Full wwPDB EM Validation Report ⓘ

Mar 23, 2026 – 06:10 AM UTC

PDB ID	:	9DM1 / pdb_00009dm1
EMDB ID	:	EMD-46995
Title	:	Mycobacterial supercomplex malate:quinone oxidoreductase assembly
Authors	:	Di Trani, J.M.; Rubinstein, J.L.
Deposited on	:	2024-09-11
Resolution	:	3.20 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:

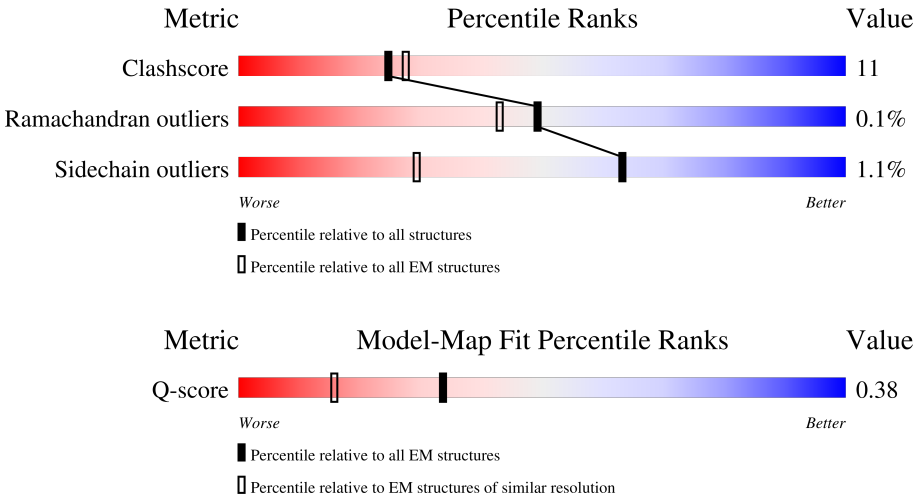
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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 3.20 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	15020 (2.70 - 3.70)

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 <=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	L	566	10% 76% 21%
1	R	566	13% 77% 20%
2	E	535	9% 81% 19%
2	F	535	9% 79% 20%

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Mol	Chain	Length	Quality of chain
3	D	216	92% 97%
3	G	216	91% 99%
4	K	312	43% 84% 16%
4	Q	312	44% 80% 19%
5	S	203	25% 82% 17%
5	X	203	26% 83% 16%
6	T	139	29% 83% 17%
6	Z	139	28% 81% 19%
7	U	79	81% 82% 18%
7	a	79	84% 94% 6%
8	V	145	74% 81% 18%
8	b	145	75% 80% 20%
9	J	100	20% 73% 19% 8%
9	P	100	23% 80% 11% 8%
10	I	223	6% 81% 18%
10	O	223	6% 79% 21%
11	W	159	39% 83% 16%
11	c	159	38% 81% 18%
12	M	382	13% 84% 15%
12	Y	382	12% 84% 16%
13	A	510	85% 94% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	CDL	R	604	-	-	X	-
16	CDL	S	301	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	CDL	T	201	-	-	X	-
16	CDL	X	301	-	-	X	-
16	CDL	X	302	-	-	X	-
16	CDL	Z	202	-	-	X	-
16	CDL	Z	203	-	-	X	-

2 Entry composition (i)

There are 24 unique types of molecules in this entry. The entry contains 51339 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 c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	552	Total	C	N	O	S	0	0
			4370	2937	695	712	26		
1	L	552	Total	C	N	O	S	0	0
			4370	2937	695	712	26		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	32	ILE	VAL	conflict	UNP A0A0K0XH24
R	47	VAL	ALA	conflict	UNP A0A0K0XH24
R	54	VAL	ILE	conflict	UNP A0A0K0XH24
R	357	THR	SER	conflict	UNP A0A0K0XH24
R	452	LEU	VAL	conflict	UNP A0A0K0XH24
R	467	THR	SER	conflict	UNP A0A0K0XH24
R	476	ILE	VAL	conflict	UNP A0A0K0XH24
R	479	VAL	ILE	conflict	UNP A0A0K0XH24
L	32	ILE	VAL	conflict	UNP A0A0K0XH24
L	47	VAL	ALA	conflict	UNP A0A0K0XH24
L	54	VAL	ILE	conflict	UNP A0A0K0XH24
L	357	THR	SER	conflict	UNP A0A0K0XH24
L	452	LEU	VAL	conflict	UNP A0A0K0XH24
L	467	THR	SER	conflict	UNP A0A0K0XH24
L	476	ILE	VAL	conflict	UNP A0A0K0XH24
L	479	VAL	ILE	conflict	UNP A0A0K0XH24

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	535	Total	C	N	O	S	0	0
			4181	2751	711	701	18		
2	F	535	Total	C	N	O	S	0	0
			4181	2751	711	701	18		

- Molecule 3 is a protein called Superoxide dismutase [Cu-Zn].

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	216	Total	C	N	O	S	0	0
			1092	645	217	229	1		
3	G	216	Total	C	N	O	S	0	0
			1092	645	217	229	1		

- Molecule 4 is a protein called Cytochrome aa3 subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Q	312	Total	C	N	O	S	0	0
			2465	1592	412	451	10		
4	K	312	Total	C	N	O	S	0	0
			2465	1592	412	451	10		

- Molecule 5 is a protein called Cytochrome aa3 subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	S	203	Total	C	N	O	S	0	0
			1560	1039	253	260	8		
5	X	203	Total	C	N	O	S	0	0
			1560	1039	253	260	8		

- 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	Z	139	Total	C	N	O	S	0	0
			1077	719	167	188	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	U	79	Total	C	N	O	S	0	0
			591	381	107	101	2		
7	a	79	Total	C	N	O	S	0	0
			591	381	107	101	2		

- Molecule 8 is a protein called Uncharacterized protein MSMEG_4692/MSMEI_4575.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	V	145	Total	C	N	O	S	0	0
			1041	658	176	205	2		
8	b	145	Total	C	N	O	S	0	0
			1041	658	176	205	2		

- Molecule 9 is a protein called Conserved transmembrane protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	P	92	Total	C	N	O	S	0	0
			736	471	136	124	5		
9	J	92	Total	C	N	O	S	0	0
			736	471	136	124	5		

- Molecule 10 is a protein called Cytochrome bc1 complex cytochrome c subunit.

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

- Molecule 11 is a protein called LpqE protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	c	158	Total	C	N	O	S	0	0
			1149	708	192	248	1		
11	W	158	Total	C	N	O	S	0	0
			1149	708	192	248	1		

- Molecule 12 is a protein called Cytochrome bc1 complex Rieske iron-sulfur subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Y	382	Total	C	N	O	S	0	0
			2977	1924	504	538	11		
12	M	382	Total	C	N	O	S	0	0
			2977	1924	504	538	11		

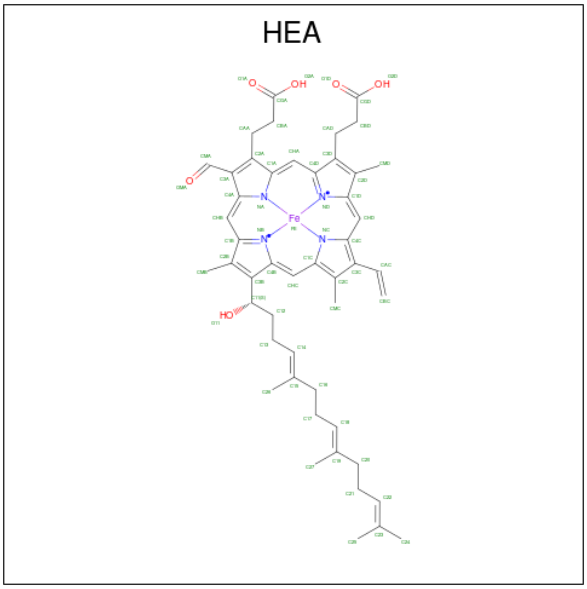
- Molecule 13 is a protein called Probable malate:quinone oxidoreductase.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	A	485	Total	C	N	O	0	0
			2377	1407	485	485		

- Molecule 14 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

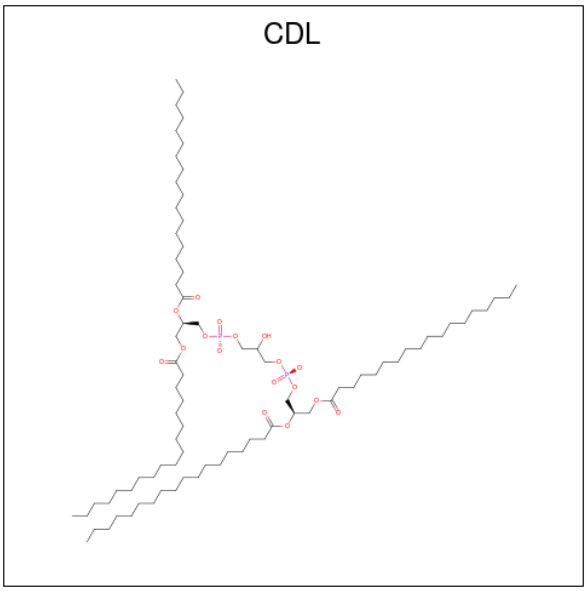
Mol	Chain	Residues	Atoms	AltConf
14	R	1	Total Cu 1 1	0
14	L	1	Total Cu 1 1	0
14	Q	2	Total Cu 2 2	0
14	K	2	Total Cu 2 2	0

- Molecule 15 is HEME-A (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



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

- Molecule 16 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
16	R	1	Total	C	O	P	0
			76	57	17	2	
16	E	1	Total	C	O	P	0
			76	57	17	2	
16	E	1	Total	C	O	P	0
			76	57	17	2	
16	F	1	Total	C	O	P	0
			76	57	17	2	
16	F	1	Total	C	O	P	0
			76	57	17	2	
16	L	1	Total	C	O	P	0
			76	57	17	2	
16	S	1	Total	C	O	P	0
			76	57	17	2	
16	T	1	Total	C	O	P	0
			76	57	17	2	
16	T	1	Total	C	O	P	0
			76	57	17	2	
16	T	1	Total	C	O	P	0
			76	57	17	2	
16	P	1	Total	C	O	P	0
			76	57	17	2	
16	X	1	Total	C	O	P	0
			76	57	17	2	
16	X	1	Total	C	O	P	0
			76	57	17	2	
16	Z	1	Total	C	O	P	0
			76	57	17	2	

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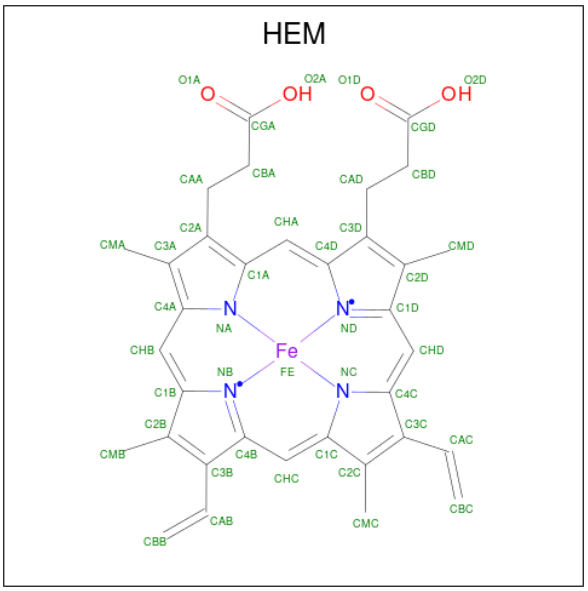
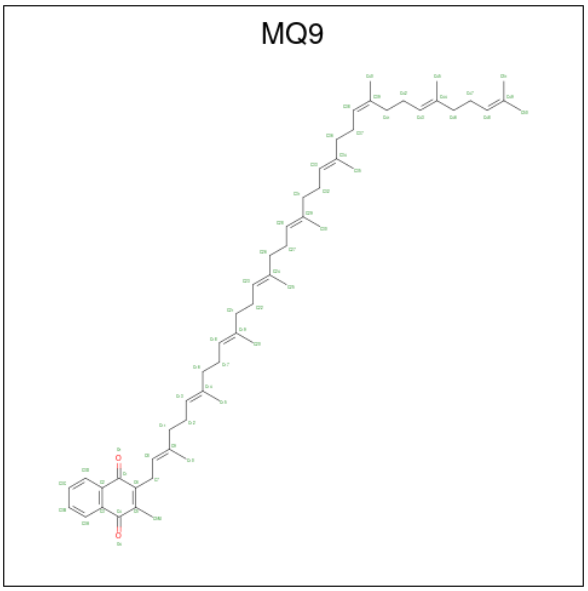
Mol	Chain	Residues	Atoms				AltConf
16	Z	1	Total 76	C 57	O 17	P 2	0
16	J	1	Total 76	C 57	O 17	P 2	0

- Molecule 17 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



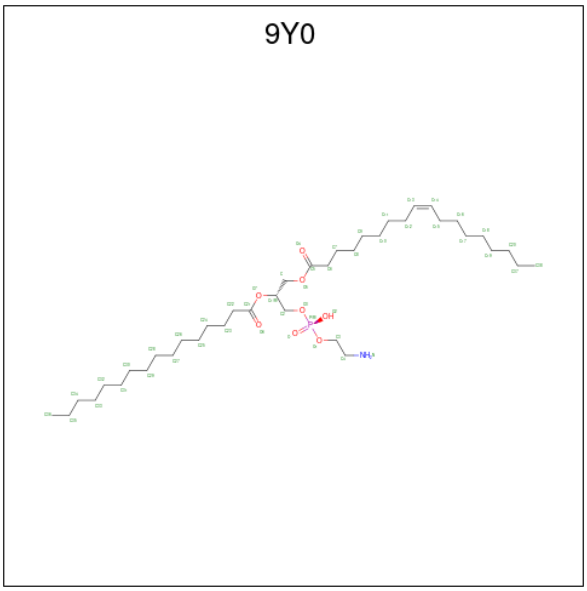
Mol	Chain	Residues	Atoms					AltConf
17	E	1	Total 42	C 33	Fe 1	N 4	O 4	0
17	E	1	Total 43	C 34	Fe 1	N 4	O 4	0
17	F	1	Total 42	C 33	Fe 1	N 4	O 4	0
17	F	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 18 is MENAQUINONE-9 (CCD ID: MQ9) (formula: $C_{56}H_{80}O_2$).



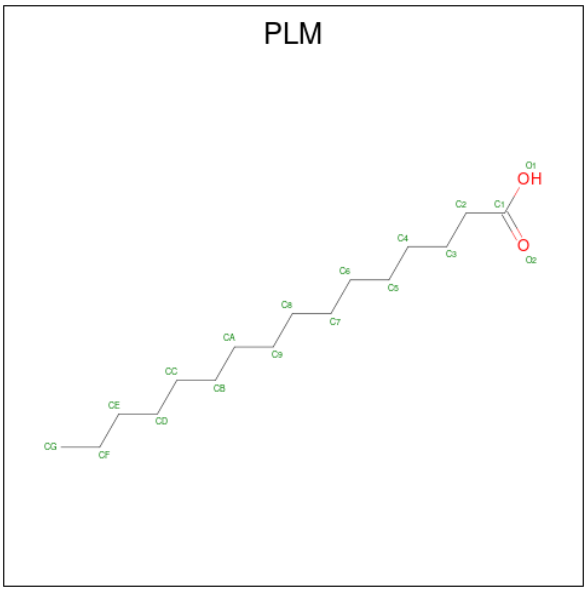
Mol	Chain	Residues	Atoms	AltConf
18	E	1	Total C O 58 56 2	0
18	E	1	Total C O 58 56 2	0
18	F	1	Total C O 58 56 2	0
18	F	1	Total C O 58 56 2	0
18	F	1	Total C O 58 56 2	0
18	F	1	Total C O 58 56 2	0
18	Z	1	Total C O 58 56 2	0
18	I	1	Total C O 58 56 2	0

- Molecule 19 is (2R)-3-(((2-aminoethoxy)(hydroxy)phosphoryl)oxy)-2-(palmitoyloxy)propyl (E)-octadec-9-enoate (CCD ID: 9Y0) (formula: $C_{39}H_{76}NO_8P$).



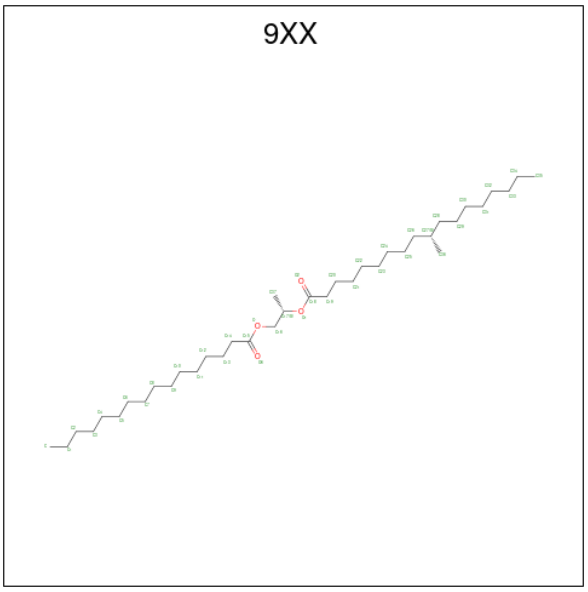
Mol	Chain	Residues	Atoms					AltConf
19	F	1	Total	C	N	O	P	0
			49	39	1	8	1	
19	S	1	Total	C	N	O	P	0
			49	39	1	8	1	
19	P	1	Total	C	N	O	P	0
			49	39	1	8	1	
19	X	1	Total	C	N	O	P	0
			49	39	1	8	1	
19	J	1	Total	C	N	O	P	0
			49	39	1	8	1	
19	J	1	Total	C	N	O	P	0
			49	39	1	8	1	

- Molecule 20 is PALMITIC ACID (CCD ID: PLM) (formula: $C_{16}H_{32}O_2$).



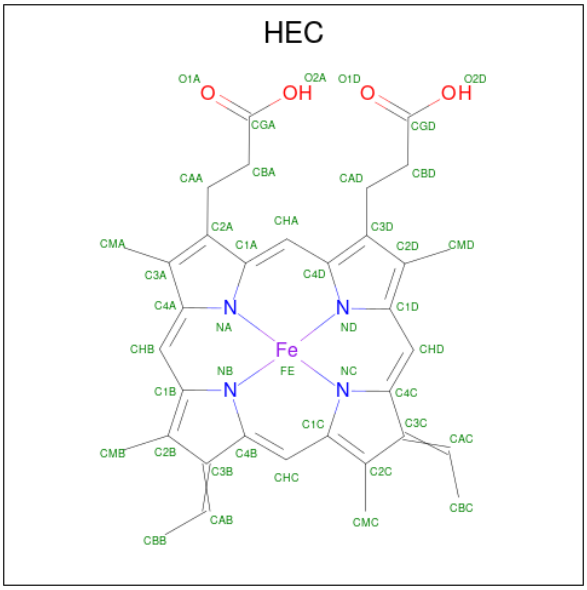
Mol	Chain	Residues	Atoms			AltConf
20	D	1	Total	C	O	0
			11	10	1	
20	G	1	Total	C	O	0
			11	10	1	
20	c	1	Total	C	O	0
			17	16	1	
20	W	1	Total	C	O	0
			17	16	1	

- Molecule 21 is (2S)-1-(hexadecanoyloxy)propan-2-yl (10S)-10-methyloctadecanoate (CCD ID: 9XX) (formula: $C_{38}H_{74}O_4$).



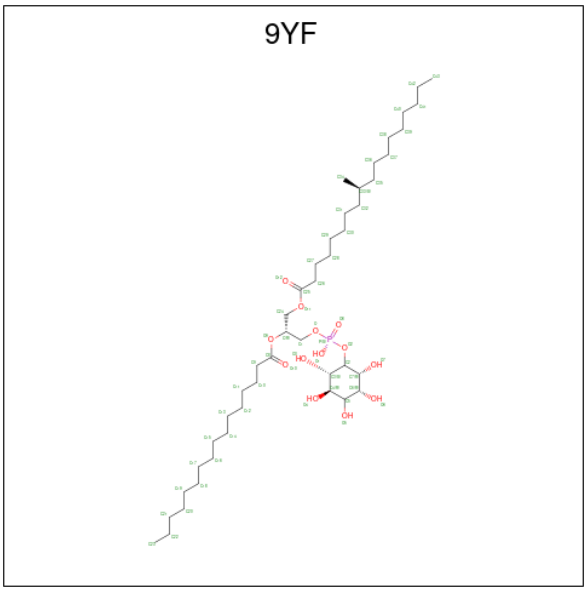
Mol	Chain	Residues	Atoms	AltConf
21	D	1	Total C O 32 28 4	0
21	G	1	Total C O 32 28 4	0
21	c	1	Total C O 42 38 4	0
21	W	1	Total C O 42 38 4	0

- Molecule 22 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



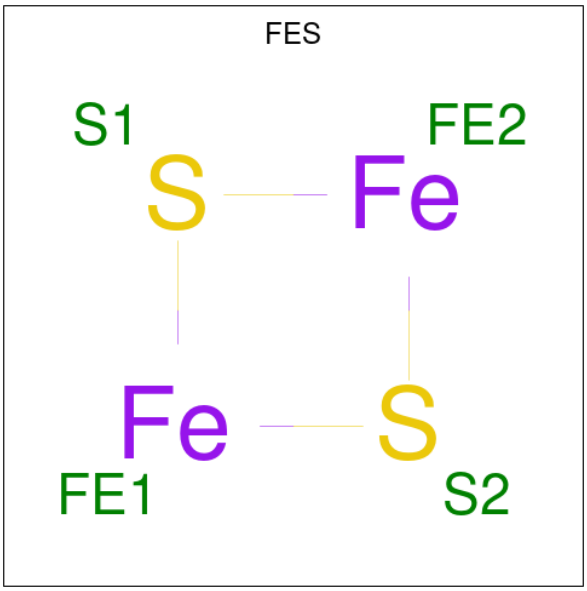
Mol	Chain	Residues	Atoms	AltConf
22	O	1	Total C Fe N O 43 34 1 4 4	0
22	O	1	Total C Fe N O 43 34 1 4 4	0
22	I	1	Total C Fe N O 43 34 1 4 4	0
22	I	1	Total C Fe N O 43 34 1 4 4	0

- Molecule 23 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: $C_{44}H_{85}O_{13}P$).



Mol	Chain	Residues	Atoms				AltConf
23	O	1	Total	C	O	P	0
			58	44	13	1	
23	c	1	Total	C	O	P	0
			58	44	13	1	
23	I	1	Total	C	O	P	0
			58	44	13	1	
23	Y	1	Total	C	O	P	0
			58	44	13	1	
23	Y	1	Total	C	O	P	0
			58	44	13	1	
23	W	1	Total	C	O	P	0
			58	44	13	1	
23	M	1	Total	C	O	P	0
			58	44	13	1	
23	M	1	Total	C	O	P	0
			58	44	13	1	

- Molecule 24 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).

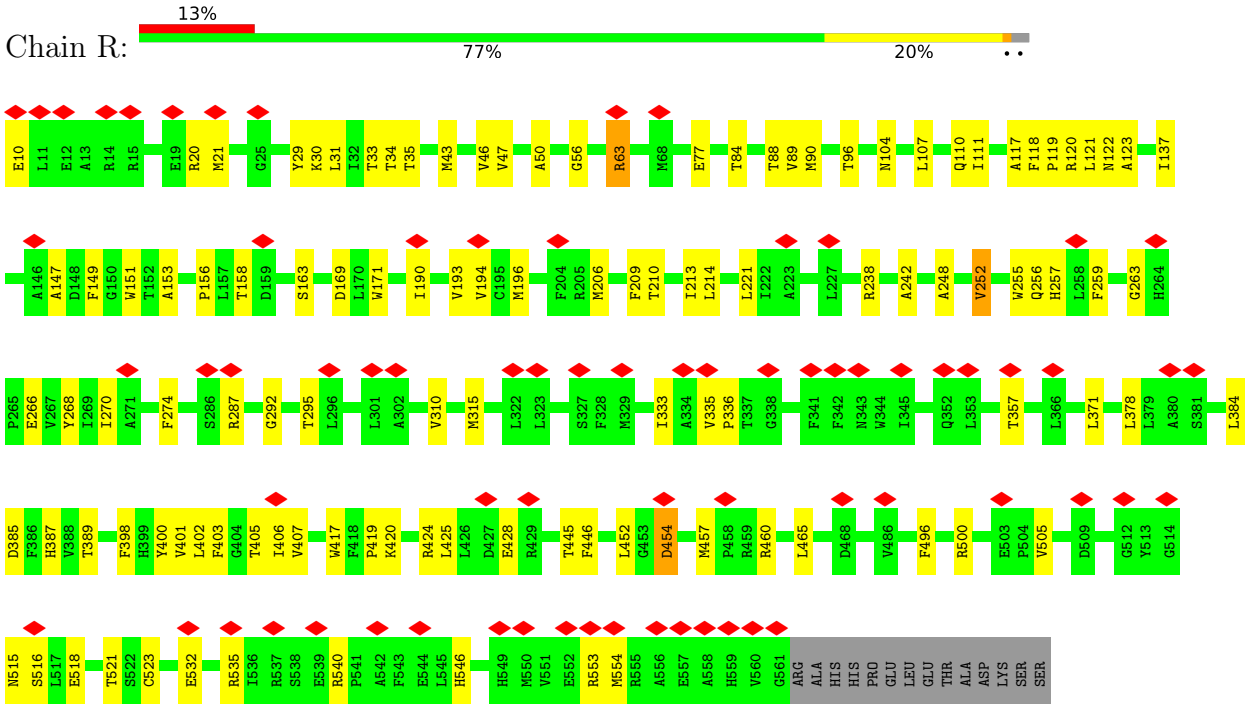


Mol	Chain	Residues	Atoms			AltConf
24	Y	1	Total 4	Fe 2	S 2	0
24	M	1	Total 4	Fe 2	S 2	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Cytochrome c oxidase subunit 1



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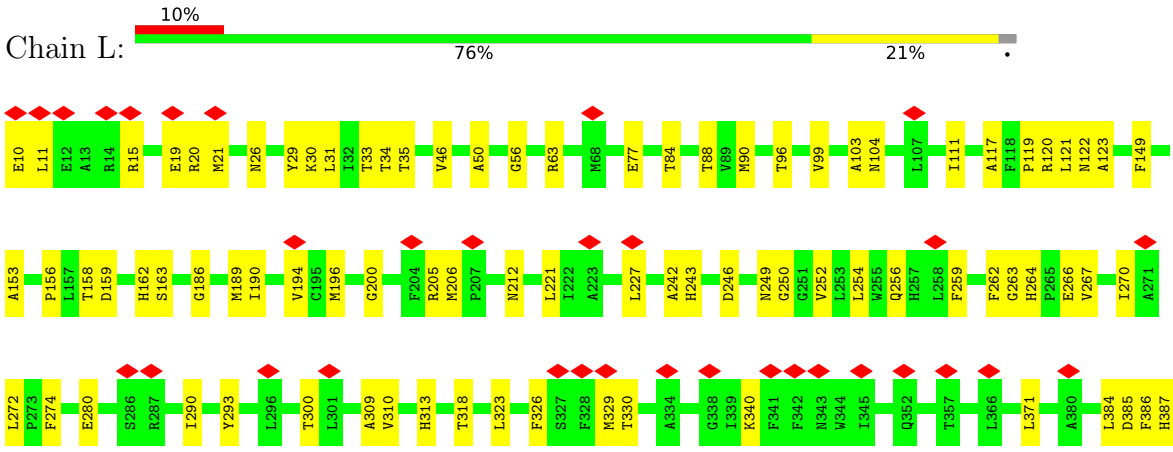
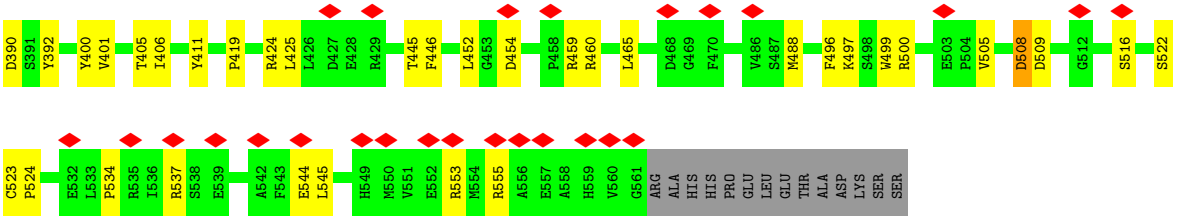
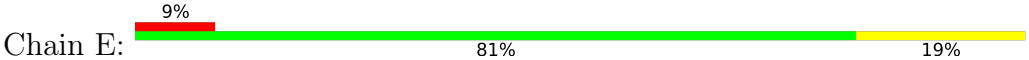
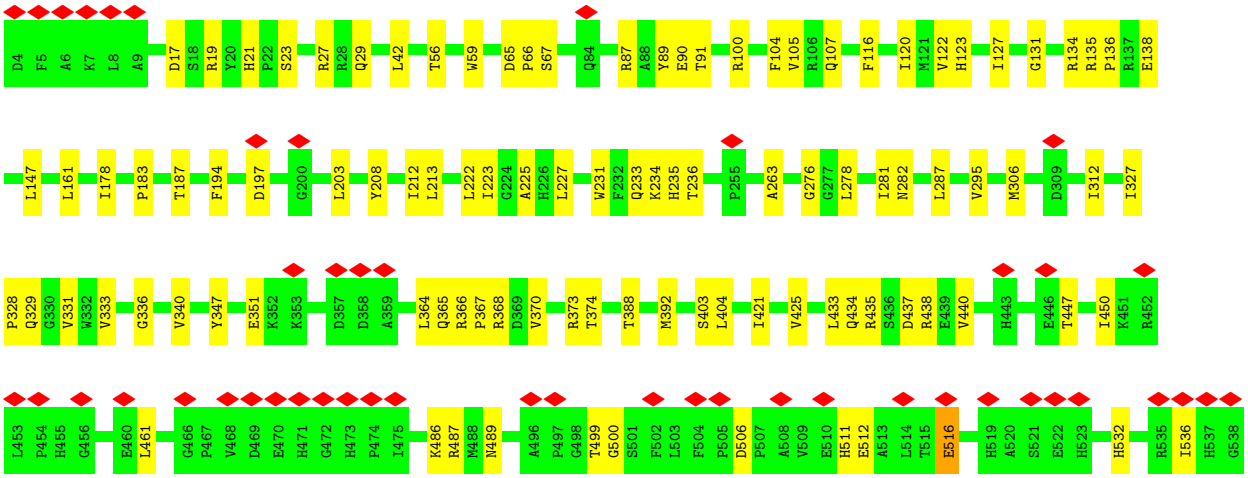


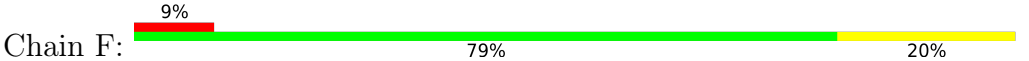


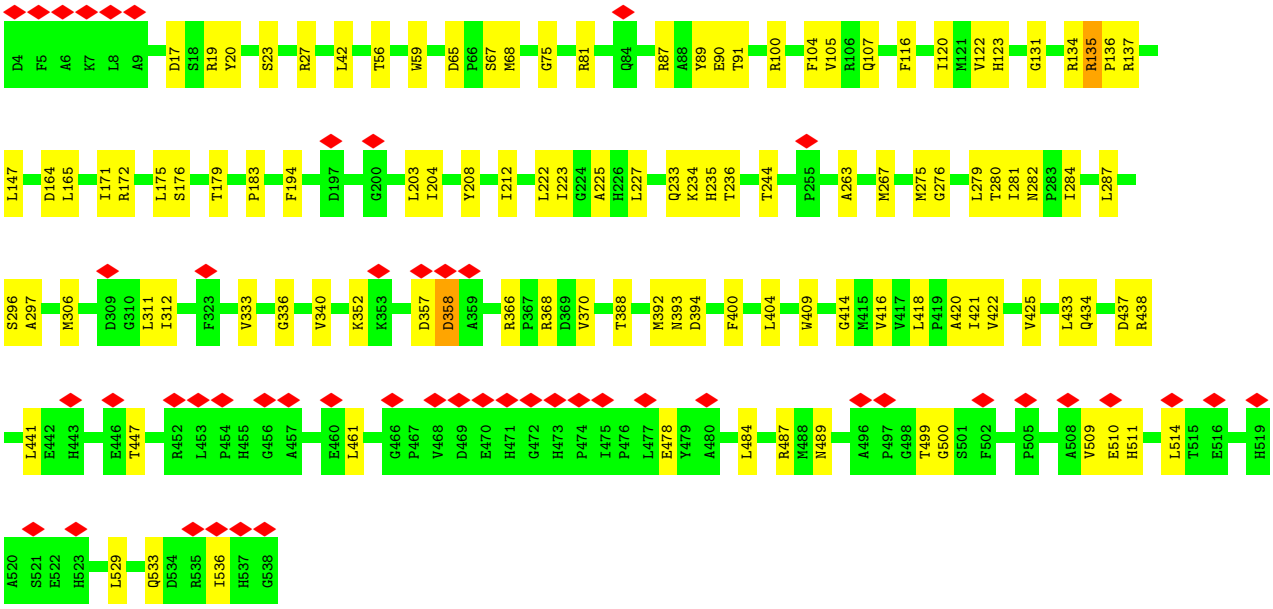
• Molecule 2: Cytochrome bc1 complex cytochrome b subunit





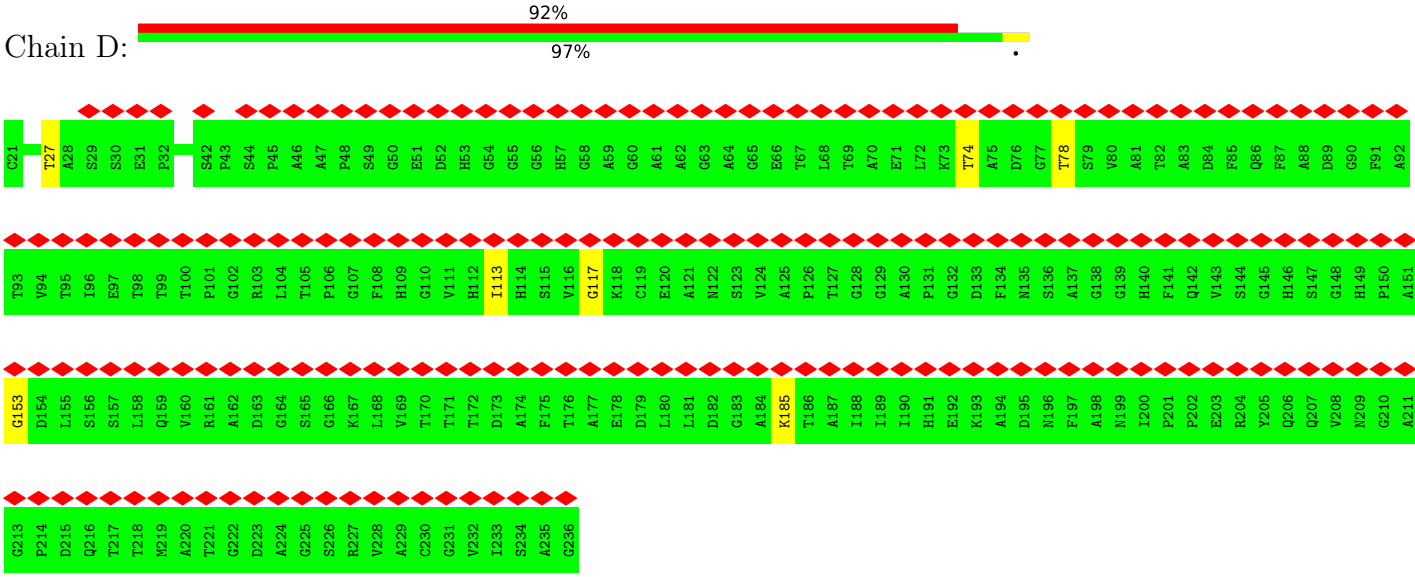
• Molecule 2: Cytochrome bc1 complex cytochrome b subunit





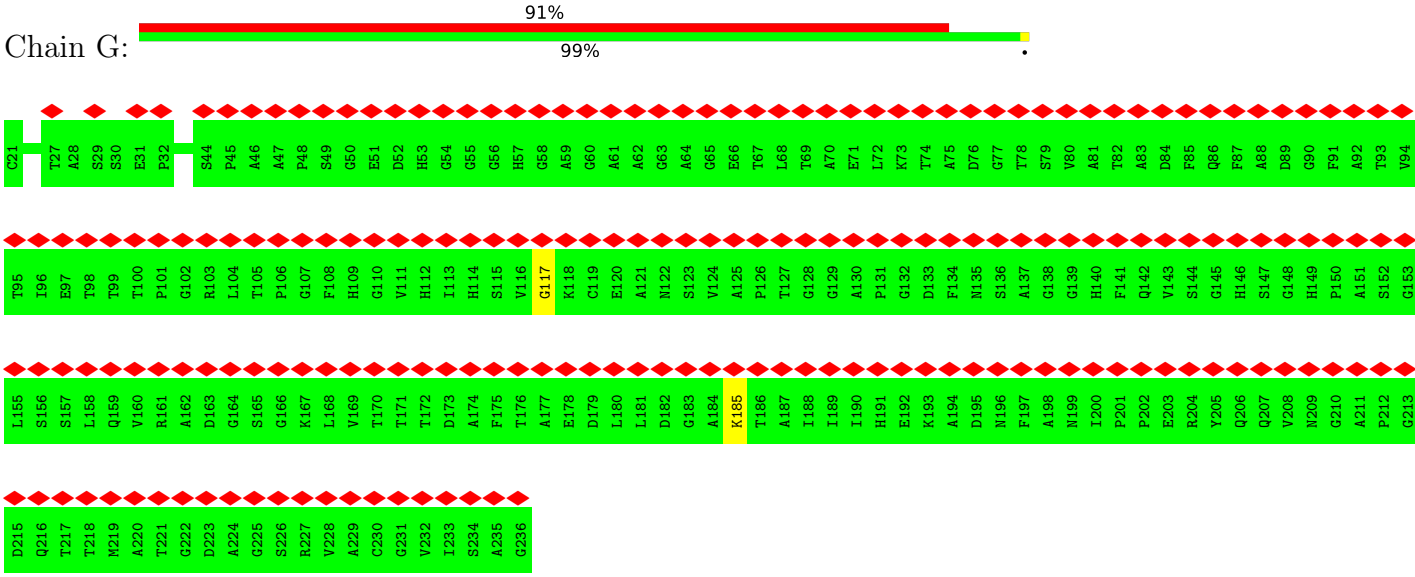
• Molecule 3: Superoxide dismutase [Cu-Zn]

Chain D:



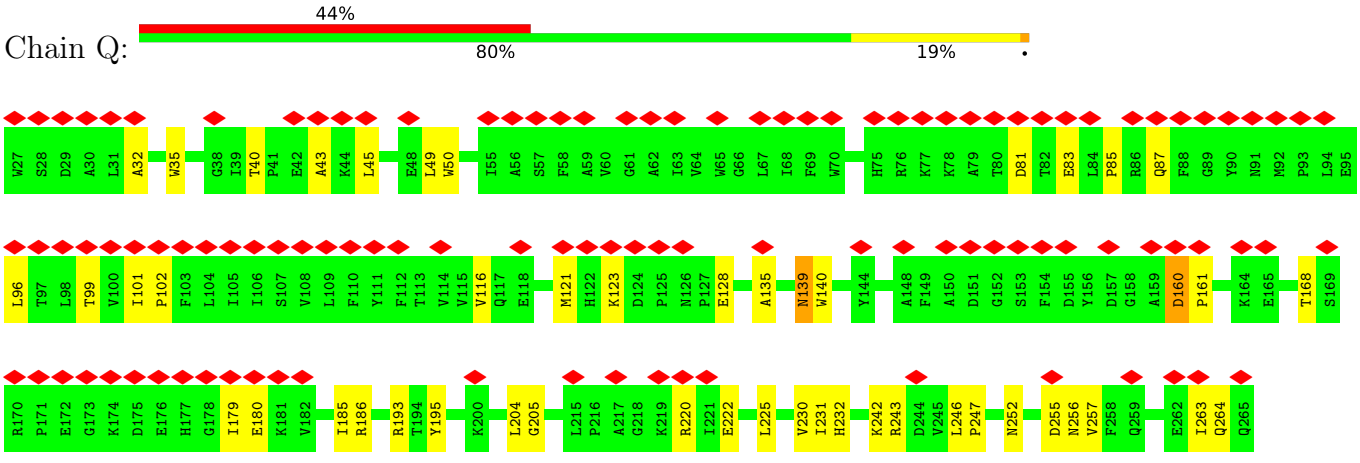
• Molecule 3: Superoxide dismutase [Cu-Zn]

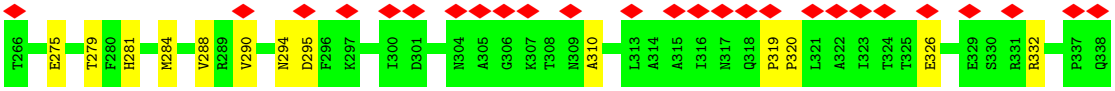
Chain G:



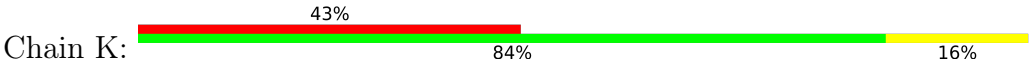
• Molecule 4: Cytochrome aa3 subunit 2

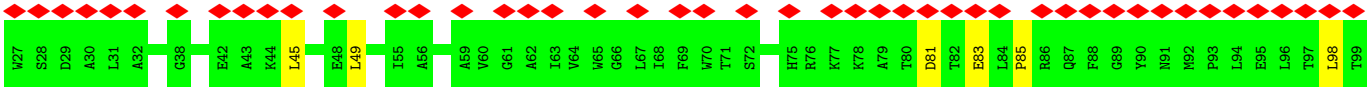
Chain Q:

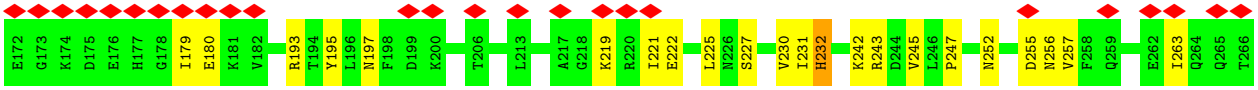


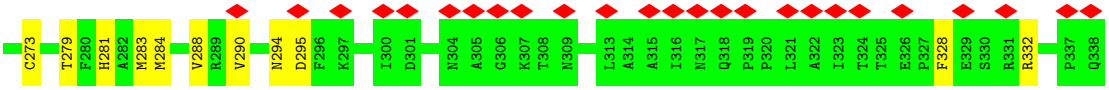


• Molecule 4: Cytochrome aa3 subunit 2

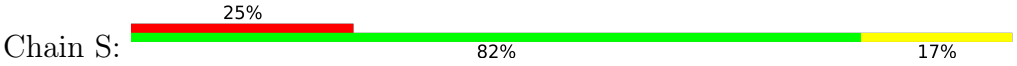


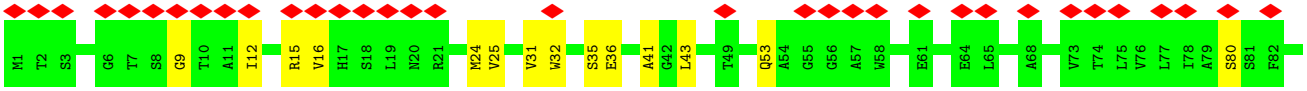


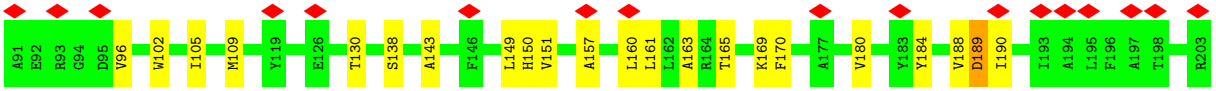




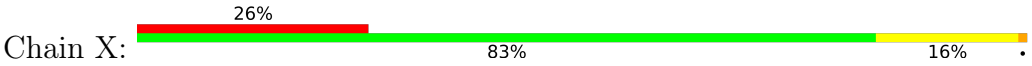
• Molecule 5: Cytochrome aa3 subunit 3

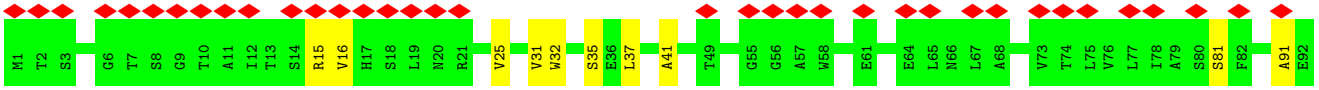


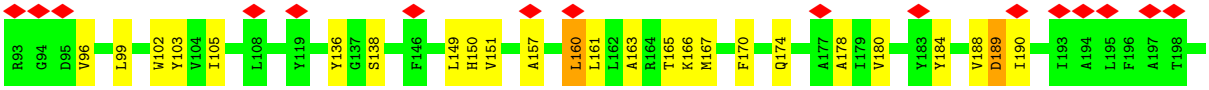




• Molecule 5: Cytochrome aa3 subunit 3

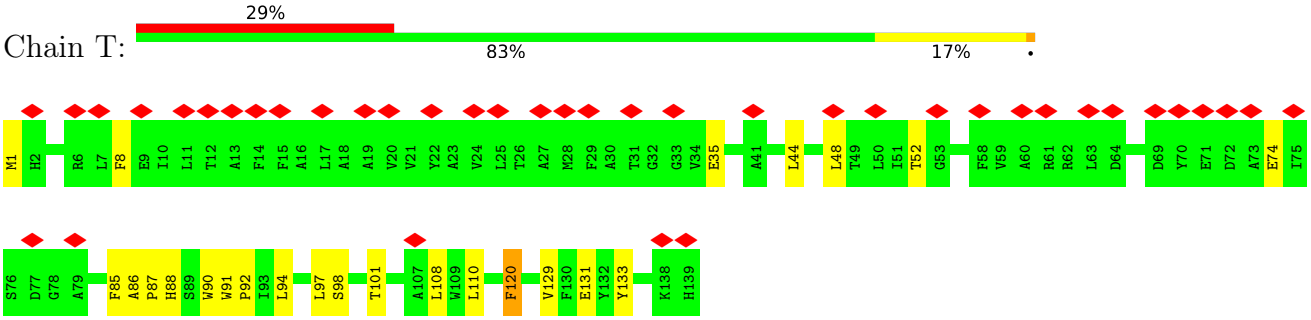






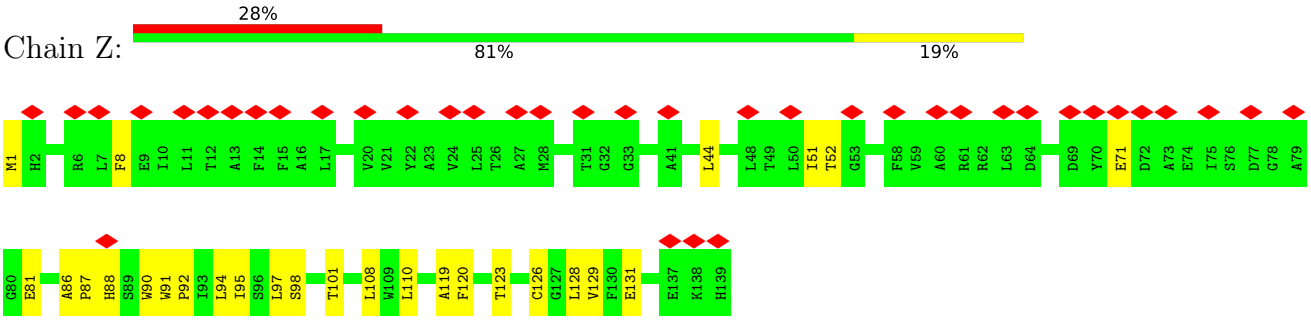
• Molecule 6: Cytochrome c oxidase polypeptide 4

Chain T:



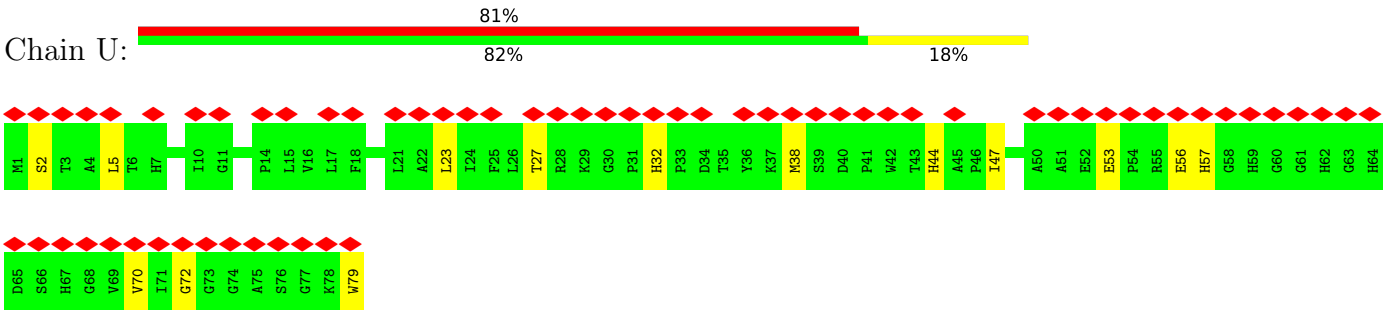
• Molecule 6: Cytochrome c oxidase polypeptide 4

Chain Z:



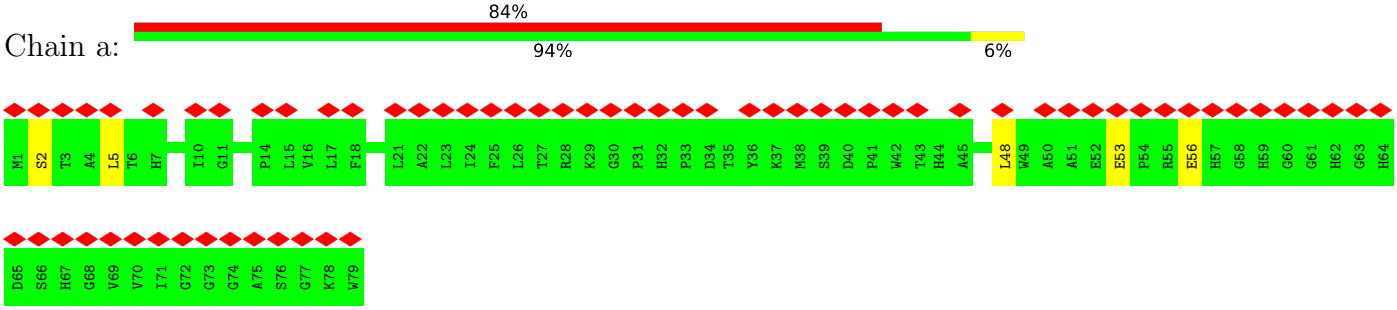
• Molecule 7: Cytochrome c oxidase subunit CtaJ

Chain U:



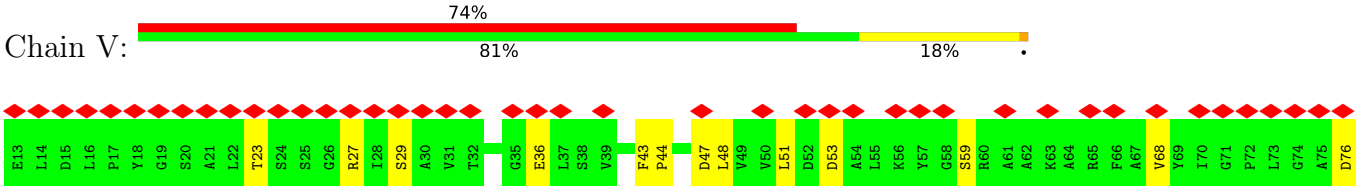
• Molecule 7: Cytochrome c oxidase subunit CtaJ

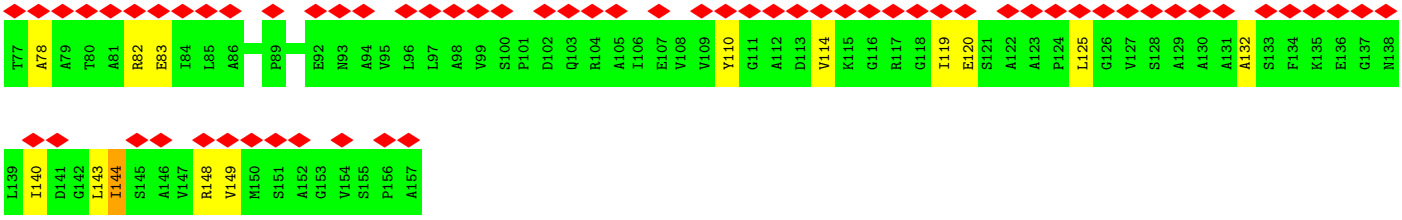
Chain a:



• Molecule 8: Uncharacterized protein MSMEG_4692/MSMEI_4575

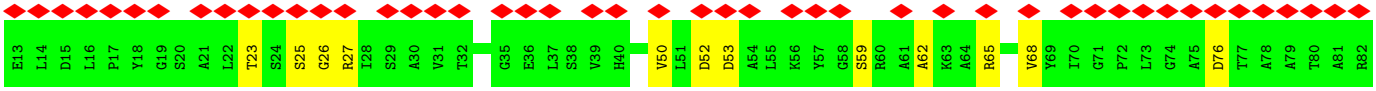
Chain V:





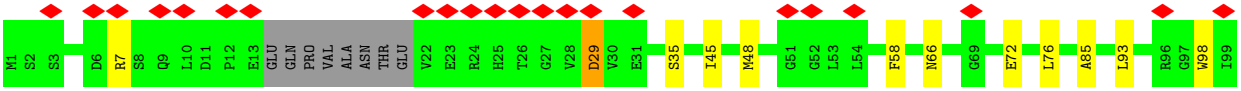
• Molecule 8: Uncharacterized protein MSMEG_4692/MSMEI_4575

Chain b:



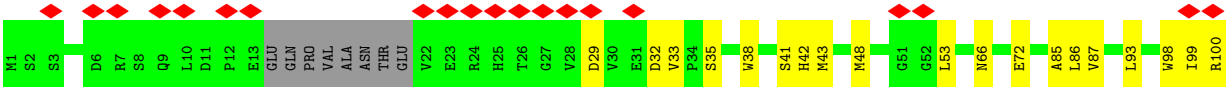
• Molecule 9: Conserved transmembrane protein

Chain P:



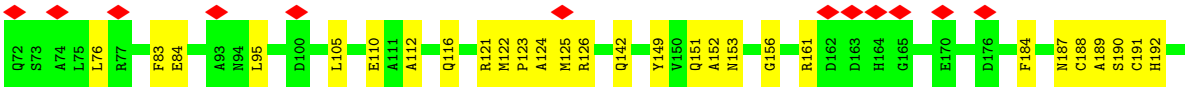
• Molecule 9: Conserved transmembrane protein

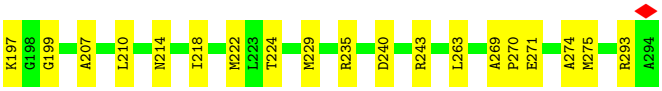
Chain J:



• Molecule 10: Cytochrome bc1 complex cytochrome c subunit

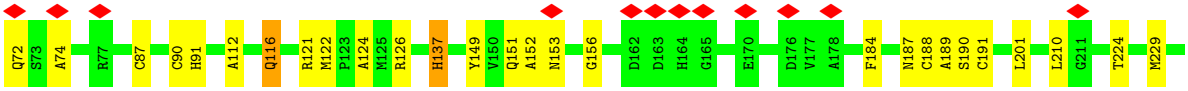
Chain O:

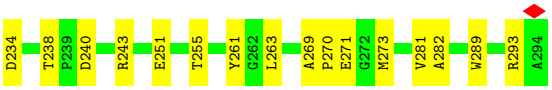




• Molecule 10: Cytochrome bc1 complex cytochrome c subunit

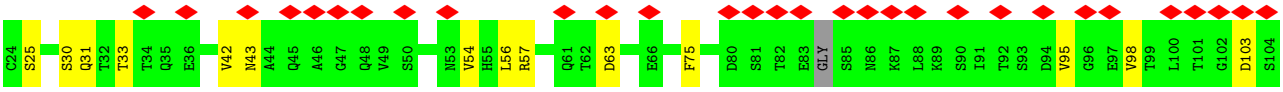
Chain I:

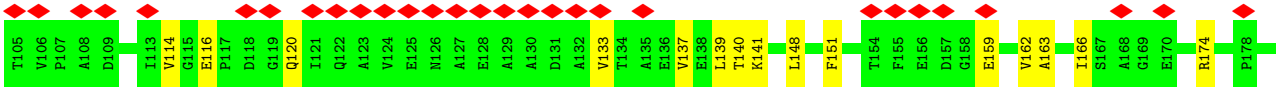




• Molecule 11: LpqE protein

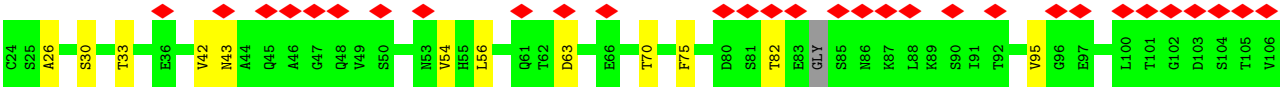
Chain c:

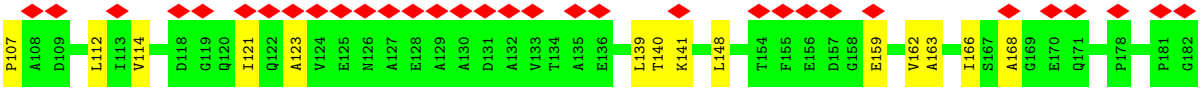




• Molecule 11: LpqE protein

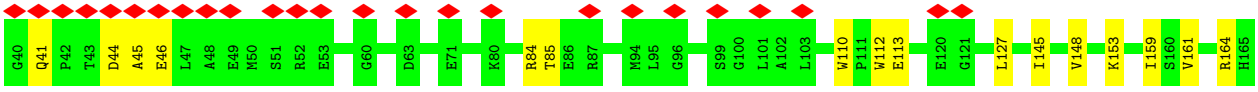
Chain W:

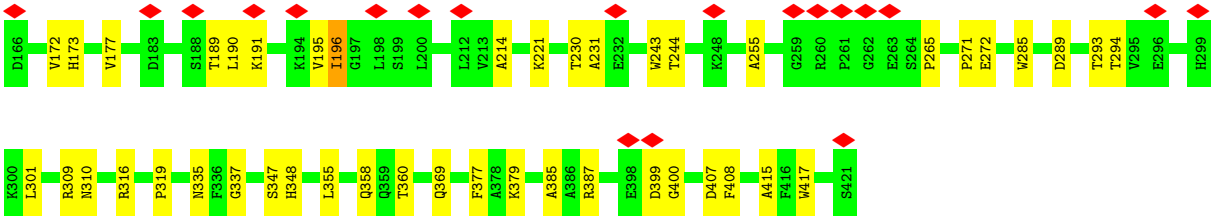




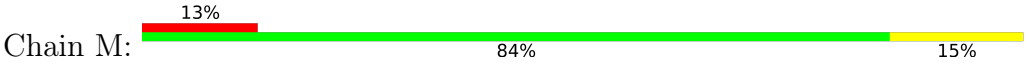
• Molecule 12: Cytochrome bc1 complex Rieske iron-sulfur subunit

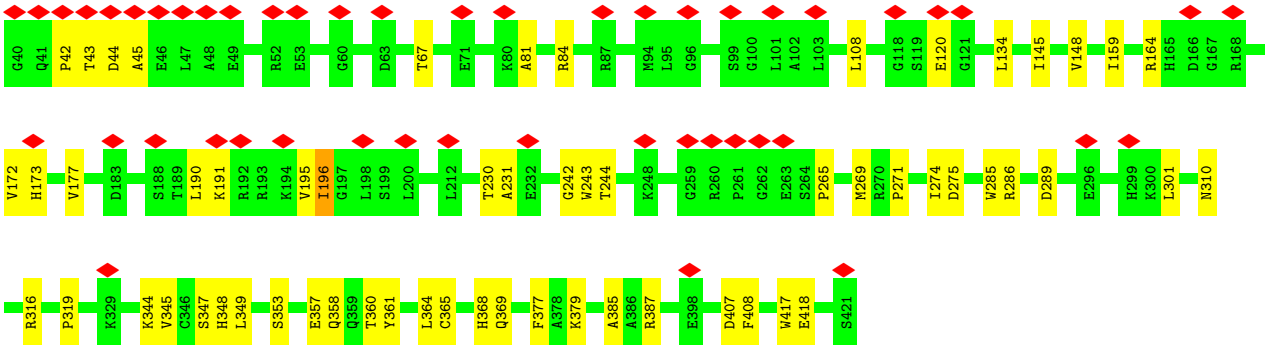
Chain Y:



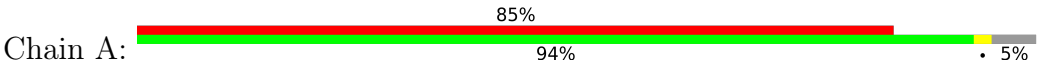


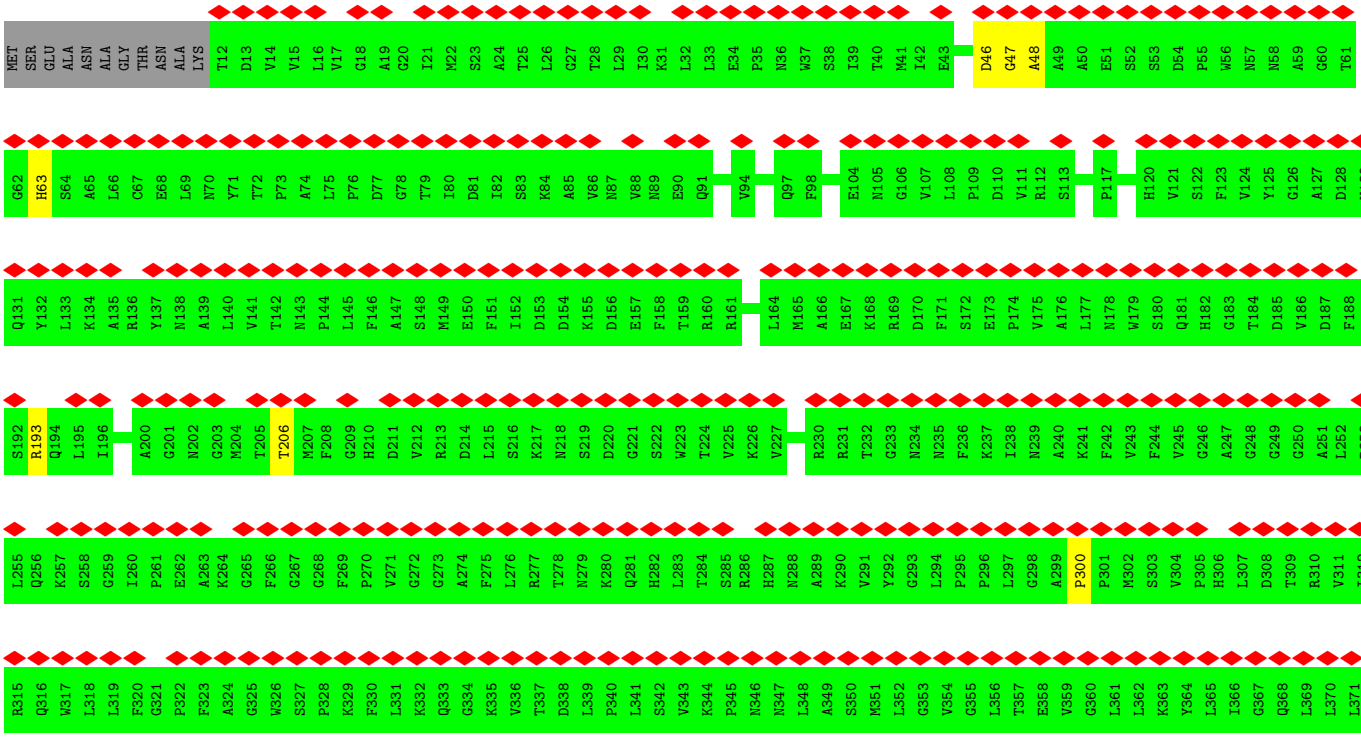
• Molecule 12: Cytochrome bc1 complex Rieske iron-sulfur subunit

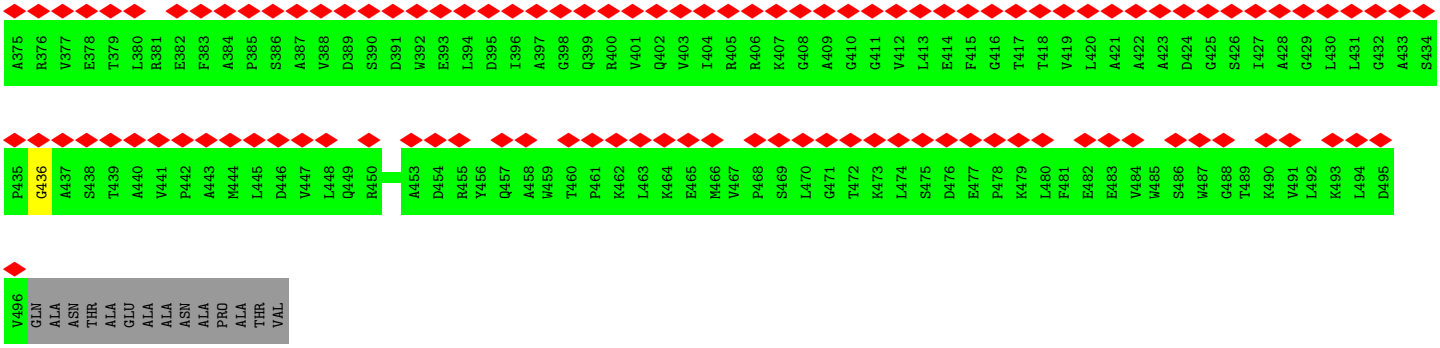




• Molecule 13: Probable malate:quinone oxidoreductase






A375 R376 V377 E378 T379 L380 R381 E382 F383 A384 P385 S386 A387 V388 D389 S390 D391 W392 E393 L394 D395 I396 A397 G398 Q399 R400 V401 Q402 V403 I404 R405 R406 K407 G408 A409 G410 G411 V412 L413 E414 F415 G416 T417 T418 V419 L420 A421 A422 A423 D424 G425 S426 I427 A428 G429 L430 L431 G432 A433 S434
P435 G436 A437 S438 T439 A440 V441 P442 A443 M444 L445 D446 V447 L448 Q449 R450 A453 D454 R455 Y456 Q457 A458 W459 T460 P461 K462 L463 K464 E465 M466 V467 P468 S469 L470 G471 T472 K473 L474 S475 D476 E477 P478 K479 L480 F481 E482 E483 V484 W485 S486 W487 G488 T489 K490 V491 L492 K493 L494 D495
V496 GLN ALA ASN THR ALA GLU ALA ALA ASN ALA PRO ALA THR VAL

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	145585	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 ($e^-/Å^2$)	41.5	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.130	Depositor
Minimum map value	-1.579	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.058	Depositor
Recommended contour level	0.335	Depositor
Map size (Å)	374.91998, 374.91998, 374.91998	wwPDB
Map dimensions	364, 364, 364	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03, 1.03, 1.03	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 9YF, PLM, FES, CDL, 9XX, HEA, HEM, HEC, CU, 9Y0, MQ9

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	L	0.18	0/4530	0.34	0/6188
1	R	0.17	0/4530	0.33	0/6188
2	E	0.21	0/4314	0.38	0/5882
2	F	0.23	0/4314	0.40	0/5882
3	D	0.14	0/1099	0.33	0/1519
3	G	0.14	0/1099	0.34	0/1519
4	K	0.18	0/2534	0.37	0/3451
4	Q	0.17	0/2534	0.34	0/3451
5	S	0.18	0/1608	0.32	0/2195
5	X	0.19	0/1608	0.32	0/2195
6	T	0.40	1/1112 (0.1%)	0.64	4/1524 (0.3%)
6	Z	0.18	0/1112	0.31	0/1524
7	U	0.15	0/613	0.27	0/836
7	a	0.15	0/613	0.28	0/836
8	V	0.16	0/1059	0.34	0/1446
8	b	0.16	0/1059	0.35	0/1446
9	J	0.16	0/757	0.29	0/1027
9	P	0.25	0/757	0.33	0/1027
10	I	0.18	0/1660	0.39	0/2250
10	O	0.38	0/1660	0.64	2/2250 (0.1%)
11	W	0.14	0/1166	0.32	0/1599
11	c	0.14	0/1166	0.33	0/1599
12	M	0.27	0/3056	0.47	0/4142
12	Y	0.20	0/3056	0.38	1/4142 (0.0%)
13	A	0.66	0/2376	1.18	1/3296 (0.0%)
All	All	0.25	1/49392 (0.0%)	0.46	8/67414 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	T	120	PHE	C-O	-7.69	1.15	1.24

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	T	120	PHE	CA-C-O	-9.20	111.05	120.90
6	T	120	PHE	CA-C-N	5.99	128.66	120.46
6	T	120	PHE	C-N-CA	5.99	128.66	120.46
13	A	300	PRO	N-CA-CB	5.61	106.33	103.19
10	O	197	LYS	N-CA-C	-5.45	103.43	110.19
10	O	274	ALA	N-CA-C	-5.37	105.51	111.36
6	T	120	PHE	CA-CB-CG	5.36	119.16	113.80
12	Y	112	TRP	CA-C-O	-5.27	115.92	121.88

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	4370	0	4346	100	0
1	R	4370	0	4345	105	0
2	E	4181	0	4202	87	0
2	F	4181	0	4199	88	0
3	D	1092	0	640	3	0
3	G	1092	0	640	1	0
4	K	2465	0	2392	36	0
4	Q	2465	0	2392	52	0
5	S	1560	0	1547	66	0
5	X	1560	0	1547	84	0
6	T	1077	0	1058	52	0
6	Z	1077	0	1058	66	0
7	U	591	0	576	10	0
7	a	591	0	576	4	0
8	V	1041	0	1052	49	0
8	b	1041	0	1052	20	0
9	J	736	0	717	14	0
9	P	736	0	717	12	0
10	I	1623	0	1564	42	0
10	O	1623	0	1564	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	W	1149	0	1110	22	0
11	c	1149	0	1110	22	0
12	M	2977	0	2984	47	0
12	Y	2977	0	2984	45	0
13	A	2377	0	1117	31	0
14	K	2	0	0	0	0
14	L	1	0	0	0	0
14	Q	2	0	0	0	0
14	R	1	0	0	0	0
15	L	120	0	108	5	0
15	R	120	0	108	4	0
16	E	152	0	192	13	0
16	F	152	0	192	20	0
16	J	76	0	96	11	0
16	L	76	0	96	18	0
16	P	76	0	96	10	0
16	R	76	0	96	22	0
16	S	76	0	96	49	0
16	T	228	0	288	49	0
16	X	152	0	192	97	0
16	Z	152	0	192	80	0
17	E	85	0	57	4	0
17	F	85	0	57	5	0
18	E	116	0	160	6	0
18	F	232	0	320	6	0
18	I	58	0	80	1	0
18	Z	58	0	80	5	0
19	F	49	0	0	0	0
19	J	98	0	0	0	0
19	P	49	0	0	0	0
19	S	49	0	0	0	0
19	X	49	0	0	0	0
20	D	11	0	16	0	0
20	G	11	0	16	0	0
20	W	17	0	31	2	0
20	c	17	0	31	0	0
21	D	32	0	0	0	0
21	G	32	0	0	0	0
21	W	42	0	0	0	0
21	c	42	0	0	0	0
22	I	86	0	64	13	0
22	O	86	0	64	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	I	58	0	0	5	0
23	M	116	0	0	0	0
23	O	58	0	0	0	0
23	W	58	0	0	1	0
23	Y	116	0	0	5	0
23	c	58	0	0	1	0
24	M	4	0	0	1	0
24	Y	4	0	0	1	0
All	All	51339	0	48217	1055	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 11.

All (1055) 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)
8:V:125:LEU:CD2	13:A:48:ALA:HB3	1.39	1.50
5:X:166:LYS:NZ	16:X:301:CDL:H112	1.28	1.48
16:Z:203:CDL:H631	23:I:304:9YF:C23	1.48	1.42
8:V:149:VAL:HG22	13:A:46:ASP:C	1.02	1.41
6:Z:120:PHE:CB	16:Z:202:CDL:H612	1.53	1.38
16:Z:203:CDL:C63	23:I:304:9YF:C23	2.03	1.37
8:V:125:LEU:HD21	13:A:48:ALA:CB	1.53	1.35
6:Z:120:PHE:HB3	16:Z:202:CDL:C61	1.58	1.34
6:T:94:LEU:HD21	16:T:201:CDL:C32	1.67	1.24
6:Z:94:LEU:HD21	16:Z:202:CDL:C32	1.68	1.21
5:X:166:LYS:HZ1	16:X:301:CDL:C11	1.54	1.21
16:X:301:CDL:H772	16:Z:203:CDL:C55	1.71	1.20
6:Z:90:TRP:CZ2	16:Z:202:CDL:HB4	1.77	1.17
6:Z:119:ALA:HB1	16:Z:203:CDL:H411	1.23	1.17
6:T:90:TRP:HZ2	16:T:201:CDL:HB4	1.05	1.16
5:X:149:LEU:HD22	16:X:302:CDL:C63	1.74	1.16
5:X:166:LYS:NZ	16:X:301:CDL:C11	2.09	1.15
16:X:301:CDL:H721	16:Z:203:CDL:C51	1.75	1.15
8:V:132:ALA:HB2	13:A:206:THR:O	1.44	1.15
16:X:301:CDL:H772	16:Z:203:CDL:H551	1.21	1.14
6:T:90:TRP:CZ2	16:T:201:CDL:HB4	1.82	1.14
8:V:125:LEU:HD23	13:A:48:ALA:N	1.61	1.14
16:X:301:CDL:H721	16:Z:203:CDL:H512	1.19	1.14
8:V:125:LEU:CD2	13:A:48:ALA:CB	2.17	1.13
6:Z:90:TRP:HZ2	16:Z:202:CDL:HB4	1.00	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:97:LEU:HD11	16:T:201:CDL:H361	1.14	1.12
6:T:97:LEU:HD11	16:T:201:CDL:C36	1.79	1.11
6:Z:97:LEU:HD11	16:Z:202:CDL:C36	1.80	1.10
6:T:94:LEU:HD21	16:T:201:CDL:H321	1.10	1.10
6:Z:94:LEU:HD21	16:Z:202:CDL:H321	1.10	1.09
5:X:149:LEU:HD22	16:X:302:CDL:H631	1.17	1.09
6:Z:97:LEU:HD11	16:Z:202:CDL:H361	1.18	1.09
8:V:149:VAL:HG22	13:A:47:GLY:N	1.73	1.03
5:X:32:TRP:CZ2	16:X:302:CDL:H382	1.93	1.02
5:S:32:TRP:CZ2	16:S:301:CDL:H382	1.94	1.02
8:V:125:LEU:HD23	13:A:48:ALA:H	0.88	1.02
5:X:32:TRP:CE2	16:X:302:CDL:H361	1.94	1.01
8:V:149:VAL:CB	13:A:46:ASP:O	2.09	1.01
1:R:121:LEU:HD13	16:S:301:CDL:CA3	1.90	1.00
5:X:32:TRP:CG	16:X:302:CDL:H331	1.95	1.00
5:X:32:TRP:CB	16:X:302:CDL:H331	1.91	1.00
8:V:149:VAL:CG2	13:A:46:ASP:C	1.79	1.00
5:S:32:TRP:CE2	16:S:301:CDL:H361	1.98	0.99
1:L:121:LEU:HD13	16:X:302:CDL:CA3	1.95	0.97
5:S:32:TRP:CB	16:S:301:CDL:H331	1.94	0.97
8:V:149:VAL:HG21	13:A:46:ASP:O	1.14	0.95
5:S:149:LEU:HB3	16:S:301:CDL:H801	1.45	0.95
4:Q:231:ILE:HD13	4:Q:246:LEU:HD23	1.49	0.95
6:Z:120:PHE:CD2	16:Z:202:CDL:H632	2.00	0.95
8:V:132:ALA:CB	13:A:206:THR:O	2.15	0.94
5:S:32:TRP:CG	16:S:301:CDL:H331	2.02	0.94
6:T:97:LEU:CD1	16:T:201:CDL:H361	1.96	0.93
16:X:301:CDL:H761	16:Z:203:CDL:H532	1.51	0.91
8:V:149:VAL:CG2	13:A:46:ASP:O	0.61	0.91
1:R:121:LEU:HD13	16:S:301:CDL:HA32	1.52	0.91
6:Z:97:LEU:CD1	16:Z:202:CDL:H361	2.01	0.90
1:L:121:LEU:HD13	16:X:302:CDL:HA32	1.53	0.90
9:P:66:ASN:ND2	12:M:385:ALA:O	2.03	0.90
6:T:98:SER:OG	16:T:201:CDL:H621	1.71	0.88
6:Z:98:SER:OG	16:Z:202:CDL:H621	1.72	0.88
8:V:149:VAL:HG23	13:A:46:ASP:O	1.06	0.87
16:Z:203:CDL:H632	23:I:304:9YF:C23	2.04	0.87
1:R:121:LEU:HB2	16:S:301:CDL:OA3	1.73	0.87
5:X:149:LEU:HB3	16:X:302:CDL:H801	1.56	0.87
7:a:53:GLU:OE1	8:b:59:SER:OG	1.93	0.87
6:T:97:LEU:CD1	16:T:201:CDL:C36	2.52	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:120:PHE:HB3	16:T:201:CDL:H612	1.55	0.87
5:X:32:TRP:CD2	16:X:302:CDL:H352	2.10	0.87
5:X:157:ALA:HB2	16:X:302:CDL:H532	1.54	0.87
5:S:32:TRP:NE1	16:S:301:CDL:H361	1.89	0.87
16:L:604:CDL:H731	16:L:604:CDL:H512	1.53	0.86
6:T:120:PHE:CB	16:T:201:CDL:H612	2.05	0.86
16:Z:203:CDL:H161	10:I:281:VAL:HG11	1.57	0.86
1:R:20:ARG:NH2	8:V:53:ASP:OD1	2.09	0.86
5:X:149:LEU:HD22	16:X:302:CDL:C64	2.05	0.86
6:Z:119:ALA:HB1	16:Z:203:CDL:C41	2.05	0.85
1:L:20:ARG:NH2	8:b:53:ASP:OD1	2.10	0.85
2:E:87:ARG:NH1	2:E:90:GLU:OE1	2.09	0.85
6:Z:97:LEU:CD1	16:Z:202:CDL:C36	2.55	0.85
5:X:32:TRP:NE1	16:X:302:CDL:H361	1.91	0.84
1:L:121:LEU:HB2	16:X:302:CDL:OA3	1.77	0.84
5:S:32:TRP:CD2	16:S:301:CDL:H352	2.13	0.84
16:L:604:CDL:H542	16:J:201:CDL:H351	1.57	0.84
1:R:389:THR:O	4:Q:242:LYS:NZ	2.11	0.84
4:Q:243:ARG:NH1	4:Q:255:ASP:O	2.11	0.84
6:T:94:LEU:HD21	16:T:201:CDL:H322	1.59	0.84
6:Z:94:LEU:HD21	16:Z:202:CDL:H322	1.60	0.83
16:X:301:CDL:C76	16:Z:203:CDL:H532	2.08	0.83
1:R:121:LEU:HD13	16:S:301:CDL:HA31	1.58	0.83
16:X:301:CDL:H772	16:Z:203:CDL:H552	1.60	0.83
5:S:149:LEU:HD23	16:S:301:CDL:H631	1.61	0.82
7:U:53:GLU:OE1	8:V:59:SER:OG	1.97	0.82
1:L:411:TYR:OH	1:L:488:MET:SD	2.37	0.82
16:R:604:CDL:HA4	16:P:201:CDL:H312	1.62	0.81
18:F:709:MQ9:H501	12:Y:214:ALA:HB1	1.62	0.81
2:F:447:THR:OG1	2:F:461:LEU:O	1.97	0.81
10:I:122:MET:O	10:I:124:ALA:N	2.14	0.81
16:Z:203:CDL:C64	23:I:304:9YF:C23	2.59	0.81
4:K:243:ARG:NH1	4:K:255:ASP:O	2.14	0.81
8:V:125:LEU:CD2	13:A:48:ALA:H	1.83	0.80
16:X:301:CDL:C77	16:Z:203:CDL:C55	2.59	0.80
8:V:23:THR:OG1	8:V:27:ARG:O	1.99	0.80
1:L:84:THR:OG1	1:L:149:PHE:O	1.98	0.80
2:E:447:THR:OG1	2:E:461:LEU:O	1.98	0.80
1:R:30:LYS:O	1:R:34:THR:N	2.16	0.79
8:V:149:VAL:HG13	13:A:47:GLY:HA3	1.63	0.79
4:K:263:ILE:HG21	4:K:290:VAL:HG21	1.62	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:66:ASN:ND2	12:Y:385:ALA:O	2.16	0.79
6:T:94:LEU:CD2	16:T:201:CDL:H321	2.04	0.79
16:X:301:CDL:C17	16:Z:203:CDL:H762	2.12	0.79
1:L:300:THR:OG1	1:L:340:LYS:NZ	2.15	0.79
16:X:301:CDL:H721	16:Z:203:CDL:H511	1.63	0.78
6:Z:94:LEU:CD2	16:Z:202:CDL:H321	2.04	0.78
6:Z:90:TRP:HZ2	16:Z:202:CDL:CB4	1.89	0.78
1:R:287:ARG:O	4:Q:87:GLN:NE2	2.17	0.78
11:c:98:VAL:HG22	11:c:137:VAL:HG12	1.65	0.78
10:I:251:GLU:O	10:I:255:THR:OG1	2.01	0.78
5:S:157:ALA:HB2	16:S:301:CDL:H532	1.65	0.78
5:X:184:TYR:OH	16:X:302:CDL:H752	1.84	0.78
1:L:30:LYS:O	1:L:34:THR:N	2.17	0.78
1:L:497:LYS:NZ	9:J:100:ARG:O	2.17	0.78
2:E:489:ASN:ND2	6:Z:131:GLU:O	2.17	0.77
12:Y:285:TRP:NE1	12:Y:289:ASP:O	2.18	0.77
5:X:32:TRP:CZ2	16:X:302:CDL:H361	2.20	0.77
5:X:184:TYR:CZ	16:X:302:CDL:H731	2.20	0.76
5:X:32:TRP:HB2	16:X:302:CDL:H331	1.66	0.76
6:Z:120:PHE:CB	16:Z:202:CDL:C61	2.36	0.76
1:L:121:LEU:HD13	16:X:302:CDL:HA31	1.65	0.76
5:X:166:LYS:CE	16:X:301:CDL:H112	2.15	0.76
6:Z:97:LEU:CD1	16:Z:202:CDL:C35	2.64	0.76
1:L:205:ARG:NH1	6:Z:71:GLU:OE2	2.19	0.76
11:c:30:SER:HG	11:c:33:THR:HG1	1.22	0.75
6:T:120:PHE:CA	16:T:201:CDL:H612	2.16	0.75
6:Z:119:ALA:CB	16:Z:203:CDL:H411	2.10	0.75
4:K:227:SER:OG	4:K:230:VAL:O	2.03	0.75
10:O:191:CYS:CB	22:O:302:HEC:HBC2	2.17	0.75
5:X:166:LYS:HZ3	16:X:301:CDL:C11	1.98	0.74
8:V:125:LEU:CG	13:A:48:ALA:HB3	2.15	0.74
4:Q:263:ILE:HG21	4:Q:290:VAL:HG21	1.67	0.74
6:T:90:TRP:HZ2	16:T:201:CDL:CB4	1.93	0.74
8:V:47:ASP:OD1	8:V:48:LEU:N	2.20	0.74
10:O:229:MET:O	12:M:358:GLN:NE2	2.21	0.74
10:O:188:CYS:HB2	22:O:302:HEC:HBB2	1.70	0.74
5:X:32:TRP:CE2	16:X:302:CDL:C36	2.70	0.74
16:X:301:CDL:H131	16:Z:203:CDL:OB7	1.87	0.74
6:T:120:PHE:CD2	16:T:201:CDL:H632	2.23	0.74
8:V:149:VAL:HG13	13:A:47:GLY:CA	2.17	0.74
5:S:184:TYR:OH	16:S:301:CDL:H752	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:X:32:TRP:CE2	16:X:302:CDL:H352	2.23	0.73
11:c:63:ASP:OD1	12:Y:399:ASP:N	2.22	0.73
12:M:285:TRP:NE1	12:M:289:ASP:O	2.20	0.73
2:F:75:GLY:O	2:F:81:ARG:NH1	2.21	0.73
1:R:553:ARG:NH2	4:Q:85:PRO:O	2.21	0.73
2:E:138:GLU:OE2	2:F:19:ARG:NE	2.22	0.73
5:S:32:TRP:HZ2	16:S:301:CDL:H382	1.48	0.73
6:Z:94:LEU:CD2	16:Z:202:CDL:C32	2.60	0.73
2:F:489:ASN:ND2	6:T:131:GLU:O	2.22	0.73
6:T:97:LEU:CD1	16:T:201:CDL:C35	2.66	0.73
2:E:365:GLN:NE2	9:J:38:TRP:O	2.21	0.72
11:c:148:LEU:HD11	12:Y:319:PRO:HB3	1.70	0.72
16:R:604:CDL:C64	20:W:201:PLM:HG1	2.18	0.72
8:V:125:LEU:CD2	13:A:48:ALA:CA	2.68	0.72
1:L:424:ARG:NH1	1:L:499:TRP:O	2.22	0.72
4:Q:275:GLU:O	4:Q:281:HIS:NE2	2.22	0.72
16:L:604:CDL:H521	16:J:201:CDL:H321	1.70	0.72
5:X:32:TRP:HZ2	16:X:302:CDL:H382	1.51	0.72
1:L:385:ASP:O	1:L:389:THR:OG1	2.08	0.72
5:S:32:TRP:CE2	16:S:301:CDL:H352	2.25	0.71
5:S:184:TYR:CZ	16:S:301:CDL:H731	2.24	0.71
11:W:148:LEU:HD11	12:M:319:PRO:HB3	1.72	0.71
2:F:42:LEU:HD13	2:F:122:VAL:HG12	1.71	0.71
5:S:32:TRP:HB2	16:S:301:CDL:H331	1.73	0.71
5:X:189:ASP:OD1	5:X:190:ILE:N	2.24	0.71
5:X:157:ALA:HB1	16:X:302:CDL:C51	2.20	0.71
1:R:515:ASN:O	1:R:516:SER:OG	2.06	0.71
5:S:149:LEU:CD2	16:S:301:CDL:H631	2.20	0.70
5:S:32:TRP:CE2	16:S:301:CDL:C36	2.74	0.70
6:T:94:LEU:CD2	16:T:201:CDL:C32	2.59	0.70
10:O:151:GLN:OE1	10:O:156:GLY:N	2.24	0.70
5:X:149:LEU:CB	16:X:302:CDL:H801	2.20	0.70
5:X:157:ALA:CB	16:X:302:CDL:H511	2.21	0.70
16:R:604:CDL:H542	16:P:201:CDL:H351	1.71	0.70
16:X:301:CDL:C77	16:Z:203:CDL:H552	2.21	0.70
2:F:500:GLY:O	12:M:84:ARG:NH2	2.24	0.70
16:Z:203:CDL:H572	10:I:282:ALA:HA	1.74	0.70
2:E:500:GLY:O	12:Y:84:ARG:NH2	2.25	0.70
1:R:10:GLU:N	1:R:10:GLU:OE1	2.24	0.70
5:X:166:LYS:HZ3	16:X:301:CDL:CA5	2.04	0.70
2:F:529:LEU:HD21	12:M:159:ILE:HG21	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:128:GLU:OE1	4:K:150:ALA:N	2.24	0.70
7:U:44:HIS:ND1	7:U:47:ILE:HD11	2.08	0.69
5:X:150:HIS:HA	16:X:302:CDL:H771	1.74	0.69
2:E:42:LEU:HD13	2:E:122:VAL:HG12	1.73	0.69
16:X:301:CDL:H111	16:X:301:CDL:HB21	1.75	0.69
16:T:203:CDL:H722	16:T:203:CDL:H132	1.75	0.69
10:O:240:ASP:OD1	10:O:243:ARG:NH2	2.25	0.69
1:L:270:ILE:HG23	1:L:406:ILE:HG21	1.75	0.69
1:R:88:THR:HG21	1:R:171:TRP:HE1	1.57	0.69
4:Q:332:ARG:NH2	11:W:26:ALA:O	2.26	0.69
16:T:202:CDL:HB21	16:T:202:CDL:H111	1.75	0.69
6:Z:120:PHE:CA	16:Z:202:CDL:H612	2.22	0.69
22:I:301:HEC:HBC3	22:I:301:HEC:HHD	1.75	0.69
1:L:10:GLU:N	1:L:10:GLU:OE1	2.25	0.69
8:V:36:GLU:OE1	8:V:36:GLU:N	2.26	0.68
6:Z:123:THR:HG23	16:Z:203:CDL:H322	1.75	0.68
2:E:235:HIS:O	12:Y:164:ARG:NH2	2.26	0.68
1:L:385:ASP:OD1	1:L:389:THR:OG1	2.09	0.68
6:Z:120:PHE:HB3	16:Z:202:CDL:H612	0.72	0.68
5:X:184:TYR:CE1	16:X:302:CDL:H732	2.29	0.68
5:X:184:TYR:CE1	16:X:302:CDL:C73	2.76	0.68
2:E:328:PRO:O	2:E:331:VAL:HG12	1.94	0.68
10:I:240:ASP:OD1	10:I:243:ARG:NH2	2.26	0.68
6:Z:120:PHE:CG	16:Z:202:CDL:C61	2.76	0.68
10:I:90:CYS:SG	22:I:301:HEC:HBC2	2.34	0.68
5:X:149:LEU:CD2	16:X:302:CDL:C64	2.71	0.68
12:M:377:PHE:O	12:M:379:LYS:N	2.27	0.68
1:R:121:LEU:CD1	16:S:301:CDL:HA32	2.24	0.68
5:S:157:ALA:CB	16:S:301:CDL:H511	2.24	0.68
6:Z:97:LEU:CD1	16:Z:202:CDL:H351	2.24	0.68
8:b:23:THR:OG1	8:b:27:ARG:O	2.11	0.68
8:b:65:ARG:NH1	8:b:90:THR:OG1	2.27	0.68
11:W:54:VAL:HG11	11:W:162:VAL:HG11	1.76	0.68
2:E:331:VAL:HG23	23:Y:502:9YF:C42	2.24	0.67
2:F:235:HIS:O	12:M:164:ARG:NH2	2.27	0.67
1:L:553:ARG:NH2	4:K:85:PRO:O	2.27	0.67
6:Z:90:TRP:CZ2	16:Z:202:CDL:CB4	2.68	0.67
10:I:151:GLN:OE1	10:I:156:GLY:N	2.27	0.67
16:R:604:CDL:H521	16:P:201:CDL:H321	1.77	0.67
5:S:32:TRP:CZ2	16:S:301:CDL:H361	2.29	0.67
8:V:125:LEU:HD23	13:A:48:ALA:CA	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:225:LEU:O	4:K:256:ASN:ND2	2.27	0.67
1:R:96:THR:OG1	1:R:266:GLU:OE2	2.12	0.67
3:D:117:GLY:N	3:D:185:LYS:O	2.28	0.67
10:O:121:ARG:NE	22:O:302:HEC:O1D	2.28	0.67
22:O:301:HEC:HBC3	22:O:301:HEC:HHD	1.77	0.67
16:X:301:CDL:C13	16:Z:203:CDL:OB7	2.43	0.67
6:Z:120:PHE:CG	16:Z:202:CDL:H611	2.29	0.67
2:E:329:GLN:OE1	12:Y:348:HIS:NE2	2.28	0.67
1:L:206:MET:O	1:L:293:TYR:OH	2.12	0.66
1:L:249:ASN:O	4:K:252:ASN:ND2	2.28	0.66
12:Y:377:PHE:O	12:Y:379:LYS:N	2.28	0.66
16:R:604:CDL:H531	16:R:604:CDL:H731	1.76	0.66
5:X:157:ALA:CB	16:X:302:CDL:C51	2.73	0.66
9:P:72:GLU:HG3	23:W:203:9YF:O10	1.95	0.66
6:Z:120:PHE:HD2	16:Z:202:CDL:H632	1.54	0.66
1:R:270:ILE:HG23	1:R:406:ILE:HG21	1.76	0.66
6:Z:123:THR:CG2	16:Z:203:CDL:H322	2.25	0.66
8:V:125:LEU:CD2	13:A:48:ALA:N	2.47	0.66
22:O:302:HEC:HHD	22:O:302:HEC:HBC3	1.77	0.65
5:X:166:LYS:HZ1	16:X:301:CDL:H112	0.64	0.65
11:c:98:VAL:HG22	11:c:137:VAL:CG1	2.26	0.65
1:R:387:HIS:NE2	1:R:454:ASP:O	2.29	0.65
2:E:136:PRO:O	2:E:233:GLN:NE2	2.28	0.65
5:S:150:HIS:HA	16:S:301:CDL:H771	1.77	0.65
8:V:149:VAL:HG22	13:A:47:GLY:CA	2.25	0.65
5:X:149:LEU:CD2	16:X:302:CDL:H631	2.11	0.65
2:F:131:GLY:O	2:F:134:ARG:NH1	2.29	0.65
2:F:425:VAL:HG11	16:F:705:CDL:H371	1.77	0.65
1:L:96:THR:OG1	1:L:266:GLU:OE2	2.13	0.65
16:E:605:CDL:H111	16:E:605:CDL:H311	1.79	0.65
1:R:117:ALA:O	5:S:15:ARG:NH2	2.30	0.65
16:T:203:CDL:H382	16:T:203:CDL:H772	1.78	0.65
5:S:184:TYR:CE1	16:S:301:CDL:C73	2.79	0.65
16:X:301:CDL:C72	16:Z:203:CDL:C51	2.66	0.65
16:X:301:CDL:C14	16:Z:203:CDL:OB7	2.44	0.65
16:F:704:CDL:H111	16:F:704:CDL:H311	1.79	0.64
16:F:705:CDL:H162	16:F:705:CDL:H771	1.77	0.64
1:L:190:ILE:HD11	6:Z:8:PHE:HZ	1.63	0.64
5:S:189:ASP:OD1	5:S:190:ILE:N	2.30	0.64
10:O:192:HIS:CE1	10:O:210:LEU:HD21	2.33	0.64
5:X:81:SER:OG	5:X:189:ASP:OD2	2.14	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:450:ILE:HG21	2:E:461:LEU:HD13	1.79	0.64
16:X:301:CDL:H141	16:Z:203:CDL:OB7	1.98	0.64
5:X:184:TYR:CZ	16:X:302:CDL:H752	2.32	0.64
1:L:21:MET:HG2	16:L:604:CDL:HA22	1.79	0.64
5:S:157:ALA:HB1	16:S:301:CDL:C51	2.28	0.64
4:K:256:ASN:OD1	4:K:257:VAL:N	2.31	0.64
17:E:602:HEM:HBB2	17:E:602:HEM:HHC	1.79	0.63
5:S:16:VAL:HG23	5:S:24:MET:HE2	1.80	0.63
5:S:43:LEU:HD23	5:S:143:ALA:HA	1.80	0.63
5:X:166:LYS:NZ	16:X:301:CDL:CA5	2.62	0.63
4:Q:225:LEU:O	4:Q:256:ASN:ND2	2.32	0.63
5:S:157:ALA:CB	16:S:301:CDL:C51	2.77	0.63
1:R:120:ARG:HB2	16:S:301:CDL:OA4	1.98	0.62
1:R:274:PHE:CD2	1:R:406:ILE:HG22	2.33	0.62
3:G:117:GLY:N	3:G:185:LYS:O	2.31	0.62
5:S:184:TYR:CE1	16:S:301:CDL:H732	2.34	0.62
16:R:604:CDL:H731	16:R:604:CDL:H512	1.81	0.62
1:R:401:VAL:O	1:R:405:THR:OG1	2.08	0.62
16:T:203:CDL:H721	16:T:203:CDL:H341	1.81	0.62
5:X:157:ALA:HB1	16:X:302:CDL:H512	1.80	0.62
6:Z:97:LEU:HD11	16:Z:202:CDL:C37	2.30	0.62
1:L:120:ARG:HB2	16:X:302:CDL:OA4	2.00	0.62
6:T:97:LEU:CD1	16:T:201:CDL:H351	2.29	0.62
16:E:606:CDL:H771	16:E:606:CDL:H162	1.80	0.62
1:L:250:GLY:O	1:L:254:LEU:N	2.29	0.62
5:X:184:TYR:CE2	16:X:302:CDL:H731	2.33	0.62
1:R:454:ASP:OD1	4:Q:35:TRP:NE1	2.33	0.62
5:S:102:TRP:CE3	5:S:105:ILE:HD11	2.35	0.62
5:X:32:TRP:CE2	16:X:302:CDL:C35	2.83	0.62
4:Q:279:THR:HG21	10:O:126:ARG:HA	1.81	0.62
10:O:122:MET:O	10:O:124:ALA:N	2.32	0.62
5:S:184:TYR:CZ	16:S:301:CDL:H752	2.35	0.61
16:R:604:CDL:H512	16:R:604:CDL:C73	2.30	0.61
1:L:252:VAL:HB	4:K:231:ILE:HD11	1.82	0.61
10:I:229:MET:O	12:Y:358:GLN:NE2	2.33	0.61
23:Y:503:9YF:C14	12:M:108:LEU:HD22	2.31	0.61
2:F:263:ALA:HB1	12:M:148:VAL:HG23	1.81	0.61
11:c:120:GLN:NE2	10:I:152:ALA:O	2.29	0.61
1:R:335:VAL:HG13	1:R:336:PRO:HD3	1.81	0.61
2:E:29:GLN:OE1	2:E:231:TRP:NE1	2.32	0.61
2:E:161:LEU:HD21	2:E:208:TYR:HA	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:113:ILE:N	3:D:153:GLY:O	2.34	0.61
11:c:54:VAL:HG11	11:c:162:VAL:HG11	1.82	0.61
10:I:269:ALA:HB3	10:I:270:PRO:HD3	1.81	0.61
1:L:326:PHE:O	1:L:330:THR:OG1	2.18	0.61
8:V:140:ILE:O	8:V:144:ILE:HD12	2.01	0.60
5:X:91:ALA:HB2	5:X:99:LEU:HD12	1.84	0.60
5:X:157:ALA:HB1	16:X:302:CDL:H511	1.81	0.60
6:Z:126:CYS:HB2	16:Z:203:CDL:H321	1.82	0.60
4:Q:45:LEU:HD21	4:Q:116:VAL:HG22	1.82	0.60
1:L:274:PHE:CD2	1:L:406:ILE:HG22	2.35	0.60
6:T:97:LEU:HD11	16:T:201:CDL:C37	2.31	0.60
18:Z:201:MQ9:H153	23:I:304:9YF:C43	2.32	0.60
4:Q:256:ASN:OD1	4:Q:257:VAL:N	2.34	0.60
9:P:48:MET:SD	16:P:201:CDL:HB61	2.42	0.60
2:F:100:ARG:NH1	23:Y:503:9YF:O12	2.34	0.60
11:c:139:LEU:O	11:c:140:THR:OG1	2.16	0.59
2:F:404:LEU:HD21	12:M:369:GLN:CG	2.32	0.59
1:L:84:THR:O	1:L:88:THR:OG1	2.18	0.59
1:L:227:LEU:HD22	1:L:262:PHE:CZ	2.37	0.59
16:X:301:CDL:C77	16:Z:203:CDL:H551	2.14	0.59
2:F:487:ARG:NH1	6:T:131:GLU:O	2.33	0.59
2:F:533:GLN:OE1	9:P:7:ARG:N	2.36	0.59
2:E:65:ASP:HB3	2:E:91:THR:HG21	1.84	0.59
8:V:148:ARG:HB3	13:A:46:ASP:CB	2.32	0.59
4:Q:193:ARG:NH2	10:O:142:GLN:OE1	2.35	0.59
2:F:87:ARG:NH1	2:F:90:GLU:OE1	2.34	0.59
11:W:159:GLU:N	11:W:159:GLU:OE1	2.36	0.59
16:T:202:CDL:HB22	16:T:202:CDL:HB4	1.84	0.59
16:X:301:CDL:H792	16:Z:203:CDL:H581	1.83	0.59
16:L:604:CDL:H731	16:L:604:CDL:H531	1.84	0.59
16:X:301:CDL:HB22	16:X:301:CDL:HB4	1.84	0.59
2:E:438:ARG:NH2	9:J:35:SER:OG	2.36	0.59
2:E:263:ALA:HB1	12:Y:148:VAL:HG23	1.84	0.58
8:V:125:LEU:HD21	13:A:48:ALA:CA	2.28	0.58
5:X:32:TRP:CZ2	16:X:302:CDL:C38	2.78	0.58
5:X:161:LEU:O	5:X:165:THR:HG23	2.02	0.58
16:F:704:CDL:H371	16:F:704:CDL:H152	1.86	0.58
5:X:41:ALA:HA	6:Z:44:LEU:HD22	1.85	0.58
6:Z:101:THR:HG22	18:Z:201:MQ9:C18	2.33	0.58
1:L:200:GLY:O	1:L:205:ARG:NH2	2.36	0.58
1:R:88:THR:HG22	1:R:151:TRP:HD1	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:35:THR:HG21	6:Z:86:ALA:O	2.03	0.58
1:L:121:LEU:CD1	16:X:302:CDL:HA32	2.29	0.58
1:R:268:TYR:OH	1:R:333:ILE:HD12	2.03	0.58
2:E:312:ILE:HD13	2:E:333:VAL:HG21	1.85	0.58
4:K:45:LEU:CD2	4:K:116:VAL:HG22	2.33	0.58
5:S:32:TRP:CZ2	16:S:301:CDL:C38	2.81	0.57
5:S:32:TRP:CE2	16:S:301:CDL:C35	2.87	0.57
11:c:56:LEU:HD12	11:c:166:ILE:CD1	2.33	0.57
1:R:378:LEU:HD23	4:Q:50:TRP:CZ3	2.38	0.57
1:R:540:ARG:NH2	1:R:554:MET:SD	2.77	0.57
8:V:125:LEU:HD21	13:A:48:ALA:HB3	0.63	0.57
9:P:29:ASP:N	9:P:29:ASP:OD1	2.37	0.57
16:X:301:CDL:C72	16:Z:203:CDL:H511	2.31	0.57
5:S:184:TYR:CE2	16:S:301:CDL:H731	2.39	0.57
2:E:17:ASP:OD1	2:E:23:SER:OG	2.18	0.57
16:T:202:CDL:C17	16:T:203:CDL:H741	2.35	0.57
16:T:203:CDL:HA62	16:T:203:CDL:H712	1.86	0.57
5:X:184:TYR:CE1	16:X:302:CDL:H731	2.40	0.57
2:E:425:VAL:HG22	16:L:604:CDL:H722	1.87	0.57
8:b:68:VAL:HG11	8:b:143:LEU:HD13	1.87	0.57
1:R:357:THR:N	1:R:428:GLU:OE2	2.38	0.57
16:E:605:CDL:H371	16:E:605:CDL:H152	1.86	0.57
2:E:19:ARG:O	2:F:233:GLN:NE2	2.37	0.57
2:E:89:TYR:OH	2:E:287:LEU:O	2.23	0.57
5:S:25:VAL:HG12	5:S:180:VAL:HG11	1.86	0.56
5:S:157:ALA:HA	16:S:301:CDL:H511	1.87	0.56
1:L:122:ASN:OD1	1:L:123:ALA:N	2.38	0.56
10:O:112:ALA:HB2	10:O:224:THR:HG21	1.87	0.56
2:E:66:PRO:O	2:E:67:SER:OG	2.23	0.56
2:E:370:VAL:O	2:E:370:VAL:HG13	2.03	0.56
2:F:422:VAL:HG22	16:F:705:CDL:H402	1.87	0.56
3:D:74:THR:N	3:D:78:THR:O	2.38	0.56
4:Q:140:TRP:NE1	4:Q:284:MET:O	2.39	0.56
4:K:279:THR:HG21	10:I:126:ARG:HA	1.87	0.56
1:R:465:LEU:HD11	4:Q:326:GLU:O	2.05	0.56
2:F:500:GLY:O	12:M:84:ARG:CZ	2.54	0.56
1:L:256:GLN:OE1	1:L:318:THR:HG21	2.05	0.56
4:K:45:LEU:HD21	4:K:116:VAL:HG22	1.87	0.56
1:R:274:PHE:CE2	1:R:406:ILE:HG22	2.40	0.56
16:Z:203:CDL:C16	10:I:281:VAL:HG11	2.33	0.56
1:L:77:GLU:OE1	4:K:332:ARG:NH2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:X:184:TYR:CD1	16:X:302:CDL:H732	2.41	0.56
16:L:604:CDL:H512	16:L:604:CDL:C73	2.33	0.56
2:F:116:PHE:CZ	2:F:120:ILE:HD11	2.41	0.55
16:X:301:CDL:H572	16:X:301:CDL:H742	1.88	0.55
2:E:65:ASP:OD1	2:F:67:SER:OG	2.23	0.55
17:F:703:HEM:HHC	17:F:703:HEM:HBB2	1.88	0.55
1:L:544:GLU:OE2	1:L:555:ARG:NH2	2.39	0.55
1:R:460:ARG:N	15:R:603:HEA:O2A	2.39	0.55
2:F:438:ARG:NH2	9:P:35:SER:OG	2.39	0.55
1:L:274:PHE:CE2	1:L:406:ILE:HG22	2.41	0.55
6:Z:123:THR:HG23	16:Z:203:CDL:H331	1.88	0.55
11:W:148:LEU:HD12	11:W:163:ALA:O	2.06	0.55
1:R:209:PHE:CZ	1:R:213:ILE:HD11	2.42	0.55
2:E:161:LEU:HD21	2:E:208:TYR:CA	2.37	0.55
4:Q:45:LEU:CD2	4:Q:116:VAL:HG22	2.35	0.55
16:R:604:CDL:HB61	16:R:604:CDL:OB4	2.06	0.55
5:S:157:ALA:HB1	16:S:301:CDL:H512	1.87	0.55
1:L:29:TYR:OH	16:Z:202:CDL:OA4	2.23	0.55
5:S:149:LEU:CB	16:S:301:CDL:H801	2.29	0.55
6:T:94:LEU:CD2	16:T:201:CDL:H322	2.30	0.55
16:T:202:CDL:H772	16:T:203:CDL:H582	1.89	0.55
11:c:159:GLU:N	11:c:159:GLU:OE1	2.40	0.55
2:E:104:PHE:HD2	18:E:604:MQ9:H502	1.72	0.55
2:E:213:LEU:HD21	17:F:703:HEM:CBC	2.36	0.55
22:O:302:HEC:HHC	22:O:302:HEC:HBB3	1.89	0.55
6:Z:90:TRP:HH2	16:Z:202:CDL:OB7	1.90	0.55
1:R:122:ASN:OD1	1:R:123:ALA:N	2.40	0.55
1:R:252:VAL:HG21	4:Q:246:LEU:HD22	1.89	0.55
5:X:32:TRP:CH2	16:X:302:CDL:H382	2.42	0.55
6:Z:98:SER:OG	16:Z:202:CDL:C62	2.53	0.55
2:E:116:PHE:CZ	2:E:120:ILE:HD11	2.43	0.55
2:E:282:ASN:ND2	17:E:602:HEM:O1A	2.38	0.55
2:E:368:ARG:O	2:E:434:GLN:NE2	2.39	0.55
1:R:156:PRO:HG3	1:R:252:VAL:HG12	1.88	0.54
11:c:148:LEU:HD12	11:c:163:ALA:O	2.06	0.54
2:E:487:ARG:NH1	6:Z:131:GLU:O	2.39	0.54
16:T:202:CDL:H572	16:T:202:CDL:H742	1.89	0.54
1:R:89:VAL:CG2	1:R:137:ILE:HD11	2.37	0.54
6:T:90:TRP:CZ2	16:T:201:CDL:CB4	2.73	0.54
6:Z:94:LEU:CD2	16:Z:202:CDL:H322	2.31	0.54
10:I:87:CYS:SG	22:I:301:HEC:HAB	2.47	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:R:604:CDL:H792	16:F:705:CDL:H391	1.90	0.54
2:F:194:PHE:CE2	2:F:203:LEU:HD22	2.43	0.54
1:L:386:PHE:O	4:K:242:LYS:NZ	2.32	0.54
4:Q:121:MET:HE1	4:Q:257:VAL:HG13	1.89	0.54
10:O:116:GLN:CG	10:O:122:MET:HE3	2.37	0.54
4:K:288:VAL:HG23	4:K:288:VAL:O	2.07	0.54
10:O:191:CYS:HB2	22:O:302:HEC:HBC2	1.89	0.54
1:R:193:VAL:HG13	1:R:206:MET:HE1	1.90	0.54
6:T:120:PHE:HA	16:T:201:CDL:H612	1.87	0.54
10:O:76:LEU:HD11	10:O:152:ALA:CB	2.38	0.54
1:L:35:THR:HG22	1:L:119:PRO:HB2	1.89	0.54
11:c:42:VAL:HG12	11:c:54:VAL:HG13	1.89	0.54
2:E:312:ILE:HA	2:E:333:VAL:HG21	1.90	0.53
16:L:604:CDL:HB61	16:L:604:CDL:OB4	2.07	0.53
1:R:46:VAL:CG1	16:P:201:CDL:H371	2.38	0.53
5:X:32:TRP:NE1	16:X:302:CDL:C36	2.68	0.53
2:F:172:ARG:NH1	2:F:176:SER:OG	2.41	0.53
5:S:184:TYR:CD1	16:S:301:CDL:H732	2.43	0.53
16:Z:203:CDL:H161	10:I:281:VAL:CG1	2.33	0.53
1:R:398:PHE:HA	1:R:401:VAL:HG22	1.90	0.53
1:L:460:ARG:N	15:L:603:HEA:O2A	2.37	0.53
16:L:604:CDL:H531	16:L:604:CDL:H712	1.91	0.53
5:X:184:TYR:CZ	16:X:302:CDL:C73	2.91	0.53
6:Z:123:THR:HG23	16:Z:203:CDL:C32	2.37	0.53
1:L:194:VAL:HG13	6:Z:1:MET:HE3	1.91	0.53
7:U:72:GLY:N	8:V:110:TYR:O	2.39	0.53
10:I:121:ARG:NE	22:I:302:HEC:O1D	2.41	0.53
1:R:21:MET:HG2	16:R:604:CDL:HA22	1.90	0.53
1:L:243:HIS:ND1	1:L:246:ASP:OD2	2.42	0.53
4:Q:40:THR:HG23	4:Q:43:ALA:H	1.73	0.53
5:X:15:ARG:O	5:X:16:VAL:HG23	2.07	0.53
2:F:404:LEU:HD21	12:M:369:GLN:HG2	1.90	0.53
5:S:157:ALA:HB1	16:S:301:CDL:H511	1.88	0.53
18:Z:201:MQ9:H511	23:c:203:9YF:C22	2.39	0.53
2:F:393:ASN:OD1	2:F:394:ASP:N	2.41	0.53
1:L:259:PHE:O	1:L:263:GLY:N	2.38	0.53
1:R:163:SER:OG	1:R:163:SER:O	2.26	0.53
2:E:367:PRO:O	2:E:374:THR:OG1	2.25	0.53
1:L:387:HIS:NE2	1:L:454:ASP:O	2.38	0.53
2:F:65:ASP:HB3	2:F:91:THR:HG21	1.91	0.53
5:X:99:LEU:C	5:X:99:LEU:HD23	2.33	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:29:ASP:OD1	9:J:29:ASP:N	2.40	0.52
2:E:336:GLY:O	2:E:340:VAL:HG23	2.09	0.52
2:E:499:THR:HG22	2:E:511:HIS:ND1	2.25	0.52
5:S:184:TYR:CE1	16:S:301:CDL:H731	2.41	0.52
16:T:202:CDL:H741	16:T:202:CDL:H611	1.92	0.52
5:X:157:ALA:HA	16:X:302:CDL:H511	1.90	0.52
4:Q:294:ASN:OD1	4:Q:295:ASP:N	2.41	0.52
9:P:45:ILE:HD12	9:P:48:MET:HE3	1.91	0.52
8:b:114:VAL:O	8:b:114:VAL:HG13	2.10	0.52
1:R:419:PRO:HG3	1:R:425:LEU:HD23	1.91	0.52
16:E:605:CDL:OB7	16:F:704:CDL:H112	2.09	0.52
2:F:368:ARG:O	2:F:434:GLN:NE2	2.38	0.52
1:L:419:PRO:HG3	1:L:425:LEU:HD23	1.90	0.52
10:O:110:GLU:OE2	10:O:161:ARG:NH2	2.38	0.52
10:O:187:ASN:O	22:O:302:HEC:HMC3	2.09	0.52
6:Z:98:SER:O	6:Z:101:THR:OG1	2.26	0.52
1:R:398:PHE:O	1:R:402:LEU:HD12	2.10	0.52
7:U:56:GLU:N	7:U:56:GLU:OE1	2.43	0.52
1:R:257:HIS:NE2	6:T:35:GLU:OE1	2.43	0.52
1:L:117:ALA:O	5:X:15:ARG:NH2	2.42	0.52
5:S:32:TRP:NE1	16:S:301:CDL:C36	2.69	0.52
10:I:187:ASN:O	22:I:302:HEC:HMC3	2.09	0.52
12:M:67:THR:HG23	12:M:67:THR:O	2.10	0.52
10:O:76:LEU:HD11	10:O:152:ALA:HB3	1.92	0.52
4:K:245:VAL:HG23	4:K:245:VAL:O	2.09	0.52
10:O:124:ALA:O	22:O:301:HEC:HAC	2.10	0.52
10:O:214:ASN:O	10:O:218:ILE:HD12	2.10	0.52
5:X:32:TRP:CZ2	16:X:302:CDL:C36	2.93	0.52
1:R:169:ASP:OD1	1:R:238:ARG:NE	2.42	0.51
16:T:202:CDL:H732	12:M:145:ILE:HD13	1.92	0.51
4:K:294:ASN:OD1	4:K:295:ASP:N	2.43	0.51
2:E:404:LEU:HD21	12:Y:369:GLN:CG	2.39	0.51
1:L:445:THR:HG23	1:L:446:PHE:CD2	2.45	0.51
1:R:104:ASN:OD1	1:R:122:ASN:ND2	2.43	0.51
1:L:496:PHE:O	1:L:500:ARG:NH2	2.43	0.51
8:V:125:LEU:CG	13:A:48:ALA:CB	2.83	0.51
5:X:157:ALA:CA	16:X:302:CDL:H511	2.40	0.51
2:E:131:GLY:O	2:E:134:ARG:NE	2.41	0.51
10:O:76:LEU:HD13	10:O:149:TYR:HA	1.93	0.51
5:X:149:LEU:CD2	16:X:302:CDL:C63	2.68	0.51
12:M:407:ASP:OD1	12:M:408:PHE:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:175:LEU:O	2:F:179:THR:OG1	2.27	0.51
5:X:189:ASP:OD1	5:X:189:ASP:C	2.54	0.51
9:J:93:LEU:O	9:J:98:TRP:N	2.40	0.51
1:R:158:THR:O	1:R:238:ARG:NH1	2.41	0.51
2:F:433:LEU:CD1	16:F:705:CDL:HA61	2.41	0.51
6:T:120:PHE:CB	16:T:201:CDL:C61	2.84	0.51
5:X:81:SER:HG	5:X:189:ASP:CG	2.16	0.51
6:Z:97:LEU:HD12	16:Z:202:CDL:C35	2.38	0.51
8:b:25:SER:OG	8:b:26:GLY:N	2.44	0.51
9:J:53:LEU:CD1	9:J:87:VAL:HG11	2.41	0.51
2:E:236:THR:HG21	2:E:364:LEU:HD21	1.92	0.51
6:T:94:LEU:HD23	16:T:201:CDL:H352	1.91	0.51
16:X:301:CDL:H741	16:X:301:CDL:H611	1.92	0.51
16:R:604:CDL:H722	2:F:425:VAL:HG22	1.93	0.51
2:F:27:ARG:HB2	12:Y:177:VAL:HG22	1.92	0.51
2:E:227:LEU:HD22	16:E:605:CDL:H782	1.93	0.51
2:E:327:ILE:CG2	2:E:331:VAL:HG11	2.40	0.51
2:E:421:ILE:HG13	16:J:201:CDL:H572	1.92	0.51
2:E:65:ASP:CB	2:E:91:THR:HG21	2.42	0.50
1:L:392:TYR:HD2	1:L:452:LEU:HD23	1.76	0.50
8:b:95:VAL:HG13	8:b:110:TYR:CE1	2.46	0.50
11:W:75:PHE:CZ	11:W:114:VAL:HG11	2.45	0.50
2:E:366:ARG:NH1	2:E:437:ASP:OD2	2.42	0.50
10:O:116:GLN:HG2	10:O:122:MET:HE3	1.92	0.50
2:F:135:ARG:HB3	2:F:136:PRO:CD	2.42	0.50
11:W:56:LEU:HD12	11:W:166:ILE:CD1	2.41	0.50
4:Q:310:ALA:CB	11:W:82:THR:HG21	2.41	0.50
6:T:97:LEU:HD12	16:T:201:CDL:C35	2.39	0.50
12:Y:407:ASP:OD1	12:Y:408:PHE:N	2.42	0.50
1:R:35:THR:HG21	6:T:86:ALA:O	2.12	0.50
1:L:508:ASP:N	1:L:508:ASP:OD1	2.44	0.50
1:L:534:PRO:HB3	1:L:545:LEU:HD12	1.94	0.50
7:a:56:GLU:OE1	7:a:56:GLU:N	2.45	0.50
1:R:89:VAL:HG21	1:R:137:ILE:HD11	1.93	0.50
1:R:496:PHE:O	1:R:500:ARG:NH2	2.44	0.50
16:Z:203:CDL:C57	10:I:282:ALA:HA	2.42	0.50
1:L:15:ARG:NH1	1:L:19:GLU:OE1	2.43	0.50
1:L:35:THR:HG22	1:L:35:THR:O	2.12	0.50
5:S:157:ALA:CA	16:S:301:CDL:H511	2.41	0.50
18:E:604:MQ9:H511	18:E:604:MQ9:H453	1.94	0.50
12:M:347:SER:O	12:M:387:ARG:NH1	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:331:VAL:CG2	23:Y:502:9YF:C42	2.90	0.50
1:L:401:VAL:HG11	15:L:602:HEA:C2C	2.42	0.50
2:E:278:LEU:O	10:I:261:TYR:N	2.40	0.49
5:S:149:LEU:CG	16:S:301:CDL:H631	2.43	0.49
1:R:406:ILE:HD11	15:R:603:HEA:CBC	2.42	0.49
2:F:306:MET:HE1	10:O:269:ALA:HA	1.94	0.49
2:F:478:GLU:OE2	9:P:7:ARG:NH1	2.44	0.49
8:V:149:VAL:HG13	13:A:47:GLY:HA2	1.92	0.49
10:O:192:HIS:ND1	10:O:210:LEU:HD21	2.27	0.49
10:I:124:ALA:O	22:I:301:HEC:HAC	2.12	0.49
12:Y:265:PRO:CG	12:Y:301:LEU:HD23	2.42	0.49
2:F:312:ILE:HG13	2:F:333:VAL:HG21	1.94	0.49
16:L:604:CDL:H612	16:J:201:CDL:H402	1.94	0.49
6:Z:108:LEU:O	6:Z:110:LEU:N	2.44	0.49
1:R:259:PHE:O	1:R:263:GLY:N	2.41	0.49
1:R:445:THR:HG23	1:R:446:PHE:CD2	2.47	0.49
16:E:605:CDL:H112	16:F:704:CDL:OB7	2.12	0.49
2:F:421:ILE:HG13	16:P:201:CDL:H572	1.94	0.49
6:T:90:TRP:HH2	16:T:201:CDL:OB7	1.95	0.49
6:T:108:LEU:O	6:T:110:LEU:N	2.45	0.49
8:V:51:LEU:HB2	8:V:144:ILE:HD11	1.93	0.49
12:M:275:ASP:OD1	12:M:275:ASP:N	2.44	0.49
6:T:98:SER:OG	16:T:201:CDL:C62	2.53	0.49
16:X:301:CDL:C17	16:Z:203:CDL:H731	2.42	0.49
10:I:184:PHE:O	10:I:188:CYS:N	2.46	0.49
12:M:159:ILE:O	12:M:159:ILE:HG22	2.12	0.49
1:R:292:GLY:O	1:R:295:THR:OG1	2.25	0.49
2:F:65:ASP:CB	2:F:91:THR:HG21	2.43	0.49
1:L:371:LEU:HD23	1:L:400:TYR:CE2	2.48	0.49
11:W:95:VAL:HG23	11:W:141:LYS:HE2	1.94	0.49
2:E:127:ILE:HD11	17:E:601:HEM:CAC	2.43	0.49
2:E:433:LEU:CD1	16:E:606:CDL:HA61	2.42	0.49
2:F:104:PHE:HD2	18:F:709:MQ9:H502	1.78	0.49
2:F:275:MET:HE1	10:O:275:MET:HE1	1.95	0.49
5:S:149:LEU:HB3	16:S:301:CDL:C80	2.32	0.49
10:O:235:ARG:NH1	11:W:168:ALA:O	2.46	0.49
22:O:301:HEC:HHD	22:O:301:HEC:CBC	2.42	0.49
4:K:135:ALA:HB3	4:K:245:VAL:HG21	1.93	0.49
6:Z:94:LEU:HD23	16:Z:202:CDL:H352	1.95	0.49
2:E:42:LEU:HD13	2:E:122:VAL:CG1	2.42	0.49
2:F:227:LEU:HD22	16:F:704:CDL:H782	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:87:VAL:HG22	16:J:201:CDL:H511	1.94	0.49
1:R:107:LEU:HD12	1:R:210:THR:HG22	1.94	0.48
2:F:17:ASP:OD2	2:F:23:SER:OG	2.18	0.48
2:F:370:VAL:O	2:F:370:VAL:HG13	2.13	0.48
11:W:42:VAL:HG12	11:W:54:VAL:HG13	1.95	0.48
5:X:167:MET:HE2	16:X:301:CDL:HA31	1.95	0.48
12:M:242:GLY:O	12:M:286:ARG:NH1	2.45	0.48
1:R:515:ASN:N	1:R:515:ASN:OD1	2.44	0.48
16:E:605:CDL:OB7	16:F:704:CDL:C11	2.61	0.48
2:F:336:GLY:O	2:F:340:VAL:HG23	2.12	0.48
10:O:122:MET:SD	22:O:301:HEC:NA	2.87	0.48
12:Y:110:TRP:HZ2	12:Y:127:LEU:HD11	1.78	0.48
11:W:139:LEU:O	11:W:140:THR:OG1	2.17	0.48
12:M:269:MET:HE1	12:M:274:ILE:HD11	1.95	0.48
1:L:96:THR:O	1:L:99:VAL:HG22	2.14	0.48
4:Q:160:ASP:N	4:Q:161:PRO:CD	2.76	0.48
5:S:161:LEU:O	5:S:165:THR:HG23	2.14	0.48
2:E:212:ILE:HD11	2:F:212:ILE:HD11	1.95	0.48
1:L:31:LEU:HD23	16:L:604:CDL:H381	1.96	0.48
5:S:9:GLY:O	5:S:169:LYS:NZ	2.30	0.48
10:O:184:PHE:O	10:O:188:CYS:N	2.45	0.48
16:X:301:CDL:H732	12:Y:145:ILE:HD13	1.95	0.48
6:Z:101:THR:HG22	18:Z:201:MQ9:H18	1.94	0.48
11:c:63:ASP:OD1	12:Y:400:GLY:N	2.46	0.48
12:Y:293:THR:HG23	12:Y:294:THR:HG23	1.96	0.48
12:M:44:ASP:OD1	12:M:45:ALA:N	2.46	0.48
2:E:27:ARG:HB2	12:M:177:VAL:HG22	1.95	0.48
12:M:265:PRO:CG	12:M:301:LEU:HD23	2.44	0.48
1:R:34:THR:HG21	1:R:43:MET:CE	2.43	0.48
1:R:194:VAL:CG1	6:T:1:MET:HE3	2.44	0.48
2:E:123:HIS:NE2	17:E:601:HEM:ND	2.62	0.48
2:F:281:ILE:HD12	10:O:271:GLU:CG	2.43	0.48
5:S:102:TRP:HE3	5:S:105:ILE:HD11	1.78	0.48
12:M:243:TRP:NE1	12:M:310:ASN:O	2.41	0.48
2:E:107:GLN:NE2	2:E:276:GLY:O	2.46	0.48
1:L:156:PRO:HG3	1:L:252:VAL:HG12	1.94	0.48
4:K:230:VAL:HG22	4:K:231:ILE:N	2.29	0.48
2:E:388:THR:HG22	2:E:392:MET:HE2	1.95	0.48
7:U:32:HIS:NE2	8:V:43:PHE:O	2.47	0.48
5:X:32:TRP:CG	16:X:302:CDL:C33	2.85	0.48
9:J:86:LEU:HD23	16:J:201:CDL:H162	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:392:TYR:CD2	1:L:452:LEU:HD23	2.49	0.47
6:T:120:PHE:HB3	16:T:201:CDL:C61	2.35	0.47
6:Z:120:PHE:HB3	16:Z:202:CDL:C62	2.38	0.47
1:R:50:ALA:CB	16:P:201:CDL:H401	2.44	0.47
1:R:221:LEU:HD22	5:S:35:SER:OG	2.14	0.47
1:R:335:VAL:HG13	1:R:336:PRO:CD	2.43	0.47
2:E:147:LEU:HD13	2:E:222:LEU:CB	2.44	0.47
2:E:365:GLN:OE1	2:E:373:ARG:NH2	2.42	0.47
2:E:506:ASP:OD2	12:Y:84:ARG:NH2	2.45	0.47
4:Q:222:GLU:OE2	4:Q:257:VAL:HG21	2.15	0.47
4:Q:275:GLU:O	4:Q:281:HIS:CE1	2.66	0.47
2:E:327:ILE:HG23	2:E:331:VAL:HG11	1.96	0.47
2:F:281:ILE:HD12	10:O:271:GLU:CD	2.39	0.47
5:S:15:ARG:HB3	5:S:24:MET:HE3	1.94	0.47
1:L:104:ASN:OD1	1:L:122:ASN:ND2	2.48	0.47
1:L:221:LEU:HD22	5:X:35:SER:OG	2.14	0.47
16:L:604:CDL:HA4	16:J:201:CDL:H312	1.96	0.47
8:V:149:VAL:CG1	13:A:47:GLY:HA2	2.43	0.47
11:W:42:VAL:O	11:W:54:VAL:HG12	2.14	0.47
5:S:189:ASP:OD1	5:S:189:ASP:C	2.57	0.47
10:O:95:LEU:HD12	10:O:105:LEU:HB2	1.95	0.47
1:R:35:THR:HG22	1:R:119:PRO:HB2	1.97	0.47
16:R:604:CDL:H312	16:R:604:CDL:H342	1.79	0.47
2:E:281:ILE:HD12	10:I:271:GLU:CD	2.39	0.47
2:E:347:TYR:OH	2:E:351:GLU:OE1	2.32	0.47
7:U:38:MET:HE3	7:U:79:TRP:CH2	2.48	0.47
1:R:378:LEU:HD23	4:Q:50:TRP:CH2	2.49	0.47
1:R:403:PHE:CZ	1:R:407:VAL:HG11	2.50	0.47
16:E:605:CDL:C11	16:F:704:CDL:OB7	2.63	0.47
2:F:279:LEU:HD22	10:O:263:LEU:HD21	1.97	0.47
11:c:56:LEU:HD12	11:c:166:ILE:HD13	1.96	0.47
1:R:406:ILE:HD11	15:R:603:HEA:HBC2	1.95	0.47
1:L:120:ARG:NH1	6:Z:131:GLU:OE1	2.44	0.47
18:Z:201:MQ9:H152	10:I:273:MET:HE3	1.97	0.47
16:F:704:CDL:H591	16:F:704:CDL:H621	1.61	0.47
4:K:197:ASN:OD1	4:K:197:ASN:N	2.48	0.47
10:I:210:LEU:HD21	22:I:302:HEC:HHB	1.95	0.47
12:M:230:THR:HG22	12:M:231:ALA:N	2.30	0.47
11:W:63:ASP:OD1	11:W:63:ASP:N	2.48	0.47
1:R:35:THR:HG22	1:R:35:THR:O	2.15	0.46
8:V:125:LEU:HD11	13:A:193:ARG:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:140:TRP:NE1	4:K:284:MET:O	2.47	0.46
6:Z:123:THR:HG23	16:Z:203:CDL:C33	2.45	0.46
22:I:302:HEC:CBB	22:I:302:HEC:HHC	2.45	0.46
12:Y:230:THR:HG23	12:Y:244:THR:HG22	1.96	0.46
12:M:271:PRO:O	12:M:316:ARG:NH1	2.48	0.46
1:R:77:GLU:OE2	4:Q:332:ARG:NH1	2.43	0.46
1:R:266:GLU:OE1	1:R:270:ILE:HD12	2.15	0.46
8:V:149:VAL:CG1	13:A:47:GLY:CA	2.92	0.46
12:Y:44:ASP:OD1	12:Y:45:ALA:N	2.48	0.46
2:E:392:MET:SD	10:I:269:ALA:HB1	2.54	0.46
2:E:440:VAL:HG21	2:E:486:LYS:HG2	1.97	0.46
5:S:160:LEU:CD2	6:T:129:VAL:HG11	2.46	0.46
5:X:91:ALA:CB	5:X:99:LEU:HD12	2.45	0.46
11:W:30:SER:HG	11:W:33:THR:HG1	1.61	0.46
2:F:282:ASN:ND2	17:F:703:HEM:O1A	2.42	0.46
1:L:46:VAL:CG1	16:J:201:CDL:H371	2.46	0.46
8:V:44:PRO:O	8:V:47:ASP:OD1	2.34	0.46
11:c:75:PHE:CZ	11:c:114:VAL:HG11	2.50	0.46
2:F:388:THR:HG22	2:F:392:MET:HE2	1.98	0.46
22:I:302:HEC:HHD	22:I:302:HEC:CBC	2.46	0.46
2:E:450:ILE:HD12	6:Z:81:GLU:OE2	2.16	0.46
1:L:186:GLY:O	1:L:190:ILE:HG22	2.16	0.46
8:b:110:TYR:OH	8:b:123:ALA:HB2	2.16	0.46
10:I:112:ALA:HB2	10:I:224:THR:HG21	1.97	0.46
10:I:234:ASP:O	10:I:238:THR:HA	2.15	0.46
1:L:33:THR:HG22	6:Z:90:TRP:HB3	1.97	0.46
8:b:76:ASP:OD1	8:b:76:ASP:N	2.46	0.46
2:F:244:THR:HG21	2:F:536:ILE:HG21	1.96	0.46
1:L:465:LEU:HD21	4:K:328:PHE:CD1	2.51	0.46
6:T:97:LEU:O	6:T:101:THR:HG23	2.15	0.46
16:X:301:CDL:H792	16:Z:203:CDL:C58	2.46	0.46
8:b:99:VAL:HG21	8:b:134:PHE:CE2	2.51	0.46
12:M:42:PRO:O	12:M:43:THR:OG1	2.32	0.46
1:R:532:GLU:OE2	8:V:23:THR:OG1	2.33	0.46
16:R:604:CDL:C64	20:W:201:PLM:CG	2.90	0.46
2:F:147:LEU:HD13	2:F:222:LEU:HB2	1.96	0.46
2:F:414:GLY:O	2:F:418:LEU:N	2.48	0.46
1:L:505:VAL:O	1:L:505:VAL:HG13	2.15	0.46
16:T:202:CDL:H622	16:T:202:CDL:H791	1.98	0.46
6:Z:120:PHE:CD2	16:Z:202:CDL:C63	2.88	0.46
2:E:194:PHE:CE2	2:E:203:LEU:HD22	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:419:PRO:CG	1:L:425:LEU:HD23	2.46	0.45
11:c:42:VAL:O	11:c:54:VAL:HG12	2.15	0.45
1:R:56:GLY:N	1:R:90:MET:HE2	2.30	0.45
1:R:84:THR:OG1	1:R:149:PHE:O	2.25	0.45
1:R:310:VAL:HG11	1:R:333:ILE:HD13	1.97	0.45
1:L:309:ALA:HB3	1:L:329:MET:HE1	1.98	0.45
12:Y:355:LEU:N	12:Y:355:LEU:HD12	2.32	0.45
1:R:77:GLU:OE2	4:Q:332:ARG:NH2	2.49	0.45
1:R:118:PHE:HB3	16:S:301:CDL:OA3	2.16	0.45
1:R:385:ASP:O	1:R:389:THR:OG1	2.10	0.45
8:V:47:ASP:OD1	8:V:47:ASP:C	2.58	0.45
11:c:57:ARG:NH1	11:c:116:GLU:O	2.46	0.45
12:Y:347:SER:O	12:Y:387:ARG:NH1	2.44	0.45
2:F:499:THR:HG22	2:F:511:HIS:ND1	2.30	0.45
1:L:264:HIS:O	1:L:267:VAL:HG22	2.16	0.45
16:L:604:CDL:H711	16:L:604:CDL:C81	2.46	0.45
12:M:349:LEU:HD12	12:M:368:HIS:CE1	2.52	0.45
12:M:364:LEU:HD12	12:M:365:CYS:H	1.82	0.45
1:R:84:THR:O	1:R:88:THR:HG23	2.16	0.45
6:T:8:PHE:CE1	6:T:52:THR:HG21	2.51	0.45
5:X:37:LEU:HD22	6:Z:51:ILE:HD12	1.99	0.45
12:Y:230:THR:HG22	12:Y:231:ALA:N	2.32	0.45
12:Y:243:TRP:NE1	12:Y:310:ASN:O	2.42	0.45
1:R:153:ALA:O	1:R:255:TRP:NE1	2.50	0.45
1:R:190:ILE:HD11	6:T:8:PHE:HZ	1.81	0.45
4:Q:32:ALA:HB1	4:Q:35:TRP:HB2	1.98	0.45
5:S:163:ALA:HB1	16:T:202:CDL:HA61	1.98	0.45
8:V:68:VAL:HG13	8:V:143:LEU:HD22	1.99	0.45
4:K:145:GLN:O	4:K:158:GLY:N	2.49	0.45
5:X:41:ALA:CA	6:Z:44:LEU:HD22	2.45	0.45
6:Z:97:LEU:HD13	16:Z:202:CDL:H351	1.97	0.45
10:I:72:GLN:OE1	10:I:74:ALA:N	2.50	0.45
12:Y:335:ASN:ND2	12:Y:337:GLY:O	2.49	0.45
1:L:20:ARG:NH1	8:b:52:ASP:OD1	2.45	0.45
1:L:111:ILE:HD12	1:L:196:MET:O	2.17	0.45
5:S:41:ALA:HA	6:T:44:LEU:HD22	1.98	0.45
6:Z:91:TRP:N	6:Z:92:PRO:CD	2.80	0.45
16:L:604:CDL:H522	16:L:604:CDL:H552	1.68	0.45
4:Q:195:TYR:CE2	4:Q:247:PRO:O	2.70	0.45
10:O:122:MET:HA	10:O:122:MET:HE2	1.99	0.45
16:X:301:CDL:H622	16:X:301:CDL:H791	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:147:LEU:HD13	2:F:222:LEU:CB	2.47	0.45
18:F:709:MQ9:H511	18:F:709:MQ9:H453	1.98	0.45
10:O:149:TYR:O	10:O:153:ASN:ND2	2.50	0.45
5:X:157:ALA:CB	16:X:302:CDL:H512	2.43	0.45
8:b:95:VAL:HG13	8:b:110:TYR:HE1	1.82	0.45
2:E:56:THR:HG22	18:E:604:MQ9:H451	1.99	0.45
2:E:392:MET:HE1	18:I:303:MQ9:C3C	2.47	0.45
16:L:604:CDL:H381	16:L:604:CDL:H412	1.72	0.45
1:R:417:TRP:NE1	1:R:518:GLU:OE2	2.46	0.44
2:F:147:LEU:HD21	2:F:223:ILE:HG13	1.98	0.44
2:F:284:ILE:O	2:F:287:LEU:O	2.35	0.44
2:F:409:TRP:CZ3	9:P:76:LEU:HD11	2.52	0.44
7:U:2:SER:O	7:U:5:LEU:N	2.51	0.44
5:X:166:LYS:NZ	16:X:301:CDL:C12	2.78	0.44
12:Y:221:LYS:HG2	23:Y:503:9YF:O6	2.16	0.44
12:M:230:THR:HG23	12:M:244:THR:HG22	1.98	0.44
12:M:358:GLN:C	12:M:360:THR:H	2.25	0.44
2:F:366:ARG:NH1	2:F:437:ASP:OD2	2.46	0.44
2:F:514:LEU:HD11	12:M:81:ALA:HB3	1.99	0.44
5:X:25:VAL:HG12	5:X:180:VAL:HG11	1.99	0.44
1:L:385:ASP:O	1:L:389:THR:CB	2.66	0.44
1:L:406:ILE:HD11	15:L:603:HEA:CBC	2.47	0.44
6:T:120:PHE:CG	16:T:201:CDL:H632	2.51	0.44
5:X:184:TYR:CD1	16:X:302:CDL:C73	2.99	0.44
1:L:310:VAL:O	1:L:310:VAL:HG13	2.16	0.44
1:L:323:LEU:HD23	4:K:117:GLN:CD	2.42	0.44
4:Q:179:ILE:HG23	4:Q:180:GLU:N	2.33	0.44
12:M:344:LYS:O	12:M:353:SER:N	2.44	0.44
2:E:213:LEU:HD21	17:F:703:HEM:HBC1	1.98	0.44
1:L:11:LEU:CD1	7:a:48:LEU:HD22	2.47	0.44
5:S:32:TRP:CZ2	16:S:301:CDL:C36	3.00	0.44
10:O:222:MET:HG3	22:O:302:HEC:HMB2	1.99	0.44
6:Z:8:PHE:CE2	6:Z:52:THR:HG21	2.52	0.44
12:Y:358:GLN:C	12:Y:360:THR:H	2.26	0.44
12:M:172:VAL:HG13	12:M:173:HIS:N	2.33	0.44
16:R:604:CDL:H751	16:R:604:CDL:H562	2.00	0.44
5:S:157:ALA:CB	16:S:301:CDL:H512	2.46	0.44
9:J:33:VAL:HG11	9:J:41:SER:OG	2.18	0.44
12:M:418:GLU:OE1	12:M:418:GLU:N	2.48	0.44
1:R:242:ALA:O	5:S:138:SER:CB	2.66	0.44
1:R:252:VAL:HG22	4:Q:252:ASN:CG	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:135:ARG:NH1	2:F:358:ASP:O	2.51	0.44
2:F:233:GLN:O	2:F:234:LYS:C	2.60	0.44
12:Y:271:PRO:O	12:Y:316:ARG:NH1	2.51	0.44
1:R:535:ARG:NH1	6:T:74:GLU:OE2	2.48	0.44
2:E:183:PRO:O	12:Y:417:TRP:CG	2.71	0.44
2:E:306:MET:HE1	10:I:269:ALA:HA	2.00	0.44
1:L:50:ALA:CB	16:J:201:CDL:H401	2.48	0.44
1:L:280:GLU:OE1	1:L:516:SER:OG	2.29	0.44
1:L:313:HIS:CD2	1:L:313:HIS:C	2.96	0.44
4:Q:230:VAL:O	4:Q:232:HIS:ND1	2.51	0.44
2:E:116:PHE:CE1	2:E:120:ILE:HD11	2.51	0.43
5:X:32:TRP:HZ2	16:X:302:CDL:C38	2.25	0.43
1:R:63:ARG:HE	1:R:63:ARG:HA	1.83	0.43
2:E:147:LEU:HD21	2:E:223:ILE:HG13	2.01	0.43
5:S:184:TYR:CD1	16:S:301:CDL:C73	3.01	0.43
10:O:83:PHE:CZ	10:O:95:LEU:HD13	2.53	0.43
1:R:248:ALA:HB3	4:Q:185:ILE:CD1	2.48	0.43
1:L:242:ALA:O	5:X:138:SER:CB	2.66	0.43
16:T:203:CDL:H411	16:T:203:CDL:H381	1.61	0.43
5:X:151:VAL:HG22	5:X:188:VAL:HG11	2.00	0.43
11:W:107:PRO:HD3	11:W:112:LEU:HD12	1.99	0.43
1:R:84:THR:HG21	1:R:147:ALA:HB3	2.00	0.43
1:R:546:HIS:NE2	8:V:29:SER:OG	2.42	0.43
2:E:500:GLY:O	12:Y:84:ARG:CZ	2.66	0.43
2:E:512:GLU:O	2:E:516:GLU:CD	2.61	0.43
2:F:340:VAL:HG22	18:F:708:MQ9:H401	2.01	0.43
1:L:290:ILE:HG23	1:L:290:ILE:O	2.18	0.43
8:V:125:LEU:HD23	13:A:48:ALA:CB	2.21	0.43
10:O:123:PRO:O	10:O:125:MET:HE1	2.19	0.43
16:X:301:CDL:H761	16:Z:203:CDL:C53	2.37	0.43
8:b:50:VAL:HG22	9:J:99:ILE:HD11	2.00	0.43
2:F:416:VAL:HG11	9:P:58:PHE:CD2	2.53	0.43
16:F:705:CDL:H542	16:F:705:CDL:H712	2.00	0.43
1:L:522:SER:OG	1:L:524:PRO:O	2.37	0.43
15:L:603:HEA:H251	16:L:604:CDL:H632	2.00	0.43
16:T:203:CDL:HA22	10:O:293:ARG:CZ	2.48	0.43
5:X:166:LYS:HZ1	16:X:301:CDL:C12	2.23	0.43
7:a:2:SER:O	7:a:5:LEU:N	2.51	0.43
11:c:56:LEU:HD11	11:c:151:PHE:HE2	1.84	0.43
22:I:302:HEC:HHC	22:I:302:HEC:HBB3	2.00	0.43
22:I:302:HEC:HHD	22:I:302:HEC:HBC3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Y:41:GLN:NE2	12:Y:46:GLU:OE2	2.52	0.43
12:M:134:LEU:HD23	12:M:134:LEU:C	2.44	0.43
2:F:422:VAL:CG2	16:F:705:CDL:H402	2.49	0.43
16:F:705:CDL:H762	16:F:705:CDL:H792	1.80	0.43
1:L:194:VAL:CG1	6:Z:1:MET:HE3	2.49	0.43
6:T:91:TRP:N	6:T:92:PRO:CD	2.81	0.43
5:X:136:TYR:CD1	5:X:136:TYR:C	2.96	0.43
1:R:110:GLN:OE1	1:R:210:THR:HG23	2.18	0.43
2:E:225:ALA:HA	16:E:605:CDL:H351	2.00	0.43
4:K:232:HIS:HB2	4:K:273:CYS:SG	2.58	0.43
1:R:384:LEU:CD1	4:Q:49:LEU:HD23	2.48	0.43
16:E:606:CDL:H722	16:Z:202:CDL:H111	2.00	0.43
2:F:171:ILE:HD12	2:F:175:LEU:HD12	2.00	0.43
8:V:78:ALA:O	8:V:82:ARG:NH1	2.51	0.43
4:K:159:ALA:C	4:K:161:PRO:HD3	2.42	0.43
4:K:195:TYR:CE1	4:K:247:PRO:O	2.72	0.43
12:Y:172:VAL:HG13	12:Y:173:HIS:N	2.33	0.43
12:Y:348:HIS:O	24:Y:501:FES:S1	2.77	0.43
1:R:452:LEU:HD11	1:R:457:MET:SD	2.59	0.43
4:Q:81:ASP:O	4:Q:83:GLU:N	2.50	0.43
4:Q:139:ASN:OD1	4:Q:205:GLY:O	2.37	0.43
8:b:68:VAL:HG13	8:b:143:LEU:HD22	2.01	0.43
11:c:95:VAL:O	11:c:141:LYS:NZ	2.40	0.43
16:R:604:CDL:H612	16:P:201:CDL:H402	2.01	0.43
2:F:400:PHE:HA	6:T:108:LEU:HD13	2.01	0.43
10:O:189:ALA:O	10:O:190:SER:C	2.62	0.43
5:X:157:ALA:HB2	16:X:302:CDL:C53	2.36	0.43
12:Y:85:THR:HG21	12:Y:153:LYS:HB3	2.01	0.43
1:R:47:VAL:CG2	16:R:604:CDL:H371	2.49	0.42
1:R:424:ARG:NH1	1:R:500:ARG:O	2.52	0.42
2:F:267:MET:HE2	12:M:148:VAL:HG21	1.99	0.42
6:T:8:PHE:CZ	6:T:52:THR:HG21	2.54	0.42
10:O:210:LEU:HD22	22:O:302:HEC:C3A	2.48	0.42
4:K:98:LEU:HD12	4:K:98:LEU:C	2.44	0.42
5:X:32:TRP:HB2	16:X:302:CDL:C33	2.44	0.42
10:I:149:TYR:O	10:I:153:ASN:ND2	2.52	0.42
1:R:193:VAL:HG11	1:R:214:LEU:HD13	2.01	0.42
2:E:134:ARG:O	2:E:135:ARG:C	2.62	0.42
2:F:123:HIS:NE2	17:F:702:HEM:ND	2.67	0.42
2:F:425:VAL:CG1	16:F:705:CDL:H371	2.46	0.42
4:Q:128:GLU:OE1	4:Q:220:ARG:N	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:151:VAL:HG22	5:S:188:VAL:HG11	2.00	0.42
5:X:96:VAL:HG22	5:X:170:PHE:HB2	2.01	0.42
5:X:160:LEU:CD2	6:Z:129:VAL:HG11	2.49	0.42
6:Z:95:ILE:CD1	6:Z:128:LEU:HD22	2.48	0.42
12:Y:190:LEU:O	12:Y:191:LYS:CG	2.67	0.42
1:R:111:ILE:HD12	1:R:196:MET:O	2.19	0.42
1:R:221:LEU:HD13	5:S:31:VAL:HG13	2.01	0.42
16:R:604:CDL:H312	16:R:604:CDL:HA61	1.82	0.42
2:F:420:ALA:HB2	16:P:201:CDL:H771	2.01	0.42
4:Q:179:ILE:O	4:Q:180:GLU:C	2.62	0.42
8:V:114:VAL:HG12	8:V:119:ILE:HG21	2.00	0.42
16:X:301:CDL:C75	16:Z:203:CDL:H532	2.50	0.42
11:W:75:PHE:CE2	11:W:114:VAL:HG11	2.54	0.42
16:E:605:CDL:H591	16:E:605:CDL:H621	1.61	0.42
2:F:311:LEU:HD23	2:F:333:VAL:HG23	1.99	0.42
12:Y:195:VAL:HG23	12:Y:196:ILE:HD12	2.01	0.42
16:R:604:CDL:H381	16:R:604:CDL:H412	1.39	0.42
15:L:602:HEA:C18	15:L:602:HEA:H261	2.48	0.42
4:Q:204:LEU:HD22	10:O:84:GLU:HB3	2.01	0.42
8:V:119:ILE:HG23	8:V:120:GLU:N	2.35	0.42
10:I:191:CYS:SG	10:I:201:LEU:HD21	2.59	0.42
12:Y:159:ILE:O	12:Y:159:ILE:HG22	2.20	0.42
1:R:454:ASP:OD1	4:Q:35:TRP:CD1	2.73	0.42
16:F:705:CDL:H391	16:T:201:CDL:C42	2.50	0.42
6:T:120:PHE:HA	16:T:201:CDL:C61	2.48	0.42
10:I:269:ALA:HB3	10:I:270:PRO:CD	2.47	0.42
11:W:70:THR:HG23	11:W:70:THR:O	2.20	0.42
12:M:364:LEU:HD12	12:M:365:CYS:N	2.35	0.42
2:E:197:ASP:OD2	12:Y:309:ARG:NH2	2.48	0.42
4:Q:96:LEU:HA	4:Q:99:THR:HG22	2.02	0.42
4:K:193:ARG:NH2	10:I:137:HIS:O	2.52	0.42
10:I:191:CYS:CB	22:I:302:HEC:HBC2	2.50	0.42
1:R:29:TYR:O	1:R:33:THR:OG1	2.32	0.42
1:R:88:THR:HG21	1:R:171:TRP:NE1	2.30	0.42
16:R:604:CDL:H611	16:R:604:CDL:H582	1.75	0.42
1:L:163:SER:OG	1:L:163:SER:O	2.36	0.42
5:S:36:GLU:OE1	5:S:150:HIS:NE2	2.41	0.42
8:b:62:ALA:O	8:b:117:ARG:NH2	2.52	0.42
16:R:604:CDL:H531	16:R:604:CDL:H712	2.02	0.42
16:L:604:CDL:H312	16:L:604:CDL:H342	1.91	0.42
8:V:76:ASP:OD1	8:V:76:ASP:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:157:ASP:OD1	4:K:158:GLY:N	2.51	0.42
11:c:174:ARG:NH1	12:Y:272:GLU:OE2	2.52	0.42
10:I:189:ALA:O	10:I:190:SER:C	2.61	0.42
1:R:31:LEU:O	1:R:34:THR:HG22	2.19	0.41
1:R:120:ARG:NH1	6:T:131:GLU:OE1	2.48	0.41
1:R:310:VAL:O	1:R:310:VAL:HG13	2.20	0.41
2:F:107:GLN:NE2	2:F:276:GLY:O	2.53	0.41
1:L:401:VAL:O	1:L:405:THR:OG1	2.11	0.41
4:Q:319:PRO:HA	4:Q:320:PRO:HD3	1.99	0.41
7:U:44:HIS:CE1	7:U:47:ILE:HD11	2.55	0.41
10:O:229:MET:HE3	22:O:302:HEC:C4B	2.50	0.41
6:Z:87:PRO:O	6:Z:88:HIS:C	2.62	0.41
12:Y:387:ARG:CZ	12:Y:415:ALA:HB2	2.50	0.41
12:M:345:VAL:O	12:M:345:VAL:HG23	2.19	0.41
2:E:404:LEU:HD21	12:Y:369:GLN:HG2	2.00	0.41
2:F:183:PRO:O	12:M:417:TRP:CG	2.74	0.41
2:F:225:ALA:HA	16:F:704:CDL:H351	2.01	0.41
16:F:704:CDL:H551	16:F:704:CDL:H581	1.70	0.41
1:L:26:ASN:OD1	1:L:26:ASN:C	2.63	0.41
1:L:56:GLY:HA2	1:L:90:MET:HE2	2.02	0.41
16:L:604:CDL:H771	16:L:604:CDL:H742	1.39	0.41
4:Q:264:GLN:OE1	4:Q:264:GLN:N	2.50	0.41
4:K:281:HIS:O	4:K:281:HIS:ND1	2.53	0.41
8:b:108:VAL:HG12	8:b:110:TYR:CE1	2.55	0.41
8:b:119:ILE:HG23	8:b:120:GLU:N	2.35	0.41
9:J:85:ALA:HB1	16:J:201:CDL:H161	2.01	0.41
11:c:42:VAL:HG22	11:c:43:ASN:N	2.34	0.41
10:I:263:LEU:HD12	10:I:263:LEU:H	1.85	0.41
2:F:68:MET:HE1	2:F:204:ILE:H	1.85	0.41
2:F:312:ILE:CG1	2:F:333:VAL:HG21	2.49	0.41
1:L:212:ASN:ND2	1:L:272:LEU:O	2.45	0.41
9:P:93:LEU:O	9:P:98:TRP:N	2.41	0.41
4:K:179:ILE:O	4:K:180:GLU:C	2.62	0.41
10:I:210:LEU:HD21	22:I:302:HEC:CHB	2.50	0.41
16:R:604:CDL:H522	16:R:604:CDL:H552	1.43	0.41
4:Q:168:THR:O	4:Q:168:THR:HG23	2.20	0.41
5:S:149:LEU:HG	16:S:301:CDL:H631	2.02	0.41
10:O:191:CYS:HB3	22:O:302:HEC:HBC2	1.99	0.41
11:W:42:VAL:HG22	11:W:43:ASN:N	2.35	0.41
12:M:195:VAL:HG23	12:M:196:ILE:HD12	2.02	0.41
2:E:59:TRP:CE3	2:E:105:VAL:HG11	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:56:THR:HA	18:F:709:MQ9:H451	2.01	0.41
18:F:701:MQ9:H403	18:F:701:MQ9:H421	1.84	0.41
4:K:219:LYS:O	4:K:221:ILE:HD12	2.20	0.41
16:Z:203:CDL:OB4	10:I:289:TRP:HD1	2.03	0.41
16:Z:203:CDL:HB22	10:I:293:ARG:HH12	1.84	0.41
10:I:122:MET:HE3	10:I:122:MET:HA	2.01	0.41
1:R:256:GLN:HB3	1:R:315:MET:SD	2.61	0.41
16:E:605:CDL:H362	16:E:605:CDL:H332	1.67	0.41
2:F:208:TYR:CE2	2:F:212:ILE:HD13	2.55	0.41
4:Q:186:ARG:NH1	5:S:53:GLN:O	2.45	0.41
10:O:199:GLY:O	10:O:207:ALA:N	2.52	0.41
12:M:190:LEU:O	12:M:191:LYS:CG	2.69	0.41
1:R:90:MET:HB3	15:R:603:HEA:CAC	2.50	0.41
2:E:532:HIS:CD2	2:E:536:ILE:HD11	2.55	0.41
2:F:235:HIS:ND1	2:F:236:THR:O	2.50	0.41
1:L:19:GLU:O	1:L:424:ARG:NH2	2.54	0.41
1:L:205:ARG:NH1	1:L:537:ARG:O	2.50	0.41
4:Q:121:MET:HE2	4:Q:123:LYS:HG3	2.01	0.41
5:S:96:VAL:HG22	5:S:170:PHE:CB	2.50	0.41
6:T:87:PRO:O	6:T:88:HIS:C	2.64	0.41
5:X:103:TYR:OH	5:X:178:ALA:O	2.38	0.41
16:X:301:CDL:H312	16:X:301:CDL:HA61	1.82	0.41
9:J:48:MET:HG2	16:J:201:CDL:HB61	2.03	0.41
1:R:420:LYS:NZ	1:R:521:THR:O	2.53	0.41
16:R:604:CDL:H512	16:R:604:CDL:H732	2.01	0.41
5:S:24:MET:HE1	6:T:85:PHE:CE1	2.56	0.41
5:X:102:TRP:CE3	5:X:105:ILE:HD11	2.55	0.41
16:X:301:CDL:H141	16:X:301:CDL:H712	2.03	0.41
18:E:603:MQ9:H421	18:E:603:MQ9:H403	1.82	0.41
2:F:59:TRP:CE3	2:F:105:VAL:HG11	2.56	0.41
2:F:89:TYR:OH	2:F:284:ILE:O	2.37	0.41
2:F:392:MET:SD	10:O:269:ALA:HB1	2.61	0.41
7:U:23:LEU:O	7:U:27:THR:OG1	2.24	0.41
7:U:56:GLU:O	7:U:57:HIS:C	2.63	0.41
22:O:301:HEC:CMB	22:O:301:HEC:HBB3	2.51	0.41
4:K:222:GLU:OE2	4:K:257:VAL:HG21	2.21	0.41
5:X:163:ALA:HB1	16:X:301:CDL:HA61	2.03	0.41
8:b:96:LEU:HD21	8:b:98:ALA:HB2	2.03	0.41
1:R:371:LEU:HD23	1:R:400:TYR:HE2	1.86	0.41
2:E:147:LEU:HD13	2:E:222:LEU:HB2	2.02	0.41
2:F:116:PHE:CE1	2:F:120:ILE:HD11	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:164:ASP:OD1	2:F:165:LEU:N	2.54	0.41
2:F:441:LEU:HD21	2:F:484:LEU:HD21	2.02	0.41
10:I:190:SER:O	12:Y:355:LEU:HD11	2.20	0.41
1:L:162:HIS:O	1:L:163:SER:OG	2.33	0.40
4:Q:288:VAL:O	4:Q:288:VAL:HG13	2.20	0.40
8:b:150:MET:O	8:b:154:VAL:HG23	2.22	0.40
11:W:56:LEU:HD12	11:W:166:ILE:HD13	2.01	0.40
11:W:148:LEU:HD11	12:M:319:PRO:CB	2.46	0.40
1:L:103:ALA:HB1	1:L:189:MET:SD	2.61	0.40
1:L:159:ASP:O	1:L:162:HIS:O	2.38	0.40
5:S:80:SER:HA	5:S:109:MET:HE3	2.03	0.40
10:I:116:GLN:HG2	10:I:122:MET:SD	2.60	0.40
11:W:121:ILE:HG22	11:W:123:ALA:H	1.86	0.40
2:E:104:PHE:CD2	18:E:604:MQ9:H502	2.54	0.40
2:E:233:GLN:O	2:E:234:LYS:C	2.62	0.40
2:E:532:HIS:NE2	2:E:536:ILE:HD11	2.36	0.40
1:L:221:LEU:HD13	5:X:31:VAL:HG13	2.03	0.40
4:Q:101:ILE:HG22	4:Q:102:PRO:HD3	2.03	0.40
10:O:116:GLN:CG	10:O:122:MET:HG2	2.52	0.40
5:X:41:ALA:HB2	6:Z:44:LEU:CB	2.51	0.40
12:M:357:GLU:O	12:M:361:TYR:N	2.55	0.40
2:E:178:ILE:HD11	2:E:312:ILE:HD11	2.03	0.40
2:F:509:VAL:HG23	2:F:510:GLU:N	2.37	0.40
1:L:122:ASN:OD1	1:L:122:ASN:C	2.65	0.40
4:Q:135:ALA:O	4:Q:232:HIS:NE2	2.53	0.40
4:Q:230:VAL:HG13	4:Q:232:HIS:HD1	1.85	0.40
6:T:48:LEU:HD23	6:T:48:LEU:C	2.46	0.40
6:T:97:LEU:HD13	16:T:201:CDL:H351	2.01	0.40
9:P:85:ALA:HB1	16:P:201:CDL:H161	2.03	0.40
4:K:81:ASP:O	4:K:83:GLU:N	2.53	0.40
16:Z:203:CDL:OB3	10:I:289:TRP:HA	2.22	0.40
11:c:103:ASP:HA	11:c:133:VAL:HG13	2.03	0.40
12:M:265:PRO:HG2	12:M:301:LEU:HD23	2.02	0.40
1:R:122:ASN:OD1	1:R:122:ASN:C	2.65	0.40
1:R:270:ILE:CG2	1:R:406:ILE:HG21	2.49	0.40
2:E:56:THR:HA	18:E:604:MQ9:H451	2.04	0.40
2:E:435:ARG:NH2	9:J:32:ASP:O	2.54	0.40
2:F:296:SER:OG	2:F:297:ALA:N	2.54	0.40
1:L:21:MET:HE2	1:L:500:ARG:HD3	2.04	0.40
1:L:153:ALA:HB1	1:L:158:THR:HG21	2.03	0.40
1:L:384:LEU:CD1	4:K:49:LEU:HD23	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:12:ILE:HG21	6:T:133:TYR:CZ	2.56	0.40
5:S:32:TRP:HZ2	16:S:301:CDL:C38	2.26	0.40
16:T:203:CDL:H712	16:T:203:CDL:CA6	2.52	0.40
12:Y:255:ALA:HB2	12:Y:285:TRP:HB3	2.04	0.40
12:M:348:HIS:O	24:M:503:FES:S2	2.80	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	L	550/566 (97%)	516 (94%)	34 (6%)	0	100	100
1	R	550/566 (97%)	518 (94%)	32 (6%)	0	100	100
2	E	533/535 (100%)	490 (92%)	43 (8%)	0	100	100
2	F	533/535 (100%)	489 (92%)	43 (8%)	1 (0%)	43	73
3	D	214/216 (99%)	193 (90%)	20 (9%)	1 (0%)	24	59
3	G	214/216 (99%)	187 (87%)	27 (13%)	0	100	100
4	K	310/312 (99%)	282 (91%)	28 (9%)	0	100	100
4	Q	310/312 (99%)	282 (91%)	28 (9%)	0	100	100
5	S	201/203 (99%)	193 (96%)	8 (4%)	0	100	100
5	X	201/203 (99%)	192 (96%)	9 (4%)	0	100	100
6	T	137/139 (99%)	129 (94%)	8 (6%)	0	100	100
6	Z	137/139 (99%)	130 (95%)	7 (5%)	0	100	100
7	U	77/79 (98%)	70 (91%)	6 (8%)	1 (1%)	9	40
7	a	77/79 (98%)	70 (91%)	7 (9%)	0	100	100
8	V	143/145 (99%)	139 (97%)	4 (3%)	0	100	100
8	b	143/145 (99%)	138 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	J	88/100 (88%)	85 (97%)	3 (3%)	0	100	100
9	P	88/100 (88%)	84 (96%)	4 (4%)	0	100	100
10	I	221/223 (99%)	199 (90%)	22 (10%)	0	100	100
10	O	221/223 (99%)	199 (90%)	22 (10%)	0	100	100
11	W	154/159 (97%)	137 (89%)	17 (11%)	0	100	100
11	c	154/159 (97%)	135 (88%)	19 (12%)	0	100	100
12	M	380/382 (100%)	344 (90%)	36 (10%)	0	100	100
12	Y	380/382 (100%)	348 (92%)	31 (8%)	1 (0%)	36	68
13	A	483/510 (95%)	474 (98%)	7 (1%)	2 (0%)	30	62
All	All	6499/6628 (98%)	6023 (93%)	470 (7%)	6 (0%)	49	79

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	135	ARG
13	A	63	HIS
12	Y	113	GLU
3	D	27	THR
13	A	436	GLY
7	U	70	VAL

5.3.2 Protein sidechains (i)

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	L	452/465 (97%)	445 (98%)	7 (2%)	57	76
1	R	452/465 (97%)	447 (99%)	5 (1%)	65	79
2	E	429/429 (100%)	423 (99%)	6 (1%)	59	77
2	F	429/429 (100%)	423 (99%)	6 (1%)	59	77
3	D	20/151 (13%)	20 (100%)	0	100	100
3	G	20/151 (13%)	20 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	K	260/266 (98%)	257 (99%)	3 (1%)	63 79
4	Q	260/266 (98%)	258 (99%)	2 (1%)	73 82
5	S	155/161 (96%)	153 (99%)	2 (1%)	61 78
5	X	155/161 (96%)	152 (98%)	3 (2%)	50 73
6	T	106/106 (100%)	106 (100%)	0	100 100
6	Z	106/106 (100%)	106 (100%)	0	100 100
7	U	59/59 (100%)	59 (100%)	0	100 100
7	a	59/59 (100%)	59 (100%)	0	100 100
8	V	107/107 (100%)	105 (98%)	2 (2%)	50 73
8	b	107/107 (100%)	106 (99%)	1 (1%)	70 81
9	J	76/83 (92%)	73 (96%)	3 (4%)	28 62
9	P	76/83 (92%)	75 (99%)	1 (1%)	61 78
10	I	163/163 (100%)	160 (98%)	3 (2%)	51 74
10	O	163/163 (100%)	162 (99%)	1 (1%)	78 84
11	W	127/127 (100%)	127 (100%)	0	100 100
11	c	127/127 (100%)	125 (98%)	2 (2%)	55 75
12	M	312/312 (100%)	310 (99%)	2 (1%)	78 84
12	Y	312/312 (100%)	309 (99%)	3 (1%)	68 80
All	All	4532/4858 (93%)	4480 (99%)	52 (1%)	63 79

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	R	63	ARG
1	R	252	VAL
1	R	454	ASP
1	R	505	VAL
1	R	523	CYS
2	E	21	HIS
2	E	100	ARG
2	E	187	THR
2	E	295	VAL
2	E	403	SER
2	E	516	GLU
2	F	20	TYR
2	F	137	ARG

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Mol	Chain	Res	Type
2	F	280	THR
2	F	352	LYS
2	F	357	ASP
2	F	358	ASP
1	L	63	ARG
1	L	388	VAL
1	L	390	ASP
1	L	459	ARG
1	L	508	ASP
1	L	509	ASP
1	L	523	CYS
4	Q	139	ASN
4	Q	160	ASP
5	S	130	THR
5	S	189	ASP
8	V	83	GLU
8	V	144	ILE
9	P	29	ASP
10	O	270	PRO
4	K	139	ASN
4	K	232	HIS
4	K	283	MET
5	X	160	LEU
5	X	174	GLN
5	X	189	ASP
8	b	83	GLU
9	J	42	HIS
9	J	43	MET
9	J	72	GLU
11	c	25	SER
11	c	31	GLN
10	I	91	HIS
10	I	116	GLN
10	I	137	HIS
12	Y	161	VAL
12	Y	189	THR
12	Y	196	ILE
12	M	120	GLU
12	M	196	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	R	80	ASN
2	E	21	HIS
2	E	443	HIS
2	F	110	HIS
1	L	76	ASN
1	L	78	GLN
1	L	249	ASN
4	Q	139	ASN
4	Q	145	GLN
4	Q	265	GLN
7	U	64	HIS
4	K	145	GLN
4	K	265	GLN
6	Z	139	HIS
11	c	31	GLN
10	I	81	GLN
10	I	94	ASN
10	I	137	HIS
10	I	142	GLN
10	I	169	GLN
12	Y	180	ASN
12	M	331	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 66 ligands modelled in this entry, 6 are monoatomic - leaving 60 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
15	HEA	L	603	1	67,67,67	1.38	9 (13%)	81,103,103	1.93	19 (23%)
23	9YF	M	501	-	58,58,58	1.08	6 (10%)	68,71,71	1.30	7 (10%)
16	CDL	T	202	-	75,75,99	0.33	0	81,87,111	0.40	0
18	MQ9	Z	201	-	59,59,59	2.36	22 (37%)	73,75,75	1.63	16 (21%)
18	MQ9	F	707	-	59,59,59	2.25	21 (35%)	73,75,75	1.73	21 (28%)
22	HEC	O	302	10	46,50,50	1.85	5 (10%)	58,82,82	1.68	5 (8%)
19	9Y0	S	302	-	48,48,48	1.16	3 (6%)	51,53,53	0.87	2 (3%)
22	HEC	I	301	-	46,50,50	1.83	5 (10%)	58,82,82	1.83	4 (6%)
23	9YF	M	502	-	58,58,58	1.09	5 (8%)	68,71,71	1.33	5 (7%)
16	CDL	L	604	-	75,75,99	0.34	0	81,87,111	0.71	3 (3%)
16	CDL	F	705	-	75,75,99	0.37	0	81,87,111	0.46	1 (1%)
21	9XX	W	202	-	41,41,41	1.10	4 (9%)	44,44,44	1.19	3 (6%)
19	9Y0	J	203	-	48,48,48	1.16	3 (6%)	51,53,53	0.77	2 (3%)
16	CDL	E	606	-	75,75,99	0.37	0	81,87,111	0.42	0
16	CDL	E	605	-	75,75,99	0.34	0	81,87,111	0.42	0
17	HEM	E	601	2	49,49,50	1.39	7 (14%)	67,81,82	1.05	2 (2%)
18	MQ9	F	701	-	59,59,59	2.44	23 (38%)	73,75,75	1.38	15 (20%)
16	CDL	T	201	-	75,75,99	1.26	9 (12%)	81,87,111	1.83	15 (18%)
17	HEM	E	602	2	50,50,50	1.42	7 (14%)	67,82,82	1.14	5 (7%)
20	PLM	D	301	3	9,10,17	0.53	0	8,9,17	0.43	0
21	9XX	G	302	3	31,31,41	1.12	3 (9%)	34,34,44	1.47	5 (14%)
19	9Y0	J	202	-	48,48,48	1.17	3 (6%)	51,53,53	0.90	2 (3%)
15	HEA	L	602	1	67,67,67	1.43	11 (16%)	81,103,103	2.38	30 (37%)
15	HEA	R	602	1	67,67,67	1.44	10 (14%)	81,103,103	2.33	30 (37%)
22	HEC	I	302	10	46,50,50	1.84	6 (13%)	58,82,82	1.68	6 (10%)
20	PLM	c	201	11	15,16,17	0.47	0	14,15,17	0.34	0
16	CDL	J	201	-	75,75,99	0.33	0	81,87,111	0.45	0
23	9YF	O	303	-	58,58,58	1.05	5 (8%)	68,71,71	1.01	3 (4%)
16	CDL	X	301	-	75,75,99	0.33	0	81,87,111	0.40	0
17	HEM	F	702	2	49,49,50	1.37	6 (12%)	67,81,82	1.03	2 (2%)
19	9Y0	X	303	-	48,48,48	1.17	3 (6%)	51,53,53	0.90	2 (3%)
18	MQ9	I	303	-	59,59,59	2.39	23 (38%)	73,75,75	1.43	18 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
16	CDL	F	704	-	75,75,99	0.34	0	81,87,111	0.42	0
16	CDL	R	604	-	75,75,99	0.34	0	81,87,111	0.60	2 (2%)
17	HEM	F	703	2	50,50,50	1.41	7 (14%)	67,82,82	1.12	3 (4%)
18	MQ9	F	709	-	59,59,59	2.43	22 (37%)	73,75,75	1.54	15 (20%)
19	9Y0	P	202	-	48,48,48	1.19	3 (6%)	51,53,53	0.95	2 (3%)
20	PLM	W	201	11	15,16,17	0.49	0	14,15,17	0.33	0
23	9YF	Y	502	-	58,58,58	1.08	7 (12%)	68,71,71	1.30	7 (10%)
15	HEA	R	603	1	67,67,67	1.37	10 (14%)	81,103,103	2.04	18 (22%)
21	9XX	c	202	11	41,41,41	0.96	3 (7%)	44,44,44	1.18	4 (9%)
24	FES	M	503	12	0,4,4	-	-	-		
23	9YF	c	203	-	58,58,58	1.01	5 (8%)	68,71,71	1.13	3 (4%)
18	MQ9	E	604	-	59,59,59	2.41	22 (37%)	73,75,75	1.53	16 (21%)
23	9YF	W	203	-	58,58,58	1.02	5 (8%)	68,71,71	1.13	3 (4%)
16	CDL	Z	203	-	75,75,99	1.32	7 (9%)	81,87,111	2.04	9 (11%)
20	PLM	G	301	3	9,10,17	0.54	0	8,9,17	0.43	0
22	HEC	O	301	10	46,50,50	1.85	6 (13%)	58,82,82	1.67	4 (6%)
23	9YF	Y	503	-	58,58,58	1.09	5 (8%)	68,71,71	1.33	5 (7%)
24	FES	Y	501	12	0,4,4	-	-	-		
23	9YF	I	304	-	58,58,58	1.04	5 (8%)	68,71,71	1.01	3 (4%)
19	9Y0	F	706	-	48,48,48	1.17	3 (6%)	51,53,53	0.87	2 (3%)
16	CDL	S	301	-	75,75,99	1.32	7 (9%)	81,87,111	1.99	9 (11%)
16	CDL	Z	202	-	75,75,99	1.26	9 (12%)	81,87,111	1.83	15 (18%)
16	CDL	T	203	-	75,75,99	0.37	0	81,87,111	0.45	0
16	CDL	P	201	-	75,75,99	0.33	0	81,87,111	0.45	0
21	9XX	D	302	-	31,31,41	1.11	3 (9%)	34,34,44	1.44	4 (11%)
18	MQ9	F	708	-	59,59,59	2.30	22 (37%)	73,75,75	1.43	9 (12%)
18	MQ9	E	603	-	59,59,59	2.44	23 (38%)	73,75,75	1.38	13 (17%)
16	CDL	X	302	-	75,75,99	1.33	7 (9%)	81,87,111	1.99	9 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	HEA	L	603	1	-	3/36/76/76	-
23	9YF	M	501	-	-	23/54/78/78	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CDL	T	202	-	-	46/86/86/110	-
18	MQ9	Z	201	-	-	11/53/73/73	0/2/2/2
18	MQ9	F	707	-	-	17/53/73/73	0/2/2/2
22	HEC	O	302	10	-	6/14/54/54	-
19	9Y0	S	302	-	-	19/52/52/52	-
22	HEC	I	301	-	-	4/14/54/54	-
23	9YF	M	502	-	-	27/54/78/78	0/1/1/1
16	CDL	L	604	-	-	48/86/86/110	-
16	CDL	F	705	-	-	44/86/86/110	-
21	9XX	W	202	-	-	15/43/43/43	-
19	9Y0	J	203	-	-	25/52/52/52	-
16	CDL	E	606	-	-	40/86/86/110	-
16	CDL	E	605	-	-	49/86/86/110	-
17	HEM	E	601	2	-	2/12/52/54	-
18	MQ9	F	701	-	-	6/53/73/73	0/2/2/2
16	CDL	T	201	-	-	34/86/86/110	-
17	HEM	E	602	2	-	2/14/54/54	-
20	PLM	D	301	3	-	3/8/8/15	-
21	9XX	G	302	3	-	10/33/33/43	-
19	9Y0	J	202	-	-	19/52/52/52	-
15	HEA	L	602	1	-	12/36/76/76	-
15	HEA	R	602	1	-	7/36/76/76	-
22	HEC	I	302	10	-	3/14/54/54	-
20	PLM	c	201	11	-	5/14/14/15	-
16	CDL	J	201	-	-	48/86/86/110	-
23	9YF	O	303	-	-	28/54/78/78	0/1/1/1
16	CDL	X	301	-	-	46/86/86/110	-
17	HEM	F	702	2	-	4/12/52/54	-
19	9Y0	X	303	-	-	17/52/52/52	-
18	MQ9	I	303	-	-	8/53/73/73	0/2/2/2
16	CDL	F	704	-	-	49/86/86/110	-
16	CDL	R	604	-	-	47/86/86/110	-
17	HEM	F	703	2	-	0/14/54/54	-
18	MQ9	F	709	-	-	12/53/73/73	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	9Y0	P	202	-	-	22/52/52/52	-
20	PLM	W	201	11	-	4/14/14/15	-
23	9YF	Y	502	-	-	23/54/78/78	0/1/1/1
15	HEA	R	603	1	-	3/36/76/76	-
21	9XX	c	202	11	-	16/43/43/43	-
24	FES	M	503	12	-	-	0/1/1/1
23	9YF	c	203	-	-	22/54/78/78	0/1/1/1
18	MQ9	E	604	-	-	11/53/73/73	0/2/2/2
23	9YF	W	203	-	-	22/54/78/78	0/1/1/1
16	CDL	Z	203	-	-	38/86/86/110	-
20	PLM	G	301	3	-	2/8/8/15	-
22	HEC	O	301	10	-	5/14/54/54	-
23	9YF	Y	503	-	-	27/54/78/78	0/1/1/1
24	FES	Y	501	12	-	-	0/1/1/1
23	9YF	I	304	-	-	27/54/78/78	0/1/1/1
19	9Y0	F	706	-	-	16/52/52/52	-
16	CDL	S	301	-	-	43/86/86/110	-
16	CDL	Z	202	-	-	34/86/86/110	-
16	CDL	T	203	-	-	47/86/86/110	-
16	CDL	P	201	-	-	48/86/86/110	-
21	9XX	D	302	-	-	9/33/33/43	-
18	MQ9	F	708	-	-	11/53/73/73	0/2/2/2
18	MQ9	E	603	-	-	6/53/73/73	0/2/2/2
16	CDL	X	302	-	-	43/86/86/110	-

All (380) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	E	604	MQ9	C6-C5	8.80	1.51	1.35
18	F	709	MQ9	C6-C5	8.77	1.50	1.35
18	F	708	MQ9	C6-C5	8.60	1.50	1.35
18	F	701	MQ9	C6-C5	8.58	1.50	1.35
18	I	303	MQ9	C6-C5	8.52	1.50	1.35
18	E	603	MQ9	C6-C5	8.50	1.50	1.35
18	Z	201	MQ9	C6-C5	8.22	1.49	1.35
18	F	707	MQ9	C6-C5	8.14	1.49	1.35
22	O	301	HEC	CAC-C3C	6.40	1.55	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	O	302	HEC	CAB-C3B	6.37	1.55	1.35
22	I	301	HEC	CAC-C3C	6.36	1.55	1.35
22	I	302	HEC	CAC-C3C	6.30	1.55	1.35
22	O	302	HEC	CAC-C3C	6.30	1.55	1.35
22	I	302	HEC	CAB-C3B	6.23	1.55	1.35
22	O	301	HEC	CAB-C3B	6.20	1.55	1.35
22	I	301	HEC	CAB-C3B	6.03	1.54	1.35
22	O	301	HEC	C3D-C2D	5.74	1.53	1.38
22	O	302	HEC	C3D-C2D	5.69	1.53	1.38
22	I	301	HEC	C3D-C2D	5.66	1.53	1.38
22	I	302	HEC	C3D-C2D	5.55	1.53	1.38
18	F	709	MQ9	C2-C1	5.09	1.58	1.48
18	E	604	MQ9	C2-C1	5.04	1.57	1.48
18	E	603	MQ9	C2-C1	5.01	1.57	1.48
18	F	701	MQ9	C2-C1	4.99	1.57	1.48
18	Z	201	MQ9	C2-C1	4.92	1.57	1.48
18	I	303	MQ9	C2-C1	4.91	1.57	1.48
18	I	303	MQ9	C3-C4	4.69	1.57	1.48
18	F	709	MQ9	C3-C4	4.68	1.57	1.48
18	E	604	MQ9	C3-C4	4.65	1.57	1.48
18	E	603	MQ9	C3-C4	4.64	1.57	1.48
18	F	701	MQ9	C3-C4	4.60	1.57	1.48
18	F	709	MQ9	C26-C24	4.59	1.60	1.51
18	F	708	MQ9	C2-C1	4.56	1.57	1.48
18	F	708	MQ9	C3-C4	4.55	1.57	1.48
18	Z	201	MQ9	C3-C4	4.51	1.56	1.48
18	E	604	MQ9	C26-C24	4.49	1.60	1.51
18	E	603	MQ9	C26-C24	4.49	1.60	1.51
18	F	707	MQ9	C26-C24	4.48	1.60	1.51
18	I	303	MQ9	C26-C24	4.46	1.60	1.51
18	F	701	MQ9	C26-C24	4.45	1.60	1.51
18	Z	201	MQ9	C26-C24	4.41	1.60	1.51
18	F	707	MQ9	C11-C9	4.34	1.60	1.51
15	R	602	HEA	C3B-C2B	4.34	1.44	1.34
18	F	707	MQ9	C3-C4	4.30	1.56	1.48
15	R	603	HEA	C3B-C2B	4.30	1.44	1.34
15	L	603	HEA	C3B-C2B	4.23	1.44	1.34
15	L	602	HEA	C3B-C2B	4.16	1.44	1.34
18	E	603	MQ9	C31-C29	4.14	1.59	1.51
18	Z	201	MQ9	C11-C9	4.12	1.59	1.51
18	F	701	MQ9	C31-C29	4.08	1.59	1.51
18	F	707	MQ9	C2-C1	4.06	1.56	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	F	708	MQ9	C26-C24	4.05	1.59	1.51
18	F	709	MQ9	C31-C29	4.05	1.59	1.51
18	E	604	MQ9	C11-C9	3.98	1.59	1.51
18	F	709	MQ9	C11-C9	3.92	1.59	1.51
17	E	602	HEM	FE-ND	3.91	2.06	1.94
21	W	202	9XX	O1-C17	-3.90	1.40	1.47
21	G	302	9XX	O1-C17	-3.87	1.40	1.47
18	I	303	MQ9	C11-C9	3.87	1.59	1.51
18	I	303	MQ9	C31-C29	3.86	1.59	1.51
21	D	302	9XX	O1-C17	-3.86	1.40	1.47
18	Z	201	MQ9	C31-C29	3.82	1.59	1.51
15	L	602	HEA	C3D-C2D	3.80	1.45	1.36
18	E	604	MQ9	C31-C29	3.80	1.59	1.51
17	F	703	HEM	FE-ND	3.77	2.06	1.94
18	E	603	MQ9	C11-C9	3.77	1.59	1.51
18	F	701	MQ9	C11-C9	3.76	1.59	1.51
21	c	202	9XX	O1-C17	-3.73	1.40	1.47
18	F	708	MQ9	C11-C9	3.73	1.59	1.51
21	W	202	9XX	O-C15	3.69	1.44	1.33
15	L	603	HEA	C3D-C2D	3.67	1.44	1.36
15	R	602	HEA	C3D-C2D	3.66	1.44	1.36
18	F	707	MQ9	C16-C14	3.64	1.58	1.51
17	E	602	HEM	FE-NB	3.61	2.06	1.94
15	R	602	HEA	C4D-C3D	3.57	1.51	1.45
15	R	603	HEA	C3D-C2D	3.50	1.44	1.36
15	R	602	HEA	C3A-C2A	3.43	1.45	1.37
15	L	602	HEA	C3A-C2A	3.43	1.45	1.37
18	F	708	MQ9	C27-C28	3.41	1.60	1.50
19	X	303	9Y0	O7-C1	-3.29	1.38	1.46
15	L	602	HEA	C4B-C3B	3.29	1.50	1.44
18	F	708	MQ9	C7-C6	3.28	1.57	1.51
18	E	603	MQ9	C22-C23	3.28	1.60	1.50
19	S	302	9Y0	O7-C1	-3.27	1.38	1.46
18	E	604	MQ9	C21-C19	3.25	1.58	1.51
18	F	709	MQ9	C21-C19	3.25	1.58	1.51
17	F	703	HEM	FE-NB	3.25	2.04	1.94
18	E	603	MQ9	C21-C19	3.25	1.58	1.51
16	Z	202	CDL	OA6-CA4	-3.25	1.39	1.46
16	T	201	CDL	OA6-CA4	-3.24	1.39	1.46
18	F	701	MQ9	C22-C23	3.24	1.60	1.50
18	F	709	MQ9	C22-C23	3.23	1.60	1.50
18	E	604	MQ9	C22-C23	3.23	1.60	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	E	601	HEM	FE-ND	3.23	2.04	1.94
17	E	601	HEM	FE-NB	3.22	2.04	1.94
18	I	303	MQ9	C22-C23	3.21	1.60	1.50
18	I	303	MQ9	C16-C14	3.20	1.57	1.51
18	I	303	MQ9	C27-C28	3.19	1.60	1.50
19	J	203	9Y0	O7-C1	-3.18	1.39	1.46
19	J	202	9Y0	O7-C1	-3.18	1.39	1.46
18	F	701	MQ9	C21-C19	3.17	1.57	1.51
19	F	706	9Y0	O7-C1	-3.17	1.39	1.46
18	E	604	MQ9	C16-C14	3.16	1.57	1.51
18	F	707	MQ9	C31-C29	3.16	1.57	1.51
18	E	603	MQ9	C41-C39	3.13	1.57	1.51
18	Z	201	MQ9	C7-C8	3.12	1.55	1.50
16	Z	203	CDL	OB8-CB7	3.12	1.42	1.33
18	F	709	MQ9	C16-C14	3.11	1.57	1.51
18	F	701	MQ9	C41-C39	3.11	1.57	1.51
18	Z	201	MQ9	C21-C19	3.11	1.57	1.51
18	Z	201	MQ9	C27-C28	3.09	1.59	1.50
15	R	602	HEA	C4B-C3B	3.08	1.50	1.44
18	E	603	MQ9	C27-C28	3.08	1.59	1.50
18	F	701	MQ9	C27-C28	3.07	1.59	1.50
16	S	301	CDL	OB8-CB7	3.07	1.42	1.33
18	Z	201	MQ9	C22-C23	3.07	1.59	1.50
17	E	601	HEM	FE-NA	3.07	2.05	1.95
17	F	702	HEM	FE-NA	3.07	2.05	1.95
18	F	708	MQ9	C22-C23	3.07	1.59	1.50
18	F	708	MQ9	C31-C29	3.07	1.57	1.51
18	I	303	MQ9	C21-C19	3.07	1.57	1.51
16	X	302	CDL	OB8-CB7	3.06	1.42	1.33
17	F	702	HEM	FE-NB	3.06	2.04	1.94
18	F	707	MQ9	C21-C19	3.05	1.57	1.51
17	F	702	HEM	FE-ND	3.04	2.04	1.94
18	F	709	MQ9	C27-C28	3.04	1.59	1.50
15	L	603	HEA	C1C-C2C	3.04	1.50	1.43
15	L	602	HEA	C4D-C3D	3.03	1.50	1.45
18	Z	201	MQ9	C16-C14	3.01	1.57	1.51
19	P	202	9Y0	O7-C1	-3.01	1.39	1.46
18	F	708	MQ9	C21-C19	3.01	1.57	1.51
17	E	602	HEM	CAB-C3B	3.01	1.55	1.47
18	F	707	MQ9	C7-C8	3.00	1.55	1.50
18	F	701	MQ9	C7-C8	3.00	1.55	1.50
18	E	604	MQ9	C27-C28	2.99	1.59	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	L	603	HEA	C3A-C2A	2.98	1.43	1.37
17	F	702	HEM	FE-NC	2.97	2.05	1.95
18	I	303	MQ9	C7-C8	2.96	1.55	1.50
18	F	708	MQ9	C7-C8	2.95	1.55	1.50
18	F	708	MQ9	C16-C14	2.94	1.57	1.51
19	J	202	9Y0	O5-C5	2.94	1.41	1.33
19	P	202	9Y0	O5-C5	2.94	1.41	1.33
18	F	701	MQ9	C16-C14	2.94	1.57	1.51
18	F	707	MQ9	C22-C23	2.93	1.59	1.50
18	E	603	MQ9	C7-C6	2.92	1.56	1.51
17	E	601	HEM	CAB-C3B	2.92	1.55	1.47
19	F	706	9Y0	O5-C5	2.92	1.41	1.33
16	Z	203	CDL	OA6-CA5	2.92	1.42	1.34
16	X	302	CDL	OA6-CA5	2.92	1.42	1.34
17	F	703	HEM	CAB-C3B	2.91	1.55	1.47
18	E	603	MQ9	C7-C8	2.90	1.55	1.50
15	L	603	HEA	C4B-C3B	2.90	1.49	1.44
23	W	203	9YF	O9-C	-2.90	1.39	1.46
15	R	603	HEA	C1C-C2C	2.90	1.49	1.43
16	X	302	CDL	CB6-CB4	2.89	1.59	1.50
16	S	301	CDL	OA6-CA5	2.89	1.42	1.34
18	F	709	MQ9	C7-C8	2.89	1.55	1.50
18	E	604	MQ9	C7-C8	2.89	1.55	1.50
16	Z	203	CDL	OB6-CB5	2.89	1.42	1.34
19	J	203	9Y0	O5-C5	2.89	1.41	1.33
17	E	601	HEM	FE-NC	2.88	2.04	1.95
18	F	701	MQ9	C7-C6	2.87	1.56	1.51
16	X	302	CDL	OB6-CB5	2.87	1.42	1.34
23	c	203	9YF	O9-C	-2.87	1.39	1.46
18	E	604	MQ9	C7-C6	2.87	1.56	1.51
23	Y	502	9YF	O9-C8	2.87	1.42	1.34
23	M	501	9YF	O9-C8	2.87	1.42	1.34
16	S	301	CDL	CB6-CB4	2.87	1.59	1.50
18	E	603	MQ9	C16-C14	2.86	1.57	1.51
18	F	709	MQ9	C7-C6	2.86	1.56	1.51
15	L	602	HEA	C1C-C2C	2.86	1.49	1.43
15	R	603	HEA	C3A-C2A	2.85	1.43	1.37
16	S	301	CDL	OB6-CB5	2.85	1.42	1.34
17	F	702	HEM	CAB-C3B	2.85	1.55	1.47
18	E	603	MQ9	C5M-C5	2.84	1.56	1.50
18	E	604	MQ9	C5M-C5	2.84	1.56	1.50
18	F	701	MQ9	C5M-C5	2.84	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	F	707	MQ9	C20-C19	2.83	1.57	1.50
16	S	301	CDL	OA8-CA7	2.83	1.41	1.33
18	F	709	MQ9	C5M-C5	2.83	1.56	1.50
23	Y	502	9YF	O11-C25	2.82	1.41	1.33
18	I	303	MQ9	C20-C19	2.82	1.57	1.50
19	X	303	9Y0	O5-C5	2.82	1.41	1.33
16	S	301	CDL	CB3-CB4	2.81	1.59	1.50
18	F	709	MQ9	C20-C19	2.80	1.57	1.50
15	R	602	HEA	C1C-C2C	2.79	1.49	1.43
16	Z	203	CDL	OA8-CA7	2.79	1.41	1.33
16	X	302	CDL	CB3-CB4	2.78	1.59	1.50
23	Y	503	9YF	O9-C	-2.78	1.40	1.46
17	F	703	HEM	CAC-C3C	2.78	1.54	1.47
18	E	604	MQ9	C20-C19	2.78	1.57	1.50
19	J	203	9Y0	O7-C21	2.78	1.42	1.34
16	X	302	CDL	OA8-CA7	2.77	1.41	1.33
19	S	302	9Y0	O5-C5	2.77	1.41	1.33
18	F	708	MQ9	C5M-C5	2.77	1.56	1.50
19	J	202	9Y0	O7-C21	2.76	1.42	1.34
18	Z	201	MQ9	C20-C19	2.76	1.57	1.50
23	M	502	9YF	O9-C	-2.76	1.40	1.46
18	I	303	MQ9	C7-C6	2.75	1.56	1.51
23	M	501	9YF	O11-C25	2.75	1.41	1.33
19	F	706	9Y0	O7-C21	2.75	1.42	1.34
16	Z	203	CDL	CB3-CB4	2.74	1.59	1.50
16	Z	203	CDL	CB6-CB4	2.74	1.59	1.50
16	T	201	CDL	CB6-CB4	2.74	1.59	1.50
16	Z	202	CDL	CB6-CB4	2.74	1.59	1.50
18	Z	201	MQ9	C7-C6	2.74	1.56	1.51
16	Z	202	CDL	OB8-CB7	2.73	1.41	1.33
18	F	701	MQ9	C20-C19	2.72	1.57	1.50
19	P	202	9Y0	O7-C21	2.72	1.42	1.34
19	X	303	9Y0	O7-C21	2.71	1.41	1.34
19	S	302	9Y0	O7-C21	2.70	1.41	1.34
18	E	603	MQ9	C20-C19	2.69	1.57	1.50
16	T	201	CDL	OB8-CB7	2.67	1.41	1.33
17	F	703	HEM	FE-NA	2.67	2.04	1.95
17	E	602	HEM	CAC-C3C	2.66	1.54	1.47
15	R	603	HEA	C4B-C3B	2.65	1.49	1.44
23	M	502	9YF	O9-C8	2.65	1.41	1.34
18	I	303	MQ9	C5M-C5	2.65	1.56	1.50
16	Z	203	CDL	OA6-CA4	-2.64	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	S	301	CDL	OA6-CA4	-2.64	1.40	1.46
23	Y	503	9YF	O9-C8	2.64	1.41	1.34
18	F	708	MQ9	C20-C19	2.64	1.57	1.50
18	F	707	MQ9	C27-C28	2.63	1.58	1.50
18	F	701	MQ9	C42-C43	2.63	1.58	1.50
16	X	302	CDL	OA6-CA4	-2.63	1.40	1.46
18	F	707	MQ9	C7-C6	2.62	1.56	1.51
18	E	603	MQ9	C42-C43	2.62	1.58	1.50
18	I	303	MQ9	C42-C43	2.60	1.58	1.50
21	c	202	9XX	O-C15	2.59	1.40	1.33
23	O	303	9YF	O9-C8	2.59	1.41	1.34
16	T	201	CDL	OB6-CB5	2.58	1.41	1.34
18	F	708	MQ9	O4-C4	-2.58	1.17	1.23
23	I	304	9YF	O9-C8	2.58	1.41	1.34
23	W	203	9YF	O11-C24	-2.58	1.39	1.45
23	W	203	9YF	O9-C8	2.57	1.41	1.34
18	F	707	MQ9	O4-C4	-2.57	1.17	1.23
18	F	709	MQ9	C41-C39	2.56	1.56	1.51
18	E	604	MQ9	C46-C44	2.54	1.56	1.51
18	I	303	MQ9	C41-C39	2.54	1.56	1.51
23	c	203	9YF	O11-C24	-2.54	1.39	1.45
18	F	709	MQ9	C46-C44	2.53	1.56	1.51
16	Z	202	CDL	OB6-CB5	2.53	1.41	1.34
17	E	602	HEM	FE-NA	2.53	2.03	1.95
23	c	203	9YF	O9-C8	2.51	1.41	1.34
21	D	302	9XX	O-C15	2.51	1.40	1.33
18	E	603	MQ9	C46-C44	2.50	1.56	1.51
18	Z	201	MQ9	C5M-C5	2.48	1.55	1.50
23	W	203	9YF	P-O2	2.48	1.66	1.59
18	E	604	MQ9	C41-C39	2.47	1.56	1.51
23	c	203	9YF	P-O2	2.46	1.66	1.59
18	F	708	MQ9	C41-C39	2.46	1.56	1.51
18	F	707	MQ9	C5M-C5	2.45	1.55	1.50
18	F	701	MQ9	C46-C44	2.45	1.56	1.51
18	F	701	MQ9	C12-C13	2.45	1.57	1.50
23	O	303	9YF	O11-C25	2.44	1.40	1.33
23	M	502	9YF	O11-C25	2.43	1.40	1.33
23	M	502	9YF	O11-C24	-2.43	1.39	1.45
23	Y	503	9YF	O11-C24	-2.43	1.39	1.45
23	I	304	9YF	O11-C25	2.42	1.40	1.33
18	E	603	MQ9	C12-C13	2.42	1.57	1.50
18	F	709	MQ9	C42-C43	2.42	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	O	303	9YF	O11-C24	-2.42	1.39	1.45
21	G	302	9XX	O-C15	2.41	1.40	1.33
23	Y	503	9YF	O11-C25	2.41	1.40	1.33
15	R	602	HEA	C1A-C2A	2.40	1.49	1.45
18	Z	201	MQ9	C46-C44	2.40	1.56	1.51
15	R	602	HEA	C1B-C2B	2.40	1.49	1.44
15	L	603	HEA	C1D-ND	-2.39	1.36	1.40
18	F	707	MQ9	O1-C1	-2.38	1.18	1.23
23	I	304	9YF	O11-C24	-2.38	1.39	1.45
15	R	603	HEA	C1D-ND	-2.38	1.36	1.40
15	L	602	HEA	C1B-C2B	2.37	1.49	1.44
18	Z	201	MQ9	C42-C43	2.37	1.57	1.50
15	R	602	HEA	C3C-C4C	2.36	1.49	1.42
18	F	701	MQ9	C43-C44	2.36	1.38	1.33
18	I	303	MQ9	C12-C13	2.36	1.57	1.50
18	E	603	MQ9	C43-C44	2.34	1.38	1.33
18	E	603	MQ9	C28-C29	2.34	1.38	1.33
18	E	604	MQ9	C12-C13	2.34	1.57	1.50
18	E	603	MQ9	O4-C4	-2.33	1.18	1.23
18	F	709	MQ9	C12-C13	2.33	1.57	1.50
15	L	602	HEA	C3C-C4C	2.32	1.49	1.42
18	F	708	MQ9	C42-C43	2.32	1.57	1.50
18	Z	201	MQ9	O4-C4	-2.32	1.18	1.23
18	E	604	MQ9	C42-C43	2.32	1.57	1.50
23	O	303	9YF	O9-C	-2.32	1.41	1.46
21	G	302	9XX	O1-C18	2.31	1.40	1.34
22	I	302	HEC	C3B-C2B	-2.30	1.33	1.41
18	Z	201	MQ9	C12-C13	2.30	1.57	1.50
18	Z	201	MQ9	C41-C39	2.30	1.56	1.51
18	F	709	MQ9	O4-C4	-2.30	1.18	1.23
18	F	701	MQ9	C28-C29	2.29	1.38	1.33
23	I	304	9YF	O9-C	-2.29	1.41	1.46
18	I	303	MQ9	C43-C44	2.28	1.38	1.33
18	I	303	MQ9	O4-C4	-2.28	1.18	1.23
18	E	604	MQ9	O4-C4	-2.28	1.18	1.23
21	D	302	9XX	O1-C18	2.27	1.40	1.34
23	Y	502	9YF	P-O2	2.27	1.66	1.59
17	F	703	HEM	FE-NC	2.27	2.02	1.95
18	F	707	MQ9	C12-C13	2.27	1.57	1.50
18	F	701	MQ9	O4-C4	-2.26	1.18	1.23
18	F	707	MQ9	C46-C44	2.26	1.56	1.51
23	M	501	9YF	P-O2	2.26	1.66	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	T	201	CDL	PA1-OA4	-2.26	1.44	1.55
21	W	202	9XX	C14-C15	2.25	1.57	1.50
15	L	602	HEA	C1D-ND	-2.25	1.36	1.40
18	E	604	MQ9	C43-C44	2.24	1.38	1.33
18	F	709	MQ9	C43-C44	2.24	1.38	1.33
18	I	303	MQ9	C28-C29	2.24	1.38	1.33
23	W	203	9YF	O11-C25	2.24	1.39	1.33
15	R	603	HEA	C3C-C4C	2.23	1.49	1.42
16	Z	202	CDL	PA1-OA4	-2.23	1.45	1.55
16	T	201	CDL	CB3-CB4	2.22	1.57	1.50
23	M	501	9YF	O4-C4	-2.22	1.37	1.43
16	Z	202	CDL	CB3-CB4	2.21	1.57	1.50
15	L	602	HEA	C1A-C2A	2.21	1.49	1.45
23	c	203	9YF	O11-C25	2.21	1.39	1.33
21	W	202	9XX	O1-C18	2.20	1.40	1.34
18	E	604	MQ9	C28-C29	2.19	1.38	1.33
23	Y	502	9YF	O4-C4	-2.19	1.37	1.43
15	R	603	HEA	C4D-C3D	2.18	1.48	1.45
23	Y	502	9YF	O11-C24	-2.18	1.40	1.45
18	F	708	MQ9	C43-C44	2.17	1.38	1.33
15	R	602	HEA	C1D-ND	-2.17	1.36	1.40
18	F	708	MQ9	C28-C29	2.16	1.38	1.33
15	R	603	HEA	C1B-C2B	2.16	1.48	1.44
15	L	603	HEA	C3C-C4C	2.15	1.49	1.42
23	Y	503	9YF	O4-C4	-2.15	1.37	1.43
18	Z	201	MQ9	C43-C44	2.15	1.38	1.33
18	F	707	MQ9	C41-C39	2.14	1.55	1.51
18	E	603	MQ9	C3C-C3B	2.14	1.42	1.38
18	Z	201	MQ9	C28-C29	2.13	1.38	1.33
18	I	303	MQ9	C46-C44	2.13	1.55	1.51
23	M	501	9YF	O11-C24	-2.12	1.40	1.45
18	E	604	MQ9	C3C-C3B	2.12	1.42	1.38
18	E	603	MQ9	C5-C4	2.11	1.52	1.47
15	L	603	HEA	C1B-C2B	2.11	1.48	1.44
18	F	708	MQ9	C51-C49	2.10	1.56	1.50
22	I	301	HEC	C3B-C2B	-2.10	1.34	1.41
18	Z	201	MQ9	C3C-C3B	2.10	1.42	1.38
23	I	304	9YF	P-O2	2.09	1.65	1.59
17	E	602	HEM	CMB-C2B	2.09	1.55	1.50
23	O	303	9YF	P-O2	2.09	1.65	1.59
22	I	302	HEC	C3C-C2C	-2.09	1.34	1.41
22	I	302	HEC	CMC-C2C	2.09	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	F	701	MQ9	C3C-C3B	2.09	1.42	1.38
17	E	602	HEM	FE-NC	2.08	2.02	1.95
16	Z	202	CDL	OA8-CA7	2.08	1.39	1.33
18	F	708	MQ9	C12-C13	2.08	1.56	1.50
18	F	708	MQ9	C6-C1	2.08	1.52	1.47
22	O	301	HEC	C3C-C2C	-2.08	1.34	1.41
23	M	502	9YF	O4-C4	-2.08	1.37	1.43
15	L	602	HEA	C1D-C2D	2.08	1.48	1.44
18	F	709	MQ9	C3C-C3B	2.07	1.42	1.38
15	R	603	HEA	C1D-C2D	2.05	1.48	1.44
16	T	201	CDL	OA6-CA5	2.05	1.40	1.34
15	L	603	HEA	C1D-C2D	2.05	1.48	1.44
23	Y	502	9YF	O9-C	-2.05	1.41	1.46
18	F	709	MQ9	C28-C29	2.04	1.37	1.33
18	I	303	MQ9	C3C-C3B	2.04	1.42	1.38
18	F	707	MQ9	C18-C19	2.04	1.37	1.33
21	c	202	9XX	O1-C18	2.04	1.40	1.34
17	E	601	HEM	CMB-C2B	2.04	1.55	1.50
22	O	301	HEC	C3B-C2B	-2.04	1.34	1.41
18	F	701	MQ9	C5-C4	2.04	1.52	1.47
16	Z	202	CDL	OA6-CA5	2.04	1.40	1.34
16	T	201	CDL	OA8-CA7	2.03	1.39	1.33
18	F	707	MQ9	C42-C43	2.03	1.56	1.50
23	M	501	9YF	O9-C	-2.03	1.41	1.46
16	Z	202	CDL	PB2-OB5	2.03	1.67	1.59
17	F	703	HEM	CMC-C2C	2.03	1.54	1.50
23	Y	502	9YF	P-O	2.03	1.67	1.59
17	E	601	HEM	CMD-C2D	2.02	1.54	1.50
22	O	301	HEC	CMD-C2D	2.02	1.54	1.50
22	O	302	HEC	C3B-C2B	-2.02	1.34	1.41
16	T	201	CDL	PB2-OB5	2.02	1.67	1.59
18	I	303	MQ9	C5-C4	2.01	1.52	1.47
22	O	302	HEC	C3C-C2C	-2.01	1.34	1.41
22	I	301	HEC	C3C-C2C	-2.01	1.34	1.41
17	F	702	HEM	CMB-C2B	2.01	1.54	1.50

All (378) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	Z	203	CDL	CB6-CB4-CB3	-9.90	88.70	111.78
16	X	302	CDL	CB6-CB4-CB3	-9.67	89.24	111.78
16	S	301	CDL	CB6-CB4-CB3	-9.67	89.25	111.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	T	201	CDL	OB6-CB4-CB6	9.23	141.47	108.34
16	Z	202	CDL	OB6-CB4-CB6	9.23	141.45	108.34
22	I	301	HEC	CBB-CAB-C3B	-8.83	109.78	127.43
16	Z	203	CDL	OB6-CB4-CB3	-8.36	78.34	108.34
15	L	602	HEA	C12-C11-C3B	8.18	124.91	112.12
15	R	602	HEA	CAD-C3D-C4D	8.14	138.88	124.70
16	S	301	CDL	OB6-CB4-CB3	-8.00	79.65	108.34
16	X	302	CDL	OB6-CB4-CB3	-7.99	79.66	108.34
22	O	301	HEC	CBB-CAB-C3B	-7.58	112.28	127.43
16	S	301	CDL	OB6-CB4-CB6	7.25	134.37	108.34
16	X	302	CDL	OB6-CB4-CB6	7.22	134.25	108.34
16	Z	203	CDL	OB6-CB4-CB6	6.88	133.03	108.34
22	O	302	HEC	CBC-CAC-C3C	-6.75	113.95	127.43
22	I	301	HEC	CBC-CAC-C3C	-6.65	114.14	127.43
22	I	302	HEC	CBC-CAC-C3C	-6.35	114.75	127.43
22	O	301	HEC	CBC-CAC-C3C	-6.22	115.00	127.43
15	L	602	HEA	C3A-C2A-C1A	-6.13	101.24	107.05
22	I	302	HEC	CBB-CAB-C3B	-6.12	115.19	127.43
15	L	602	HEA	CAD-C3D-C4D	5.95	135.07	124.70
23	Y	503	9YF	O6-C6-C7	5.94	124.37	110.38
15	R	602	HEA	C3A-C2A-C1A	-5.93	101.43	107.05
23	M	502	9YF	O6-C6-C7	5.91	124.30	110.38
22	O	302	HEC	CBB-CAB-C3B	-5.84	115.75	127.43
15	R	603	HEA	C3A-C2A-C1A	-5.58	101.76	107.05
15	L	603	HEA	C3A-C2A-C1A	-5.53	101.81	107.05
15	R	602	HEA	C12-C11-C3B	5.48	120.69	112.12
23	Y	502	9YF	O9-C8-C9	5.36	123.08	111.48
23	M	501	9YF	O9-C8-C9	5.36	123.08	111.48
21	G	302	9XX	O1-C18-C19	4.90	122.08	111.48
15	R	603	HEA	C3D-C4D-ND	4.69	114.88	110.35
18	Z	201	MQ9	C7-C8-C9	-4.66	118.80	126.83
15	L	602	HEA	O11-C11-C3B	-4.65	102.72	111.26
16	T	201	CDL	OB6-CB4-CB3	-4.65	91.67	108.34
16	Z	202	CDL	OB6-CB4-CB3	-4.64	91.69	108.34
21	D	302	9XX	O1-C18-C19	4.61	121.45	111.48
23	W	203	9YF	O9-C8-C9	4.53	121.28	111.48
23	c	203	9YF	O9-C8-C9	4.53	121.28	111.48
16	Z	203	CDL	OA6-CA5-C11	4.51	121.25	111.48
16	T	201	CDL	OB6-CB5-C51	4.51	121.24	111.48
16	Z	202	CDL	OB6-CB5-C51	4.51	121.23	111.48
18	F	707	MQ9	C15-C14-C16	4.49	123.02	115.23
15	L	603	HEA	C3D-C4D-ND	4.46	114.66	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	L	602	HEA	CMC-C2C-C3C	4.41	136.91	126.55
15	R	603	HEA	C2A-C1A-NA	4.40	114.57	110.32
16	Z	202	CDL	OA6-CA5-C11	4.39	120.97	111.48
16	T	201	CDL	OA6-CA5-C11	4.35	120.89	111.48
15	L	603	HEA	C2A-C1A-NA	4.33	114.50	110.32
15	L	602	HEA	C2A-C1A-NA	4.24	114.41	110.32
21	W	202	9XX	O1-C18-C19	4.22	120.61	111.48
15	R	602	HEA	CAD-C3D-C2D	-4.21	119.99	127.87
19	J	202	9Y0	O7-C21-C22	4.16	120.48	111.48
15	R	603	HEA	CMC-C2C-C3C	4.15	136.31	126.55
16	S	301	CDL	OB6-CB5-C51	4.14	120.44	111.48
16	X	302	CDL	OB6-CB5-C51	4.13	120.42	111.48
15	R	603	HEA	CHA-C1A-C2A	-4.13	118.35	124.86
15	R	602	HEA	CMC-C2C-C3C	4.05	136.07	126.55
15	R	603	HEA	CHA-C4D-C3D	-4.03	118.89	124.77
23	Y	503	9YF	O9-C8-C9	4.01	120.16	111.48
15	R	603	HEA	C12-C11-C3B	-3.99	105.88	112.12
23	M	502	9YF	O9-C8-C9	3.99	120.12	111.48
19	X	303	9Y0	O7-C21-C22	3.97	120.07	111.48
15	L	602	HEA	CMC-C2C-C1C	-3.97	119.38	125.42
15	R	602	HEA	C4D-C3D-C2D	-3.96	101.12	106.89
15	L	602	HEA	C3D-C4D-ND	3.95	114.17	110.35
15	L	603	HEA	CHA-C1A-C2A	-3.93	118.66	124.86
15	L	603	HEA	CHA-C4D-C3D	-3.90	119.09	124.77
19	F	706	9Y0	O7-C21-C22	3.89	119.89	111.48
15	R	602	HEA	C2A-C1A-NA	3.85	114.04	110.32
19	S	302	9Y0	O7-C21-C22	3.82	119.75	111.48
18	F	707	MQ9	C45-C44-C46	3.78	121.80	115.23
23	I	304	9YF	O9-C8-C9	3.77	119.63	111.48
16	Z	203	CDL	OB6-CB5-C51	3.76	119.62	111.48
23	O	303	9YF	O9-C8-C9	3.75	119.59	111.48
23	Y	503	9YF	O11-C25-C26	3.74	123.24	111.83
15	L	602	HEA	CHA-C1A-C2A	-3.73	118.97	124.86
23	M	502	9YF	O11-C25-C26	3.73	123.20	111.83
16	S	301	CDL	OA6-CA5-C11	3.71	119.50	111.48
16	X	302	CDL	OA6-CA5-C11	3.70	119.49	111.48
15	R	602	HEA	C3D-C4D-ND	3.69	113.92	110.35
15	R	602	HEA	CHA-C1A-C2A	-3.69	119.04	124.86
15	R	603	HEA	CMC-C2C-C1C	-3.68	119.81	125.42
15	L	602	HEA	C4D-C3D-C2D	-3.67	101.55	106.89
22	O	302	HEC	C4D-ND-C1D	3.66	111.78	105.82
21	c	202	9XX	O1-C18-C19	3.64	119.36	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	I	302	HEC	C4D-ND-C1D	3.64	111.76	105.82
15	R	603	HEA	CAD-C3D-C4D	3.59	130.95	124.70
15	R	602	HEA	C26-C15-C14	-3.56	114.48	123.63
18	F	707	MQ9	C11-C9-C8	3.56	129.16	121.17
18	F	708	MQ9	C50-C49-C48	-3.54	112.03	122.66
22	I	301	HEC	C4D-ND-C1D	3.53	111.58	105.82
15	R	603	HEA	C4D-C3D-C2D	-3.52	101.76	106.89
19	P	202	9Y0	O7-C21-C22	3.47	118.98	111.48
15	L	602	HEA	C26-C15-C16	3.44	121.20	115.23
18	E	604	MQ9	C12-C13-C14	-3.44	119.75	127.62
18	F	708	MQ9	C8-C7-C6	3.43	120.54	112.08
15	L	602	HEA	OMA-CMA-C3A	-3.40	117.94	125.62
18	F	709	MQ9	C12-C13-C14	-3.40	119.83	127.62
15	L	603	HEA	C4D-C3D-C2D	-3.36	102.00	106.89
15	R	602	HEA	OMA-CMA-C3A	-3.35	118.07	125.62
18	F	709	MQ9	C30-C29-C31	3.34	121.02	115.23
22	O	301	HEC	C4D-ND-C1D	3.33	111.25	105.82
15	R	603	HEA	CAA-C2A-C1A	3.33	131.62	124.85
15	R	602	HEA	C26-C15-C16	3.30	120.96	115.23
18	F	709	MQ9	C17-C18-C19	-3.29	120.08	127.62
16	T	201	CDL	CB6-CB4-CB3	-3.29	104.11	111.78
18	F	708	MQ9	C15-C14-C16	3.29	120.93	115.23
16	T	201	CDL	CA4-OA6-CA5	-3.29	109.93	117.80
18	Z	201	MQ9	C40-C39-C41	-3.28	109.53	115.23
16	Z	202	CDL	CB6-CB4-CB3	-3.28	104.14	111.78
23	Y	502	9YF	O11-C25-C26	3.27	121.79	111.83
23	M	501	9YF	O11-C25-C26	3.26	121.79	111.83
18	E	604	MQ9	C17-C18-C19	-3.26	120.16	127.62
16	Z	202	CDL	CA4-OA6-CA5	-3.26	110.00	117.80
15	R	602	HEA	CMC-C2C-C1C	-3.25	120.47	125.42
18	F	708	MQ9	C51-C49-C50	3.24	122.03	114.59
15	L	603	HEA	CAA-C2A-C1A	3.20	131.37	124.85
23	I	304	9YF	O11-C25-C26	3.20	121.60	111.83
23	O	303	9YF	O11-C25-C26	3.20	121.58	111.83
18	Z	201	MQ9	C42-C43-C44	-3.19	120.33	127.62
18	E	604	MQ9	C32-C33-C34	-3.19	120.33	127.62
15	L	603	HEA	CAD-C3D-C4D	3.17	130.23	124.70
15	L	602	HEA	C26-C15-C14	-3.17	115.49	123.63
18	E	603	MQ9	C17-C18-C19	-3.16	120.38	127.62
18	F	707	MQ9	C8-C7-C6	3.16	119.87	112.08
15	L	603	HEA	CMC-C2C-C3C	3.16	133.98	126.55
18	F	709	MQ9	C32-C33-C34	-3.15	120.41	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	R	602	HEA	C3C-C2C-C1C	-3.15	103.46	107.17
16	L	604	CDL	OA5-PA1-OA3	-3.13	96.51	108.94
18	F	701	MQ9	C17-C18-C19	-3.13	120.45	127.62
19	P	202	9Y0	C29-C28-C27	3.11	130.10	114.37
19	J	203	9Y0	O7-C21-C22	3.11	118.20	111.48
16	L	604	CDL	OA2-PA1-OA3	3.09	121.20	108.94
21	G	302	9XX	O-C15-C14	3.06	121.16	111.83
18	F	709	MQ9	C35-C34-C36	3.06	120.54	115.23
15	R	603	HEA	CAA-CBA-CGA	-3.06	105.56	113.67
18	E	604	MQ9	C30-C29-C31	3.05	120.52	115.23
15	L	603	HEA	C3C-C2C-C1C	-3.03	103.60	107.17
18	Z	201	MQ9	C17-C18-C19	-3.01	120.74	127.62
21	D	302	9XX	O-C15-C14	3.00	120.98	111.83
18	Z	201	MQ9	C12-C13-C14	-2.98	120.79	127.62
18	F	707	MQ9	O1-C1-C2	-2.94	116.86	121.57
15	L	602	HEA	C3C-C2C-C1C	-2.94	103.71	107.17
16	T	201	CDL	OB8-CB7-C71	2.91	120.71	111.83
18	F	707	MQ9	C20-C19-C21	2.91	120.28	115.23
18	Z	201	MQ9	C5M-C5-C6	-2.90	119.69	124.45
16	Z	202	CDL	OB8-CB7-C71	2.89	120.66	111.83
18	E	604	MQ9	C35-C34-C36	2.88	120.23	115.23
15	R	603	HEA	C3C-C4C-NC	2.87	112.22	109.80
15	L	603	HEA	CMD-C2D-C1D	-2.87	120.56	125.03
16	Z	203	CDL	OB8-CB7-C71	2.85	120.52	111.83
18	E	604	MQ9	C15-C14-C16	2.85	120.17	115.23
15	L	602	HEA	C17-C18-C19	-2.85	121.11	127.62
18	F	709	MQ9	C27-C28-C29	-2.84	121.12	127.62
18	F	708	MQ9	C42-C41-C39	2.83	122.58	113.19
19	X	303	9Y0	O5-C5-C6	2.83	120.48	111.83
18	E	604	MQ9	C27-C28-C29	-2.82	121.16	127.62
18	E	604	MQ9	C7-C8-C9	-2.82	121.97	126.83
18	I	303	MQ9	C7-C8-C9	-2.82	121.97	126.83
18	F	701	MQ9	C42-C43-C44	-2.82	121.17	127.62
15	R	602	HEA	C3B-C4B-NB	2.82	113.08	109.84
18	F	709	MQ9	C15-C14-C16	2.81	120.11	115.23
18	Z	201	MQ9	C22-C23-C24	-2.81	121.19	127.62
15	L	602	HEA	CHA-C4D-C3D	-2.81	120.68	124.77
18	E	603	MQ9	C42-C43-C44	-2.81	121.19	127.62
17	E	602	HEM	C3B-C2B-C1B	2.80	108.52	106.41
19	J	202	9Y0	O5-C5-C6	2.80	120.38	111.83
15	R	603	HEA	C3C-C2C-C1C	-2.80	103.87	107.17
16	T	201	CDL	OA8-CA7-C31	2.79	120.34	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	Z	202	CDL	OA6-CA5-OA7	-2.78	117.19	123.70
18	F	708	MQ9	C42-C43-C44	-2.78	121.26	127.62
19	F	706	9Y0	O5-C5-C6	2.77	120.30	111.83
16	Z	202	CDL	OA8-CA7-C31	2.77	120.29	111.83
16	X	302	CDL	OB8-CB7-C71	2.77	120.29	111.83
18	I	303	MQ9	C5M-C5-C6	-2.77	119.89	124.45
18	Z	201	MQ9	C32-C33-C34	-2.77	121.29	127.62
18	F	707	MQ9	C22-C23-C24	-2.76	121.31	127.62
18	F	709	MQ9	C7-C8-C9	-2.76	122.08	126.83
16	S	301	CDL	OB8-CB7-C71	2.75	120.23	111.83
16	T	201	CDL	OA6-CA5-OA7	-2.75	117.27	123.70
15	L	603	HEA	C3C-C4C-NC	2.74	112.11	109.80
16	Z	203	CDL	OA8-CA7-C31	2.72	120.14	111.83
17	F	703	HEM	C3B-C2B-C1B	2.72	108.45	106.41
18	Z	201	MQ9	C7-C6-C5	-2.72	120.22	124.89
15	R	602	HEA	C3C-C4C-NC	2.72	112.09	109.80
18	F	701	MQ9	C20-C19-C21	2.71	119.93	115.23
18	F	708	MQ9	C27-C26-C24	2.71	122.16	113.19
15	L	603	HEA	CAA-CBA-CGA	-2.71	106.48	113.67
18	E	603	MQ9	C20-C19-C21	2.70	119.92	115.23
15	L	602	HEA	C3C-C4C-NC	2.69	112.07	109.80
19	S	302	9Y0	O5-C5-C6	2.69	120.04	111.83
15	R	602	HEA	CAA-C2A-C1A	2.69	130.31	124.85
18	F	707	MQ9	C35-C34-C36	2.68	119.89	115.23
16	X	302	CDL	OA8-CA7-C31	2.68	120.00	111.83
15	L	602	HEA	CAA-C2A-C1A	2.66	130.27	124.85
21	c	202	9XX	O-C15-C14	2.66	119.95	111.83
15	L	603	HEA	CMD-C2D-C3D	2.66	133.35	126.15
16	S	301	CDL	OA8-CA7-C31	2.66	119.93	111.83
18	F	707	MQ9	C31-C29-C28	-2.65	115.21	121.17
19	J	203	9Y0	O5-C5-C6	2.64	119.90	111.83
23	c	203	9YF	O11-C25-C26	2.64	119.89	111.83
18	Z	201	MQ9	C35-C34-C36	2.63	119.80	115.23
15	L	602	HEA	C27-C19-C20	2.63	119.79	115.23
18	F	707	MQ9	C5M-C5-C6	-2.62	120.15	124.45
23	W	203	9YF	O11-C25-C26	2.60	119.75	111.83
21	G	302	9XX	C17-O1-C18	-2.58	114.07	117.78
17	E	602	HEM	CHD-C4C-NC	2.57	127.26	124.45
18	Z	201	MQ9	C30-C29-C31	2.57	119.69	115.23
15	R	602	HEA	C27-C19-C20	2.57	119.69	115.23
18	F	707	MQ9	C7-C6-C5	-2.57	120.49	124.89
16	S	301	CDL	OB4-PB2-OB3	-2.56	100.52	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	X	302	CDL	OB4-PB2-OB3	-2.56	100.53	112.44
18	I	303	MQ9	C12-C13-C14	-2.56	121.76	127.62
16	Z	203	CDL	OA4-PA1-OA3	-2.55	100.59	112.44
15	R	602	HEA	CMD-C2D-C1D	-2.55	121.06	125.03
18	Z	201	MQ9	C25-C24-C26	2.54	119.64	115.23
18	F	707	MQ9	C7-C8-C9	-2.54	122.45	126.83
18	E	604	MQ9	C20-C19-C21	2.54	119.63	115.23
15	L	602	HEA	CAD-CBD-CGD	-2.54	106.94	113.67
18	I	303	MQ9	C32-C33-C34	-2.53	121.83	127.62
15	L	602	HEA	C3B-C4B-NB	2.53	112.75	109.84
16	T	201	CDL	OA8-CA7-OA9	-2.52	117.33	123.63
16	T	201	CDL	OB6-CB5-OB7	-2.52	117.82	123.70
18	F	709	MQ9	C20-C19-C21	2.51	119.58	115.23
18	E	604	MQ9	C40-C39-C41	-2.51	110.87	115.23
16	Z	202	CDL	OB6-CB5-OB7	-2.51	117.84	123.70
15	R	603	HEA	CMD-C2D-C1D	-2.50	121.12	125.03
18	Z	201	MQ9	C11-C9-C8	2.50	126.78	121.17
22	I	301	HEC	C2A-C1A-NA	-2.50	107.91	110.32
22	O	302	HEC	C2A-C1A-NA	-2.50	107.91	110.32
16	Z	202	CDL	OA8-CA7-OA9	-2.50	117.39	123.63
15	L	602	HEA	CMD-C2D-C1D	-2.49	121.14	125.03
18	F	701	MQ9	C5M-C5-C6	-2.49	120.36	124.45
18	F	701	MQ9	C27-C28-C29	-2.49	121.93	127.62
22	I	302	HEC	CHC-C4B-C3B	2.49	129.41	125.21
18	E	603	MQ9	C27-C28-C29	-2.48	121.94	127.62
18	I	303	MQ9	C30-C29-C28	-2.48	117.25	123.63
17	F	703	HEM	C3B-C4B-NB	-2.48	107.69	109.47
16	Z	202	CDL	OA4-PA1-OA3	-2.48	100.92	112.44
18	E	603	MQ9	C7-C6-C5	-2.48	120.64	124.89
15	R	602	HEA	C17-C18-C19	-2.48	121.96	127.62
23	Y	503	9YF	O3-C3-C4	-2.47	104.56	110.38
18	E	604	MQ9	C45-C44-C43	-2.47	117.29	123.63
18	F	707	MQ9	C40-C39-C41	-2.46	110.95	115.23
16	T	201	CDL	OA4-PA1-OA3	-2.46	100.99	112.44
18	F	707	MQ9	C10-C9-C11	-2.46	110.96	115.23
16	Z	203	CDL	OB4-PB2-OB3	-2.46	101.02	112.44
18	E	603	MQ9	C5M-C5-C6	-2.45	120.42	124.45
15	R	602	HEA	C4B-C3B-C2B	-2.44	103.34	107.44
17	F	703	HEM	C1B-NB-C4B	2.44	108.09	105.21
18	F	701	MQ9	C32-C33-C34	-2.43	122.05	127.62
23	M	502	9YF	O3-C3-C4	-2.43	104.64	110.38
18	F	701	MQ9	C7-C6-C5	-2.43	120.73	124.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	Z	201	MQ9	C45-C44-C46	2.42	119.44	115.23
17	E	602	HEM	C1B-NB-C4B	2.42	108.08	105.21
18	E	603	MQ9	C22-C23-C24	-2.42	122.08	127.62
15	R	603	HEA	CHA-C1A-NA	2.42	127.08	124.45
18	I	303	MQ9	C20-C19-C21	2.41	119.41	115.23
21	W	202	9XX	O-C15-O6	2.40	129.63	123.63
15	L	602	HEA	CAD-C3D-C2D	-2.40	123.37	127.87
23	M	501	9YF	C7-C2-C3	-2.40	107.53	110.86
22	I	302	HEC	C2A-C1A-NA	-2.40	108.01	110.32
18	E	603	MQ9	C32-C33-C34	-2.39	122.15	127.62
23	M	501	9YF	C30-C31-C32	2.39	122.62	113.62
15	R	603	HEA	CMD-C2D-C3D	2.39	132.60	126.15
18	Z	201	MQ9	C15-C14-C16	2.39	119.37	115.23
23	Y	502	9YF	C7-C2-C3	-2.38	107.55	110.86
18	F	701	MQ9	C22-C23-C24	-2.38	122.18	127.62
23	Y	502	9YF	C30-C31-C32	2.37	122.56	113.62
18	I	303	MQ9	C22-C23-C24	-2.37	122.19	127.62
15	L	602	HEA	C4B-C3B-C2B	-2.37	103.45	107.44
18	F	709	MQ9	C22-C23-C24	-2.37	122.20	127.62
18	I	303	MQ9	C51-C49-C50	2.36	120.02	114.59
18	E	604	MQ9	C22-C23-C24	-2.36	122.23	127.62
23	Y	502	9YF	O4-C4-C3	-2.34	104.86	110.38
17	E	602	HEM	C3B-C4B-NB	-2.34	107.79	109.47
23	M	501	9YF	O4-C4-C3	-2.33	104.87	110.38
18	F	708	MQ9	O1-C1-C2	-2.33	117.84	121.57
18	F	707	MQ9	C46-C44-C43	-2.33	115.93	121.17
16	T	201	CDL	OB4-PB2-OB3	-2.33	101.61	112.44
16	X	302	CDL	OA4-PA1-OA3	-2.33	101.62	112.44
18	E	603	MQ9	C7-C8-C9	-2.32	122.83	126.83
18	F	707	MQ9	C16-C14-C13	-2.32	115.96	121.17
18	I	303	MQ9	C15-C14-C16	2.31	119.24	115.23
18	F	709	MQ9	C45-C44-C43	-2.31	117.69	123.63
16	S	301	CDL	OA4-PA1-OA3	-2.31	101.70	112.44
18	F	701	MQ9	C25-C24-C26	2.31	119.23	115.23
16	Z	202	CDL	OB4-PB2-OB3	-2.30	101.74	112.44
22	I	302	HEC	CHD-C4C-C3C	2.30	129.09	125.21
15	R	602	HEA	CHD-C1D-ND	2.29	127.19	124.37
21	D	302	9XX	C17-O1-C18	-2.28	114.49	117.78
15	L	603	HEA	C25-C23-C24	2.28	119.83	114.59
18	F	707	MQ9	C12-C11-C9	2.27	120.72	113.19
18	E	603	MQ9	C25-C24-C26	2.27	119.17	115.23
18	I	303	MQ9	C7-C6-C5	-2.27	120.99	124.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	R	602	HEA	CBD-CAD-C3D	2.27	118.81	112.53
18	F	701	MQ9	C7-C8-C9	-2.27	122.92	126.83
18	F	709	MQ9	C40-C39-C41	-2.27	111.29	115.23
15	R	602	HEA	CHA-C1A-NA	2.27	126.92	124.45
22	O	302	HEC	CHC-C4B-C3B	2.27	129.03	125.21
21	c	202	9XX	O1-C17-C37	2.26	113.02	107.96
18	F	701	MQ9	C15-C14-C16	2.26	119.14	115.23
18	I	303	MQ9	C35-C34-C36	2.25	119.14	115.23
15	R	602	HEA	CAA-CBA-CGA	-2.25	107.69	113.67
23	I	304	9YF	O5-C5-C4	-2.25	105.08	110.38
23	M	501	9YF	O9-C8-O10	-2.25	118.45	123.70
23	Y	502	9YF	O9-C8-O10	-2.24	118.46	123.70
23	O	303	9YF	O5-C5-C4	-2.24	105.10	110.38
18	F	707	MQ9	C7-C6-C1	2.22	120.92	118.58
23	W	203	9YF	C7-C2-C3	-2.22	107.78	110.86
17	E	601	HEM	C4D-ND-C1D	2.21	107.83	105.21
22	O	301	HEC	C2A-C1A-NA	-2.21	108.19	110.32
18	E	603	MQ9	C15-C14-C16	2.20	119.05	115.23
17	F	702	HEM	C4D-ND-C1D	2.20	107.82	105.21
18	Z	201	MQ9	C20-C19-C21	2.20	119.05	115.23
23	M	501	9YF	O11-C24-C	2.20	114.74	108.40
15	R	603	HEA	C25-C23-C24	2.20	119.64	114.59
18	E	604	MQ9	C42-C43-C44	-2.20	122.60	127.62
15	L	603	HEA	CHA-C1A-NA	2.19	126.84	124.45
17	E	601	HEM	C3D-C4D-ND	-2.19	107.77	110.17
17	F	702	HEM	C3D-C4D-ND	-2.18	107.78	110.17
23	Y	502	9YF	O11-C24-C	2.18	114.67	108.40
18	I	303	MQ9	C42-C43-C44	-2.17	122.66	127.62
18	I	303	MQ9	C40-C39-C41	-2.16	111.47	115.23
18	F	701	MQ9	C12-C13-C14	-2.16	122.68	127.62
18	I	303	MQ9	C25-C24-C26	2.16	118.97	115.23
18	I	303	MQ9	C32-C31-C29	-2.16	106.04	113.19
15	L	602	HEA	CMD-C2D-C3D	2.16	131.98	126.15
23	c	203	9YF	C7-C2-C3	-2.15	107.87	110.86
15	R	602	HEA	C25-C23-C24	2.15	119.54	114.59
21	D	302	9XX	O1-C17-C16	2.15	111.16	106.21
18	I	303	MQ9	C10-C9-C11	2.14	118.95	115.23
15	L	602	HEA	CAA-CBA-CGA	-2.14	107.98	113.67
15	R	602	HEA	CHB-C4A-NA	2.14	126.78	124.45
15	L	602	HEA	CBD-CAD-C3D	2.13	118.43	112.53
15	L	602	HEA	C25-C23-C24	2.13	119.49	114.59
15	L	603	HEA	C12-C11-C3B	-2.13	108.79	112.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	M	502	9YF	C7-C6-C5	2.12	114.55	110.83
21	G	302	9XX	O1-C17-C16	2.11	111.07	106.21
18	I	303	MQ9	C17-C18-C19	-2.11	122.80	127.62
16	R	604	CDL	OB4-PB2-OB5	-2.11	98.02	107.57
21	W	202	9XX	O6-C15-C14	-2.11	115.54	123.78
18	F	707	MQ9	C32-C31-C29	-2.11	106.21	113.19
18	E	603	MQ9	C12-C13-C14	-2.10	122.83	127.62
23	Y	503	9YF	C7-C6-C5	2.09	114.50	110.83
15	R	602	HEA	CHC-C1C-C2C	-2.09	121.36	127.43
18	F	709	MQ9	C7-C6-C5	-2.08	121.32	124.89
16	R	604	CDL	OA5-PA1-OA3	-2.07	100.73	108.94
15	L	602	HEA	CHB-C4A-NA	2.07	126.70	124.45
15	R	602	HEA	CHD-C1D-C2D	-2.06	121.09	126.95
18	F	707	MQ9	C25-C24-C26	2.06	118.81	115.23
15	L	602	HEA	CHC-C1C-C2C	-2.06	121.44	127.43
21	c	202	9XX	C25-C26-C27	-2.06	109.12	115.97
18	E	604	MQ9	C10-C9-C11	2.06	118.80	115.23
18	F	709	MQ9	C10-C9-C11	2.06	118.80	115.23
18	E	604	MQ9	C5M-C5-C6	-2.05	121.08	124.45
16	Z	202	CDL	C58-C57-C56	-2.05	104.02	114.37
18	F	701	MQ9	C35-C34-C36	2.04	118.77	115.23
16	L	604	CDL	OB4-PB2-OB5	-2.04	98.33	107.57
16	T	201	CDL	C58-C57-C56	-2.04	104.07	114.37
15	L	603	HEA	CHB-C1B-C2B	-2.04	121.81	125.03
18	E	603	MQ9	C30-C29-C28	-2.03	118.41	123.63
15	R	602	HEA	CHB-C1B-C2B	-2.03	121.82	125.03
16	T	201	CDL	C56-C55-C54	-2.03	104.13	114.37
16	Z	202	CDL	C56-C55-C54	-2.02	104.14	114.37
17	E	602	HEM	CHC-C1C-NC	2.02	126.66	124.45
16	F	705	CDL	OA6-CA5-C11	2.02	115.85	111.48
15	L	603	HEA	OMA-CMA-C3A	-2.02	121.06	125.62
18	E	604	MQ9	C7-C6-C5	-2.02	121.43	124.89
18	F	701	MQ9	C30-C29-C31	2.02	118.73	115.23
18	F	701	MQ9	C30-C29-C28	-2.01	118.45	123.63
18	F	709	MQ9	C25-C24-C26	2.01	118.71	115.23
18	I	303	MQ9	C31-C29-C28	2.01	125.67	121.17
21	G	302	9XX	O1-C18-O2	-2.01	119.02	123.70
18	F	707	MQ9	C30-C29-C31	2.00	118.71	115.23
18	F	708	MQ9	C31-C29-C28	2.00	125.66	121.17

There are no chirality outliers.

All (1218) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	R	602	HEA	C2D-C3D-CAD-CBD
15	R	602	HEA	C4D-C3D-CAD-CBD
15	L	602	HEA	C12-C11-C3B-C2B
16	R	604	CDL	CA3-OA5-PA1-OA2
16	R	604	CDL	CA3-OA5-PA1-OA3
16	R	604	CDL	CA3-OA5-PA1-OA4
16	R	604	CDL	C11-CA5-OA6-CA4
16	R	604	CDL	CB2-OB2-PB2-OB3
16	R	604	CDL	C51-CB5-OB6-CB4
16	E	605	CDL	O1-C1-CB2-OB2
16	E	605	CDL	CA2-C1-CB2-OB2
16	E	605	CDL	CA2-OA2-PA1-OA3
16	E	605	CDL	CA2-OA2-PA1-OA5
16	E	605	CDL	CA3-OA5-PA1-OA2
16	E	605	CDL	C1-CB2-OB2-PB2
16	E	605	CDL	CB2-OB2-PB2-OB3
16	E	605	CDL	CB2-OB2-PB2-OB4
16	E	605	CDL	CB2-OB2-PB2-OB5
16	E	605	CDL	CB3-OB5-PB2-OB2
16	E	605	CDL	CB3-OB5-PB2-OB3
16	E	605	CDL	CB4-CB3-OB5-PB2
16	E	606	CDL	CA2-OA2-PA1-OA5
16	E	606	CDL	CA3-OA5-PA1-OA2
16	E	606	CDL	CA3-OA5-PA1-OA4
16	E	606	CDL	CB2-OB2-PB2-OB4
16	E	606	CDL	CB2-OB2-PB2-OB5
16	E	606	CDL	CB3-OB5-PB2-OB4
16	F	704	CDL	O1-C1-CB2-OB2
16	F	704	CDL	CA2-C1-CB2-OB2
16	F	704	CDL	CA2-OA2-PA1-OA3
16	F	704	CDL	CA2-OA2-PA1-OA5
16	F	704	CDL	CA3-OA5-PA1-OA2
16	F	704	CDL	C1-CB2-OB2-PB2
16	F	704	CDL	CB2-OB2-PB2-OB3
16	F	704	CDL	CB2-OB2-PB2-OB4
16	F	704	CDL	CB2-OB2-PB2-OB5
16	F	704	CDL	CB3-OB5-PB2-OB2
16	F	704	CDL	CB3-OB5-PB2-OB3
16	F	704	CDL	CB4-CB3-OB5-PB2
16	F	705	CDL	CA2-OA2-PA1-OA3
16	F	705	CDL	CA2-OA2-PA1-OA4
16	F	705	CDL	CA2-OA2-PA1-OA5
16	F	705	CDL	CA3-OA5-PA1-OA2

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Mol	Chain	Res	Type	Atoms
16	F	705	CDL	CA3-OA5-PA1-OA4
16	F	705	CDL	CB3-OB5-PB2-OB2
16	F	705	CDL	CB3-OB5-PB2-OB3
16	F	705	CDL	CB3-OB5-PB2-OB4
16	L	604	CDL	CA3-OA5-PA1-OA2
16	L	604	CDL	CA3-OA5-PA1-OA4
16	L	604	CDL	C11-CA5-OA6-CA4
16	L	604	CDL	C31-CA7-OA8-CA6
16	L	604	CDL	CB2-OB2-PB2-OB3
16	L	604	CDL	CB2-OB2-PB2-OB5
16	L	604	CDL	OB7-CB5-OB6-CB4
16	S	301	CDL	CA3-OA5-PA1-OA2
16	S	301	CDL	CA3-OA5-PA1-OA3
16	S	301	CDL	CB2-OB2-PB2-OB3
16	S	301	CDL	CB2-OB2-PB2-OB4
16	S	301	CDL	CB2-OB2-PB2-OB5
16	S	301	CDL	CB3-OB5-PB2-OB2
16	S	301	CDL	CB3-OB5-PB2-OB3
16	S	301	CDL	CB3-OB5-PB2-OB4
16	S	301	CDL	OB7-CB5-OB6-CB4
16	T	201	CDL	CA3-OA5-PA1-OA2
16	T	201	CDL	CA3-OA5-PA1-OA3
16	T	201	CDL	OA6-CA4-CA6-OA8
16	T	201	CDL	C11-CA5-OA6-CA4
16	T	201	CDL	C51-CB5-OB6-CB4
16	T	202	CDL	CA2-OA2-PA1-OA4
16	T	202	CDL	CA2-OA2-PA1-OA5
16	T	202	CDL	OA6-CA4-CA6-OA8
16	T	202	CDL	CB3-OB5-PB2-OB2
16	T	202	CDL	CB3-OB5-PB2-OB4
16	T	202	CDL	C51-CB5-OB6-CB4
16	T	203	CDL	O1-C1-CA2-OA2
16	T	203	CDL	CA2-C1-CB2-OB2
16	T	203	CDL	OA7-CA5-OA6-CA4
16	T	203	CDL	C11-CA5-OA6-CA4
16	T	203	CDL	CB3-OB5-PB2-OB2
16	T	203	CDL	CB3-OB5-PB2-OB3
16	P	201	CDL	CA2-OA2-PA1-OA3
16	P	201	CDL	CA2-OA2-PA1-OA4
16	P	201	CDL	CA2-OA2-PA1-OA5
16	P	201	CDL	CB2-OB2-PB2-OB3
16	P	201	CDL	CB2-OB2-PB2-OB4

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Mol	Chain	Res	Type	Atoms
16	P	201	CDL	CB2-OB2-PB2-OB5
16	X	301	CDL	CA2-OA2-PA1-OA4
16	X	301	CDL	CA2-OA2-PA1-OA5
16	X	301	CDL	OA6-CA4-CA6-OA8
16	X	301	CDL	CB3-OB5-PB2-OB2
16	X	301	CDL	CB3-OB5-PB2-OB4
16	X	301	CDL	C51-CB5-OB6-CB4
16	X	302	CDL	CA3-OA5-PA1-OA2
16	X	302	CDL	CA3-OA5-PA1-OA3
16	X	302	CDL	CB2-OB2-PB2-OB3
16	X	302	CDL	CB2-OB2-PB2-OB4
16	X	302	CDL	CB2-OB2-PB2-OB5
16	X	302	CDL	CB3-OB5-PB2-OB2
16	X	302	CDL	CB3-OB5-PB2-OB3
16	X	302	CDL	CB3-OB5-PB2-OB4
16	X	302	CDL	OB7-CB5-OB6-CB4
16	Z	202	CDL	CA3-OA5-PA1-OA2
16	Z	202	CDL	CA3-OA5-PA1-OA3
16	Z	202	CDL	OA6-CA4-CA6-OA8
16	Z	202	CDL	C11-CA5-OA6-CA4
16	Z	202	CDL	C51-CB5-OB6-CB4
16	Z	203	CDL	O1-C1-CB2-OB2
16	Z	203	CDL	CA2-OA2-PA1-OA3
16	Z	203	CDL	CA2-OA2-PA1-OA4
16	Z	203	CDL	CA2-OA2-PA1-OA5
16	Z	203	CDL	OA7-CA5-OA6-CA4
16	Z	203	CDL	C11-CA5-OA6-CA4
16	J	201	CDL	CA2-OA2-PA1-OA3
16	J	201	CDL	CA2-OA2-PA1-OA4
16	J	201	CDL	CA2-OA2-PA1-OA5
16	J	201	CDL	CB2-OB2-PB2-OB3
16	J	201	CDL	CB2-OB2-PB2-OB4
16	J	201	CDL	CB2-OB2-PB2-OB5
18	E	603	MQ9	C9-C11-C12-C13
19	F	706	9Y0	C22-C21-O7-C1
19	F	706	9Y0	O6-C21-O7-C1
19	S	302	9Y0	O1-C3-C4-N
19	P	202	9Y0	C22-C21-O7-C1
19	P	202	9Y0	O1-C3-C4-N
19	P	202	9Y0	C3-O1-P-O
19	X	303	9Y0	O1-C3-C4-N
19	J	202	9Y0	C22-C21-O7-C1

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Mol	Chain	Res	Type	Atoms
19	J	202	9Y0	O6-C21-O7-C1
19	J	202	9Y0	C2-O3-P-O
19	J	202	9Y0	C2-O3-P-O1
19	J	202	9Y0	C2-O3-P-O2
19	J	203	9Y0	O1-C3-C4-N
21	D	302	9XX	C19-C18-O1-C17
21	G	302	9XX	C19-C18-O1-C17
21	c	202	9XX	O-C16-C17-O1
21	c	202	9XX	C37-C17-O1-C18
21	c	202	9XX	C19-C18-O1-C17
21	c	202	9XX	O2-C18-O1-C17
21	W	202	9XX	O-C16-C17-O1
22	O	301	HEC	C2B-C3B-CAB-CBB
22	O	301	HEC	C4B-C3B-CAB-CBB
22	O	301	HEC	C2C-C3C-CAC-CBC
22	O	301	HEC	C4C-C3C-CAC-CBC
22	O	302	HEC	C2B-C3B-CAB-CBB
22	O	302	HEC	C4B-C3B-CAB-CBB
22	O	302	HEC	C2C-C3C-CAC-CBC
22	O	302	HEC	C4C-C3C-CAC-CBC
22	I	301	HEC	C2B-C3B-CAB-CBB
22	I	301	HEC	C4B-C3B-CAB-CBB
22	I	301	HEC	C2C-C3C-CAC-CBC
22	I	301	HEC	C4C-C3C-CAC-CBC
22	I	302	HEC	C2C-C3C-CAC-CBC
22	I	302	HEC	C4C-C3C-CAC-CBC
23	O	303	9YF	C-C1-O-P
23	O	303	9YF	C9-C8-O9-C
23	c	203	9YF	C2-O2-P-O
23	c	203	9YF	C2-O2-P-O8
23	c	203	9YF	C1-O-P-O1
23	c	203	9YF	C1-O-P-O2
23	c	203	9YF	C1-O-P-O8
23	c	203	9YF	C9-C8-O9-C
23	I	304	9YF	C-C1-O-P
23	I	304	9YF	C9-C8-O9-C
23	Y	502	9YF	C1-O-P-O1
23	Y	502	9YF	C1-O-P-O2
23	Y	502	9YF	C9-C8-O9-C
23	Y	503	9YF	C1-O-P-O8
23	Y	503	9YF	C9-C8-O9-C
23	W	203	9YF	C2-O2-P-O

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Mol	Chain	Res	Type	Atoms
23	W	203	9YF	C2-O2-P-O8
23	W	203	9YF	C1-O-P-O1
23	W	203	9YF	C1-O-P-O2
23	W	203	9YF	C1-O-P-O8
23	W	203	9YF	C9-C8-O9-C
23	M	501	9YF	C1-O-P-O1
23	M	501	9YF	C1-O-P-O2
23	M	501	9YF	C9-C8-O9-C
23	M	502	9YF	C1-O-P-O8
23	M	502	9YF	C9-C8-O9-C
16	R	604	CDL	OA9-CA7-OA8-CA6
16	L	604	CDL	OA9-CA7-OA8-CA6
21	W	202	9XX	O6-C15-O-C16
16	R	604	CDL	C31-CA7-OA8-CA6
16	T	201	CDL	OA9-CA7-OA8-CA6
16	T	202	CDL	OA9-CA7-OA8-CA6
16	T	203	CDL	OA9-CA7-OA8-CA6
16	T	203	CDL	OB9-CB7-OB8-CB6
16	X	301	CDL	OA9-CA7-OA8-CA6
16	Z	202	CDL	OA9-CA7-OA8-CA6
16	Z	203	CDL	OA9-CA7-OA8-CA6
16	Z	203	CDL	OB9-CB7-OB8-CB6
23	O	303	9YF	O12-C25-O11-C24
23	I	304	9YF	O12-C25-O11-C24
23	Y	502	9YF	O12-C25-O11-C24
23	M	501	9YF	O12-C25-O11-C24
16	R	604	CDL	OA7-CA5-OA6-CA4
16	R	604	CDL	OB7-CB5-OB6-CB4
16	E	605	CDL	OB7-CB5-OB6-CB4
16	E	606	CDL	OB7-CB5-OB6-CB4
16	F	704	CDL	OB7-CB5-OB6-CB4
16	F	705	CDL	OA7-CA5-OA6-CA4
16	L	604	CDL	OA7-CA5-OA6-CA4
16	T	201	CDL	OA7-CA5-OA6-CA4
16	T	201	CDL	OB7-CB5-OB6-CB4
16	T	202	CDL	OB7-CB5-OB6-CB4
16	X	301	CDL	OB7-CB5-OB6-CB4
16	Z	202	CDL	OA7-CA5-OA6-CA4
16	Z	202	CDL	OB7-CB5-OB6-CB4
19	P	202	9Y0	O6-C21-O7-C1
21	D	302	9XX	O2-C18-O1-C17
21	G	302	9XX	O2-C18-O1-C17

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Mol	Chain	Res	Type	Atoms
23	O	303	9YF	O10-C8-O9-C
23	c	203	9YF	O10-C8-O9-C
23	I	304	9YF	O10-C8-O9-C
23	Y	502	9YF	O10-C8-O9-C
23	Y	503	9YF	O10-C8-O9-C
23	W	203	9YF	O10-C8-O9-C
23	M	501	9YF	O10-C8-O9-C
23	M	502	9YF	O10-C8-O9-C
16	T	202	CDL	C31-CA7-OA8-CA6
16	T	203	CDL	C31-CA7-OA8-CA6
16	X	301	CDL	C31-CA7-OA8-CA6
16	Z	203	CDL	C71-CB7-OB8-CB6
19	X	303	9Y0	C6-C5-O5-C
19	J	202	9Y0	C6-C5-O5-C
21	W	202	9XX	C14-C15-O-C16
23	O	303	9YF	C26-C25-O11-C24
23	I	304	9YF	C26-C25-O11-C24
23	Y	502	9YF	C26-C25-O11-C24
23	M	501	9YF	C26-C25-O11-C24
16	E	605	CDL	C51-CB5-OB6-CB4
16	F	704	CDL	C51-CB5-OB6-CB4
16	F	705	CDL	C11-CA5-OA6-CA4
16	L	604	CDL	C51-CB5-OB6-CB4
16	S	301	CDL	C51-CB5-OB6-CB4
16	X	302	CDL	C51-CB5-OB6-CB4
15	L	602	HEA	C26-C15-C16-C17
18	F	707	MQ9	C15-C14-C16-C17
15	L	602	HEA	C14-C15-C16-C17
18	F	707	MQ9	C13-C14-C16-C17
23	Y	503	9YF	O12-C25-O11-C24
23	M	502	9YF	O12-C25-O11-C24
16	T	201	CDL	C31-CA7-OA8-CA6
16	T	203	CDL	C71-CB7-OB8-CB6
16	Z	202	CDL	C31-CA7-OA8-CA6
16	Z	203	CDL	C31-CA7-OA8-CA6
19	F	706	9Y0	C6-C5-O5-C
19	S	302	9Y0	C6-C5-O5-C
23	Y	503	9YF	C26-C25-O11-C24
23	M	502	9YF	C26-C25-O11-C24
19	F	706	9Y0	O4-C5-O5-C
19	X	303	9Y0	O4-C5-O5-C
19	J	202	9Y0	O4-C5-O5-C

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Mol	Chain	Res	Type	Atoms
19	S	302	9Y0	O6-C21-O7-C1
16	E	606	CDL	O1-C1-CB2-OB2
16	T	201	CDL	O1-C1-CB2-OB2
16	T	203	CDL	O1-C1-CB2-OB2
16	P	201	CDL	O1-C1-CA2-OA2
16	P	201	CDL	O1-C1-CB2-OB2
16	Z	202	CDL	O1-C1-CB2-OB2
16	J	201	CDL	O1-C1-CA2-OA2
16	J	201	CDL	O1-C1-CB2-OB2
23	c	203	9YF	C26-C25-O11-C24
23	W	203	9YF	C26-C25-O11-C24
19	S	302	9Y0	O4-C5-O5-C
16	E	606	CDL	C51-CB5-OB6-CB4
16	T	202	CDL	C11-CA5-OA6-CA4
16	X	301	CDL	C11-CA5-OA6-CA4
19	S	302	9Y0	C22-C21-O7-C1
19	X	303	9Y0	C22-C21-O7-C1
16	T	202	CDL	OA7-CA5-OA6-CA4
16	X	301	CDL	OA7-CA5-OA6-CA4
15	R	603	HEA	C15-C16-C17-C18
15	L	603	HEA	C15-C16-C17-C18
18	E	603	MQ9	C44-C46-C47-C48
18	E	604	MQ9	C29-C31-C32-C33
18	E	604	MQ9	C39-C41-C42-C43
18	F	701	MQ9	C9-C11-C12-C13
18	F	701	MQ9	C44-C46-C47-C48
18	F	707	MQ9	C9-C11-C12-C13
18	F	707	MQ9	C14-C16-C17-C18
18	F	708	MQ9	C14-C16-C17-C18
18	F	709	MQ9	C29-C31-C32-C33
18	F	709	MQ9	C39-C41-C42-C43
18	Z	201	MQ9	C9-C11-C12-C13
18	Z	201	MQ9	C14-C16-C17-C18
18	Z	201	MQ9	C29-C31-C32-C33
18	Z	201	MQ9	C44-C46-C47-C48
18	I	303	MQ9	C14-C16-C17-C18
16	T	203	CDL	C38-C39-C40-C41
16	P	201	CDL	C1-CA2-OA2-PA1
16	J	201	CDL	C1-CA2-OA2-PA1
15	L	602	HEA	C3D-CAD-CBD-CGD
16	F	705	CDL	C76-C77-C78-C79
19	J	202	9Y0	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
16	E	605	CDL	C31-CA7-OA8-CA6
16	F	704	CDL	C31-CA7-OA8-CA6
16	L	604	CDL	C74-C75-C76-C77
23	c	203	9YF	O12-C25-O11-C24
23	W	203	9YF	O12-C25-O11-C24
16	R	604	CDL	C38-C39-C40-C41
16	E	605	CDL	C59-C60-C61-C62
16	F	704	CDL	C59-C60-C61-C62
16	E	606	CDL	C76-C77-C78-C79
16	E	605	CDL	OA9-CA7-OA8-CA6
16	F	704	CDL	OA9-CA7-OA8-CA6
19	X	303	9Y0	O6-C21-O7-C1
16	T	201	CDL	CA2-C1-CB2-OB2
16	P	201	CDL	CA2-C1-CB2-OB2
16	Z	202	CDL	CA2-C1-CB2-OB2
16	Z	203	CDL	CA2-C1-CB2-OB2
16	J	201	CDL	CA2-C1-CB2-OB2
16	R	604	CDL	C71-CB7-OB8-CB6
16	L	604	CDL	C71-CB7-OB8-CB6
16	S	301	CDL	C31-CA7-OA8-CA6
16	X	302	CDL	C31-CA7-OA8-CA6
19	J	203	9Y0	C6-C5-O5-C
16	R	604	CDL	C52-C53-C54-C55
16	P	201	CDL	C55-C56-C57-C58
16	J	201	CDL	C55-C56-C57-C58
16	E	606	CDL	C58-C59-C60-C61
19	P	202	9Y0	C23-C24-C25-C26
16	F	705	CDL	C57-C58-C59-C60
16	T	201	CDL	O1-C1-CA2-OA2
16	Z	202	CDL	O1-C1-CA2-OA2
16	E	605	CDL	C33-C34-C35-C36
16	F	704	CDL	C33-C34-C35-C36
19	P	202	9Y0	C27-C28-C29-C30
16	E	606	CDL	C11-CA5-OA6-CA4
16	P	201	CDL	C51-CB5-OB6-CB4
16	J	201	CDL	C51-CB5-OB6-CB4
16	T	201	CDL	OB6-CB4-CB6-OB8
16	P	201	CDL	OB6-CB4-CB6-OB8
16	Z	202	CDL	OB6-CB4-CB6-OB8
16	J	201	CDL	OB6-CB4-CB6-OB8
23	Y	502	9YF	C11-C10-C9-C8
23	M	501	9YF	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
16	Z	203	CDL	CB7-C71-C72-C73
18	E	603	MQ9	C40-C39-C41-C42
19	P	202	9Y0	C29-C30-C31-C32
16	S	301	CDL	CB7-C71-C72-C73
16	X	302	CDL	CB7-C71-C72-C73
15	L	602	HEA	C4D-C3D-CAD-CBD
18	E	604	MQ9	C9-C11-C12-C13
18	E	604	MQ9	C44-C46-C47-C48
18	F	707	MQ9	C24-C26-C27-C28
18	F	707	MQ9	C29-C31-C32-C33
18	F	707	MQ9	C39-C41-C42-C43
18	F	707	MQ9	C44-C46-C47-C48
18	F	708	MQ9	C29-C31-C32-C33
18	F	709	MQ9	C9-C11-C12-C13
18	F	709	MQ9	C44-C46-C47-C48
18	Z	201	MQ9	C39-C41-C42-C43
16	L	604	CDL	C31-C32-C33-C34
16	R	604	CDL	CB7-C71-C72-C73
16	L	604	CDL	CA5-C11-C12-C13
16	T	201	CDL	CA5-C11-C12-C13
16	Z	202	CDL	CA5-C11-C12-C13
19	J	203	9Y0	C21-C22-C23-C24
21	W	202	9XX	C12-C13-C14-C15
23	Y	503	9YF	C25-C26-C27-C28
23	M	502	9YF	C25-C26-C27-C28
16	R	604	CDL	OB9-CB7-OB8-CB6
16	L	604	CDL	OB9-CB7-OB8-CB6
16	S	301	CDL	OA9-CA7-OA8-CA6
16	X	302	CDL	OA9-CA7-OA8-CA6
23	c	203	9YF	C33-C35-C36-C37
23	W	203	9YF	C33-C35-C36-C37
16	L	604	CDL	CB7-C71-C72-C73
16	S	301	CDL	CA5-C11-C12-C13
16	T	202	CDL	CB7-C71-C72-C73
16	X	301	CDL	CB7-C71-C72-C73
16	X	302	CDL	CA5-C11-C12-C13
19	J	203	9Y0	O4-C5-O5-C
16	R	604	CDL	C31-C32-C33-C34
16	R	604	CDL	C58-C59-C60-C61
16	E	606	CDL	OA7-CA5-OA6-CA4
16	L	604	CDL	C61-C62-C63-C64
16	P	201	CDL	OB7-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
16	J	201	CDL	OB7-CB5-OB6-CB4
16	T	203	CDL	CB2-C1-CA2-OA2
16	P	201	CDL	CB2-C1-CA2-OA2
16	J	201	CDL	CB2-C1-CA2-OA2
16	L	604	CDL	C38-C39-C40-C41
16	Z	203	CDL	CB5-C51-C52-C53
21	W	202	9XX	C19-C18-O1-C17
16	F	705	CDL	C78-C79-C80-C81
18	I	303	MQ9	C34-C36-C37-C38
23	Y	503	9YF	C9-C10-C11-C12
23	M	502	9YF	C9-C10-C11-C12
15	L	602	HEA	C2D-C3D-CAD-CBD
19	X	303	9Y0	C21-C22-C23-C24
16	T	201	CDL	CB6-CB4-OB6-CB5
16	Z	202	CDL	CB6-CB4-OB6-CB5
16	E	606	CDL	C78-C79-C80-C81
19	F	706	9Y0	C22-C23-C24-C25
21	W	202	9XX	O2-C18-O1-C17
16	E	605	CDL	C11-CA5-OA6-CA4
16	F	704	CDL	C11-CA5-OA6-CA4
18	E	603	MQ9	C38-C39-C41-C42
16	F	704	CDL	C55-C56-C57-C58
16	E	605	CDL	C55-C56-C57-C58
21	G	302	9XX	C17-C16-O-C15
16	T	201	CDL	C12-C13-C14-C15
16	Z	202	CDL	C12-C13-C14-C15
19	J	203	9Y0	C9-C10-C11-C12
21	W	202	9XX	C28-C29-C30-C31
23	Y	503	9YF	C26-C27-C28-C29
23	M	502	9YF	C26-C27-C28-C29
16	R	604	CDL	C35-C36-C37-C38
16	L	604	CDL	C75-C76-C77-C78
23	Y	503	9YF	C35-C36-C37-C38
23	Y	503	9YF	C37-C38-C39-C40
23	M	502	9YF	C35-C36-C37-C38
16	R	604	CDL	C55-C56-C57-C58
16	P	201	CDL	C60-C61-C62-C63
16	J	201	CDL	C60-C61-C62-C63
21	c	202	9XX	C31-C32-C33-C34
23	M	502	9YF	C37-C38-C39-C40
16	S	301	CDL	C71-CB7-OB8-CB6
16	X	302	CDL	C71-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
16	R	604	CDL	C75-C76-C77-C78
16	E	605	CDL	OA7-CA5-OA6-CA4
16	F	704	CDL	OA7-CA5-OA6-CA4
16	T	203	CDL	C73-C74-C75-C76
16	Z	203	CDL	C37-C38-C39-C40
16	E	605	CDL	C56-C57-C58-C59
16	F	704	CDL	C56-C57-C58-C59
16	T	203	CDL	C56-C57-C58-C59
16	F	705	CDL	C51-CB5-OB6-CB4
16	P	201	CDL	C11-CA5-OA6-CA4
16	J	201	CDL	C11-CA5-OA6-CA4
16	Z	203	CDL	C52-C53-C54-C55
19	S	302	9Y0	C21-C22-C23-C24
16	E	605	CDL	C75-C76-C77-C78
16	F	704	CDL	C75-C76-C77-C78
16	S	301	CDL	C35-C36-C37-C38
16	T	202	CDL	C59-C60-C61-C62
16	P	201	CDL	C75-C76-C77-C78
16	X	301	CDL	C59-C60-C61-C62
16	X	302	CDL	C35-C36-C37-C38
16	Z	203	CDL	C31-C32-C33-C34
16	J	201	CDL	C75-C76-C77-C78
19	J	203	9Y0	C6-C7-C8-C9
16	T	203	CDL	C32-C33-C34-C35
16	R	604	CDL	C53-C54-C55-C56
16	P	201	CDL	C32-C33-C34-C35
16	J	201	CDL	C32-C33-C34-C35
19	J	202	9Y0	C16-C17-C18-C19
23	Y	502	9YF	C10-C11-C12-C13
16	X	302	CDL	C74-C75-C76-C77
23	M	501	9YF	C10-C11-C12-C13
21	D	302	9XX	C14-C15-O-C16
16	E	605	CDL	CA3-CA4-CA6-OA8
16	F	704	CDL	CA3-CA4-CA6-OA8
16	F	705	CDL	C34-C35-C36-C37
16	S	301	CDL	C74-C75-C76-C77
16	T	203	CDL	C74-C75-C76-C77
19	F	706	9Y0	C15-C16-C17-C18
19	P	202	9Y0	C9-C10-C11-C12
19	P	202	9Y0	C21-C22-C23-C24
16	L	604	CDL	C55-C56-C57-C58
16	T	201	CDL	C51-C52-C53-C54

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Mol	Chain	Res	Type	Atoms
16	P	201	CDL	C31-C32-C33-C34
16	Z	202	CDL	C51-C52-C53-C54
16	Z	203	CDL	C32-C33-C34-C35
16	J	201	CDL	C31-C32-C33-C34
19	J	202	9Y0	C15-C16-C17-C18
21	W	202	9XX	C31-C32-C33-C34
16	F	705	CDL	C52-C53-C54-C55
16	Z	203	CDL	C35-C36-C37-C38
16	L	604	CDL	C76-C77-C78-C79
16	S	301	CDL	C31-C32-C33-C34
16	P	201	CDL	CB7-C71-C72-C73
16	J	201	CDL	CB7-C71-C72-C73
19	P	202	9Y0	C5-C6-C7-C8
16	E	606	CDL	C34-C35-C36-C37
16	F	705	CDL	C37-C38-C39-C40
16	S	301	CDL	C72-C73-C74-C75
16	T	203	CDL	C53-C54-C55-C56
16	X	302	CDL	C31-C32-C33-C34
16	X	302	CDL	C72-C73-C74-C75
17	E	602	HEM	C3D-CAD-CBD-CGD
16	F	705	CDL	C12-C13-C14-C15
16	L	604	CDL	C37-C38-C39-C40
16	P	201	CDL	C54-C55-C56-C57
16	P	201	CDL	C56-C57-C58-C59
16	R	604	CDL	C32-C33-C34-C35
16	L	604	CDL	C52-C53-C54-C55
16	Z	203	CDL	C11-C12-C13-C14
16	Z	203	CDL	C59-C60-C61-C62
16	J	201	CDL	C54-C55-C56-C57
16	J	201	CDL	C56-C57-C58-C59
23	O	303	9YF	C35-C36-C37-C38
23	I	304	9YF	C35-C36-C37-C38
16	S	301	CDL	OB9-CB7-OB8-CB6
16	X	302	CDL	OB9-CB7-OB8-CB6
16	E	606	CDL	C52-C53-C54-C55
16	P	201	CDL	OA7-CA5-OA6-CA4
16	J	201	CDL	OA7-CA5-OA6-CA4
18	F	701	MQ9	C40-C39-C41-C42
16	R	604	CDL	C37-C38-C39-C40
16	E	606	CDL	C37-C38-C39-C40
16	E	606	CDL	C53-C54-C55-C56
16	L	604	CDL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
16	T	201	CDL	C76-C77-C78-C79
16	Z	202	CDL	C76-C77-C78-C79
23	I	304	9YF	C26-C27-C28-C29
16	F	705	CDL	C31-CA7-OA8-CA6
23	O	303	9YF	C26-C27-C28-C29
23	Y	503	9YF	C27-C28-C29-C30
23	M	502	9YF	C27-C28-C29-C30
16	S	301	CDL	C11-C12-C13-C14
16	X	301	CDL	C11-C12-C13-C14
16	X	302	CDL	C11-C12-C13-C14
23	Y	502	9YF	C28-C29-C30-C31
23	M	501	9YF	C28-C29-C30-C31
16	T	202	CDL	C11-C12-C13-C14
16	T	203	CDL	C11-C12-C13-C14
23	Y	503	9YF	C11-C12-C13-C14
16	X	301	CDL	C52-C53-C54-C55
23	M	502	9YF	C11-C12-C13-C14
16	T	202	CDL	C52-C53-C54-C55
19	F	706	9Y0	C29-C30-C31-C32
19	J	203	9Y0	C22-C23-C24-C25
23	Y	503	9YF	C19-C20-C21-C22
23	M	502	9YF	C19-C20-C21-C22
16	E	606	CDL	CB5-C51-C52-C53
16	P	201	CDL	CA7-C31-C32-C33
16	J	201	CDL	CA7-C31-C32-C33
16	F	705	CDL	OB7-CB5-OB6-CB4
16	L	604	CDL	C32-C33-C34-C35
19	F	706	9Y0	C16-C17-C18-C19
19	J	203	9Y0	C24-C25-C26-C27
16	X	302	CDL	C60-C61-C62-C63
16	E	605	CDL	CA7-C31-C32-C33
16	F	704	CDL	CA7-C31-C32-C33
23	O	303	9YF	C11-C10-C9-C8
23	I	304	9YF	C11-C10-C9-C8
16	L	604	CDL	C53-C54-C55-C56
16	S	301	CDL	C60-C61-C62-C63
16	Z	202	CDL	C31-C32-C33-C34
16	Z	203	CDL	C73-C74-C75-C76
23	c	203	9YF	C17-C18-C19-C20
23	W	203	9YF	C17-C18-C19-C20
16	T	201	CDL	C31-C32-C33-C34
16	F	705	CDL	C59-C60-C61-C62

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Mol	Chain	Res	Type	Atoms
19	P	202	9Y0	C6-C7-C8-C9
20	c	201	PLM	C5-C6-C7-C8
23	Y	502	9YF	C33-C35-C36-C37
23	M	501	9YF	C33-C35-C36-C37
16	E	605	CDL	CB7-C71-C72-C73
16	F	704	CDL	CB7-C71-C72-C73
16	L	604	CDL	CB5-C51-C52-C53
19	S	302	9Y0	C18-C19-C20-C37
23	c	203	9YF	C15-C16-C17-C18
23	W	203	9YF	C15-C16-C17-C18
18	E	603	MQ9	C39-C41-C42-C43
18	F	708	MQ9	C39-C41-C42-C43
16	P	201	CDL	C52-C53-C54-C55
16	J	201	CDL	C52-C53-C54-C55
16	S	301	CDL	OA6-CA4-CA6-OA8
16	X	302	CDL	OA6-CA4-CA6-OA8
16	F	704	CDL	C12-C13-C14-C15
16	L	604	CDL	C12-C13-C14-C15
16	P	201	CDL	C57-C58-C59-C60
16	Z	203	CDL	C56-C57-C58-C59
16	J	201	CDL	C57-C58-C59-C60
16	E	605	CDL	C12-C13-C14-C15
16	F	705	CDL	C56-C57-C58-C59
19	J	202	9Y0	C6-C7-C8-C9
16	E	605	CDL	C34-C35-C36-C37
16	F	704	CDL	C34-C35-C36-C37
16	T	202	CDL	C55-C56-C57-C58
20	W	201	PLM	C2-C3-C4-C5
16	P	201	CDL	C74-C75-C76-C77
16	X	301	CDL	C55-C56-C57-C58
16	J	201	CDL	C74-C75-C76-C77
16	E	606	CDL	CA2-C1-CB2-OB2
16	F	705	CDL	OA9-CA7-OA8-CA6
21	c	202	9XX	C1-C2-C3-C4
16	T	201	CDL	C59-C60-C61-C62
16	X	301	CDL	C75-C76-C77-C78
16	Z	202	CDL	C59-C60-C61-C62
16	T	202	CDL	C75-C76-C77-C78
19	F	706	9Y0	C6-C7-C8-C9
19	P	202	9Y0	C14-C15-C16-C17
16	E	605	CDL	OB5-CB3-CB4-CB6
16	F	704	CDL	OB5-CB3-CB4-CB6

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Mol	Chain	Res	Type	Atoms
23	O	303	9YF	C24-C-C1-O
23	I	304	9YF	C24-C-C1-O
16	E	605	CDL	C32-C33-C34-C35
16	F	704	CDL	C32-C33-C34-C35
16	X	301	CDL	C38-C39-C40-C41
16	X	301	CDL	CA5-C11-C12-C13
23	Y	503	9YF	C31-C32-C33-C35
23	Y	503	9YF	C32-C33-C35-C36
23	M	502	9YF	C31-C32-C33-C35
23	M	502	9YF	C32-C33-C35-C36
16	T	202	CDL	C38-C39-C40-C41
16	P	201	CDL	C73-C74-C75-C76
16	J	201	CDL	C73-C74-C75-C76
21	D	302	9XX	O6-C15-O-C16
19	J	202	9Y0	C29-C30-C31-C32
16	X	302	CDL	C76-C77-C78-C79
16	T	202	CDL	CA5-C11-C12-C13
16	S	301	CDL	C76-C77-C78-C79
19	J	203	9Y0	C16-C17-C18-C19
16	F	704	CDL	C71-C72-C73-C74
16	T	203	CDL	C31-C32-C33-C34
16	E	605	CDL	C71-C72-C73-C74
16	E	605	CDL	CB3-CB4-CB6-OB8
16	F	704	CDL	CB3-CB4-CB6-OB8
16	S	301	CDL	CB3-CB4-CB6-OB8
16	T	202	CDL	CA3-CA4-CA6-OA8
16	P	201	CDL	CA3-CA4-CA6-OA8
16	P	201	CDL	CB3-CB4-CB6-OB8
16	X	301	CDL	CA3-CA4-CA6-OA8
16	X	302	CDL	CB3-CB4-CB6-OB8
16	J	201	CDL	CA3-CA4-CA6-OA8
16	J	201	CDL	CB3-CB4-CB6-OB8
18	F	708	MQ9	C34-C36-C37-C38
19	X	303	9Y0	O5-C-C1-C2
23	c	203	9YF	C1-C-C24-O11
23	W	203	9YF	C1-C-C24-O11
16	R	604	CDL	C72-C73-C74-C75
21	G	302	9XX	C14-C15-O-C16
16	Z	203	CDL	C72-C73-C74-C75
16	J	201	CDL	C76-C77-C78-C79
23	Y	502	9YF	C26-C27-C28-C29
16	P	201	CDL	C76-C77-C78-C79

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Mol	Chain	Res	Type	Atoms
23	M	501	9YF	C26-C27-C28-C29
16	T	201	CDL	CB5-C51-C52-C53
16	Z	202	CDL	CB5-C51-C52-C53
16	Z	203	CDL	CA7-C31-C32-C33
19	P	202	9Y0	C26-C27-C28-C29
18	F	701	MQ9	C38-C39-C41-C42
18	Z	201	MQ9	C12-C11-C9-C8
16	T	203	CDL	C57-C58-C59-C60
16	X	302	CDL	C34-C35-C36-C37
16	E	605	CDL	C72-C73-C74-C75
16	F	704	CDL	C72-C73-C74-C75
16	T	202	CDL	C72-C73-C74-C75
16	X	301	CDL	C72-C73-C74-C75
16	S	301	CDL	C34-C35-C36-C37
23	Y	502	9YF	C12-C13-C14-C15
23	M	501	9YF	C12-C13-C14-C15
16	E	605	CDL	CB6-CB4-OB6-CB5
16	F	704	CDL	CB6-CB4-OB6-CB5
21	c	202	9XX	C28-C29-C30-C31
21	c	202	9XX	C24-C25-C26-C27
19	X	303	9Y0	C14-C15-C16-C17
21	W	202	9XX	C20-C21-C22-C23
21	c	202	9XX	C7-C8-C9-C10
16	E	605	CDL	OA5-CA3-CA4-OA6
16	E	606	CDL	OA5-CA3-CA4-OA6
16	F	704	CDL	OA5-CA3-CA4-OA6
16	S	301	CDL	OA5-CA3-CA4-OA6
16	X	302	CDL	OA5-CA3-CA4-OA6
19	F	706	9Y0	O7-C1-C2-O3
16	E	606	CDL	C54-C55-C56-C57
16	X	302	CDL	C77-C78-C79-C80
16	J	201	CDL	C59-C60-C61-C62
16	R	604	CDL	C59-C60-C61-C62
16	S	301	CDL	C77-C78-C79-C80
16	P	201	CDL	C34-C35-C36-C37
16	P	201	CDL	C59-C60-C61-C62
16	X	301	CDL	C36-C37-C38-C39
16	J	201	CDL	C34-C35-C36-C37
16	L	604	CDL	C33-C34-C35-C36
16	T	202	CDL	C36-C37-C38-C39
16	T	203	CDL	C71-C72-C73-C74
23	W	203	9YF	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
20	G	301	PLM	C4-C5-C6-C7
23	c	203	9YF	C27-C28-C29-C30
16	F	705	CDL	OB6-CB4-CB6-OB8
16	Z	203	CDL	OB6-CB4-CB6-OB8
19	X	303	9Y0	O5-C-C1-O7
19	J	203	9Y0	O5-C-C1-O7
16	R	604	CDL	C11-C12-C13-C14
19	J	203	9Y0	C32-C33-C34-C35
16	T	202	CDL	C14-C15-C16-C17
16	T	203	CDL	C77-C78-C79-C80
16	X	301	CDL	C14-C15-C16-C17
16	X	301	CDL	C54-C55-C56-C57
16	L	604	CDL	C78-C79-C80-C81
16	J	201	CDL	C61-C62-C63-C64
23	Y	503	9YF	C40-C41-C42-C43
23	M	502	9YF	C40-C41-C42-C43
16	T	202	CDL	C54-C55-C56-C57
16	R	604	CDL	C39-C40-C41-C42
16	P	201	CDL	C61-C62-C63-C64
19	X	303	9Y0	C6-C7-C8-C9
23	c	203	9YF	C20-C21-C22-C23
23	W	203	9YF	C20-C21-C22-C23
18	I	303	MQ9	C15-C14-C16-C17
23	M	501	9YF	C18-C19-C20-C21
23	Y	503	9YF	C31-C32-C33-C34
23	Y	503	9YF	C34-C33-C35-C36
23	M	502	9YF	C31-C32-C33-C34
23	M	502	9YF	C34-C33-C35-C36
16	T	203	CDL	C54-C55-C56-C57
23	Y	502	9YF	C18-C19-C20-C21
16	T	201	CDL	CB4-CB3-OB5-PB2
16	T	202	CDL	C1-CB2-OB2-PB2
16	X	301	CDL	C1-CB2-OB2-PB2
16	Z	202	CDL	CB4-CB3-OB5-PB2
23	Y	502	9YF	C-C1-O-P
23	M	501	9YF	C-C1-O-P
16	R	604	CDL	C54-C55-C56-C57
19	X	303	9Y0	C18-C19-C20-C37
19	J	203	9Y0	C26-C27-C28-C29
20	W	201	PLM	C9-CA-CB-CC
16	E	606	CDL	C39-C40-C41-C42
16	F	705	CDL	C58-C59-C60-C61

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Mol	Chain	Res	Type	Atoms
16	T	202	CDL	C76-C77-C78-C79
16	Z	202	CDL	C33-C34-C35-C36
19	S	302	9Y0	C6-C7-C8-C9
19	X	303	9Y0	C27-C28-C29-C30
16	R	604	CDL	C60-C61-C62-C63
16	T	201	CDL	C33-C34-C35-C36
16	X	301	CDL	C76-C77-C78-C79
16	R	604	CDL	C78-C79-C80-C81
16	S	301	CDL	C39-C40-C41-C42
16	X	302	CDL	C39-C40-C41-C42
16	E	606	CDL	OA5-CA3-CA4-CA6
16	T	202	CDL	OB5-CB3-CB4-CB6
16	X	301	CDL	OB5-CB3-CB4-CB6
16	R	604	CDL	C72-C71-CB7-OB8
21	c	202	9XX	O1-C18-C19-C20
21	G	302	9XX	C26-C27-C28-C29
16	E	605	CDL	C78-C79-C80-C81
16	F	704	CDL	C78-C79-C80-C81
23	O	303	9YF	C20-C21-C22-C23
23	I	304	9YF	C20-C21-C22-C23
16	T	201	CDL	C36-C37-C38-C39
16	T	203	CDL	C61-C62-C63-C64
16	T	203	CDL	C52-C53-C54-C55
16	Z	203	CDL	C38-C39-C40-C41
23	Y	503	9YF	C16-C17-C18-C19
23	M	502	9YF	C16-C17-C18-C19
16	Z	202	CDL	C36-C37-C38-C39
18	Z	201	MQ9	C12-C11-C9-C10
21	c	202	9XX	O-C16-C17-C37
21	W	202	9XX	O-C16-C17-C37
16	R	604	CDL	C77-C78-C79-C80
15	R	602	HEA	C15-C16-C17-C18
16	L	604	CDL	CB3-CB4-CB6-OB8
16	S	301	CDL	CA3-CA4-CA6-OA8
16	X	302	CDL	CA3-CA4-CA6-OA8
18	F	701	MQ9	C39-C41-C42-C43
19	S	302	9Y0	O5-C-C1-C2
19	J	203	9Y0	O5-C-C1-C2
23	O	303	9YF	C1-C-C24-O11
23	I	304	9YF	C1-C-C24-O11
16	E	605	CDL	C76-C77-C78-C79
16	F	704	CDL	C53-C54-C55-C56

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Mol	Chain	Res	Type	Atoms
16	F	704	CDL	C76-C77-C78-C79
16	E	606	CDL	CA5-C11-C12-C13
16	T	202	CDL	CA7-C31-C32-C33
16	X	301	CDL	CA7-C31-C32-C33
16	E	605	CDL	C53-C54-C55-C56
16	S	301	CDL	C59-C60-C61-C62
16	X	302	CDL	C59-C60-C61-C62
16	R	604	CDL	CB5-C51-C52-C53
16	R	604	CDL	OA5-CA3-CA4-OA6
16	F	705	CDL	OA5-CA3-CA4-OA6
16	T	203	CDL	OB5-CB3-CB4-OB6
19	S	302	9Y0	C14-C15-C16-C17
16	T	201	CDL	CB7-C71-C72-C73
16	S	301	CDL	C61-C62-C63-C64
16	E	605	CDL	C31-C32-C33-C34
16	X	302	CDL	C61-C62-C63-C64
16	L	604	CDL	C72-C71-CB7-OB8
16	Z	202	CDL	CB7-C71-C72-C73
16	E	606	CDL	OB6-CB4-CB6-OB8
16	L	604	CDL	OB6-CB4-CB6-OB8
19	S	302	9Y0	O5-C-C1-O7
16	F	704	CDL	C31-C32-C33-C34
16	L	604	CDL	C35-C36-C37-C38
19	X	303	9Y0	C29-C30-C31-C32
23	M	502	9YF	C15-C16-C17-C18
16	R	604	CDL	C73-C74-C75-C76
23	Y	503	9YF	C15-C16-C17-C18
18	I	303	MQ9	C13-C14-C16-C17
16	R	604	CDL	C51-C52-C53-C54
20	c	201	PLM	CA-CB-CC-CD
23	Y	503	9YF	C14-C15-C16-C17
21	G	302	9XX	O6-C15-O-C16
16	E	605	CDL	C61-C62-C63-C64
23	M	502	9YF	C14-C15-C16-C17
16	F	704	CDL	C61-C62-C63-C64
16	F	705	CDL	C61-C62-C63-C64
18	F	708	MQ9	C9-C11-C12-C13
18	F	708	MQ9	C19-C21-C22-C23
19	S	302	9Y0	C29-C30-C31-C32
16	E	606	CDL	C57-C58-C59-C60
19	S	302	9Y0	C27-C28-C29-C30
23	I	304	9YF	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
23	W	203	9YF	C9-C10-C11-C12
16	T	201	CDL	CB2-C1-CA2-OA2
16	Z	202	CDL	CB2-C1-CA2-OA2
23	O	303	9YF	C27-C28-C29-C30
23	c	203	9YF	C9-C10-C11-C12
16	L	604	CDL	C56-C57-C58-C59
16	T	203	CDL	OB5-CB3-CB4-CB6
16	J	201	CDL	C36-C37-C38-C39
16	P	201	CDL	C36-C37-C38-C39
16	R	604	CDL	C12-C13-C14-C15
16	X	302	CDL	C71-C72-C73-C74
23	O	303	9YF	C39-C40-C41-C42
23	I	304	9YF	C39-C40-C41-C42
16	F	705	CDL	C52-C51-CB5-OB6
16	S	301	CDL	C71-C72-C73-C74
16	Z	203	CDL	C54-C55-C56-C57
18	Z	201	MQ9	C20-C19-C21-C22
16	P	201	CDL	C12-C13-C14-C15
16	J	201	CDL	C12-C13-C14-C15
16	L	604	CDL	C73-C74-C75-C76
20	D	301	PLM	C4-C5-C6-C7
16	T	202	CDL	OB5-CB3-CB4-OB6
16	T	203	CDL	OA5-CA3-CA4-OA6
16	X	301	CDL	OB5-CB3-CB4-OB6
23	Y	502	9YF	O9-C-C1-O
23	M	501	9YF	O9-C-C1-O
16	F	705	CDL	C39-C40-C41-C42
16	R	604	CDL	CB3-CB4-CB6-OB8
16	F	705	CDL	CB3-CB4-CB6-OB8
16	T	201	CDL	CA3-CA4-CA6-OA8
16	T	201	CDL	CB3-CB4-CB6-OB8
16	Z	202	CDL	CA3-CA4-CA6-OA8
16	Z	202	CDL	CB3-CB4-CB6-OB8
18	F	707	MQ9	C19-C21-C22-C23
17	E	602	HEM	C4B-C3B-CAB-CBB
21	W	202	9XX	C1-C2-C3-C4
19	J	202	9Y0	C19-C20-C37-C38
16	E	605	CDL	OB6-CB4-CB6-OB8
16	F	704	CDL	OB6-CB4-CB6-OB8
16	Z	203	CDL	C78-C79-C80-C81
19	J	202	9Y0	C5-C6-C7-C8
16	X	301	CDL	C73-C74-C75-C76

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Mol	Chain	Res	Type	Atoms
16	T	202	CDL	C73-C74-C75-C76
21	G	302	9XX	C5-C6-C7-C8
21	c	202	9XX	C19-C20-C21-C22
18	F	707	MQ9	C20-C19-C21-C22
16	F	705	CDL	O1-C1-CB2-OB2
16	X	302	CDL	C33-C34-C35-C36
16	S	301	CDL	C33-C34-C35-C36
16	E	606	CDL	C51-C52-C53-C54
21	D	302	9XX	C17-C16-O-C15
16	T	203	CDL	C58-C59-C60-C61
16	E	605	CDL	OA5-CA3-CA4-CA6
16	F	704	CDL	OA5-CA3-CA4-CA6
16	S	301	CDL	OA5-CA3-CA4-CA6
16	X	302	CDL	OA5-CA3-CA4-CA6
23	Y	502	9YF	C19-C20-C21-C22
16	L	604	CDL	C39-C40-C41-C42
21	D	302	9XX	C26-C27-C28-C29
23	Y	503	9YF	C12-C13-C14-C15
23	M	502	9YF	C12-C13-C14-C15
23	M	501	9YF	C19-C20-C21-C22
19	J	203	9Y0	C30-C31-C32-C33
21	c	202	9XX	C6-C7-C8-C9
16	E	606	CDL	C77-C78-C79-C80
16	T	202	CDL	CB4-CB3-OB5-PB2
16	X	301	CDL	CB4-CB3-OB5-PB2
16	T	203	CDL	C59-C60-C61-C62
16	E	606	CDL	C59-C60-C61-C62
19	P	202	9Y0	C18-C19-C20-C37
16	E	605	CDL	OB5-CB3-CB4-OB6
16	F	704	CDL	OB5-CB3-CB4-OB6
23	O	303	9YF	O9-C-C1-O
23	I	304	9YF	O9-C-C1-O
23	Y	503	9YF	O9-C-C1-O
23	M	502	9YF	O9-C-C1-O
21	D	302	9XX	C20-C21-C22-C23
23	Y	503	9YF	C33-C35-C36-C37
23	M	502	9YF	C33-C35-C36-C37
16	R	604	CDL	OB6-CB4-CB6-OB8
16	E	605	CDL	OA6-CA4-CA6-OA8
16	F	704	CDL	OA6-CA4-CA6-OA8
16	S	301	CDL	OB6-CB4-CB6-OB8
16	P	201	CDL	OA6-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
16	X	302	CDL	OB6-CB4-CB6-OB8
16	J	201	CDL	OA6-CA4-CA6-OA8
23	O	303	9YF	O9-C-C24-O11
23	I	304	9YF	O9-C-C24-O11
16	X	301	CDL	C33-C34-C35-C36
16	T	202	CDL	C33-C34-C35-C36
20	G	301	PLM	C7-C8-C9-CA
16	E	606	CDL	C61-C62-C63-C64
23	O	303	9YF	C33-C35-C36-C37
23	I	304	9YF	C33-C35-C36-C37
23	c	203	9YF	C39-C40-C41-C42
23	W	203	9YF	C39-C40-C41-C42
16	L	604	CDL	C60-C61-C62-C63
16	R	604	CDL	CB2-OB2-PB2-OB5
16	E	605	CDL	CB3-OB5-PB2-OB4
16	E	606	CDL	CA2-OA2-PA1-OA3
16	F	704	CDL	CB3-OB5-PB2-OB4
16	F	705	CDL	CB2-OB2-PB2-OB4
16	S	301	CDL	CA3-OA5-PA1-OA4
16	T	201	CDL	CA2-OA2-PA1-OA3
16	T	201	CDL	CB2-OB2-PB2-OB3
16	T	202	CDL	CB2-OB2-PB2-OB3
16	T	202	CDL	CB2-OB2-PB2-OB4
16	T	202	CDL	CB2-OB2-PB2-OB5
16	T	202	CDL	CB3-OB5-PB2-OB3
16	T	203	CDL	CA3-OA5-PA1-OA2
16	T	203	CDL	CA3-OA5-PA1-OA3
16	T	203	CDL	CA3-OA5-PA1-OA4
16	T	203	CDL	CB3-OB5-PB2-OB4
16	X	301	CDL	CB2-OB2-PB2-OB3
16	X	301	CDL	CB2-OB2-PB2-OB4
16	X	301	CDL	CB2-OB2-PB2-OB5
16	X	301	CDL	CB3-OB5-PB2-OB3
16	X	302	CDL	CA3-OA5-PA1-OA4
16	Z	202	CDL	CA2-OA2-PA1-OA3
16	Z	202	CDL	CB2-OB2-PB2-OB3
16	Z	203	CDL	CA3-OA5-PA1-OA2
16	Z	203	CDL	CA3-OA5-PA1-OA3
16	Z	203	CDL	CA3-OA5-PA1-OA4
19	P	202	9Y0	C2-O3-P-O1
19	P	202	9Y0	C2-O3-P-O2
19	J	203	9Y0	C2-O3-P-O

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Mol	Chain	Res	Type	Atoms
23	O	303	9YF	C1-O-P-O1
23	O	303	9YF	C1-O-P-O2
23	I	304	9YF	C1-O-P-O1
18	F	707	MQ9	C12-C11-C9-C8
18	Z	201	MQ9	C18-C19-C21-C22
16	R	604	CDL	C1-CA2-OA2-PA1
16	E	606	CDL	C1-CA2-OA2-PA1
16	E	606	CDL	C1-CB2-OB2-PB2
16	F	705	CDL	C1-CA2-OA2-PA1
16	S	301	CDL	C1-CA2-OA2-PA1
16	S	301	CDL	C1-CB2-OB2-PB2
16	X	302	CDL	C1-CA2-OA2-PA1
16	X	302	CDL	C1-CB2-OB2-PB2
16	Z	203	CDL	C1-CA2-OA2-PA1
20	c	201	PLM	CC-CD-CE-CF
15	L	602	HEA	C12-C11-C3B-C4B
19	F	706	9Y0	C30-C31-C32-C33
16	F	705	CDL	C73-C74-C75-C76
19	P	202	9Y0	C25-C26-C27-C28
23	O	303	9YF	C29-C30-C31-C32
23	I	304	9YF	C29-C30-C31-C32
23	M	501	9YF	C25-C26-C27-C28
16	E	605	CDL	C60-C61-C62-C63
16	F	704	CDL	C60-C61-C62-C63
19	S	302	9Y0	C22-C23-C24-C25
19	S	302	9Y0	C13-C14-C15-C16
23	Y	502	9YF	C25-C26-C27-C28
16	T	202	CDL	C35-C36-C37-C38
16	X	301	CDL	C35-C36-C37-C38
23	O	303	9YF	C18-C19-C20-C21
16	T	203	CDL	CA6-CA4-OA6-CA5
23	I	304	9YF	C18-C19-C20-C21
23	Y	502	9YF	C16-C17-C18-C19
16	R	604	CDL	OA5-CA3-CA4-CA6
19	F	706	9Y0	C-C1-C2-O3
23	M	501	9YF	C16-C17-C18-C19
21	G	302	9XX	C36-C27-C28-C29
19	P	202	9Y0	C11-C12-C13-C14
19	X	303	9Y0	C13-C14-C15-C16
19	J	203	9Y0	C11-C12-C13-C14
18	F	707	MQ9	C12-C11-C9-C10
18	F	709	MQ9	C35-C34-C36-C37

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Mol	Chain	Res	Type	Atoms
16	L	604	CDL	C77-C78-C79-C80
16	F	705	CDL	C1-CB2-OB2-PB2
23	c	203	9YF	O9-C-C24-O11
23	W	203	9YF	O9-C-C24-O11
16	T	203	CDL	C55-C56-C57-C58
20	D	301	PLM	C7-C8-C9-CA
23	Y	502	9YF	C40-C41-C42-C43
23	M	501	9YF	C40-C41-C42-C43
18	F	707	MQ9	C16-C17-C18-C19
19	F	706	9Y0	C19-C20-C37-C38
18	I	303	MQ9	C29-C31-C32-C33
16	R	604	CDL	C71-C72-C73-C74
16	F	705	CDL	C54-C55-C56-C57
21	G	302	9XX	C20-C21-C22-C23
18	F	709	MQ9	C40-C39-C41-C42
18	F	707	MQ9	C18-C19-C21-C22
16	F	705	CDL	C38-C39-C40-C41
16	T	202	CDL	C53-C54-C55-C56
16	X	301	CDL	C53-C54-C55-C56
21	D	302	9XX	C36-C27-C28-C29
16	P	201	CDL	C37-C38-C39-C40
23	M	501	9YF	C35-C36-C37-C38
16	J	201	CDL	C37-C38-C39-C40
23	Y	502	9YF	C35-C36-C37-C38
16	J	201	CDL	C12-C11-CA5-OA6
19	J	203	9Y0	C14-C15-C16-C17
18	F	708	MQ9	C15-C14-C16-C17
16	P	201	CDL	C12-C11-CA5-OA6
18	F	709	MQ9	C33-C34-C36-C37
16	T	201	CDL	OB5-CB3-CB4-OB6
16	Z	202	CDL	OB5-CB3-CB4-OB6
19	X	303	9Y0	C22-C23-C24-C25
19	J	202	9Y0	C7-C8-C9-C10
16	Z	203	CDL	C57-C58-C59-C60
19	S	302	9Y0	C5-C6-C7-C8
18	F	708	MQ9	C40-C39-C41-C42
16	J	201	CDL	C38-C39-C40-C41
16	X	302	CDL	C57-C58-C59-C60
16	P	201	CDL	C38-C39-C40-C41
16	S	301	CDL	C57-C58-C59-C60
19	P	202	9Y0	C16-C17-C18-C19
23	O	303	9YF	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
23	M	501	9YF	C37-C38-C39-C40
23	I	304	9YF	C37-C38-C39-C40
23	Y	502	9YF	C37-C38-C39-C40
16	T	202	CDL	C13-C14-C15-C16
16	X	301	CDL	C13-C14-C15-C16
22	O	301	HEC	C2D-C3D-CAD-CBD
23	Y	503	9YF	C29-C30-C31-C32
23	M	502	9YF	C29-C30-C31-C32
16	R	604	CDL	C33-C34-C35-C36
16	F	705	CDL	C77-C78-C79-C80
15	R	602	HEA	CAA-CBA-CGA-O1A
16	T	203	CDL	C14-C15-C16-C17
15	L	602	HEA	CAD-CBD-CGD-O1D
18	F	709	MQ9	C38-C39-C41-C42
21	c	202	9XX	O2-C18-C19-C20
19	P	202	9Y0	C24-C25-C26-C27
15	L	603	HEA	CAA-CBA-CGA-O1A
19	J	202	9Y0	O7-C1-C2-O3
16	E	605	CDL	CB5-C51-C52-C53
16	F	704	CDL	CB5-C51-C52-C53
15	R	602	HEA	CAD-CBD-CGD-O1D
18	E	604	MQ9	C40-C39-C41-C42
16	T	202	CDL	OA5-CA3-CA4-CA6
16	X	301	CDL	OA5-CA3-CA4-CA6
19	F	706	9Y0	C7-C8-C9-C10
15	R	602	HEA	CAA-CBA-CGA-O2A
15	L	602	HEA	CAA-CBA-CGA-O1A
16	J	201	CDL	C11-C12-C13-C14
23	c	203	9YF	C31-C32-C33-C35
23	W	203	9YF	C31-C32-C33-C35
16	P	201	CDL	C11-C12-C13-C14
15	R	603	HEA	CAA-CBA-CGA-O1A
16	E	605	CDL	C11-C12-C13-C14
16	T	203	CDL	C39-C40-C41-C42
16	F	704	CDL	C11-C12-C13-C14
19	S	302	9Y0	C7-C8-C9-C10
18	F	701	MQ9	C15-C14-C16-C17
18	F	708	MQ9	C13-C14-C16-C17
20	D	301	PLM	C2-C3-C4-C5
20	c	201	PLM	C7-C8-C9-CA
16	X	302	CDL	C55-C56-C57-C58
19	J	203	9Y0	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
23	I	304	9YF	C30-C31-C32-C33
16	Z	203	CDL	C14-C15-C16-C17
16	S	301	CDL	C55-C56-C57-C58
20	c	201	PLM	C8-C9-CA-CB
15	L	602	HEA	CAD-CBD-CGD-O2D
16	L	604	CDL	C59-C60-C61-C62
23	O	303	9YF	C30-C31-C32-C33
18	E	604	MQ9	C35-C34-C36-C37
18	Z	201	MQ9	C30-C29-C31-C32
15	R	602	HEA	CAD-CBD-CGD-O2D
15	L	602	HEA	CAA-CBA-CGA-O2A
16	L	604	CDL	C1-CA2-OA2-PA1
16	L	604	CDL	C1-CB2-OB2-PB2
16	L	604	CDL	CB4-CB3-OB5-PB2
15	L	603	HEA	CAA-CBA-CGA-O2A
16	T	203	CDL	C13-C14-C15-C16
16	F	705	CDL	CB7-C71-C72-C73
16	E	606	CDL	CB3-CB4-CB6-OB8
18	I	303	MQ9	C9-C11-C12-C13
15	R	603	HEA	CAA-CBA-CGA-O2A
20	W	201	PLM	CC-CD-CE-CF
16	T	202	CDL	OA5-CA3-CA4-OA6
16	X	301	CDL	OA5-CA3-CA4-OA6
18	F	709	MQ9	C30-C29-C31-C32
16	R	604	CDL	C72-C71-CB7-OB9
19	F	706	9Y0	C11-C12-C13-C14
21	W	202	9XX	O1-C18-C19-C20
16	X	301	CDL	C56-C57-C58-C59
16	T	203	CDL	CA7-C31-C32-C33
16	T	202	CDL	C56-C57-C58-C59
17	F	702	HEM	CAD-CBD-CGD-O2D
16	F	705	CDL	C60-C61-C62-C63
16	Z	203	CDL	C13-C14-C15-C16
16	F	705	CDL	OA5-CA3-CA4-CA6
16	T	203	CDL	OA5-CA3-CA4-CA6
21	W	202	9XX	C3-C4-C5-C6
18	F	708	MQ9	C38-C39-C41-C42
18	Z	201	MQ9	C28-C29-C31-C32
16	R	604	CDL	CB4-CB3-OB5-PB2
16	E	605	CDL	C1-CA2-OA2-PA1
16	F	704	CDL	C1-CA2-OA2-PA1
16	P	201	CDL	CA4-CA3-OA5-PA1

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Mol	Chain	Res	Type	Atoms
16	J	201	CDL	CA4-CA3-OA5-PA1
16	T	203	CDL	C35-C36-C37-C38
19	J	202	9Y0	C24-C25-C26-C27
16	T	201	CDL	C78-C79-C80-C81
16	P	201	CDL	C14-C15-C16-C17
16	Z	202	CDL	C78-C79-C80-C81
16	J	201	CDL	C14-C15-C16-C17
23	W	203	9YF	C13-C14-C15-C16
16	F	705	CDL	C33-C34-C35-C36
23	c	203	9YF	C13-C14-C15-C16
18	E	604	MQ9	C20-C19-C21-C22
16	T	203	CDL	C75-C76-C77-C78
20	W	201	PLM	C7-C8-C9-CA
16	E	606	CDL	C72-C73-C74-C75
16	T	203	CDL	C52-C51-CB5-OB6
19	P	202	9Y0	C-C1-O7-C21
19	S	302	9Y0	C10-C11-C12-C13
16	T	201	CDL	C32-C33-C34-C35
16	Z	202	CDL	C32-C33-C34-C35
16	L	604	CDL	C57-C58-C59-C60
18	I	303	MQ9	C12-C11-C9-C10
19	J	203	9Y0	O7-C1-C2-O3
18	F	709	MQ9	C24-C26-C27-C28
18	F	707	MQ9	C45-C44-C46-C47
18	F	709	MQ9	C20-C19-C21-C22
21	W	202	9XX	C2-C3-C4-C5
16	L	604	CDL	C72-C71-CB7-OB9
17	F	702	HEM	CAD-CBD-CGD-O1D
23	Y	503	9YF	O11-C25-C26-C27
23	M	502	9YF	O11-C25-C26-C27
19	J	202	9Y0	C11-C12-C13-C14
19	J	203	9Y0	C23-C24-C25-C26
19	J	203	9Y0	C13-C14-C15-C16
18	E	604	MQ9	C24-C26-C27-C28
16	Z	203	CDL	C58-C59-C60-C61
23	c	203	9YF	C2-O2-P-O1
23	W	203	9YF	C2-O2-P-O1
18	F	707	MQ9	C25-C24-C26-C27
16	E	606	CDL	OA9-CA7-OA8-CA6
16	X	301	CDL	O1-C1-CB2-OB2
23	I	304	9YF	O9-C8-C9-C10
16	Z	203	CDL	C71-C72-C73-C74

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Mol	Chain	Res	Type	Atoms
16	S	301	CDL	C12-C11-CA5-OA6
16	X	302	CDL	C12-C11-CA5-OA6
23	O	303	9YF	O11-C25-C26-C27
23	O	303	9YF	O9-C8-C9-C10
23	I	304	9YF	O11-C25-C26-C27
23	Y	502	9YF	O9-C8-C9-C10
23	M	501	9YF	O9-C8-C9-C10
18	E	603	MQ9	C15-C14-C16-C17
16	Z	202	CDL	C74-C75-C76-C77
22	I	302	HEC	C3A-C2A-CAA-CBA
16	T	201	CDL	C74-C75-C76-C77
17	E	601	HEM	CAA-CBA-CGA-O2A
23	c	203	9YF	C31-C32-C33-C34
23	W	203	9YF	C31-C32-C33-C34
16	L	604	CDL	C12-C11-CA5-OA6
16	T	203	CDL	CB3-CB4-CB6-OB8
17	F	702	HEM	CAA-CBA-CGA-O1A
18	E	604	MQ9	C12-C11-C9-C10
16	J	201	CDL	C32-C31-CA7-OA8
23	Y	503	9YF	C18-C19-C20-C21
17	E	601	HEM	CAA-CBA-CGA-O1A
21	W	202	9XX	C24-C25-C26-C27
19	F	706	9Y0	C31-C32-C33-C34
23	M	502	9YF	C18-C19-C20-C21
16	P	201	CDL	C32-C31-CA7-OA8
21	c	202	9XX	C10-C11-C12-C13
16	T	202	CDL	CA2-C1-CB2-OB2
16	X	301	CDL	CA2-C1-CB2-OB2
18	F	708	MQ9	C31-C32-C33-C34
19	J	203	9Y0	C18-C19-C20-C37
21	c	202	9XX	C26-C27-C28-C29
16	T	202	CDL	CB3-CB4-OB6-CB5
16	T	202	CDL	CB6-CB4-OB6-CB5
16	T	203	CDL	CA3-CA4-OA6-CA5
16	X	301	CDL	CB3-CB4-OB6-CB5
16	X	301	CDL	CB6-CB4-OB6-CB5
19	P	202	9Y0	C2-C1-O7-C21
16	T	202	CDL	O1-C1-CB2-OB2
16	E	606	CDL	C31-CA7-OA8-CA6
18	F	707	MQ9	C30-C29-C31-C32
18	F	709	MQ9	C12-C11-C9-C10
16	R	604	CDL	C57-C58-C59-C60

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Mol	Chain	Res	Type	Atoms
16	S	301	CDL	C12-C11-CA5-OA7
16	X	302	CDL	C12-C11-CA5-OA7
16	P	201	CDL	C32-C31-CA7-OA9
16	J	201	CDL	C32-C31-CA7-OA9
16	Z	203	CDL	CB4-CB6-OB8-CB7
16	P	201	CDL	C52-C51-CB5-OB6
16	J	201	CDL	C52-C51-CB5-OB6
19	X	303	9Y0	C32-C33-C34-C35
18	E	604	MQ9	C11-C12-C13-C14
19	J	203	9Y0	O5-C5-C6-C7
17	F	702	HEM	CAA-CBA-CGA-O2A
16	L	604	CDL	C12-C11-CA5-OA7
23	Y	502	9YF	O10-C8-C9-C10
23	M	501	9YF	O10-C8-C9-C10
16	E	606	CDL	C36-C37-C38-C39
22	O	302	HEC	CAA-CBA-CGA-O2A
23	O	303	9YF	O12-C25-C26-C27
23	I	304	9YF	O12-C25-C26-C27
18	I	303	MQ9	C31-C32-C33-C34
19	J	203	9Y0	C1-C2-O3-P
18	E	604	MQ9	C33-C34-C36-C37
23	I	304	9YF	C12-C13-C14-C15
23	O	303	9YF	C12-C13-C14-C15
15	L	602	HEA	O11-C11-C3B-C4B
23	I	304	9YF	O10-C8-C9-C10
16	F	705	CDL	O1-C1-CA2-OA2
21	D	302	9XX	C11-C12-C13-C14
23	O	303	9YF	O10-C8-C9-C10
19	S	302	9Y0	O7-C21-C22-C23
23	O	303	9YF	C11-C12-C13-C14
23	I	304	9YF	C11-C12-C13-C14
22	O	302	HEC	CAA-CBA-CGA-O1A
19	J	203	9Y0	O4-C5-C6-C7
21	G	302	9XX	C12-C13-C14-C15
19	J	202	9Y0	C11-C10-C9-C8
16	E	606	CDL	C52-C51-CB5-OB6
19	X	303	9Y0	O7-C21-C22-C23
16	L	604	CDL	C51-C52-C53-C54
16	F	705	CDL	CB5-C51-C52-C53
16	P	201	CDL	C52-C51-CB5-OB7
16	J	201	CDL	C52-C51-CB5-OB7

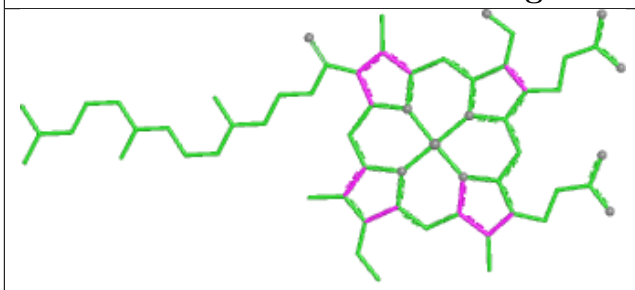
There are no ring outliers.

42 monomers are involved in 403 short contacts:

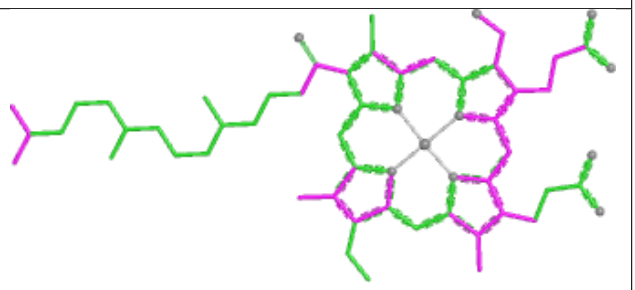
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	L	603	HEA	3	0
16	T	202	CDL	9	0
18	Z	201	MQ9	5	0
22	O	302	HEC	11	0
22	I	301	HEC	4	0
16	L	604	CDL	18	0
16	F	705	CDL	10	0
16	E	606	CDL	3	0
16	E	605	CDL	10	0
17	E	601	HEM	2	0
18	F	701	MQ9	1	0
16	T	201	CDL	33	0
17	E	602	HEM	2	0
15	L	602	HEA	2	0
22	I	302	HEC	9	0
16	J	201	CDL	11	0
16	X	301	CDL	43	0
17	F	702	HEM	1	0
18	I	303	MQ9	1	0
16	F	704	CDL	10	0
16	R	604	CDL	22	0
17	F	703	HEM	4	0
18	F	709	MQ9	4	0
20	W	201	PLM	2	0
23	Y	502	9YF	2	0
15	R	603	HEA	4	0
24	M	503	FES	1	0
23	c	203	9YF	1	0
18	E	604	MQ9	5	0
23	W	203	9YF	1	0
16	Z	203	CDL	44	0
22	O	301	HEC	5	0
23	Y	503	9YF	3	0
24	Y	501	FES	1	0
23	I	304	9YF	5	0
16	S	301	CDL	49	0
16	Z	202	CDL	36	0
16	T	203	CDL	9	0
16	P	201	CDL	10	0
18	F	708	MQ9	1	0
18	E	603	MQ9	1	0
16	X	302	CDL	54	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 then 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.

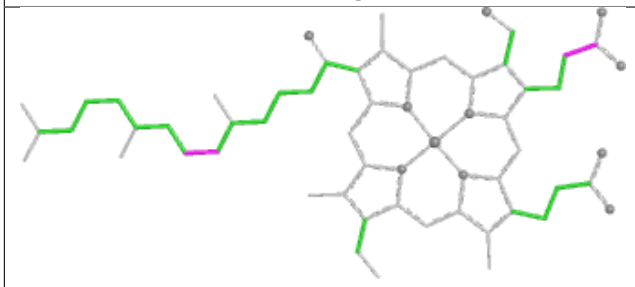
Ligand HEA L 603



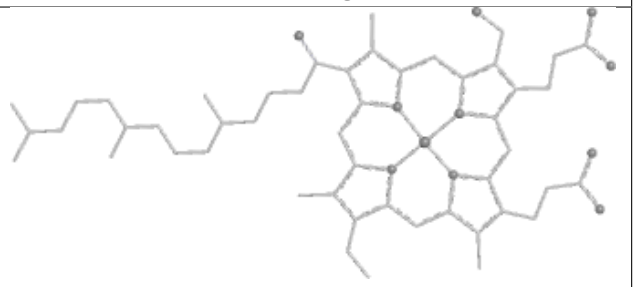
Bond lengths



Bond angles

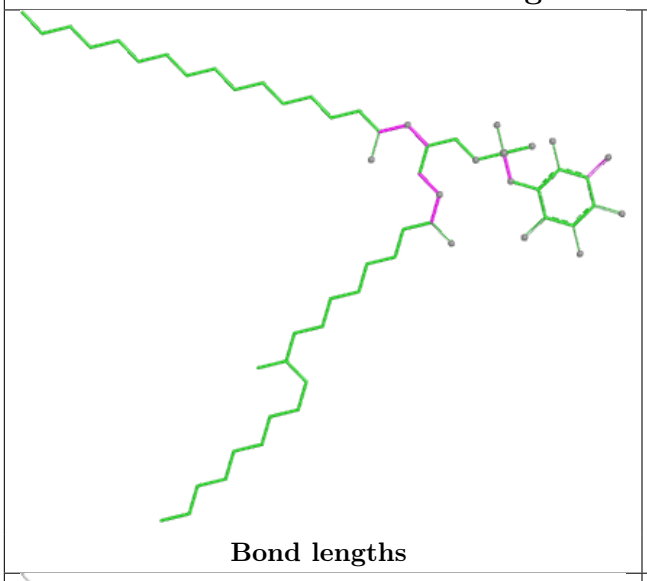


Torsions

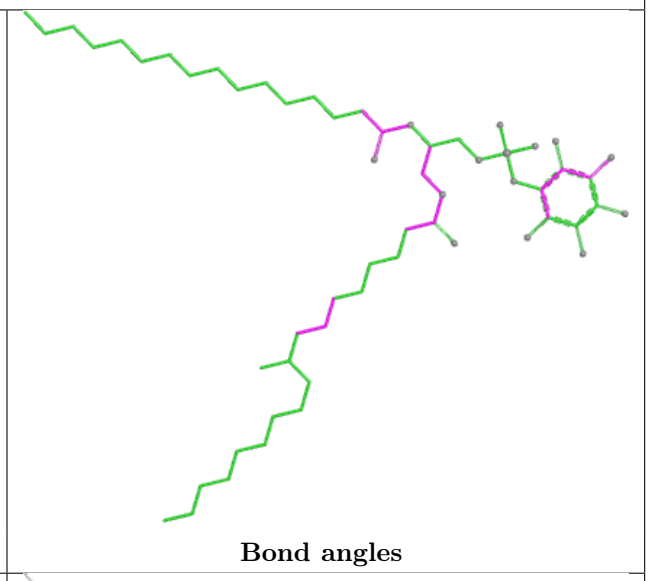


Rings

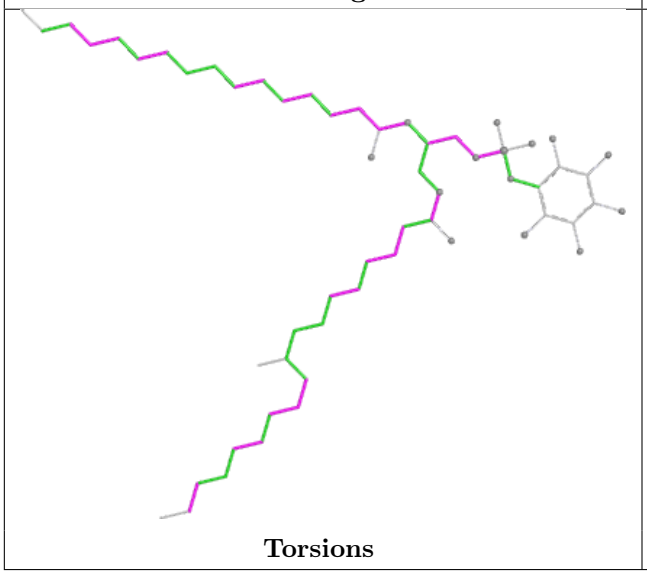
Ligand 9YF M 501



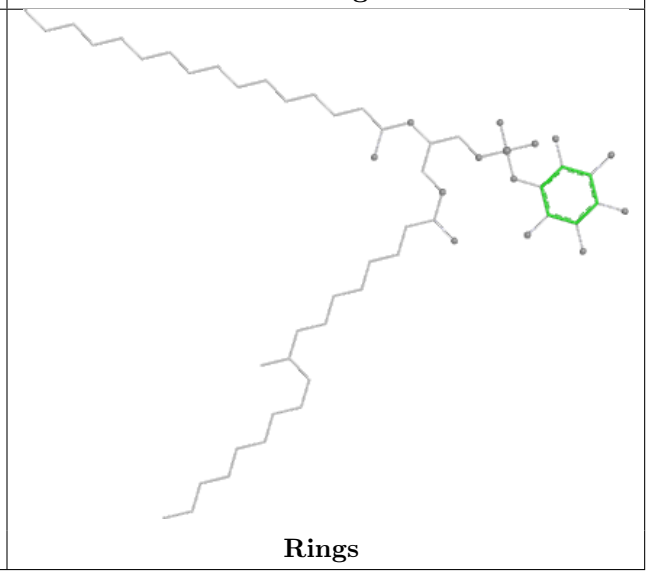
Bond lengths



Bond angles

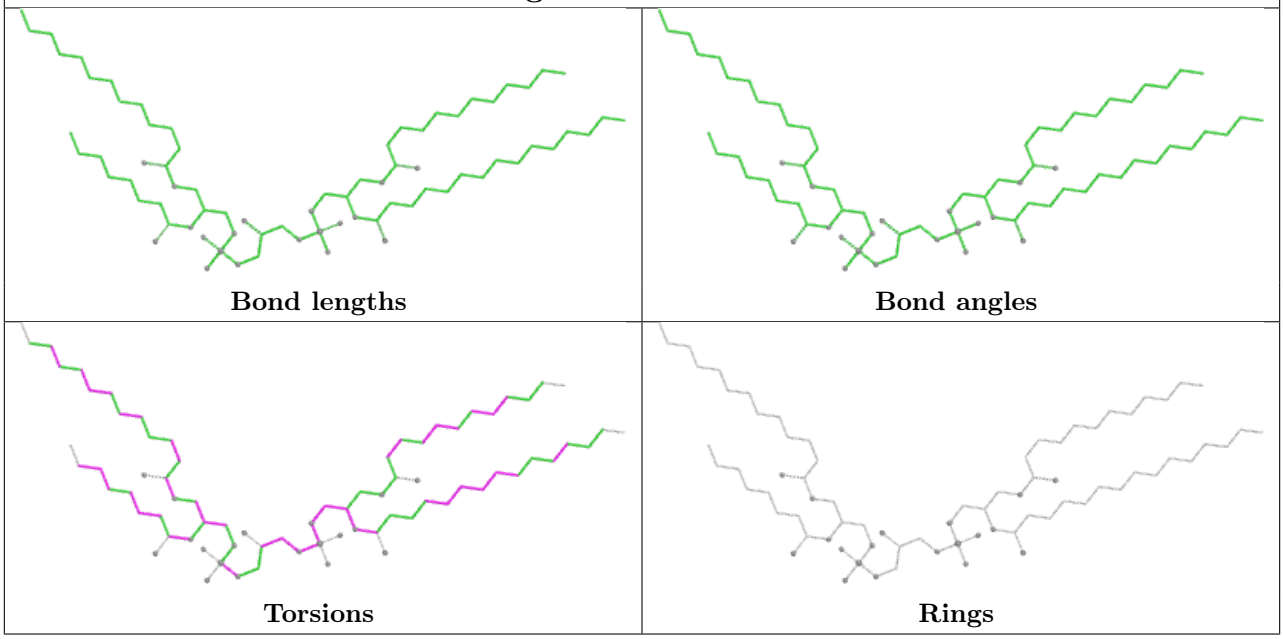


Torsions

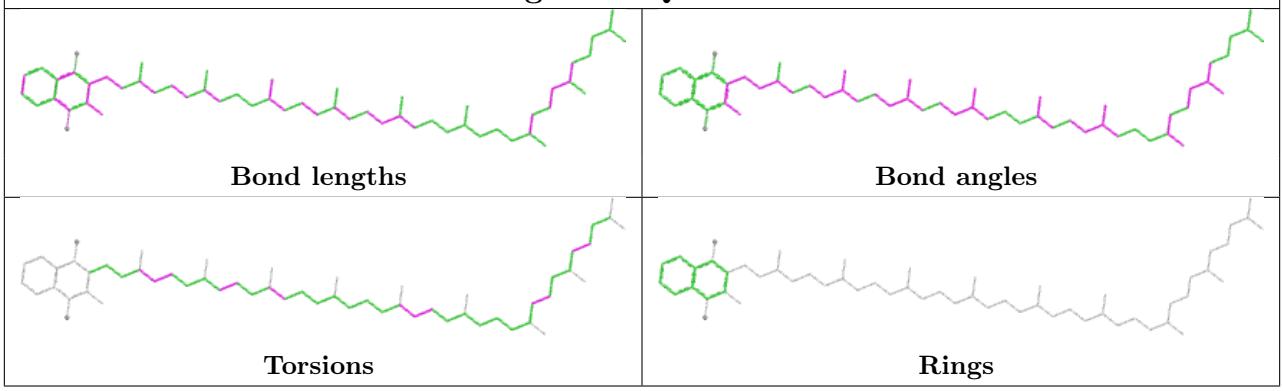


Rings

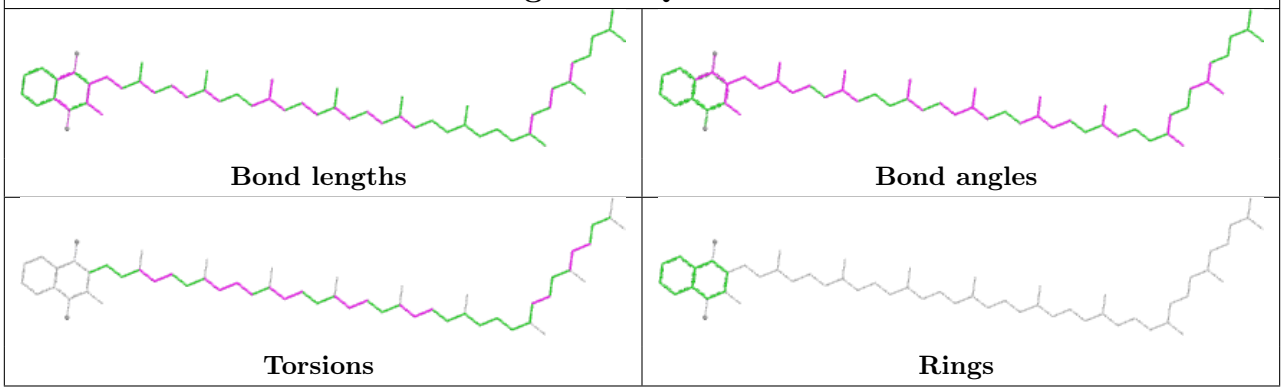
Ligand CDL T 202



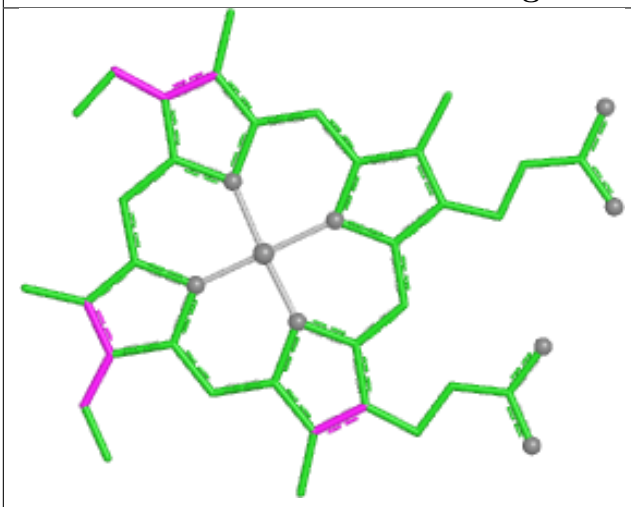
Ligand MQ9 Z 201



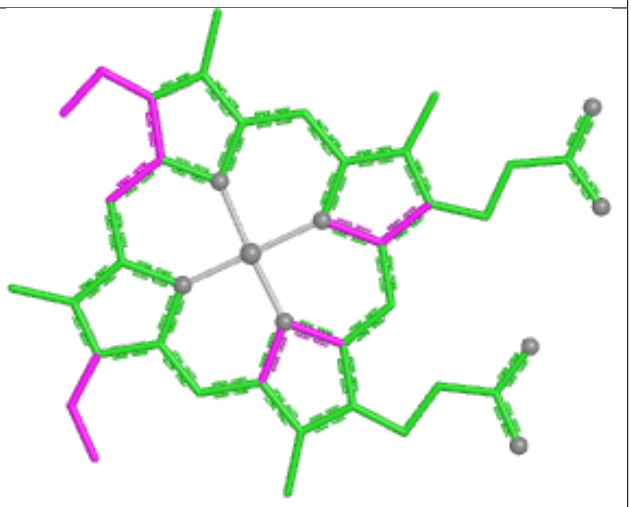
Ligand MQ9 F 707



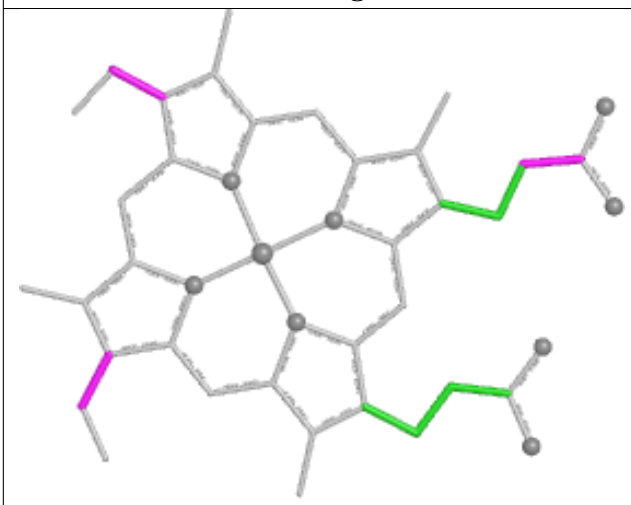
Ligand HEC O 302



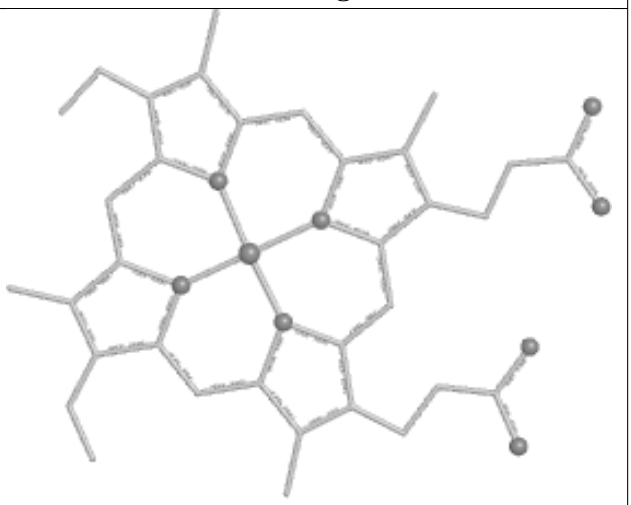
Bond lengths



Bond angles

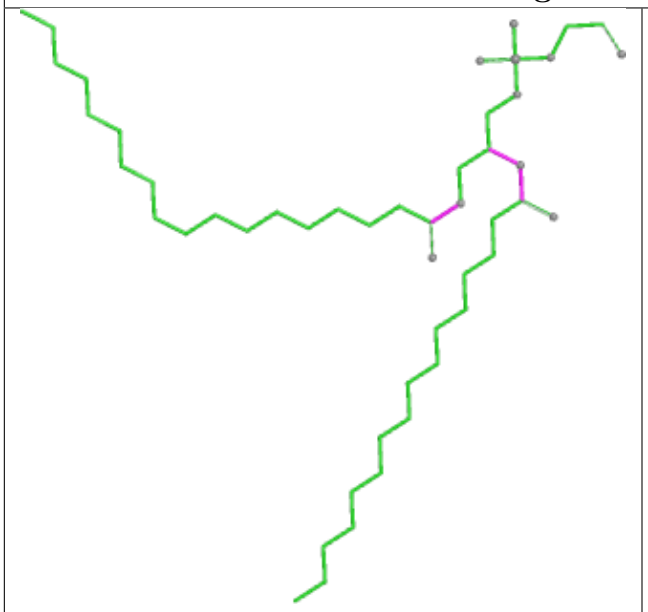


Torsions

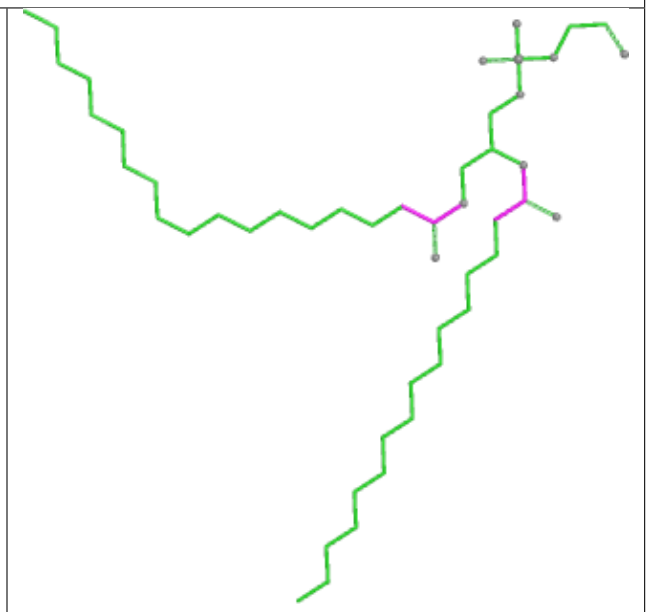


Rings

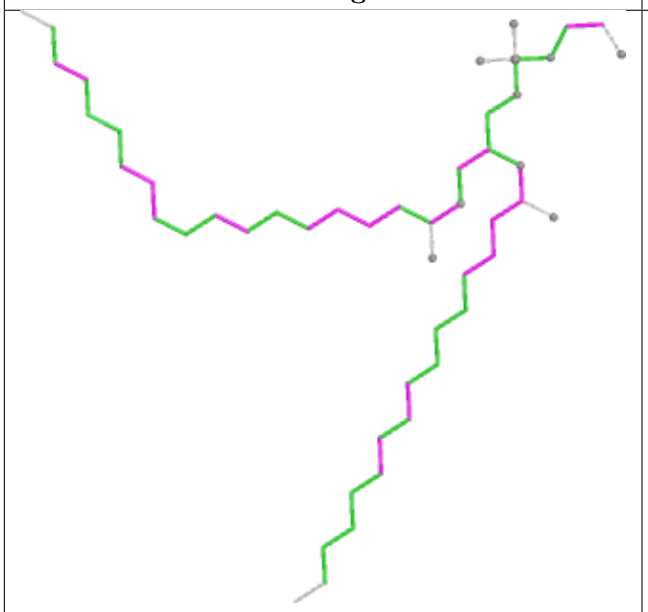
Ligand 9Y0 S 302



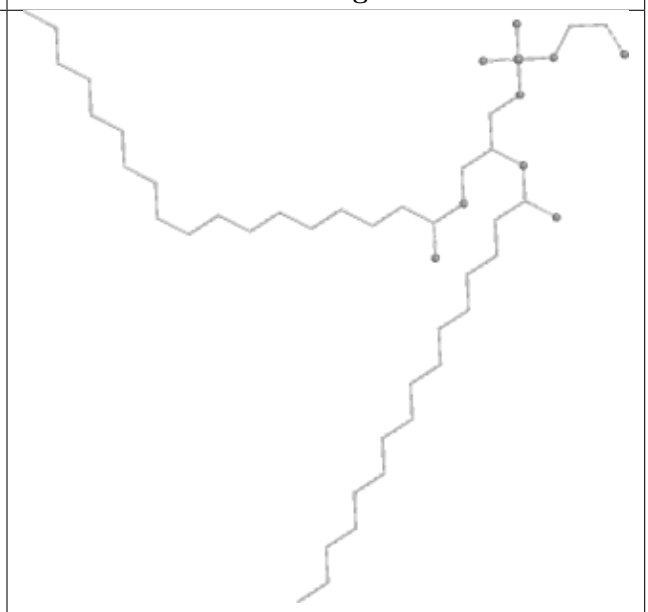
Bond lengths



Bond angles

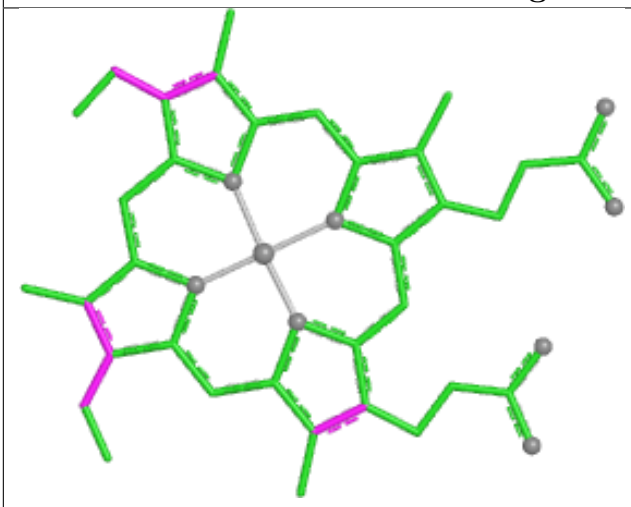


Torsions



Rings

Ligand HEC I 301



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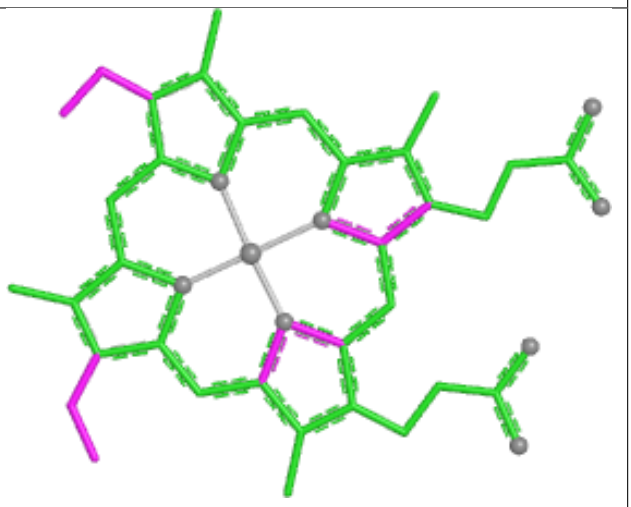
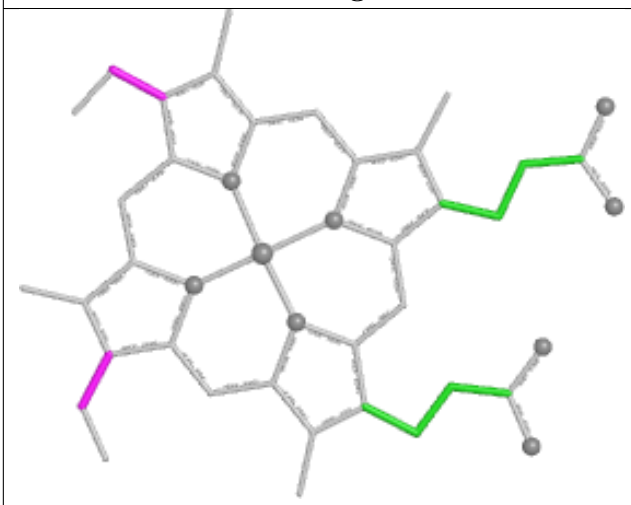
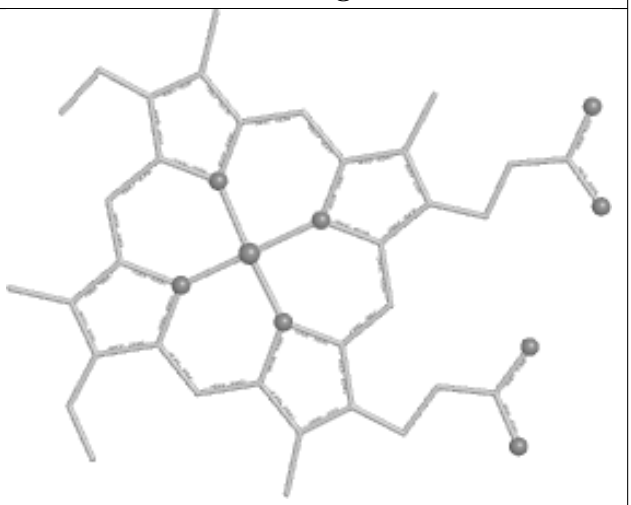


Bond angles

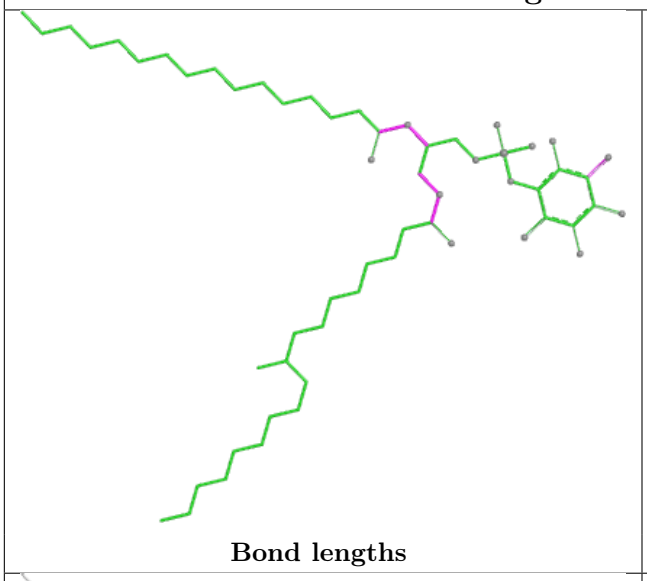


Torsions



Rings

Ligand 9YF M 502



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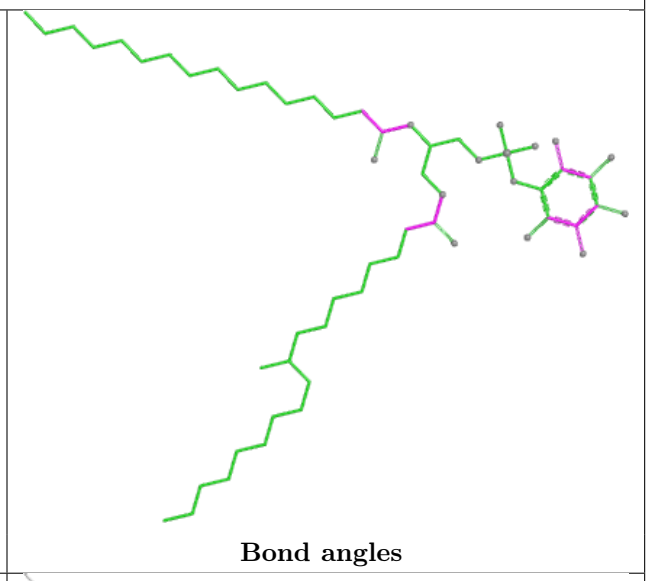
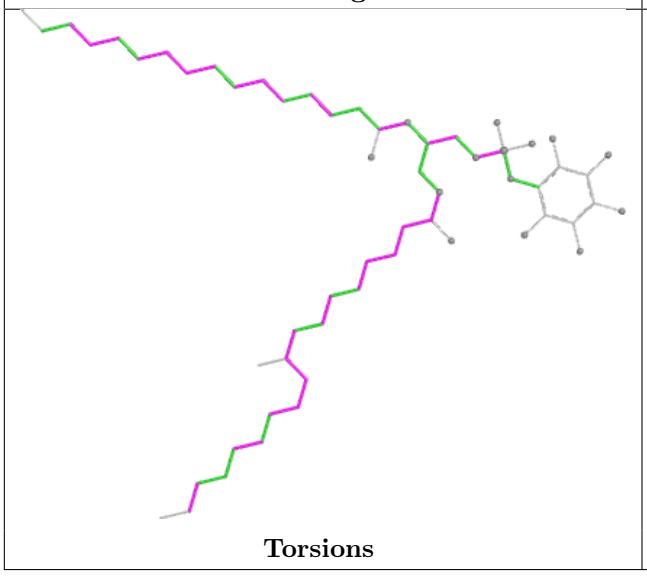


Bond angles



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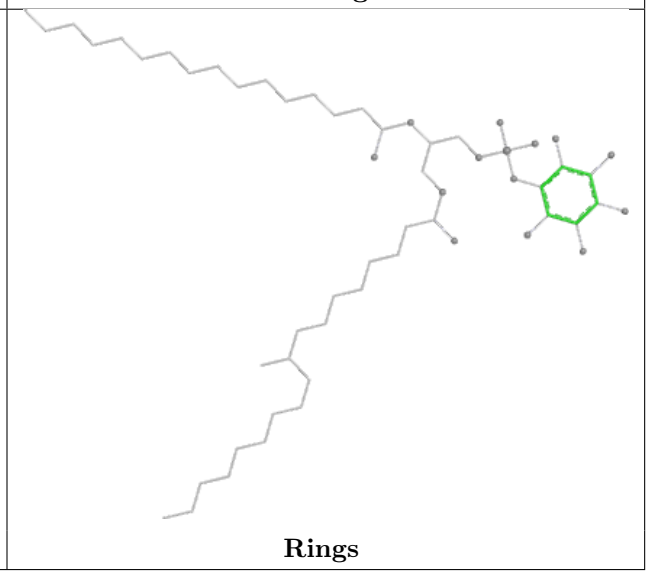
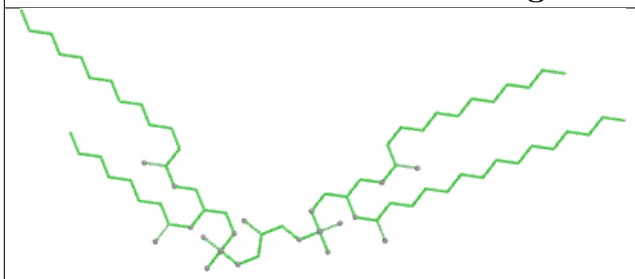


Rings

Ligand CDL L 604



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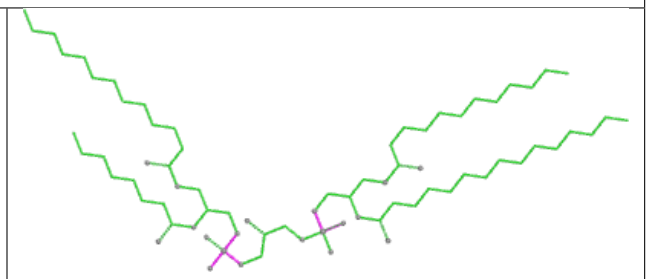
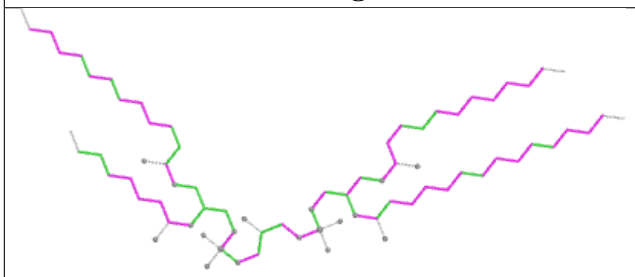


Bond angles



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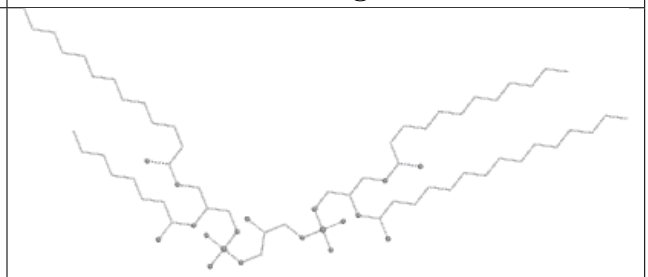
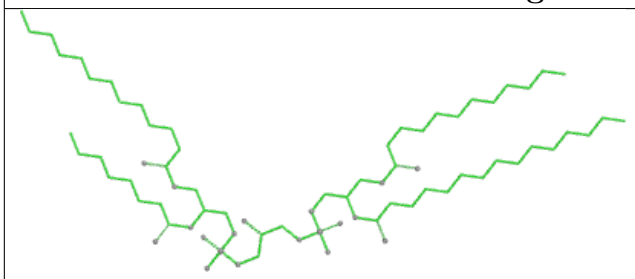


Rings

Ligand CDL F 705



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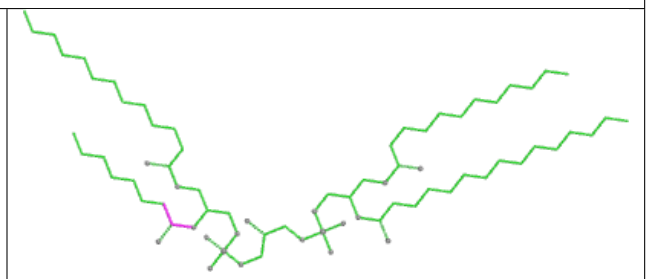
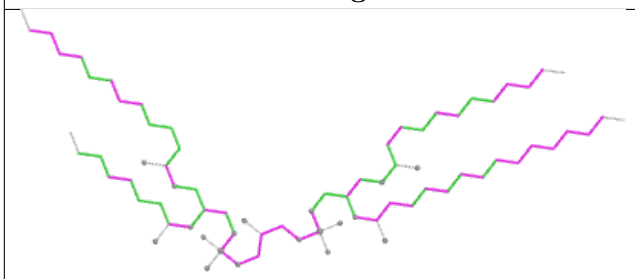


Bond angles



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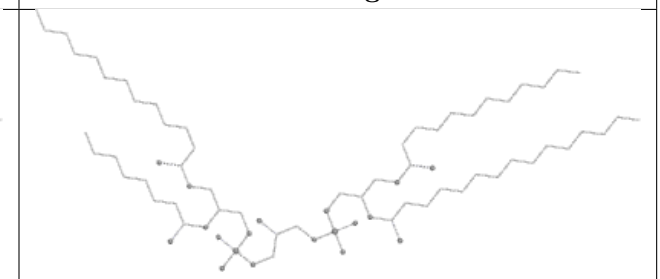
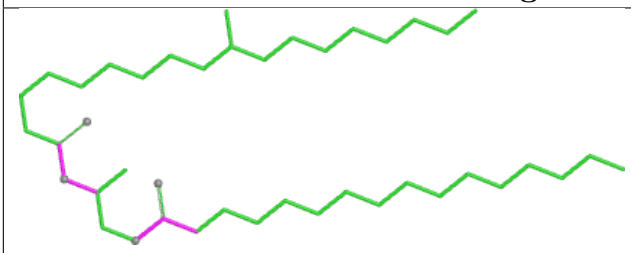


Rings

Ligand 9XX W 202



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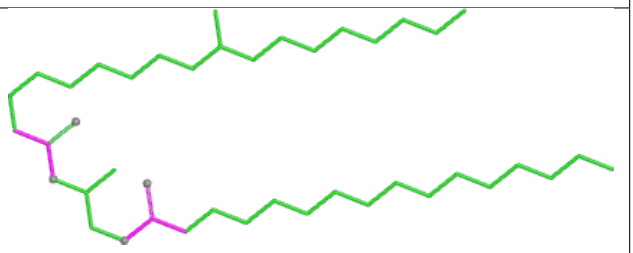
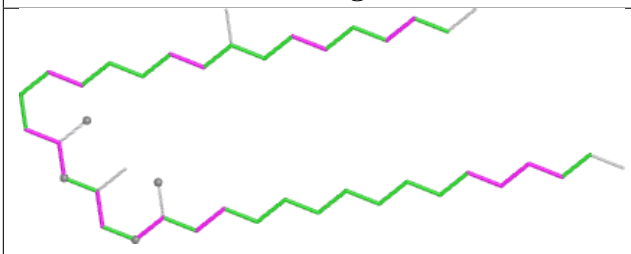


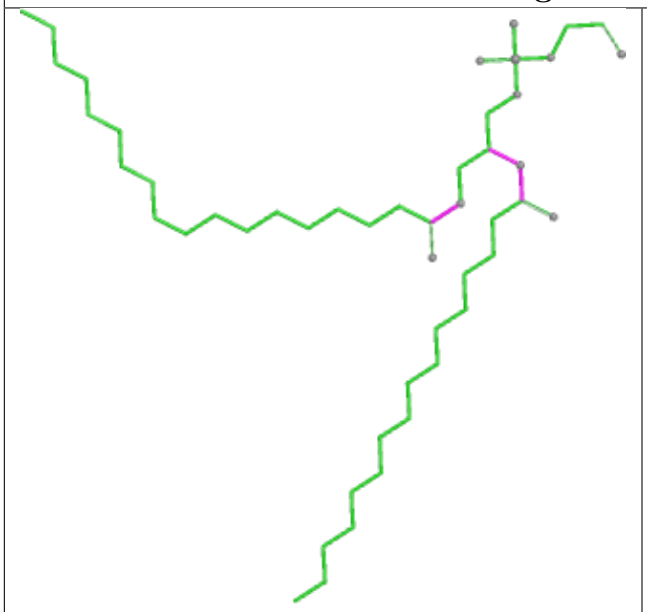
Bond angles



Torsions

Rings

Ligand 9Y0 J 203



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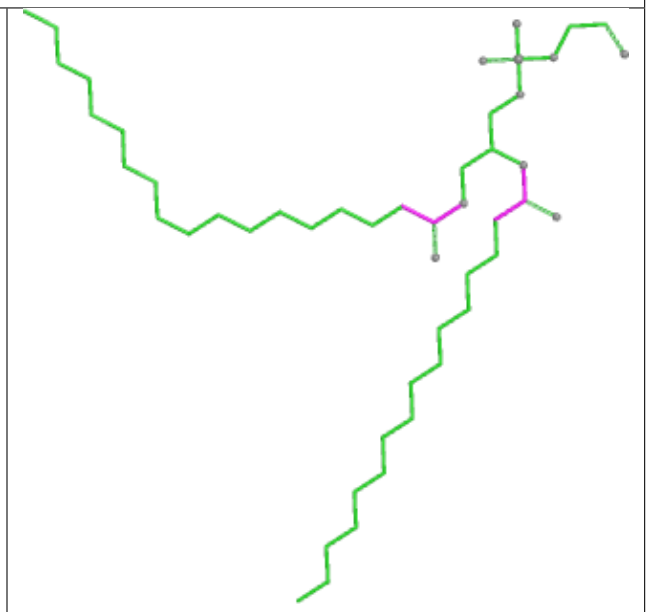

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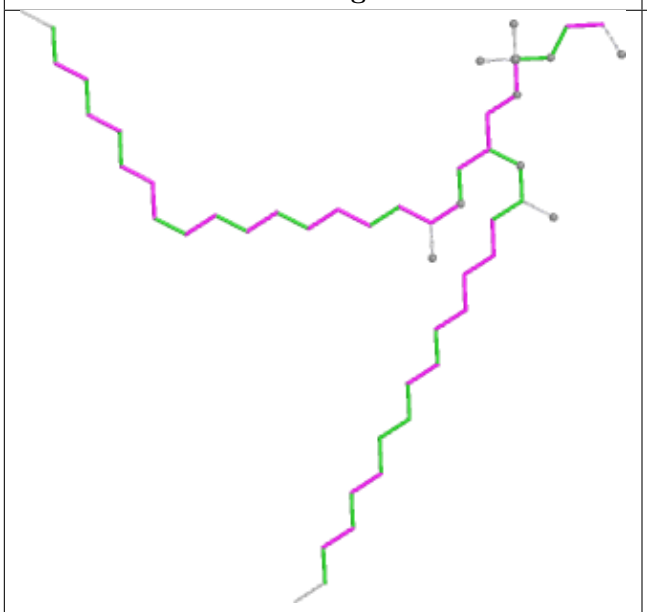

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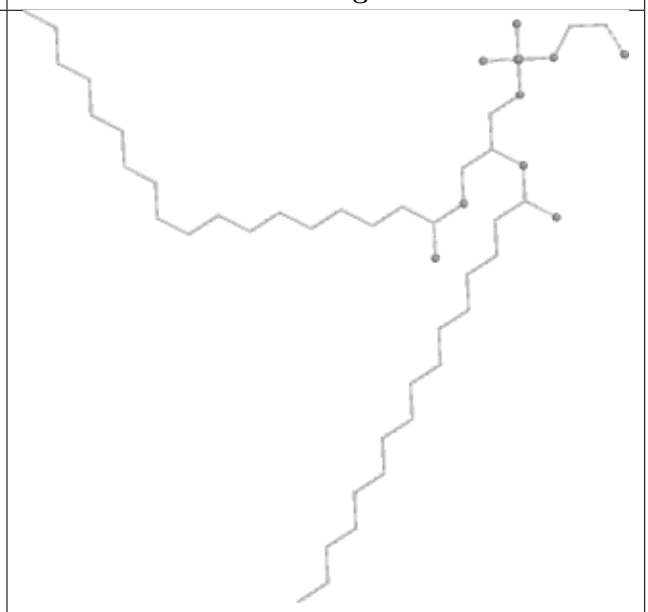
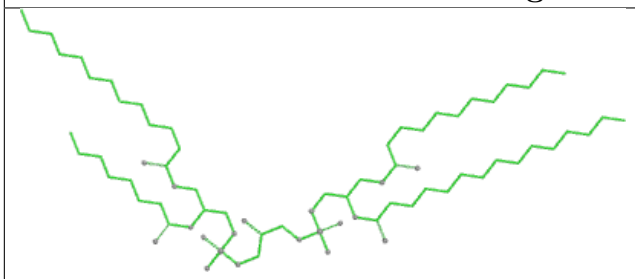


Rings

Ligand CDL E 606



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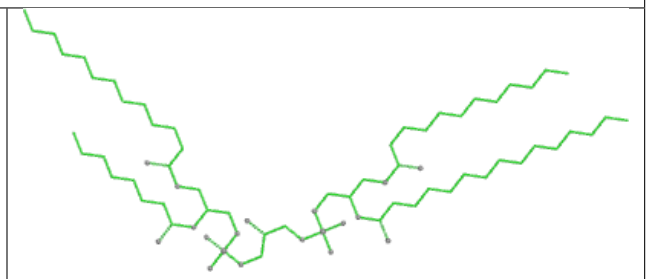
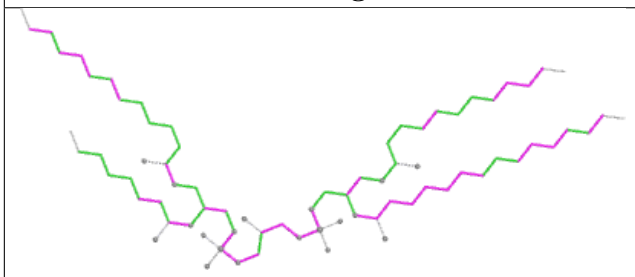


Bond angles



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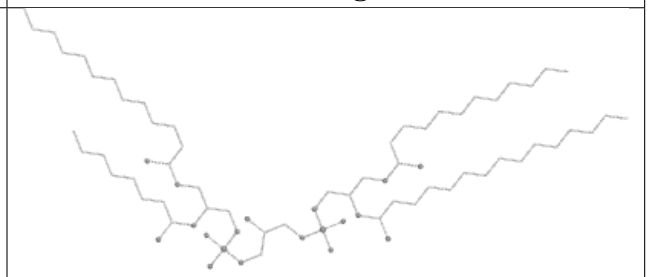
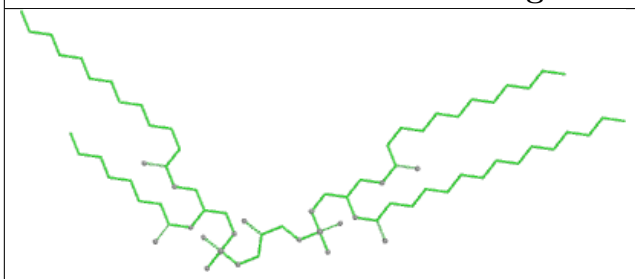


Rings

Ligand CDL E 605



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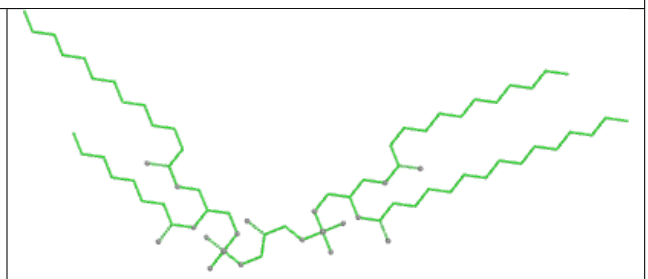

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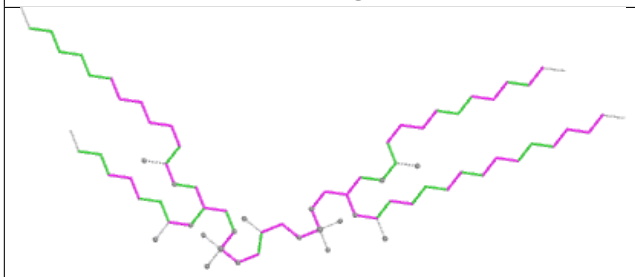

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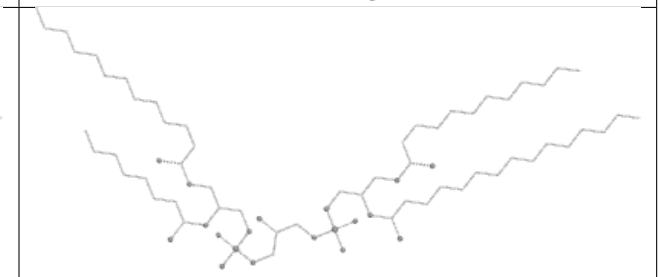
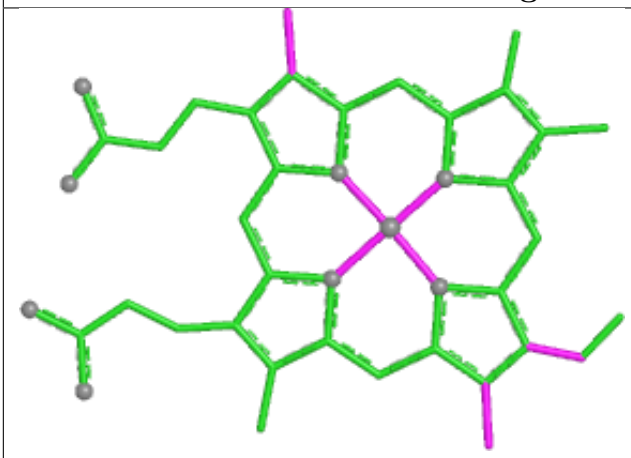


Rings

Ligand HEM E 601



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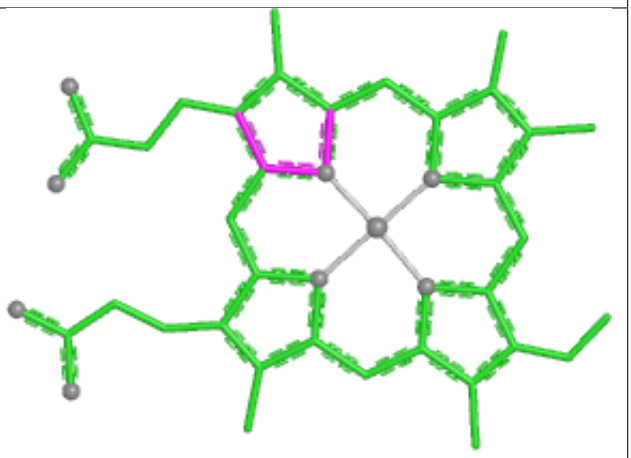

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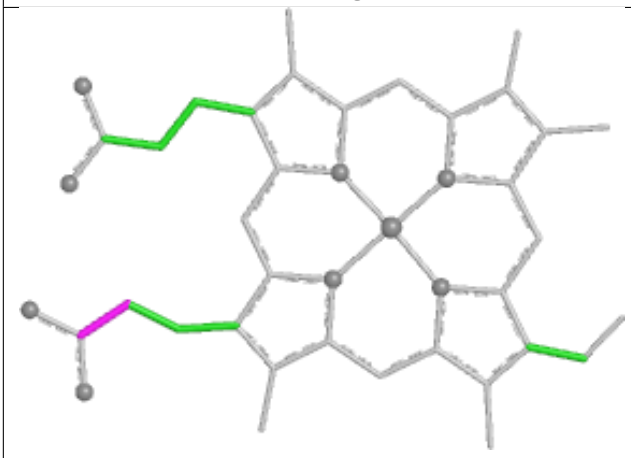

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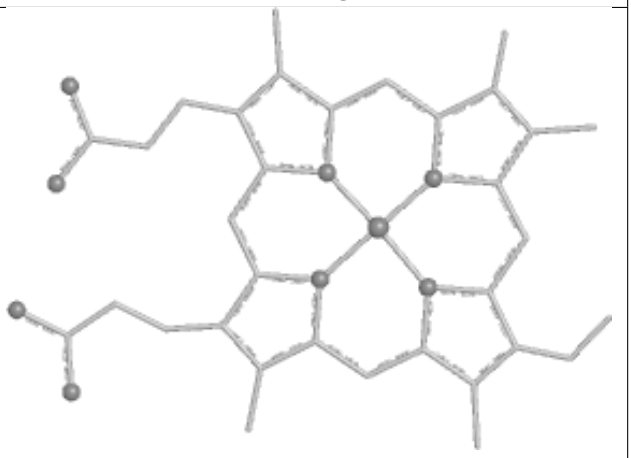
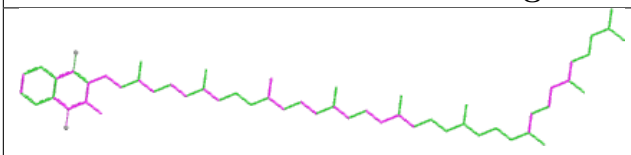


Rings

Ligand MQ9 F 701



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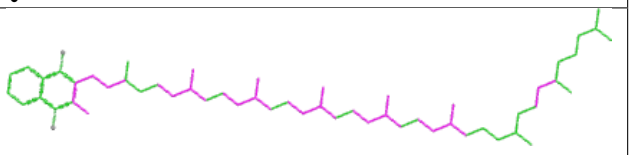
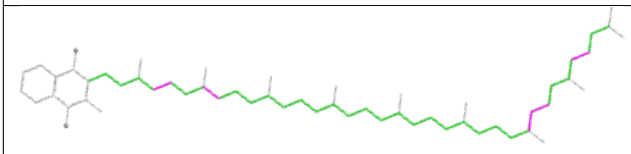


Bond angles



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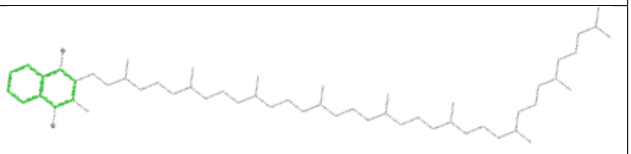
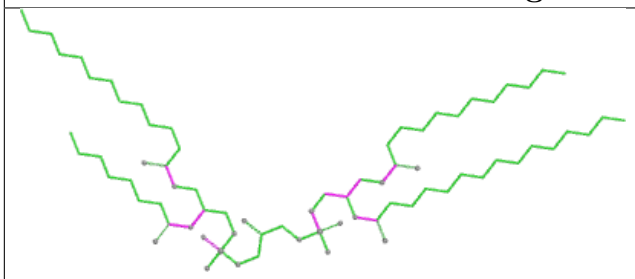


Rings

Ligand CDL T 201



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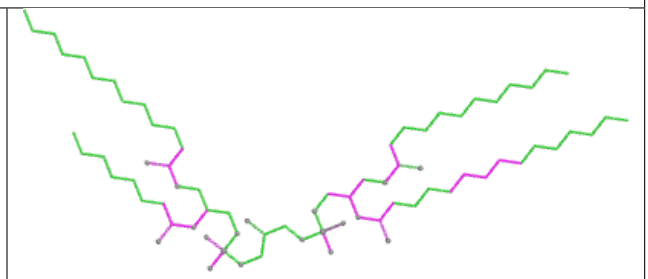
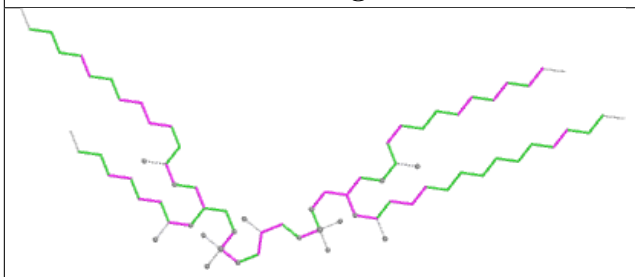


Bond angles



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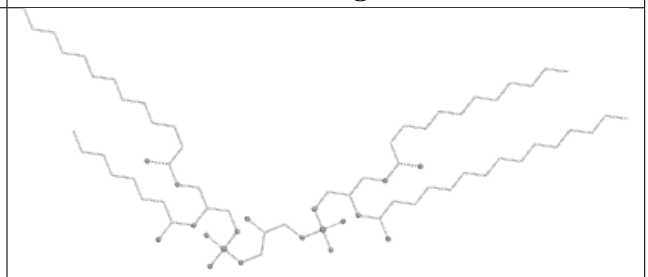
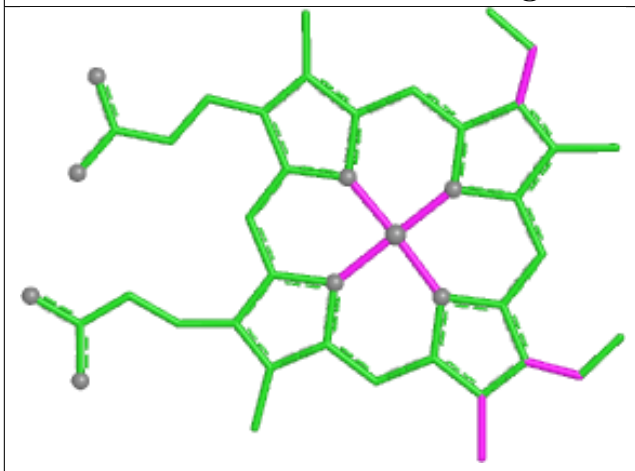


Rings

Ligand HEM E 602



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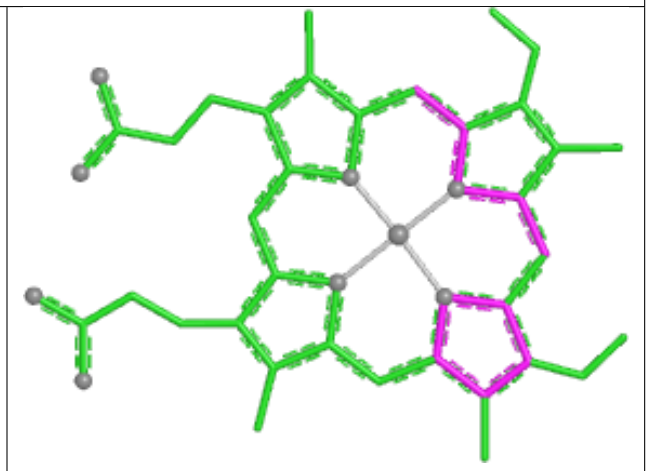
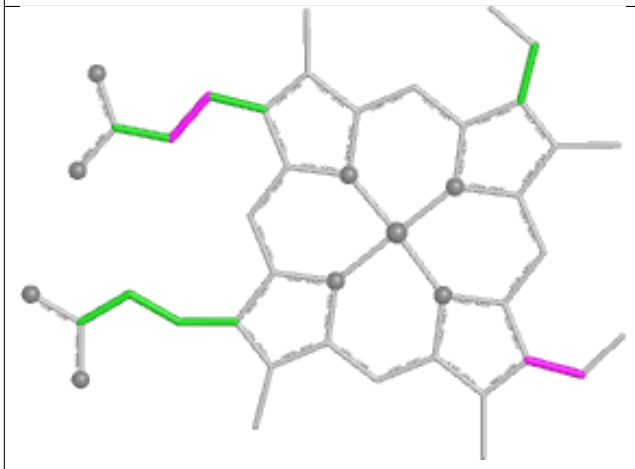


Bond angles



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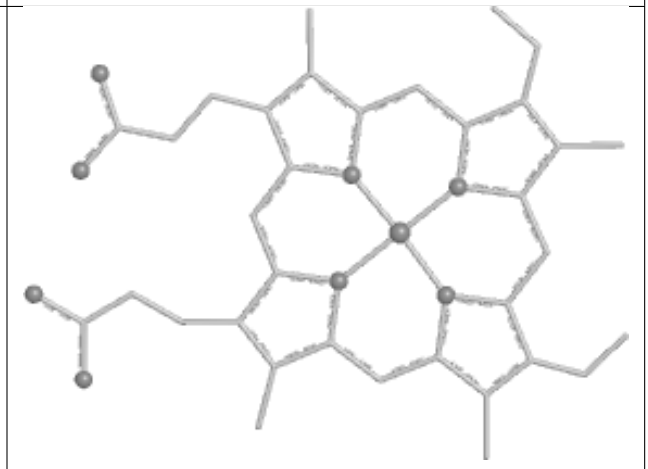
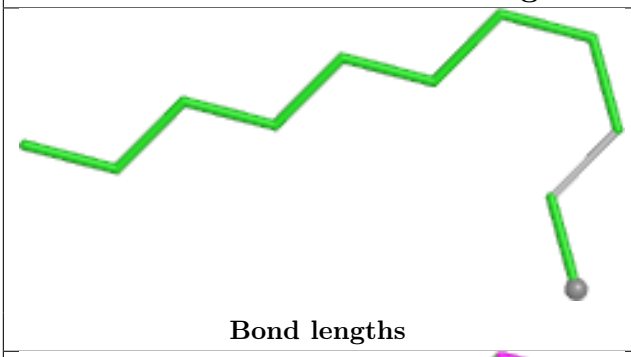


Rings

Ligand PLM D 301



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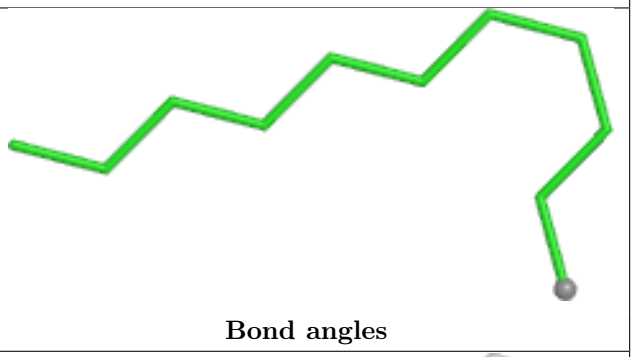
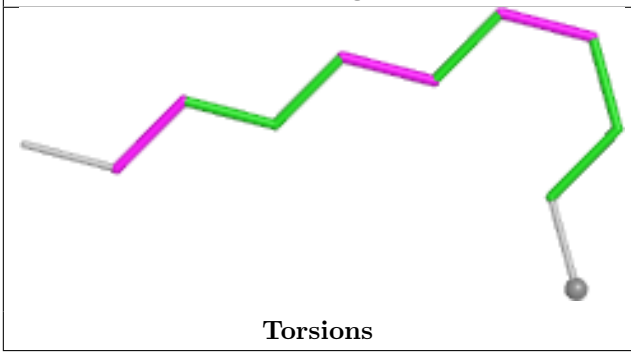
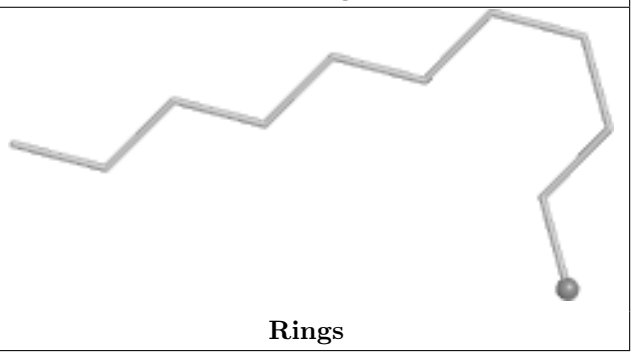


Bond angles

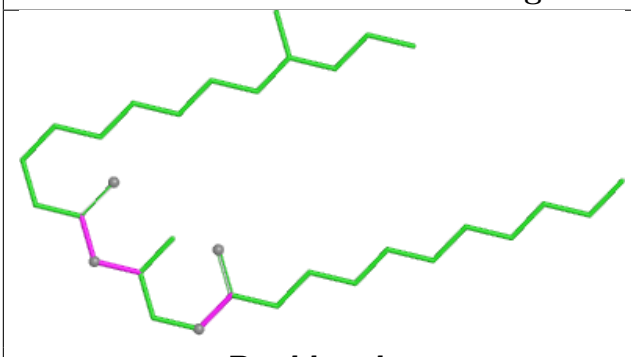


Torsions

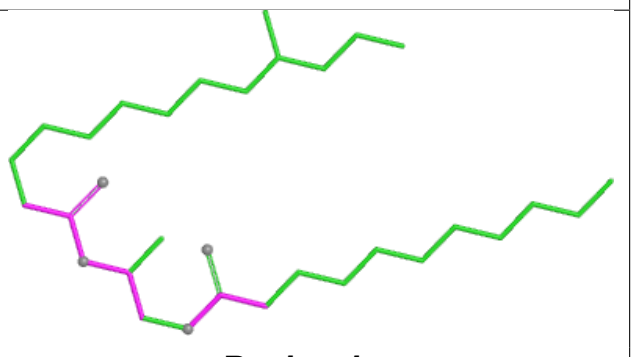


Rings

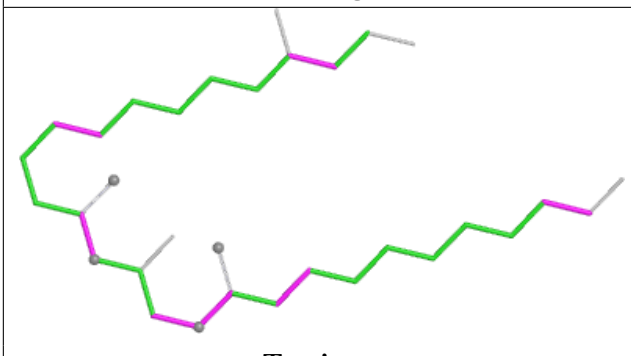
Ligand 9XX G 302



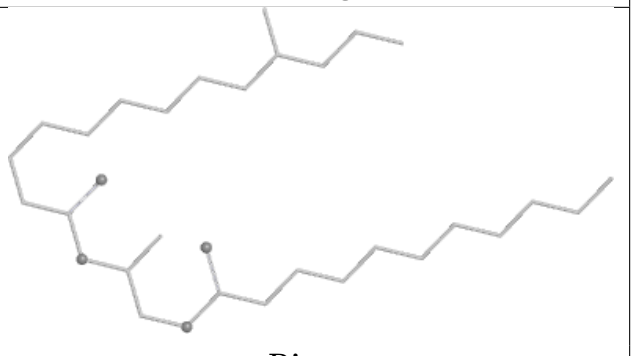
Bond lengths



Bond angles

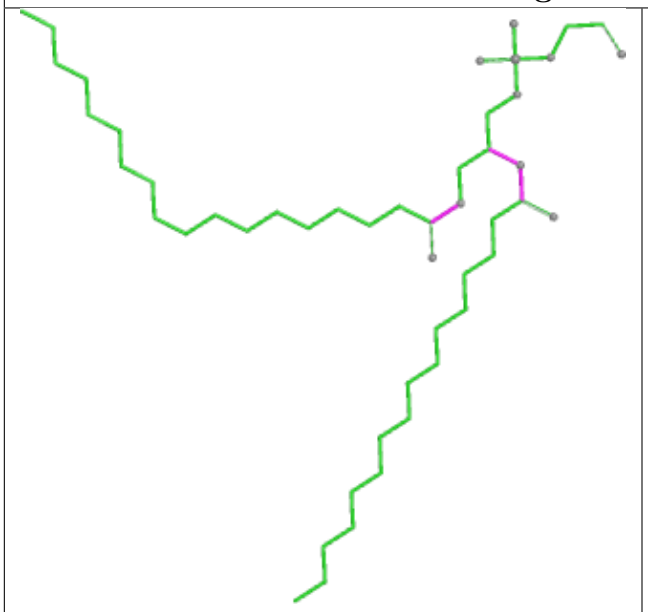


Torsions



Rings

Ligand 9Y0 J 202



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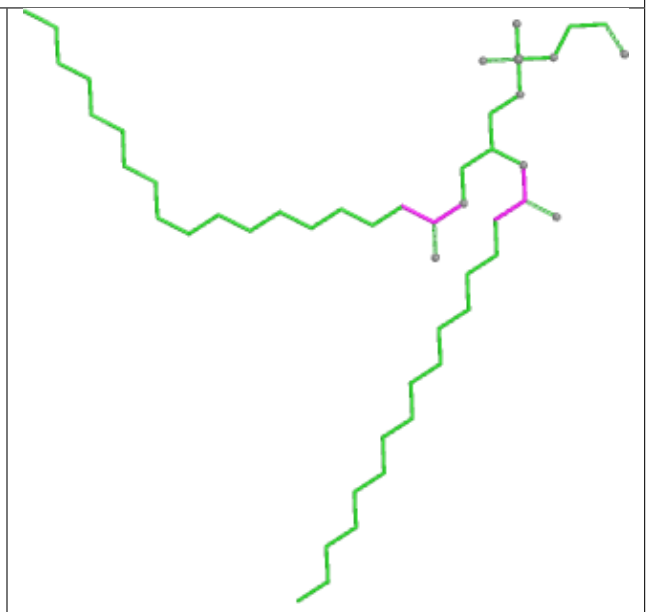

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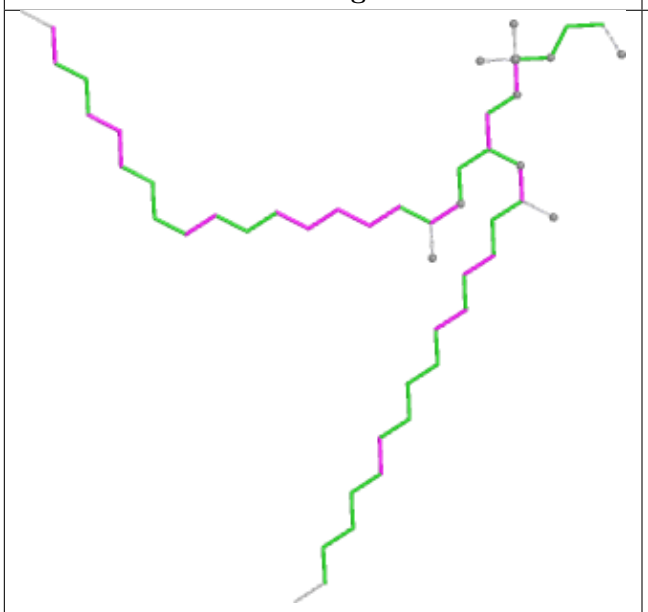

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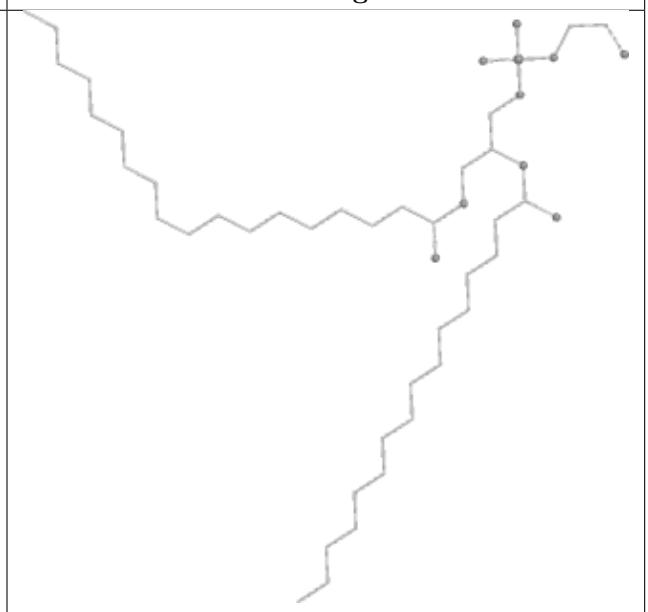
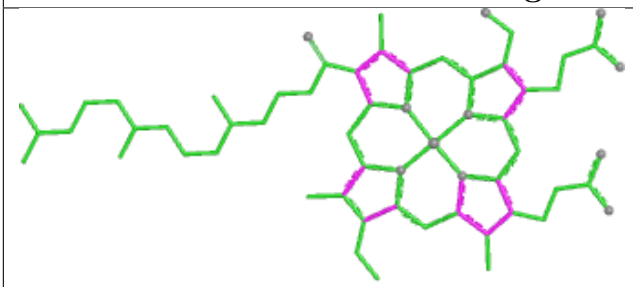


Rings

Ligand HEA L 602



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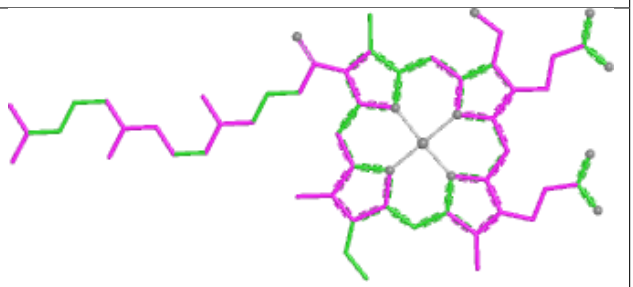

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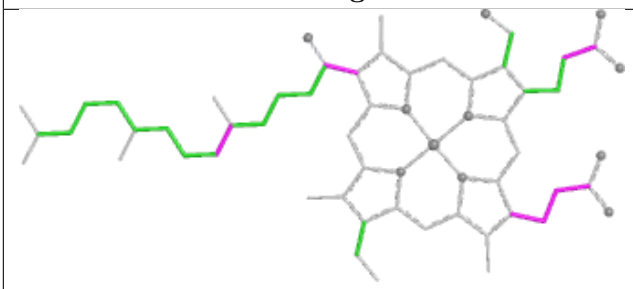
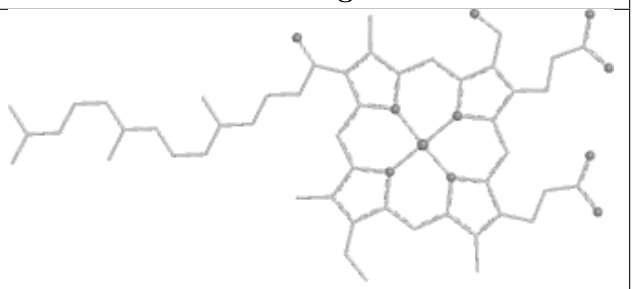
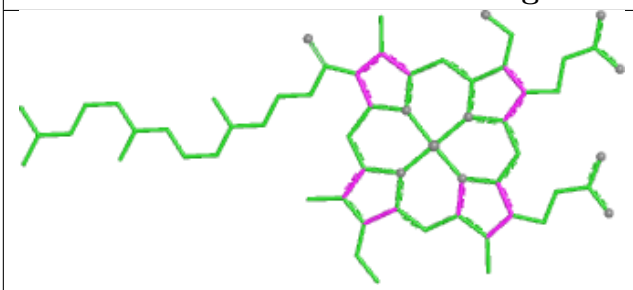


Torsions



Rings

Ligand HEA R 602



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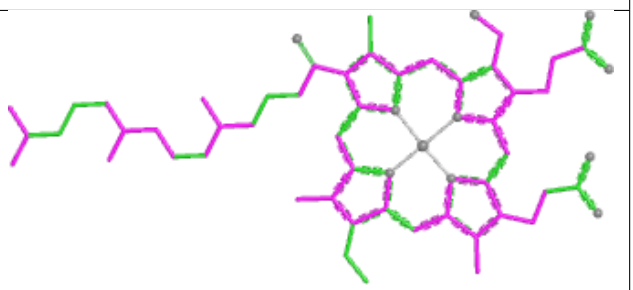

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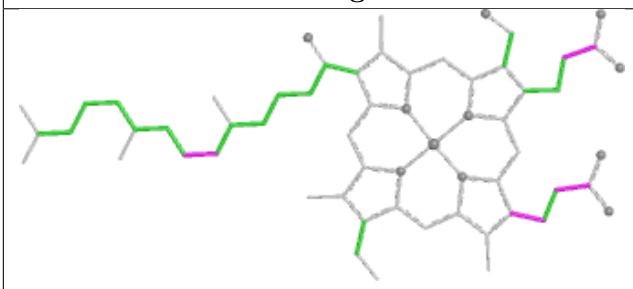

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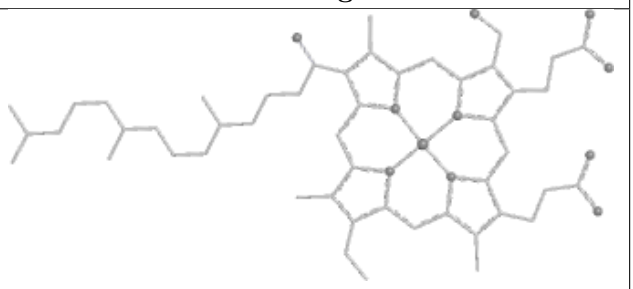
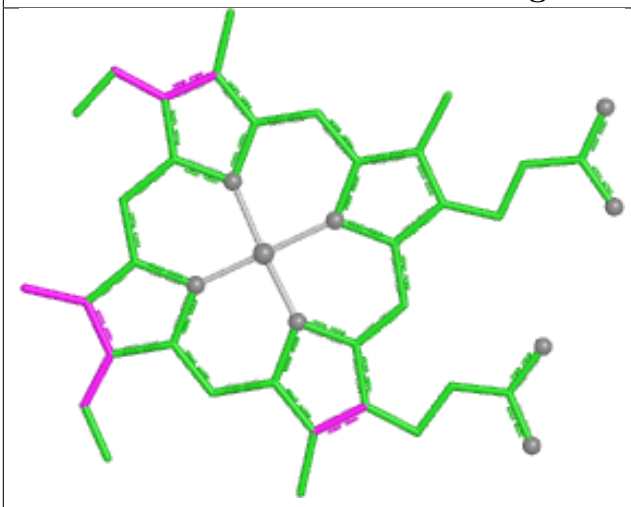


Rings

Ligand HEC I 302



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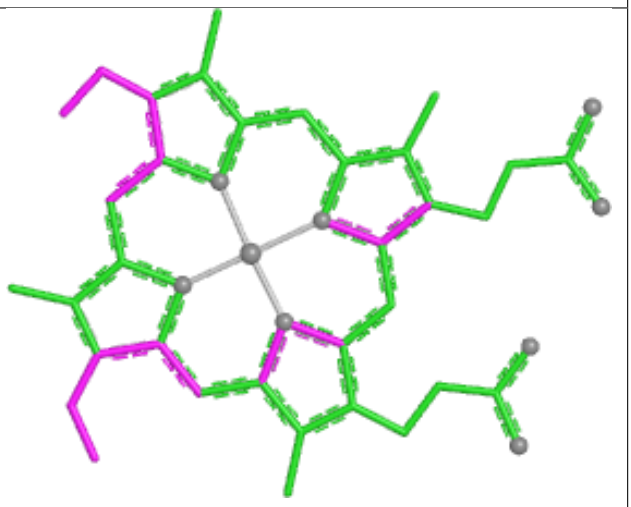

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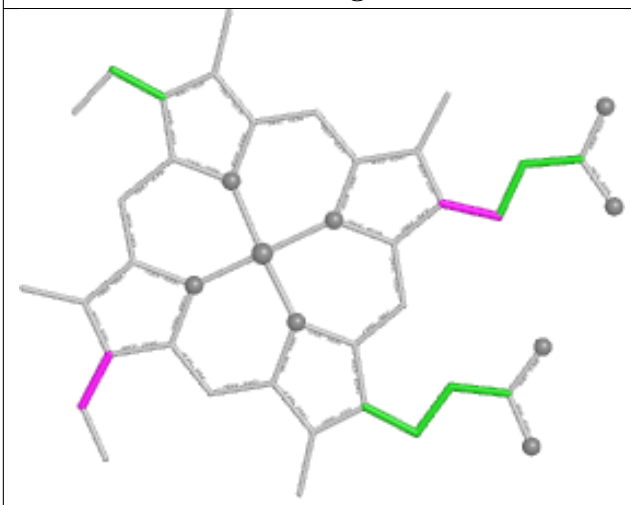

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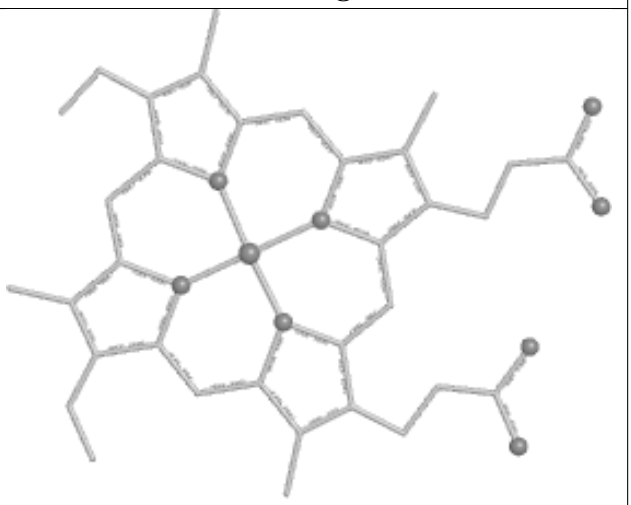
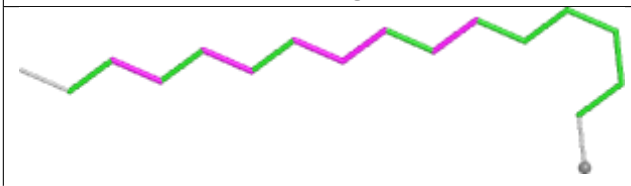


Rings

Ligand PLM c 201

Bond lengths

Bond angles



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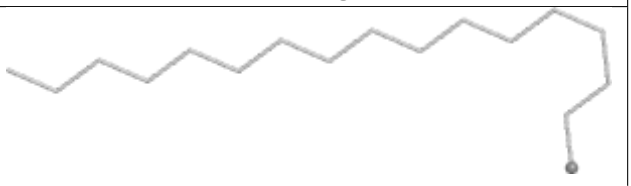
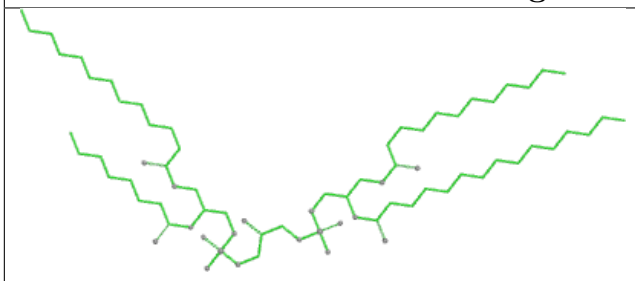


Rings

Ligand CDL J 201



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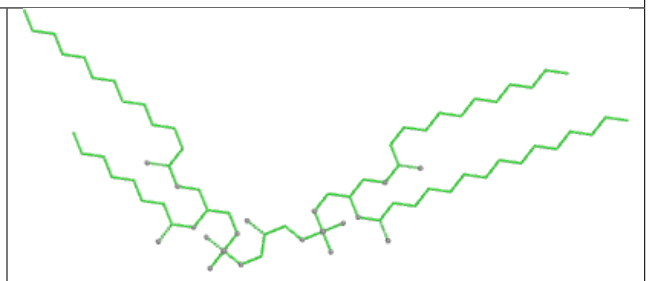
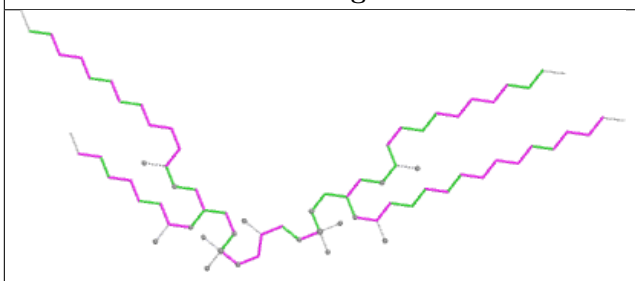


Bond angles



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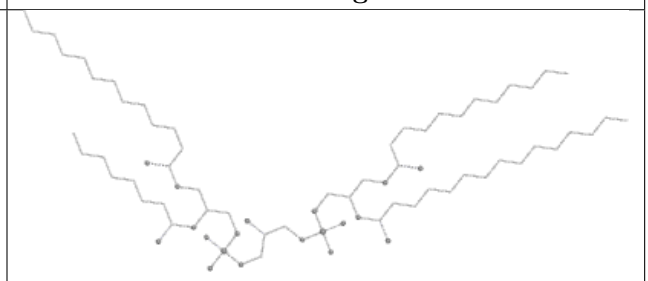
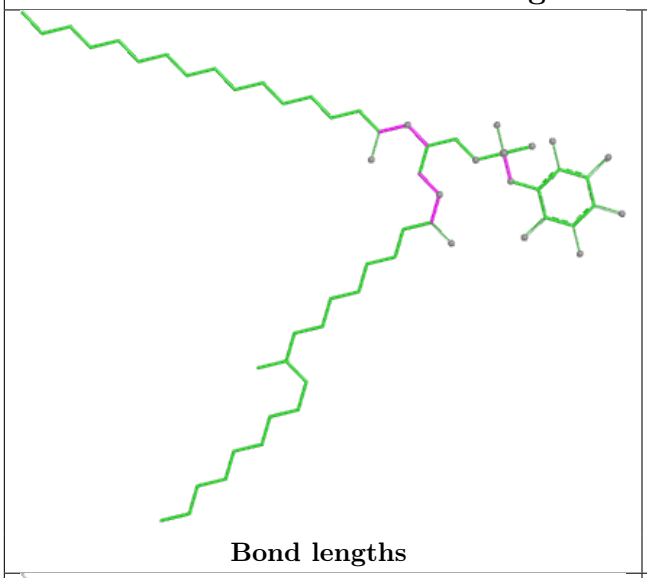


Rings

Ligand 9YF O 303



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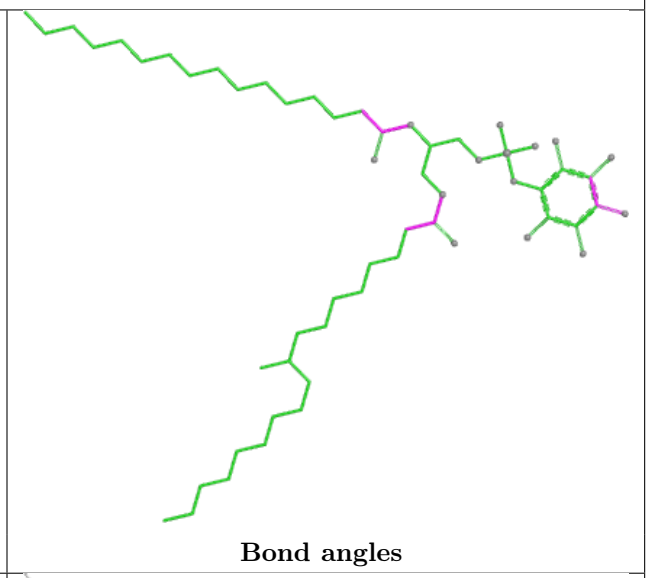
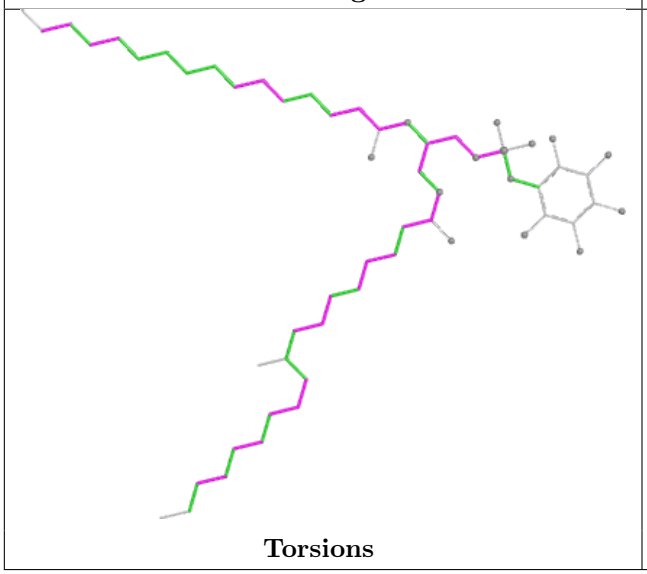


Bond angles



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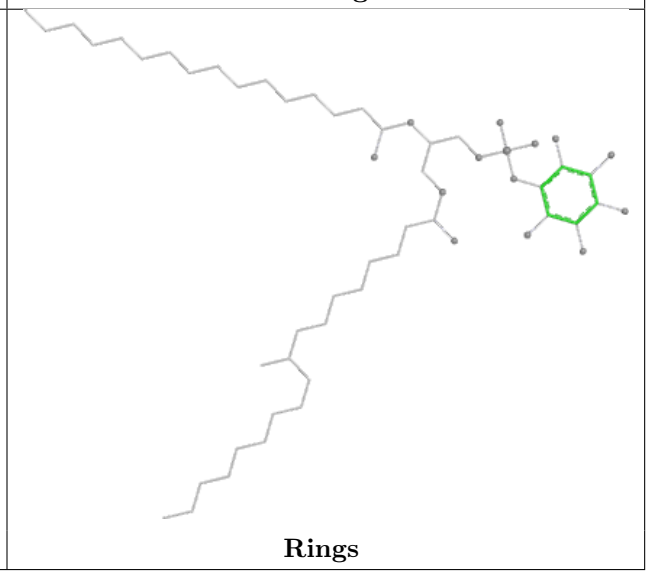
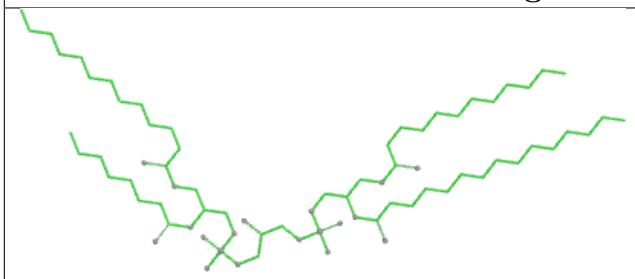


Rings

Ligand CDL X 301



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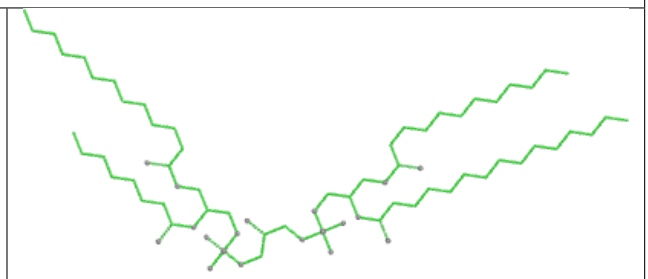

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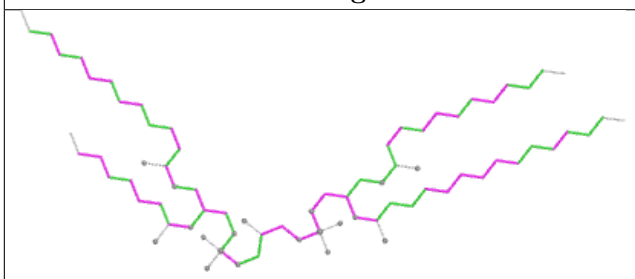

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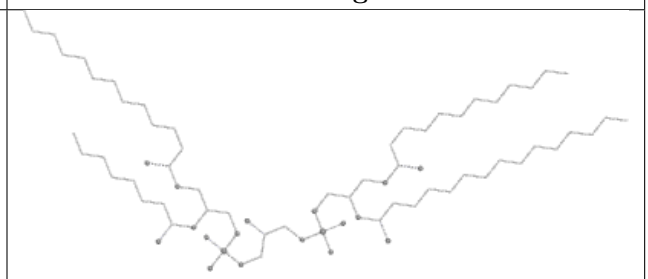
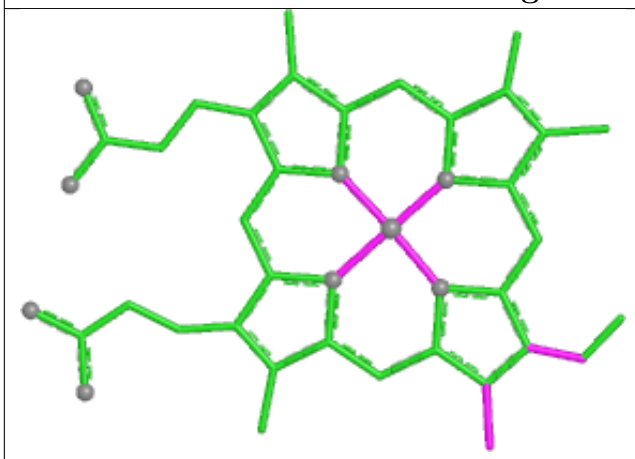


Rings

Ligand HEM F 702



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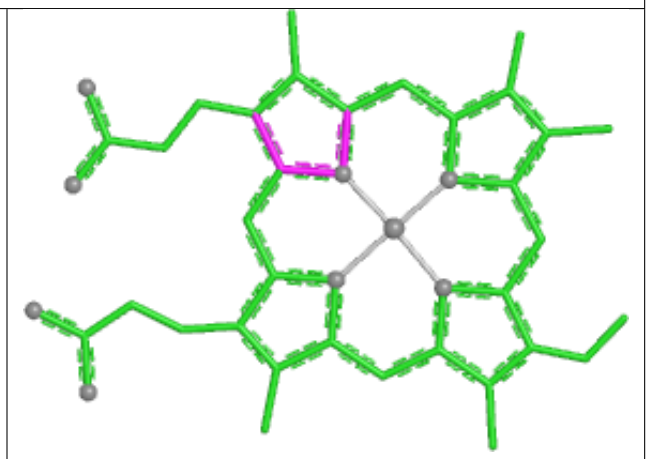

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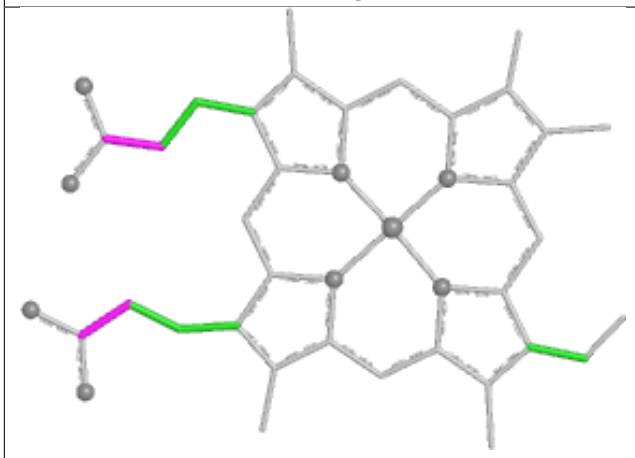

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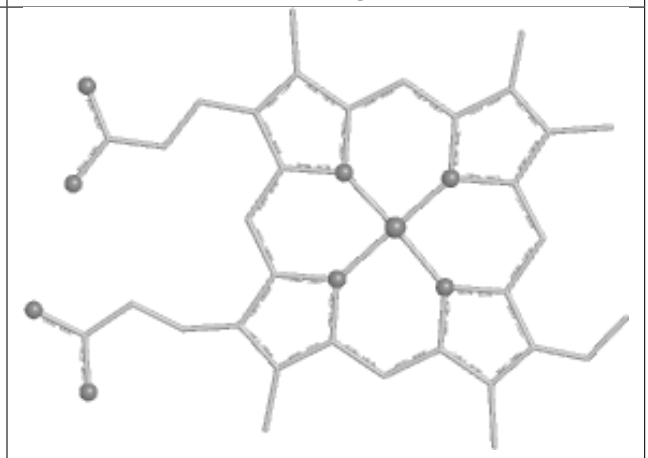
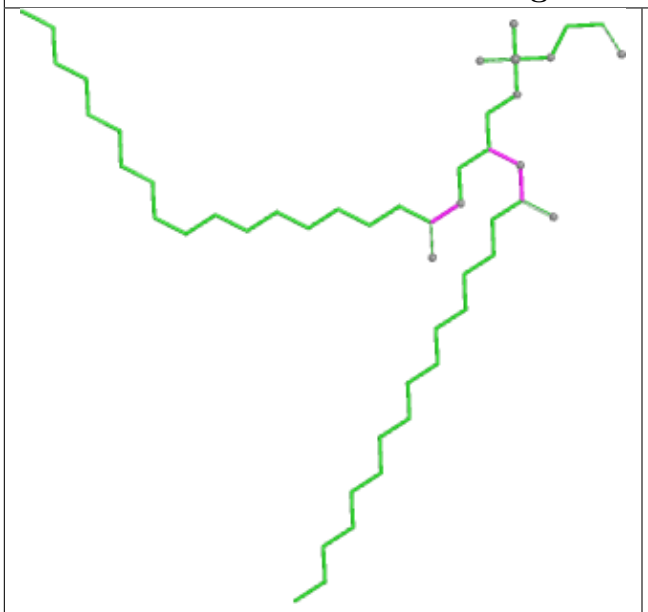


Rings

Ligand 9Y0 X 303



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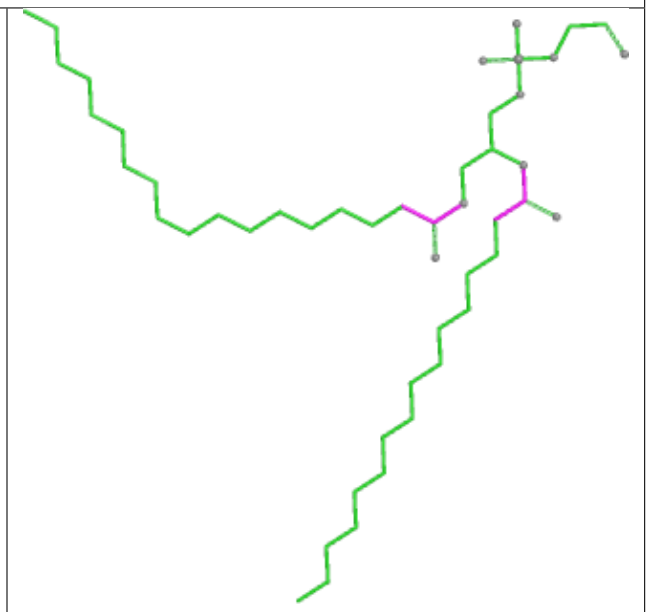
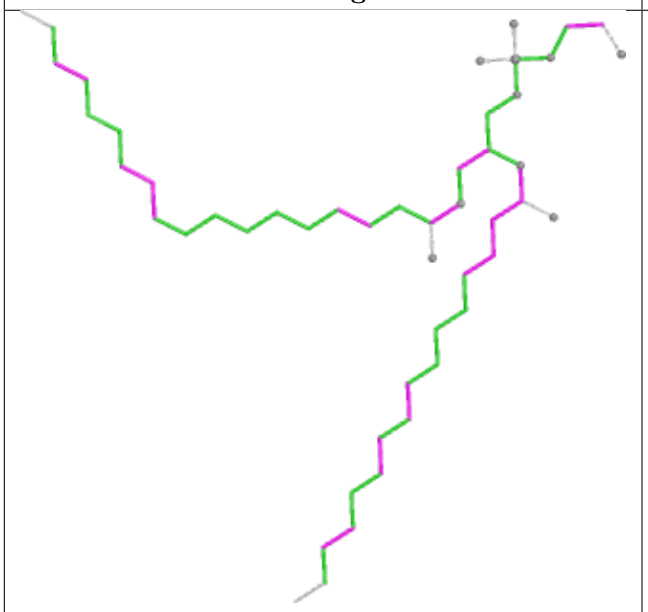


Bond angles



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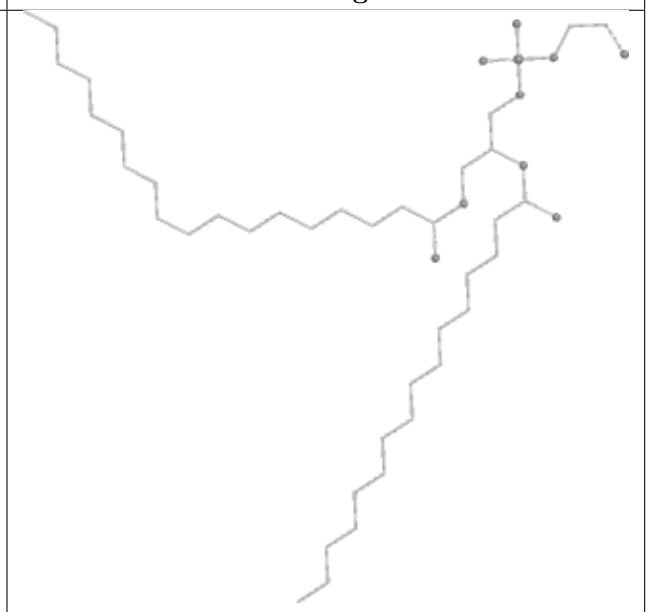
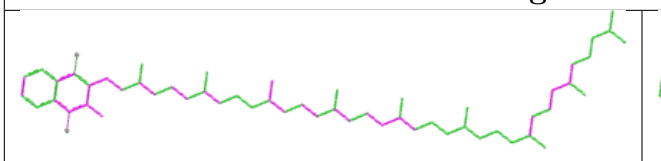


Rings

Ligand MQ9 I 303



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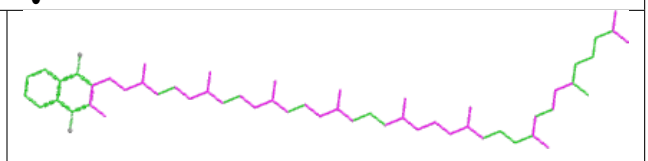
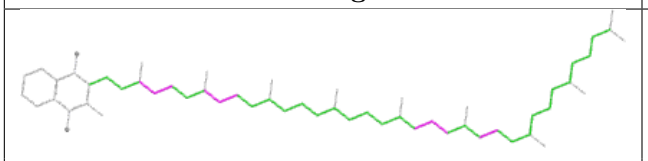
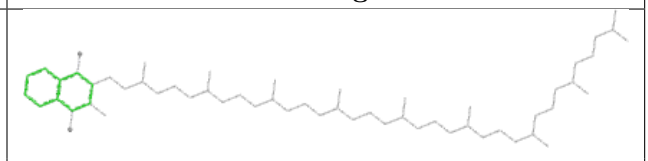


Bond angles

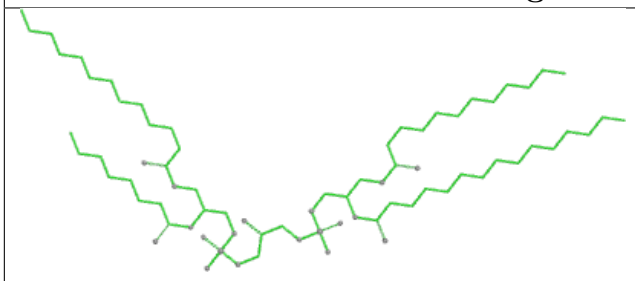


Torsions



Rings

Ligand CDL F 704



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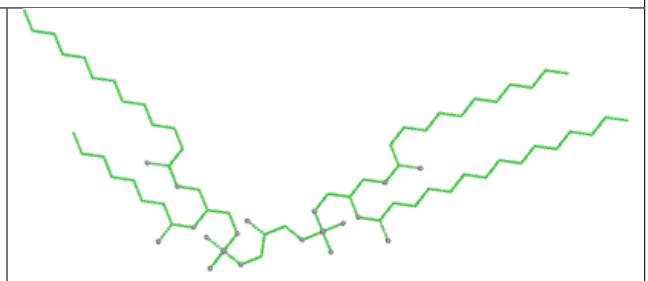
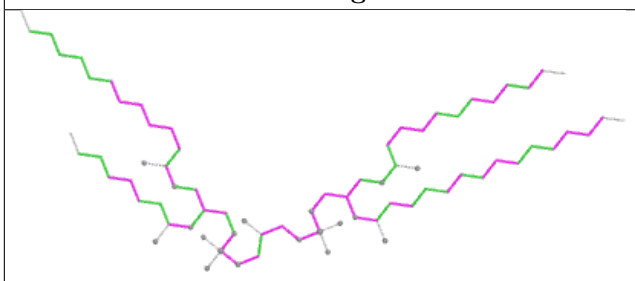
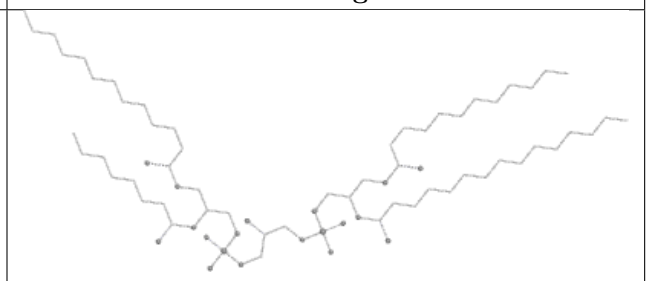


Bond angles

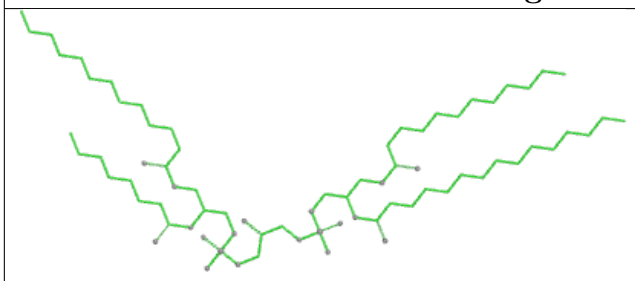


Torsions



Rings

Ligand CDL R 604



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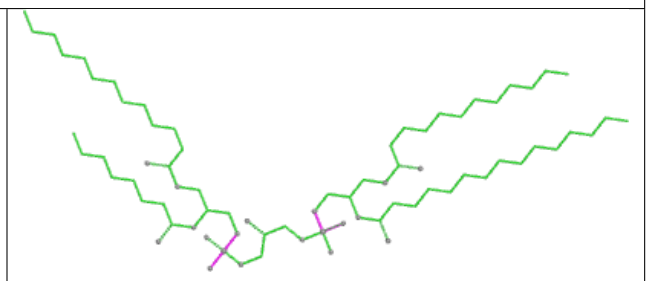
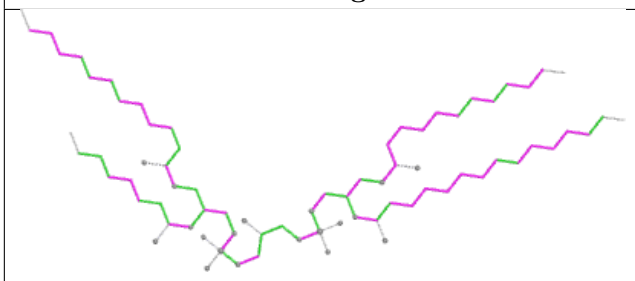


Bond angles



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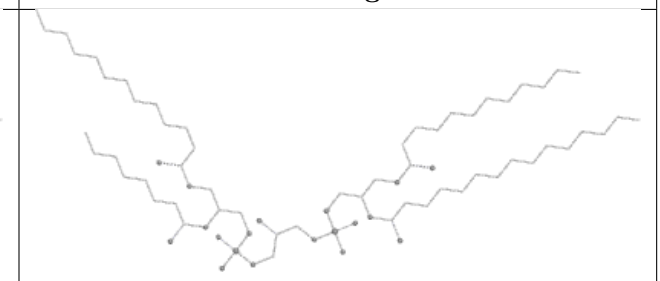
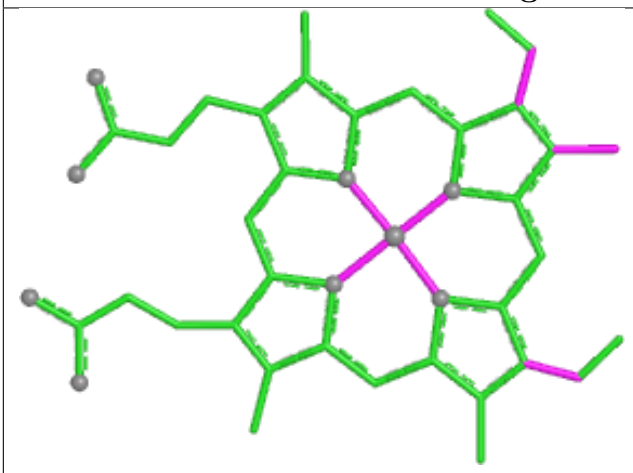
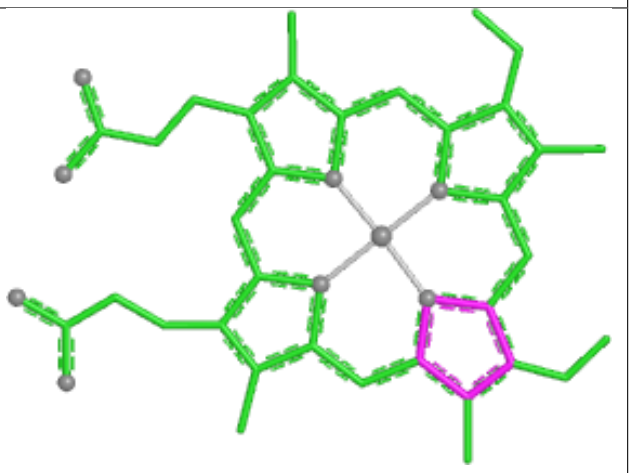


Rings

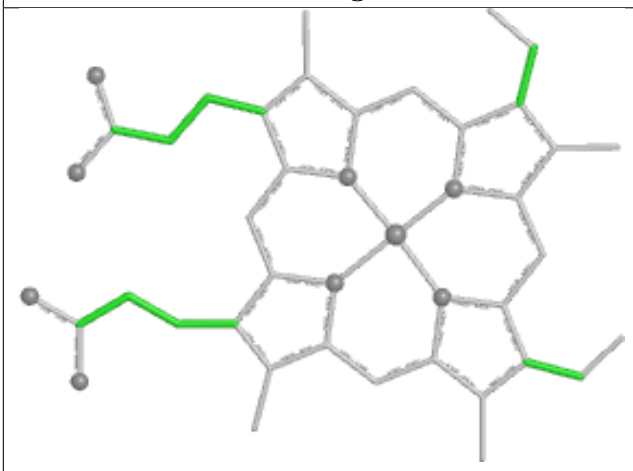
Ligand HEM F 703



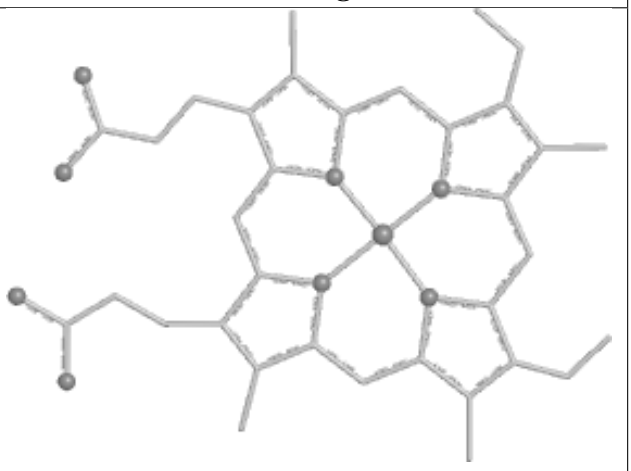
Bond lengths



Bond angles

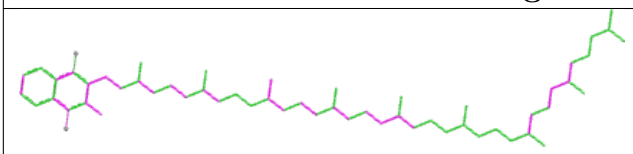


Torsions



Rings

Ligand MQ9 F 709



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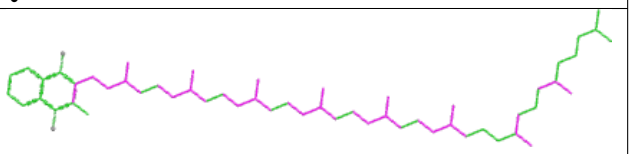

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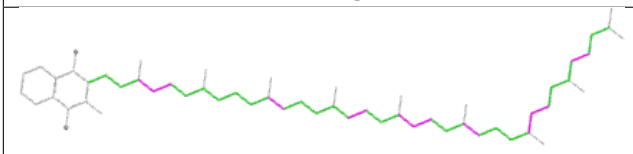
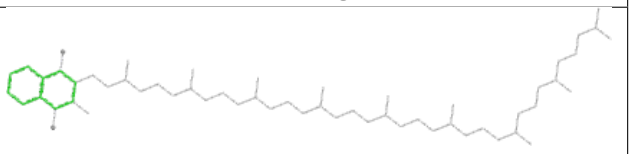
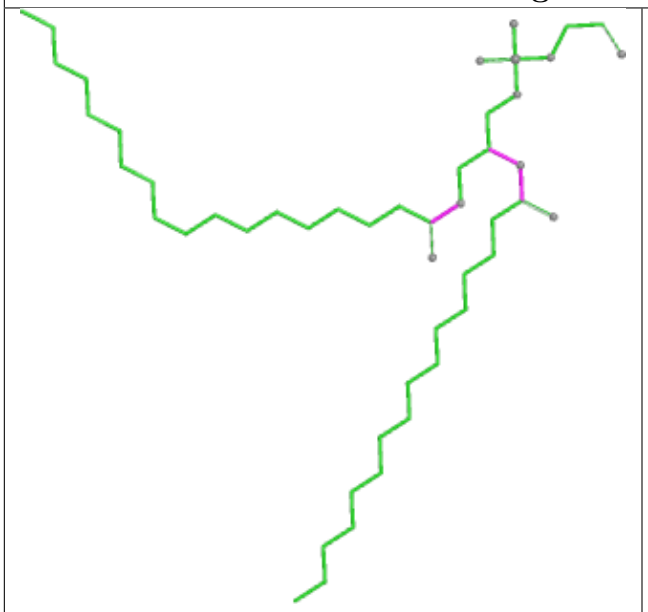


Torsions



Rings

Ligand 9Y0 P 202



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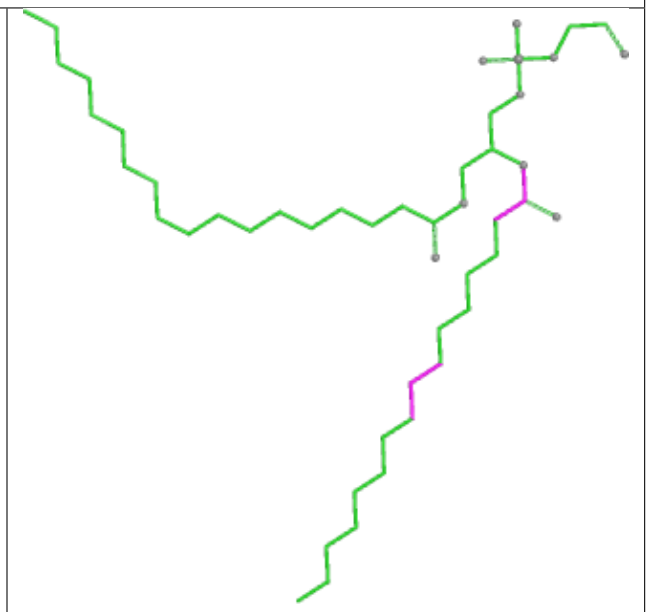
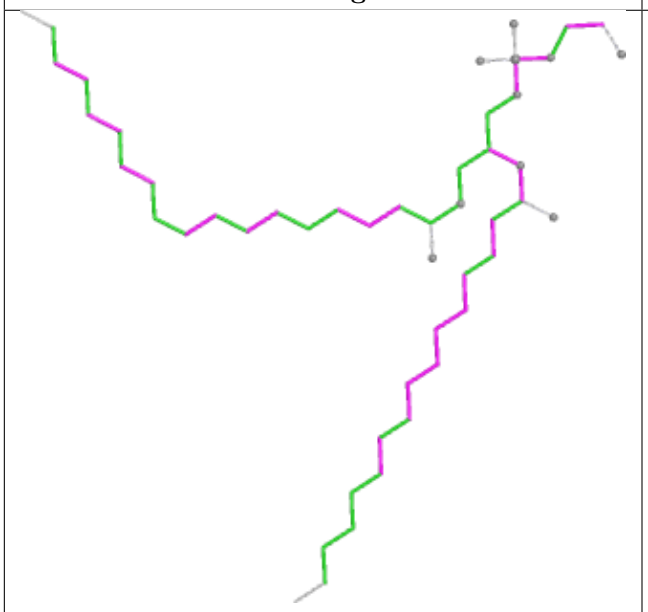


Bond angles



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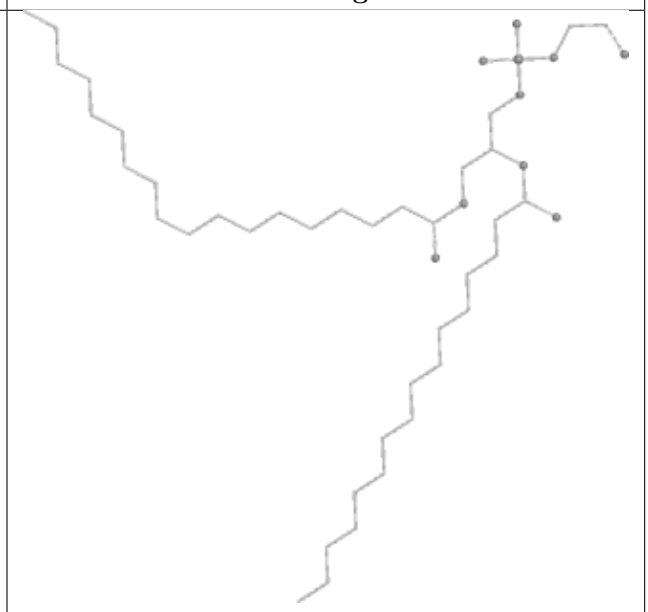
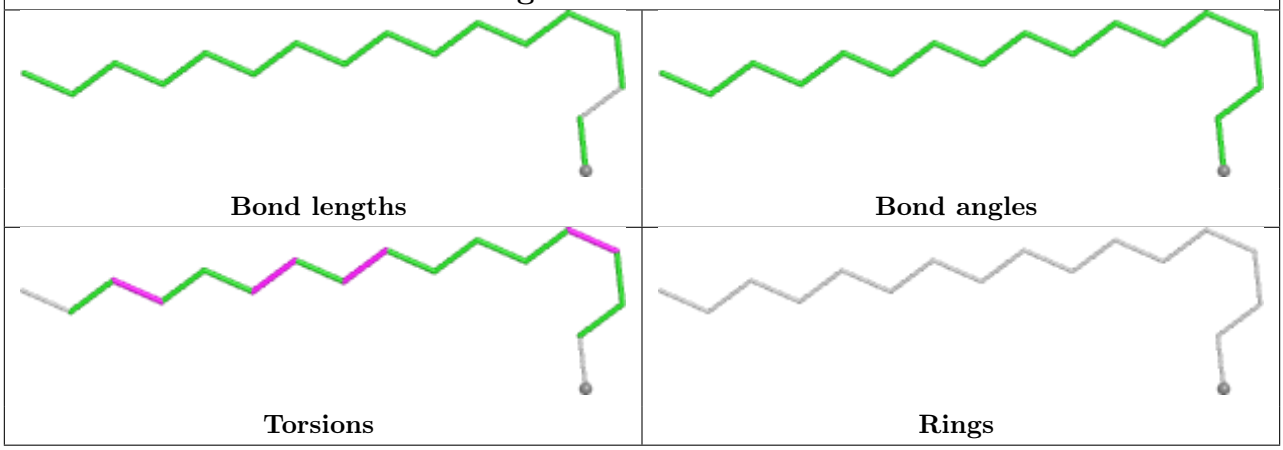
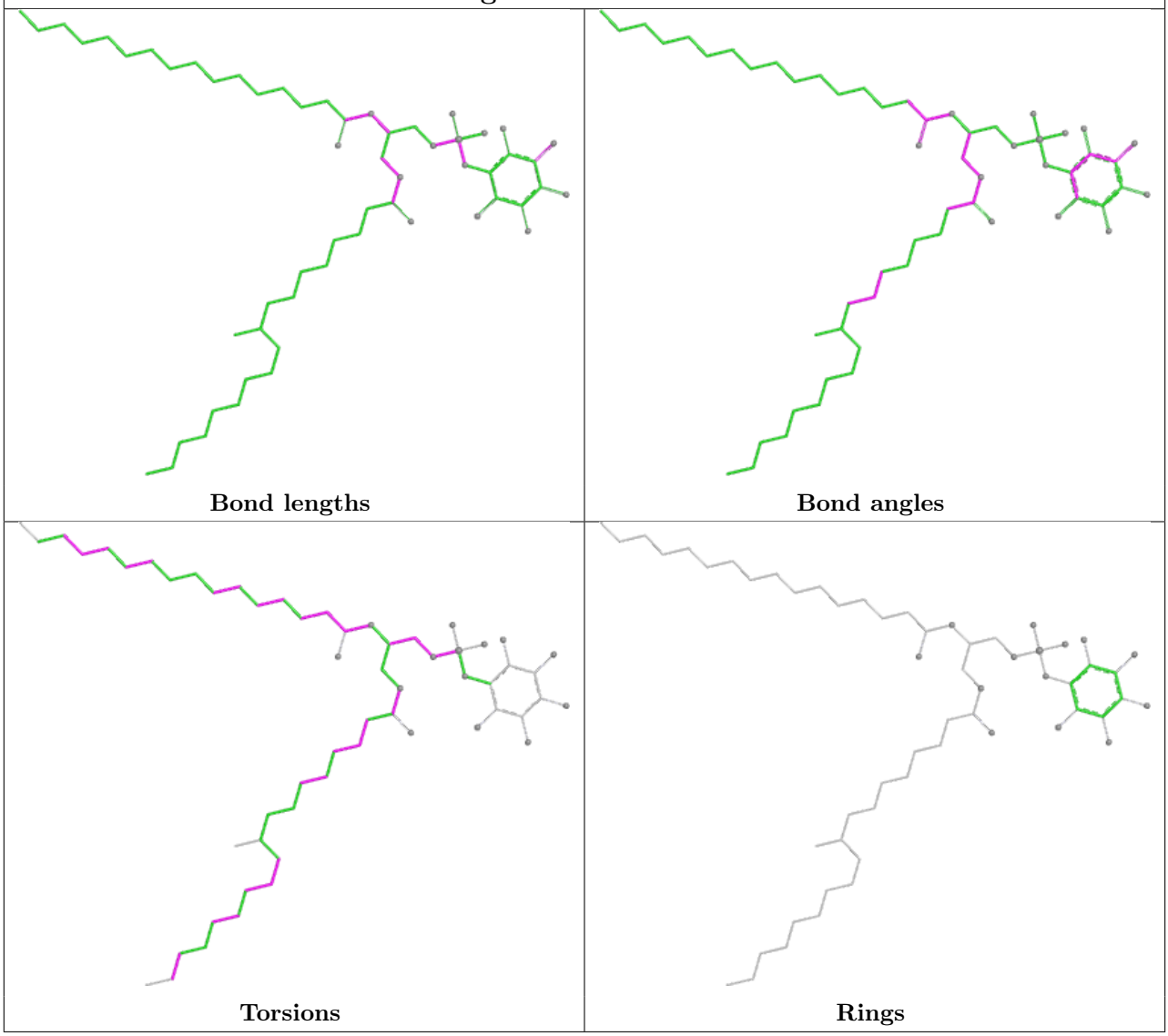


Rings

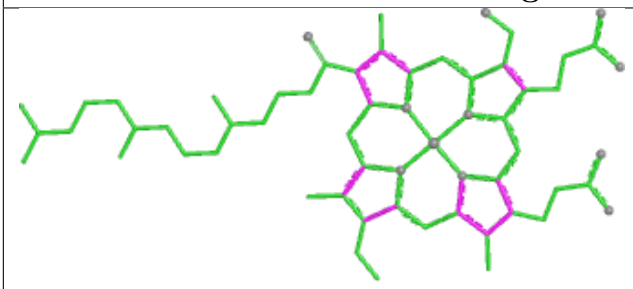
Ligand PLM W 201



Ligand 9YF Y 502



Ligand HEA R 603



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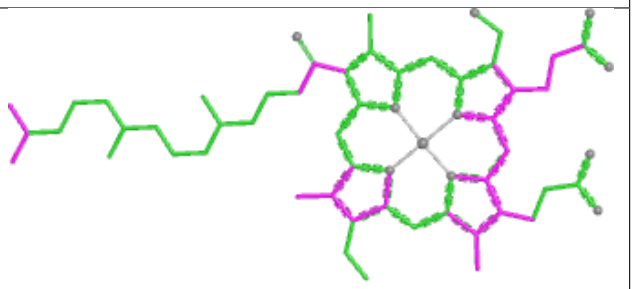
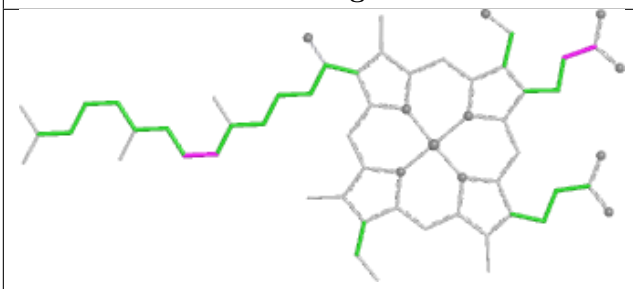


Bond angles



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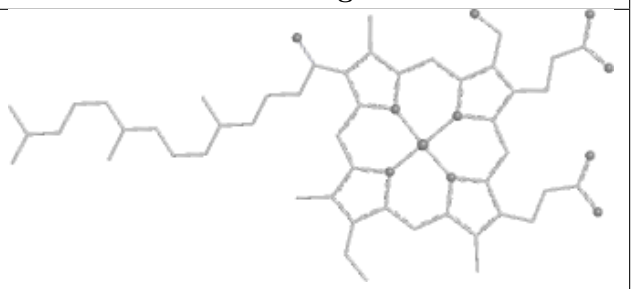
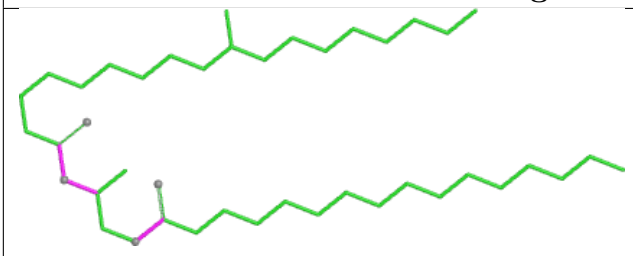


Rings

Ligand 9XX c 202



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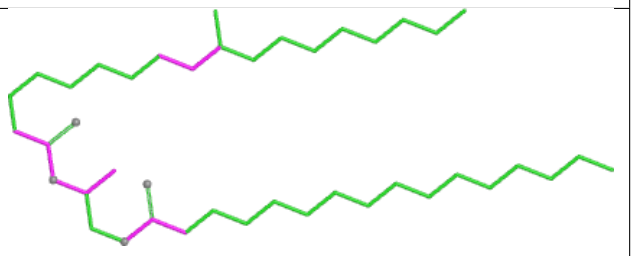

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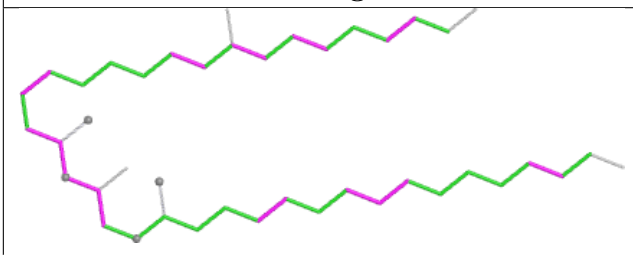

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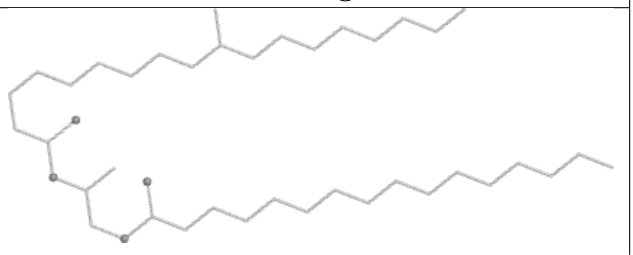
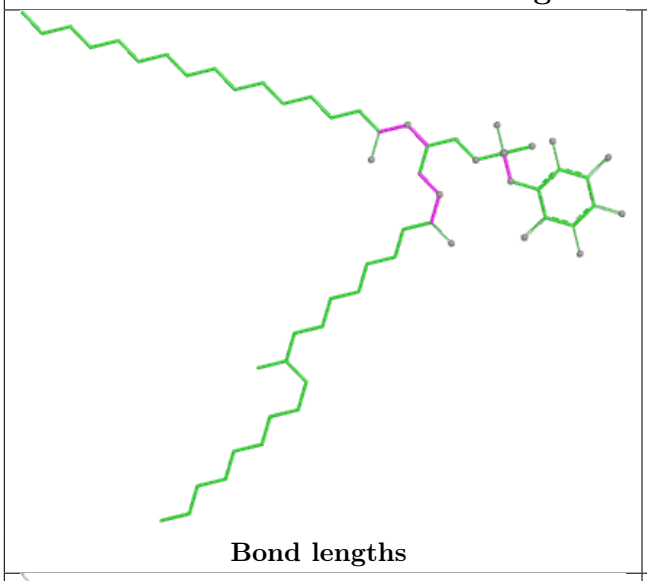


Rings

Ligand 9YF c 203



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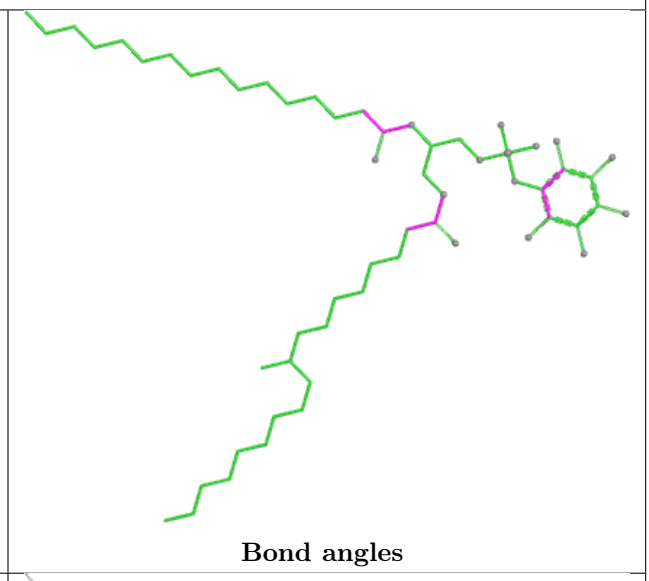
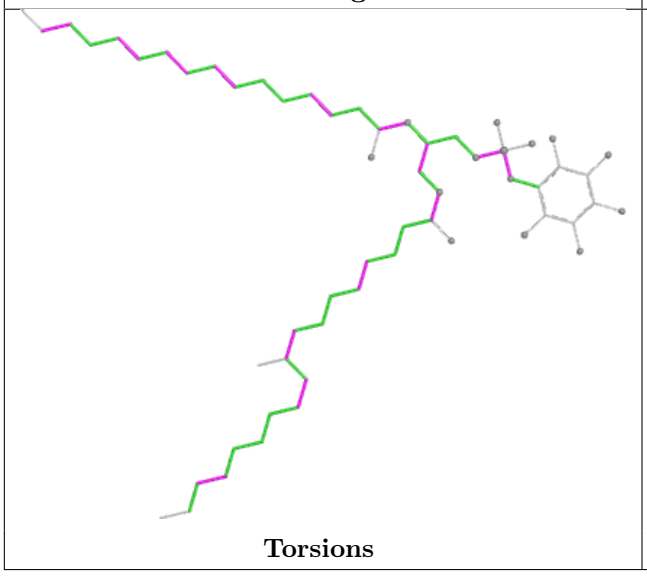


Bond angles



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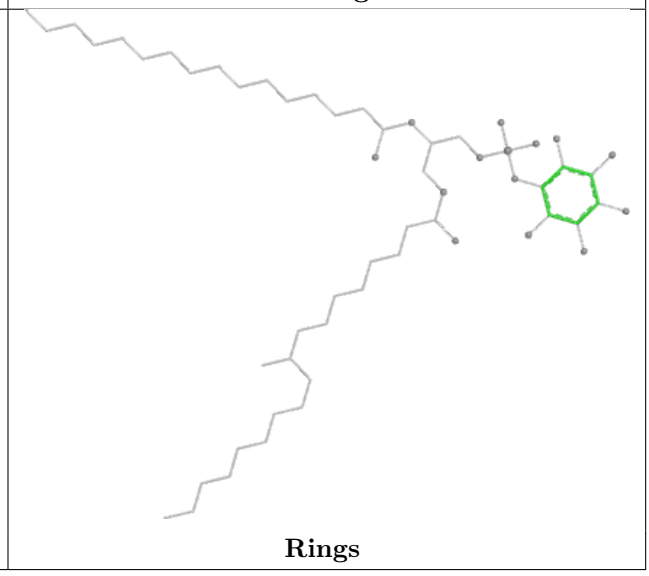
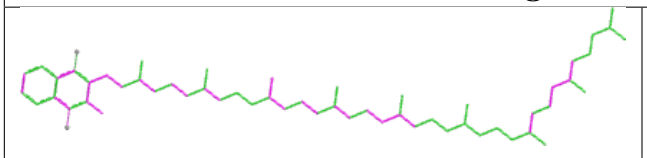


Rings

Ligand MQ9 E 604



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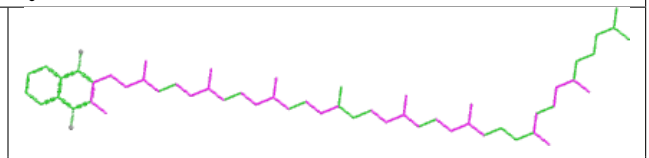
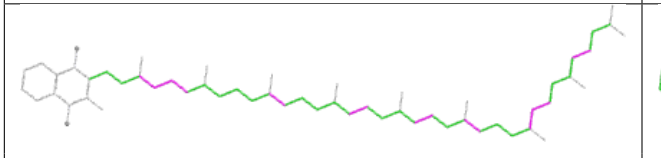


Bond angles



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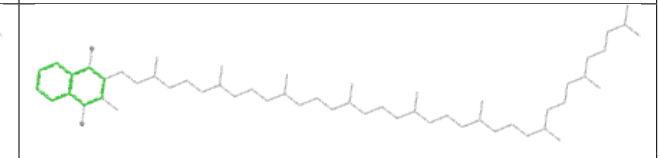
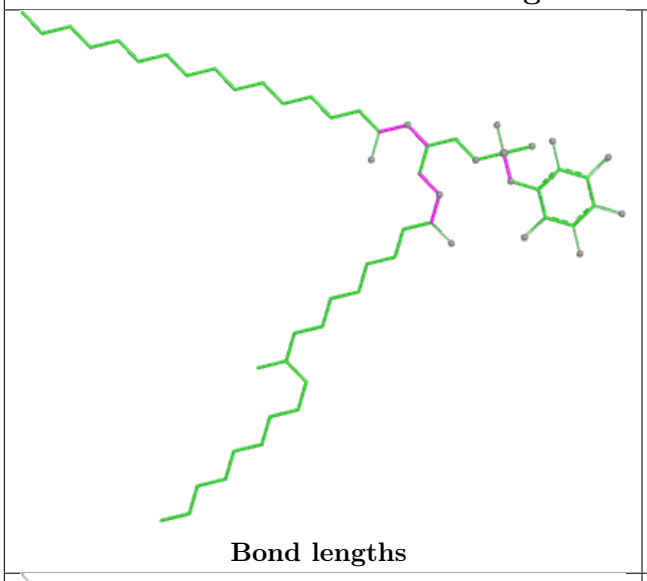


Rings

Ligand 9YF W 203



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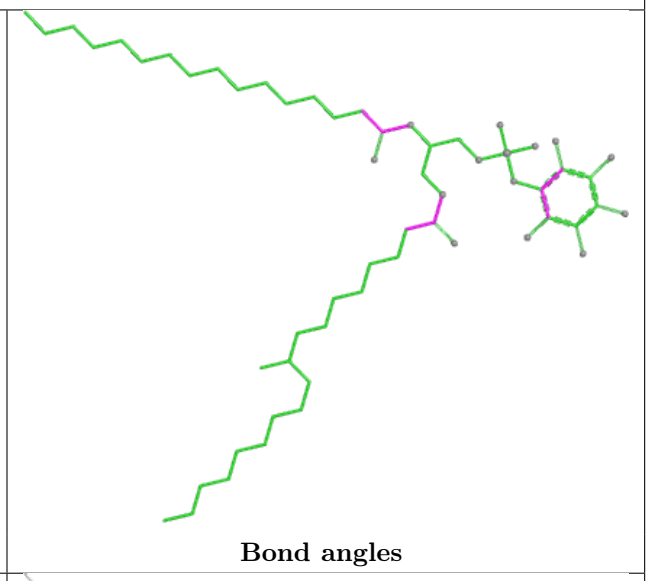
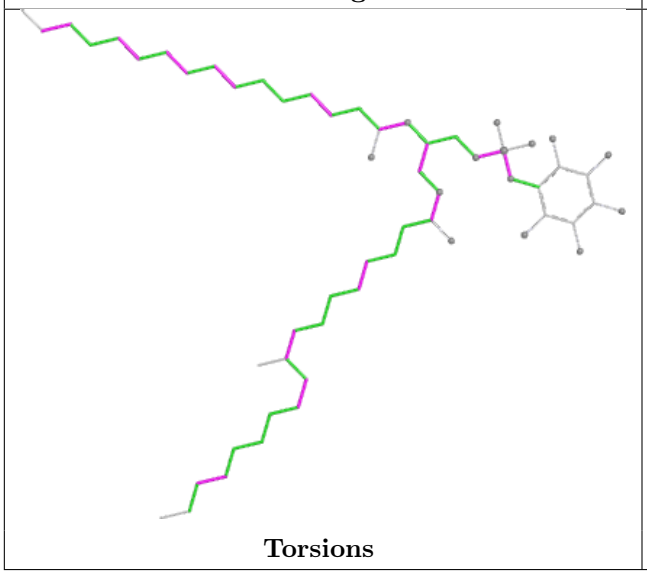


Bond angles



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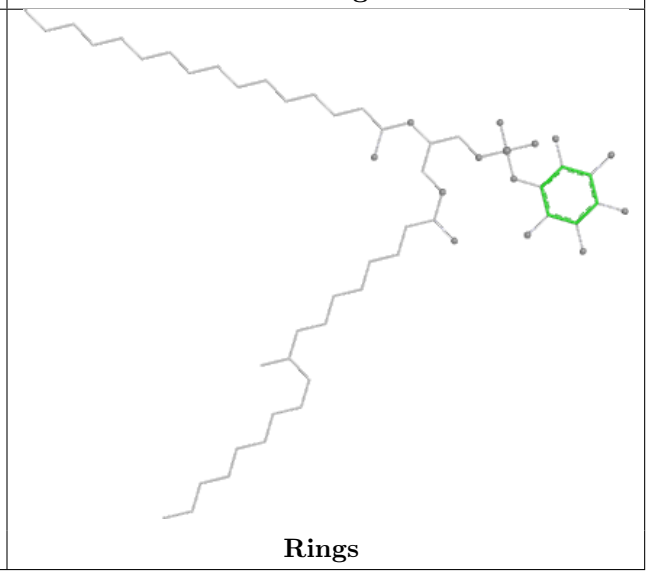
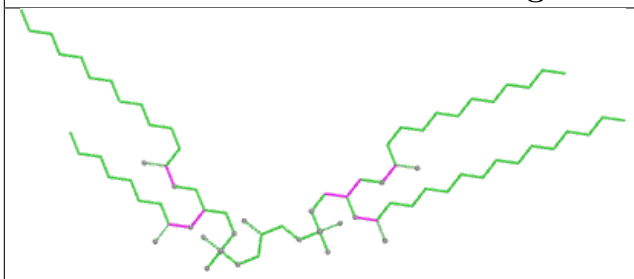


Rings

Ligand CDL Z 203



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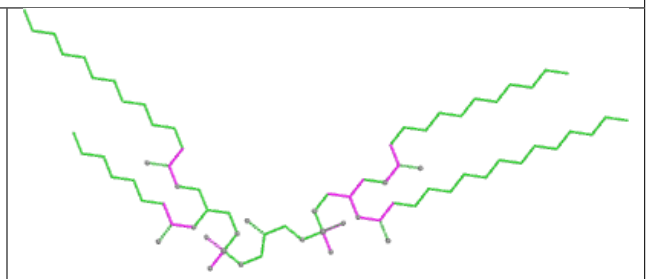

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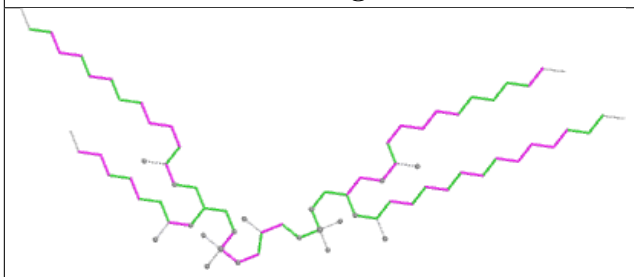

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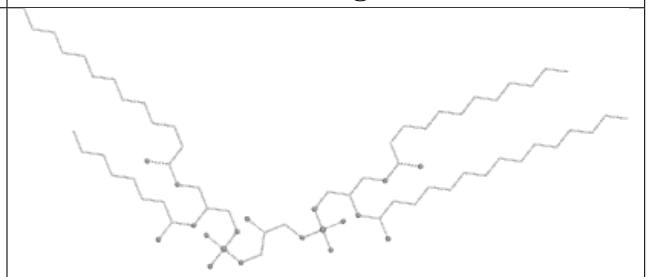


Rings

Ligand PLM G 301

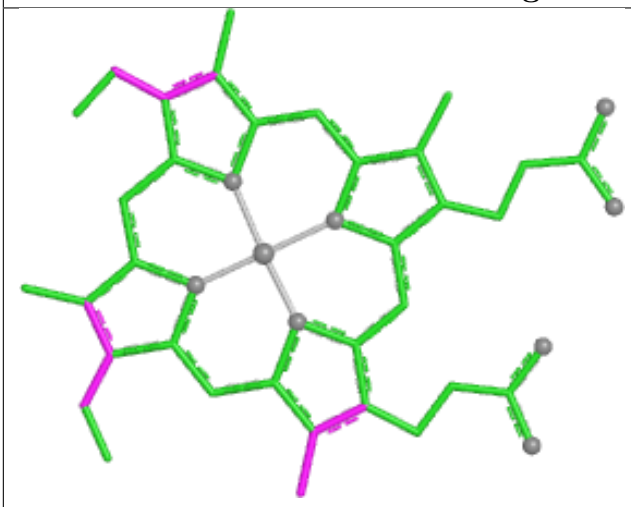
Bond lengths

Bond angles

Torsions

Rings

Ligand HEC O 301



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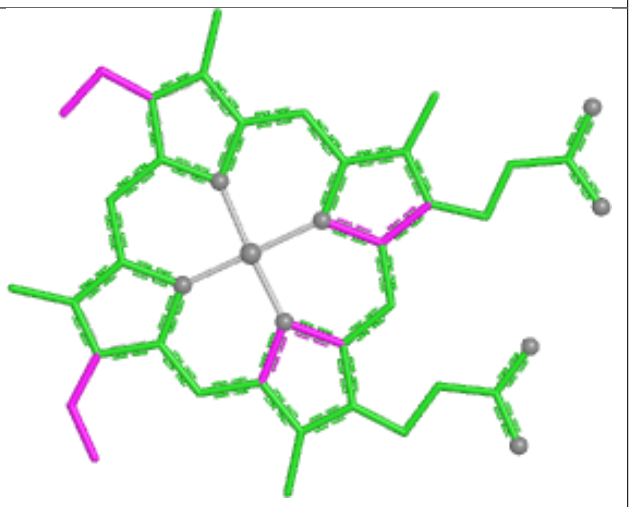

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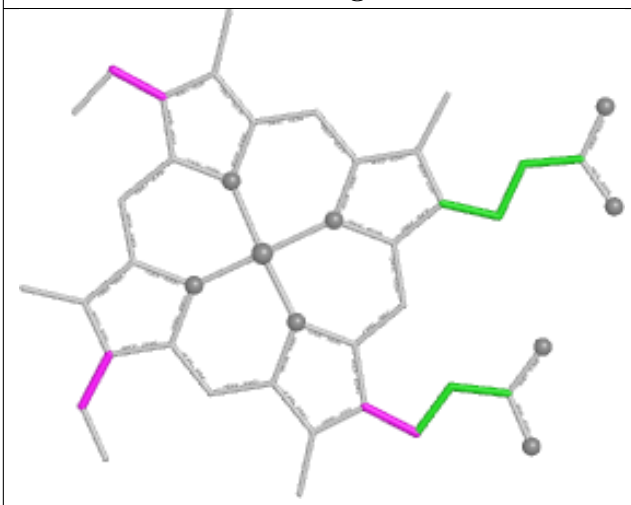

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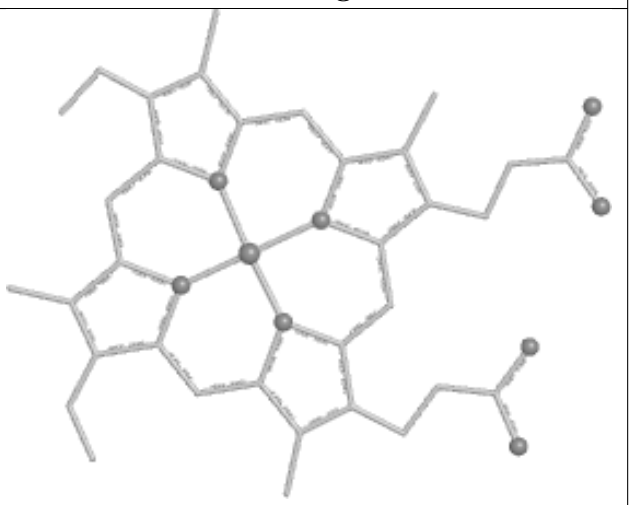
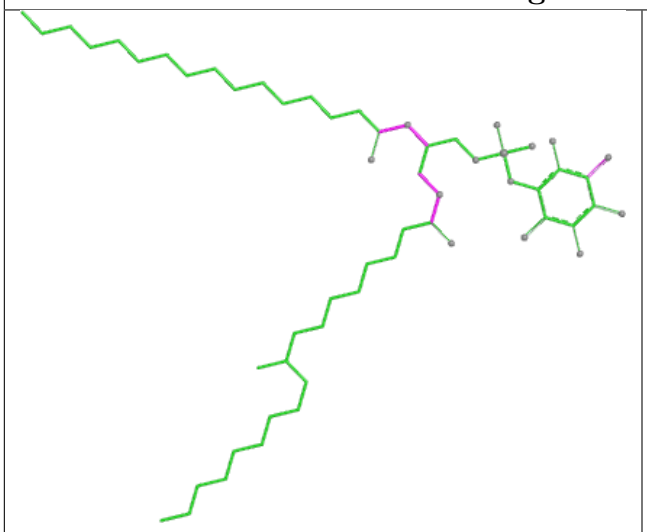


Rings

Ligand 9YF Y 503



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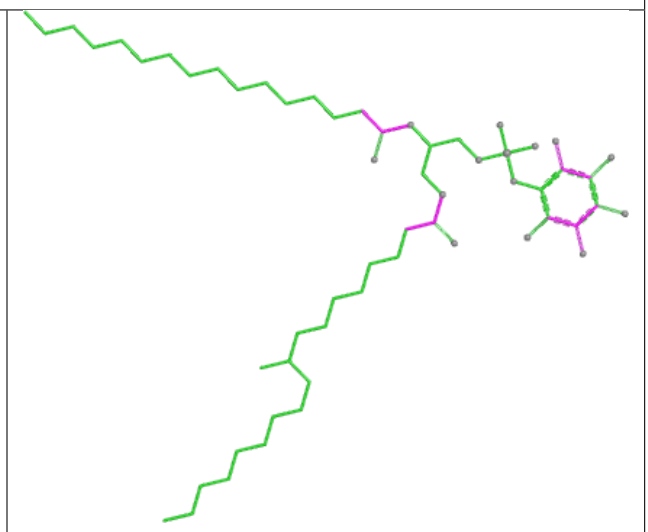

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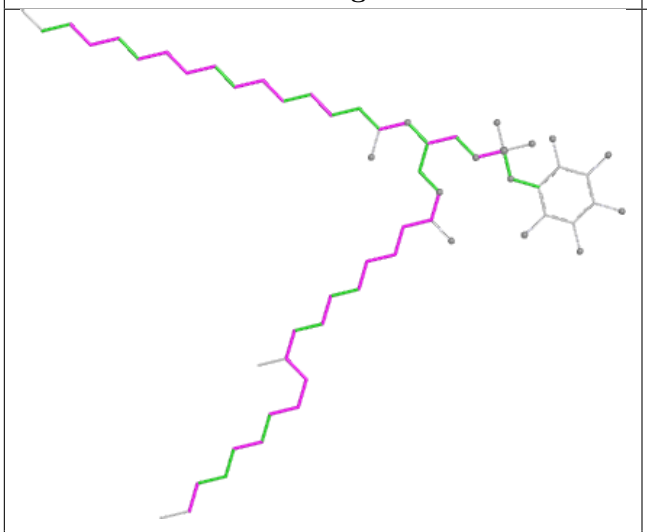

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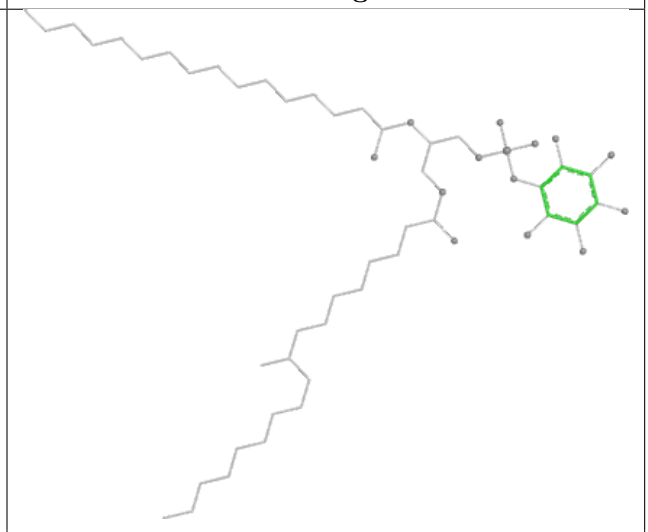
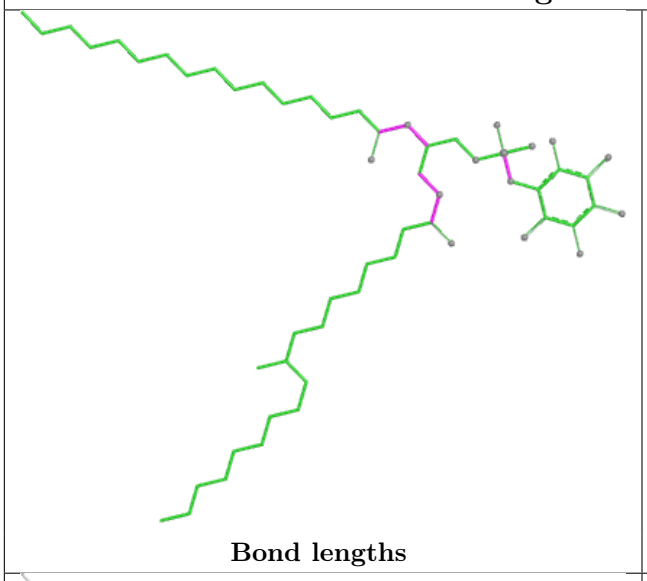


Rings

Ligand 9YF I 304



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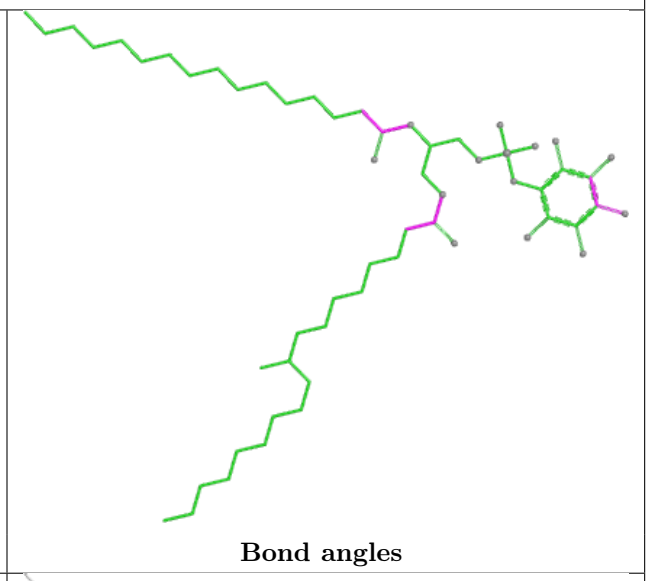
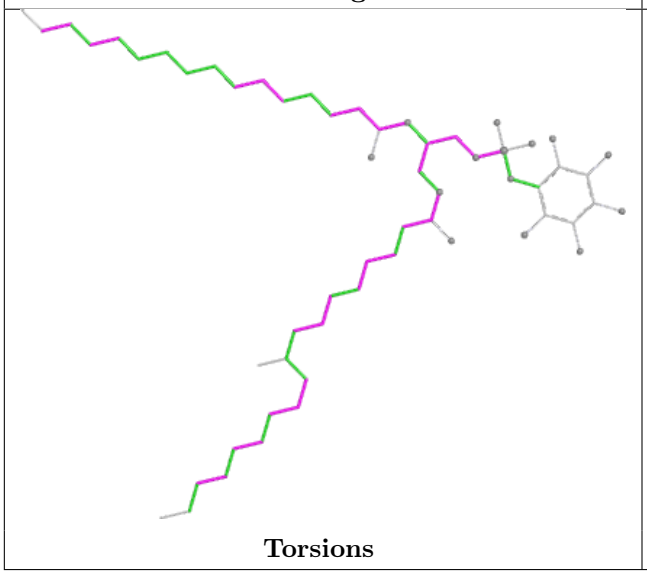


Bond angles



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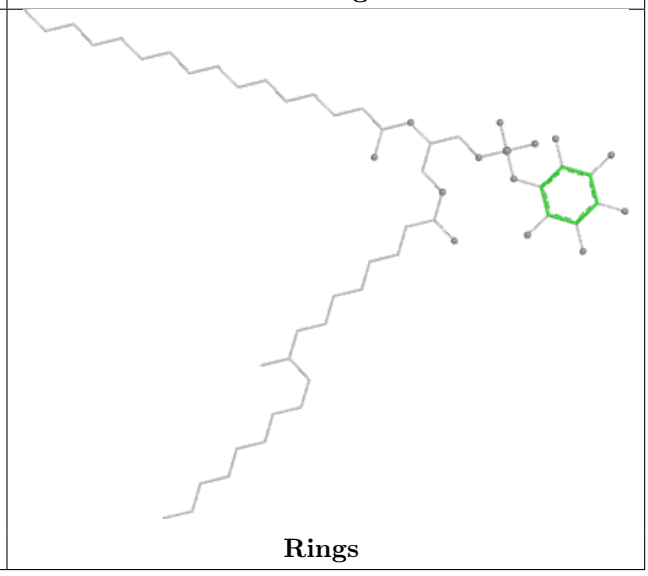
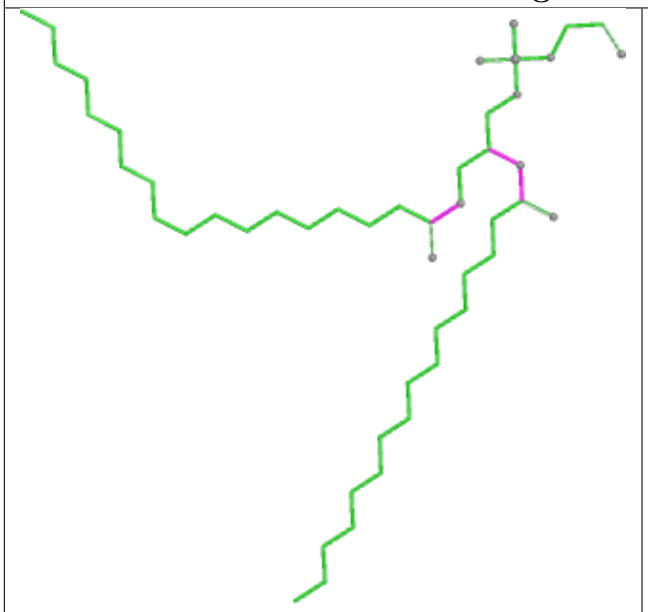


Rings

Ligand 9Y0 F 706



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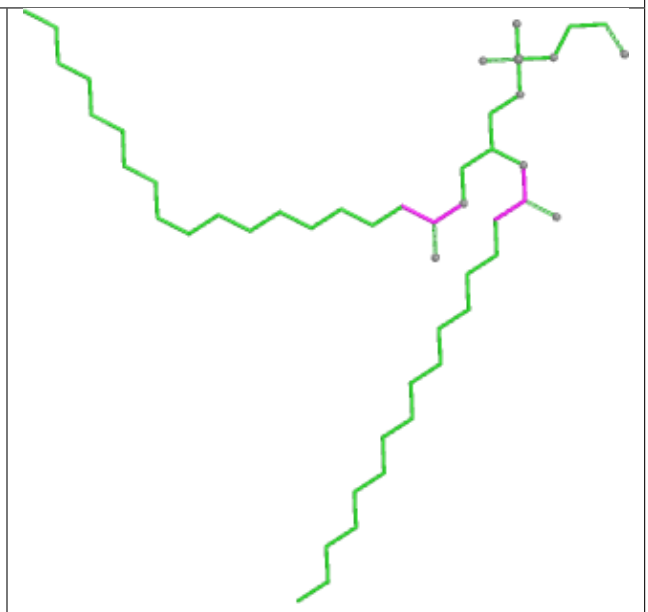
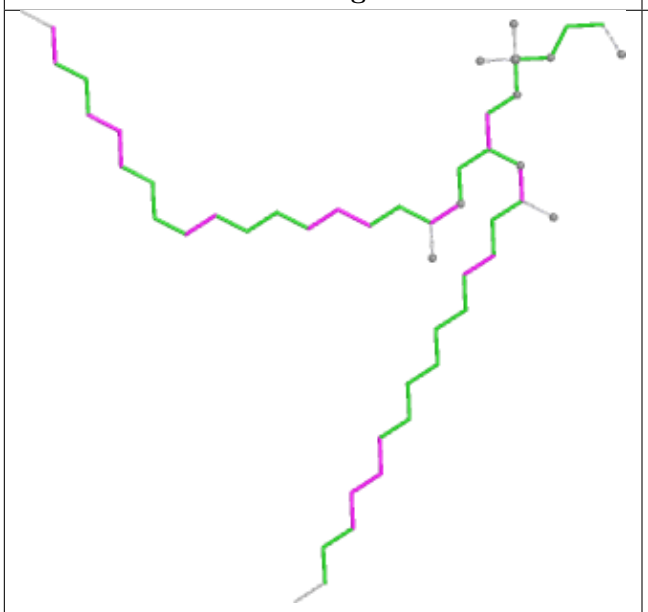


Bond angles



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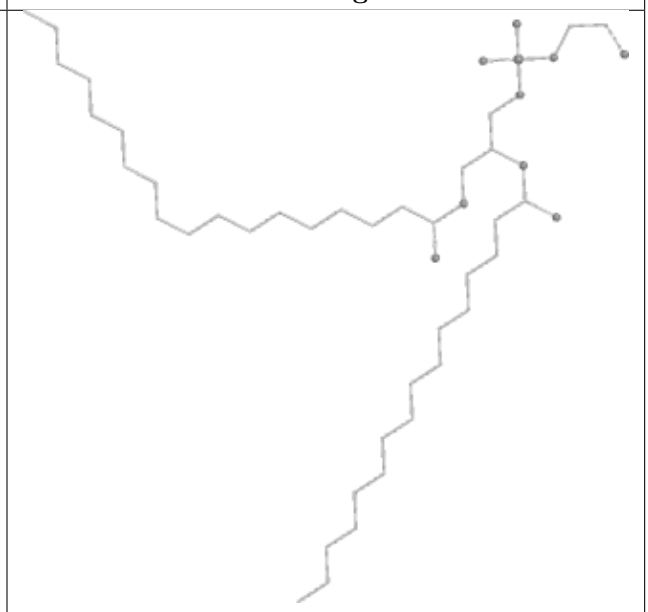
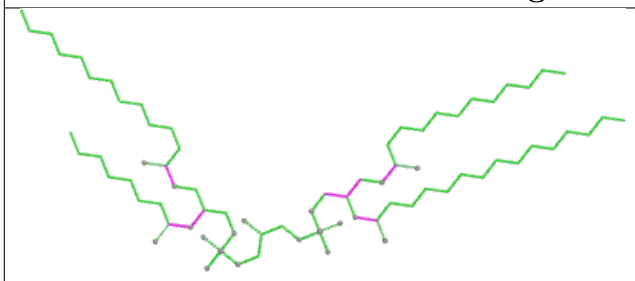


Rings

Ligand CDL S 301



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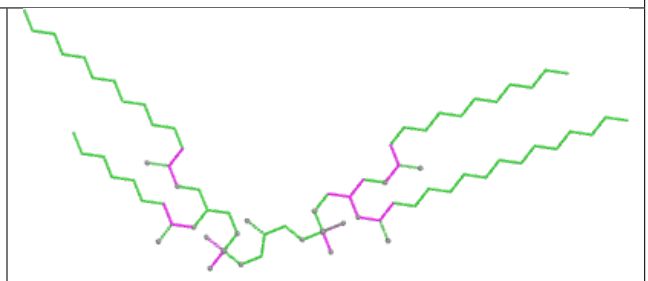
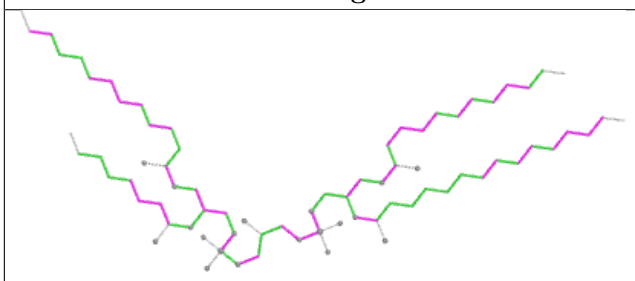
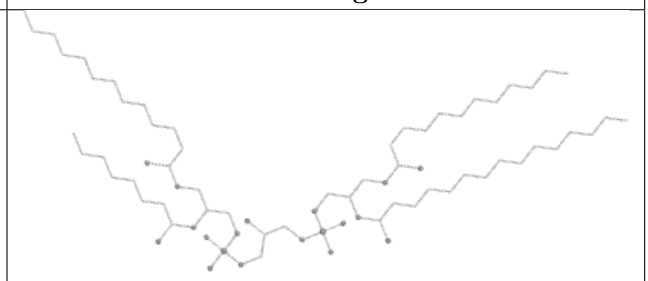


Bond angles

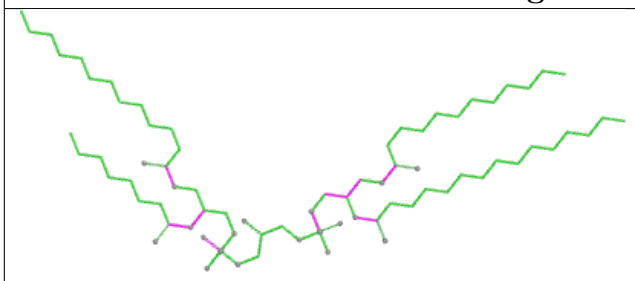


Torsions

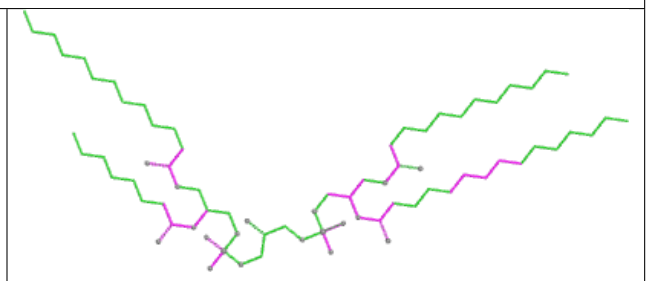


Rings

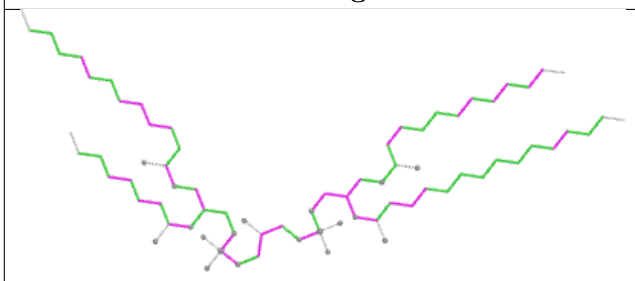
Ligand CDL Z 202



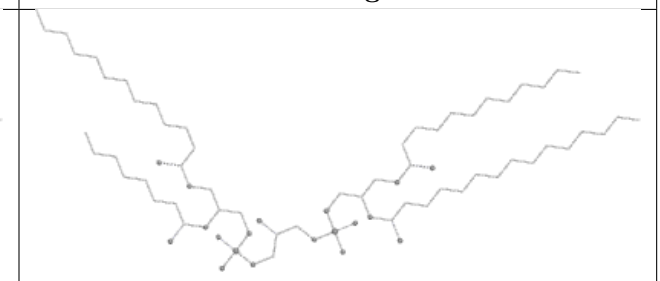
Bond lengths



Bond angles

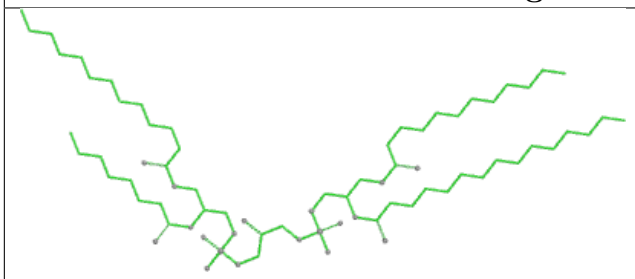


Torsions

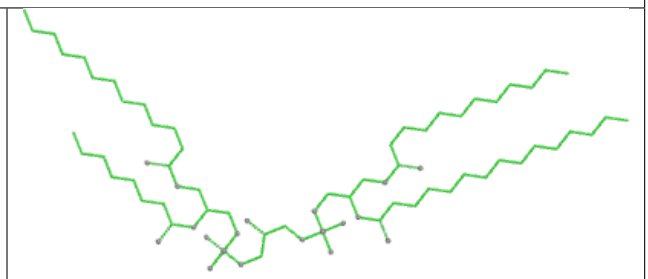


Rings

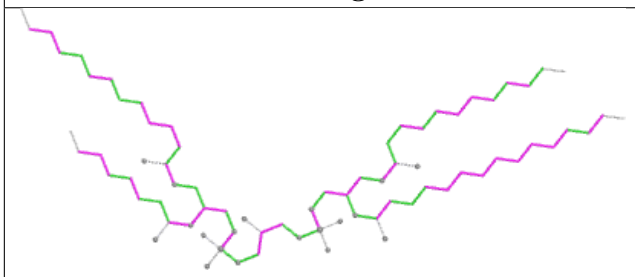
Ligand CDL T 203



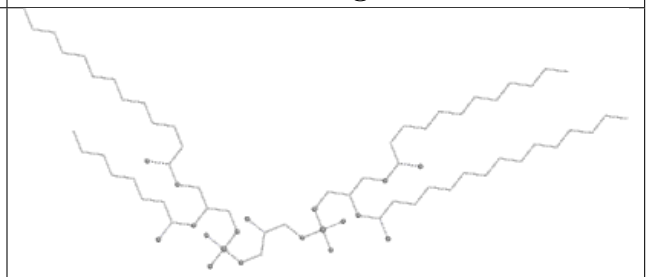
Bond lengths



Bond angles

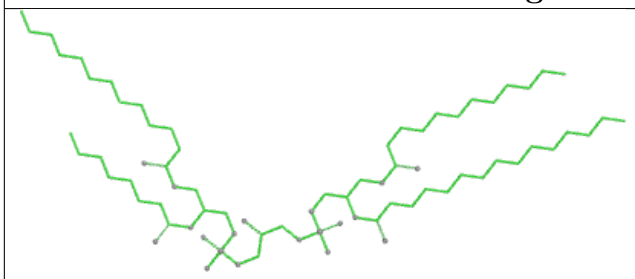


Torsions

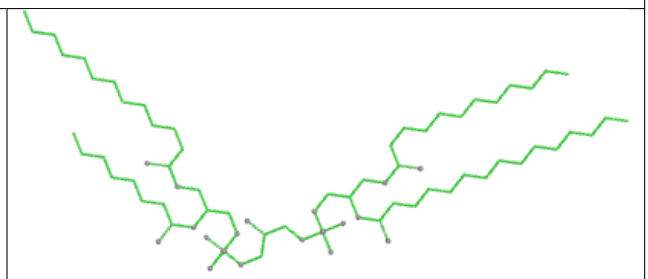


Rings

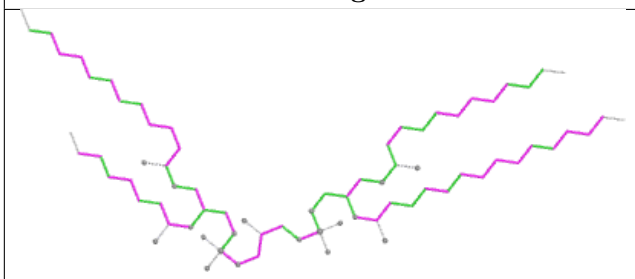
Ligand CDL P 201



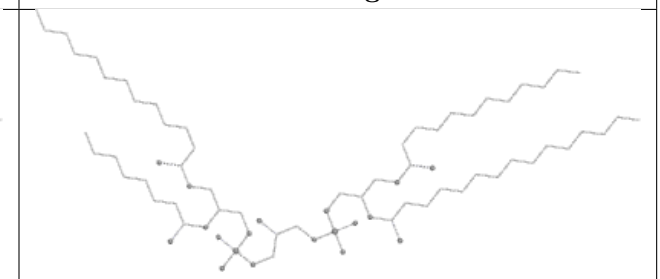
Bond lengths



Bond angles

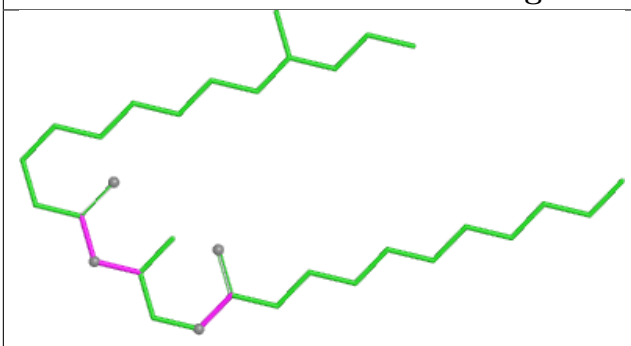


Torsions

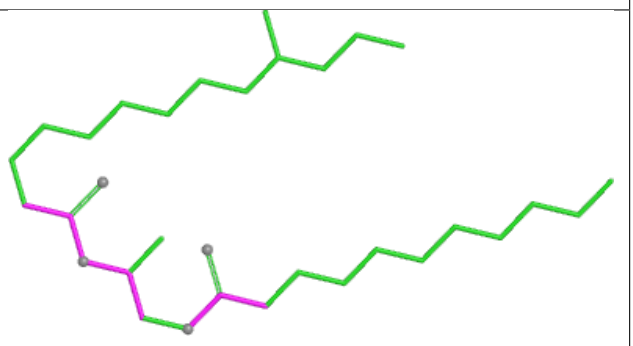


Rings

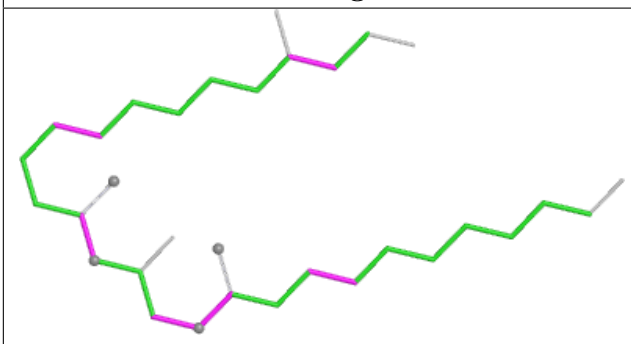
Ligand 9XX D 302



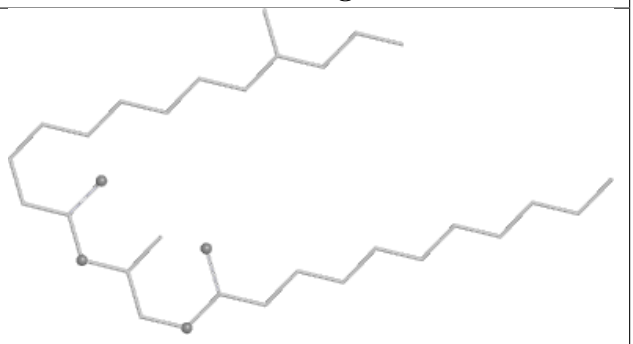
Bond lengths



Bond angles

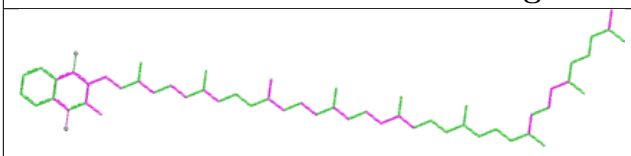


Torsions

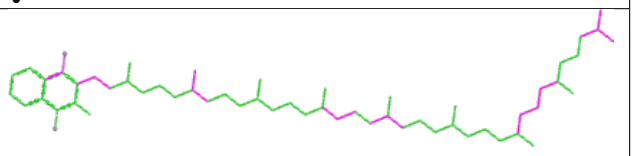


Rings

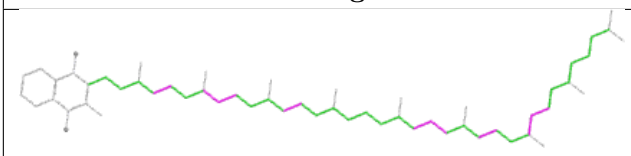
Ligand MQ9 F 708



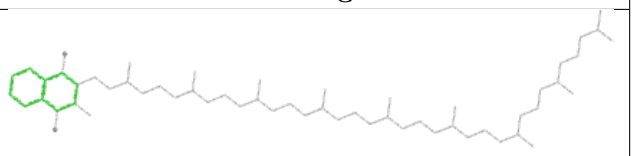
Bond lengths



Bond angles

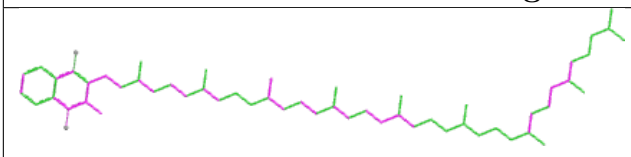


Torsions

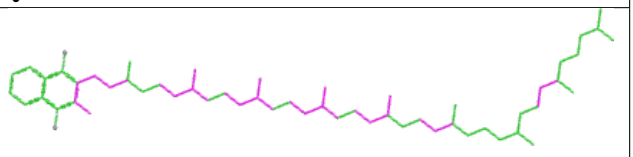


Rings

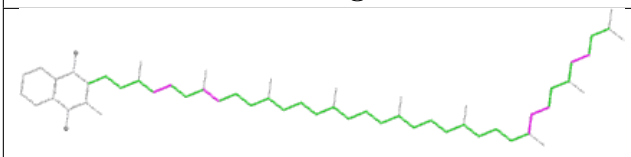
Ligand MQ9 E 603



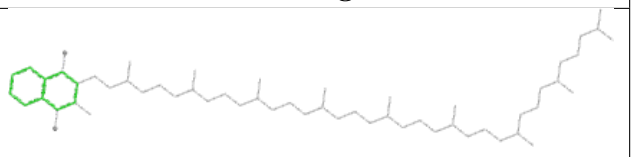
Bond lengths



Bond angles

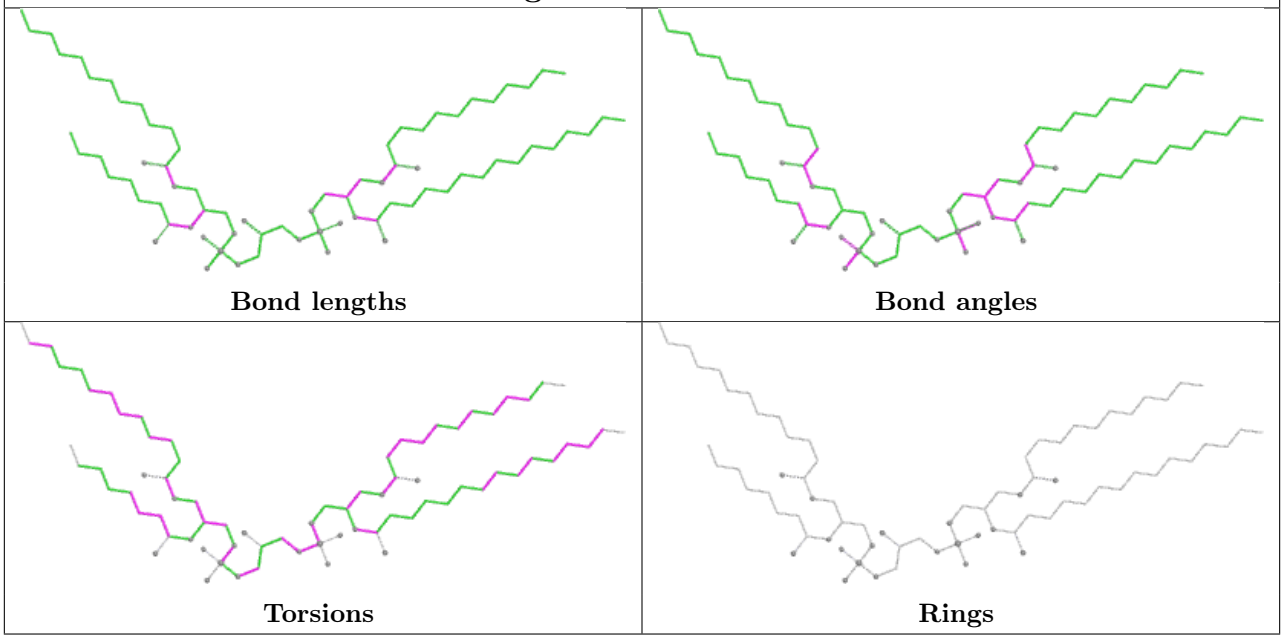


Torsions



Rings

Ligand CDL X 302



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

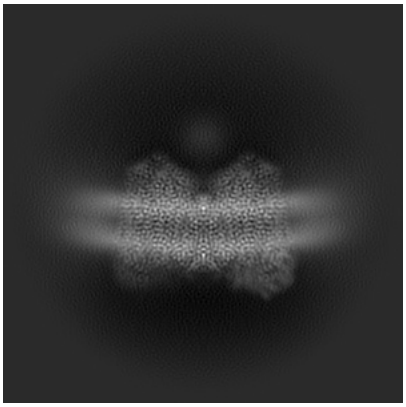
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-46995. These allow visual inspection of the internal detail of the map and identification of artifacts.

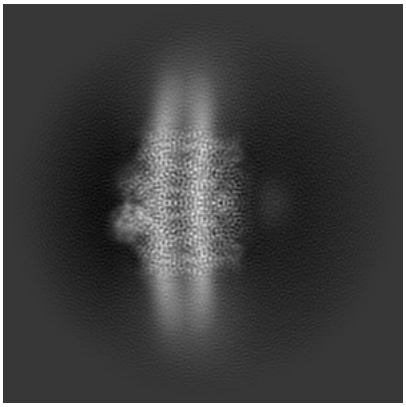
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

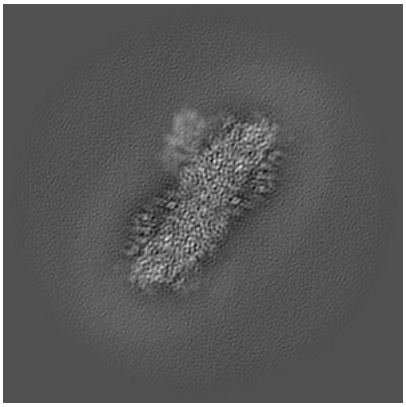
6.1.1 Primary map



X



Y

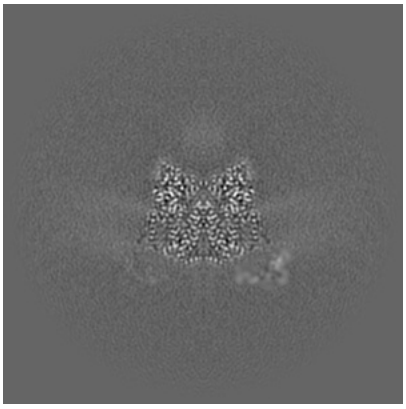


Z

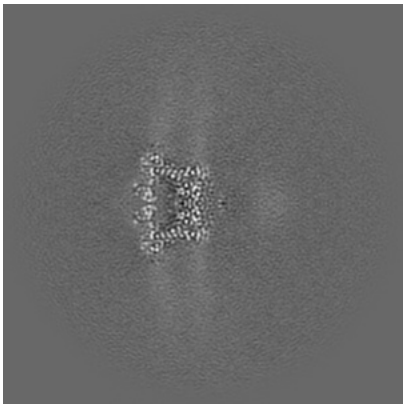
The images above show the map projected in three orthogonal directions.

6.2 Central slices

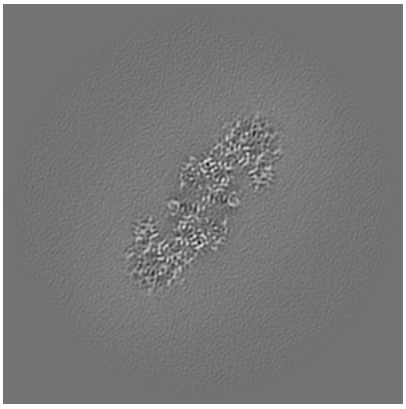
6.2.1 Primary map



X Index: 182



Y Index: 182

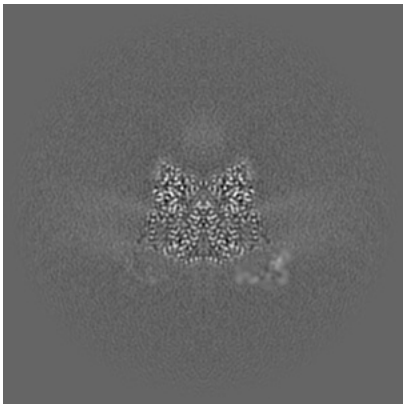


Z Index: 182

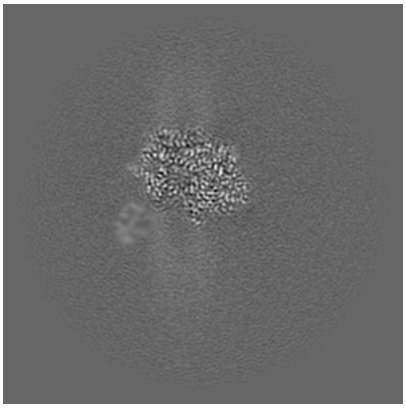
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

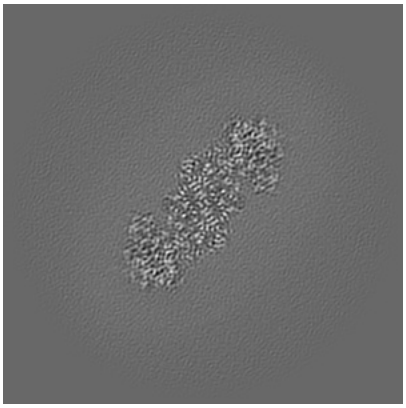
6.3.1 Primary map



X Index: 182



Y Index: 219

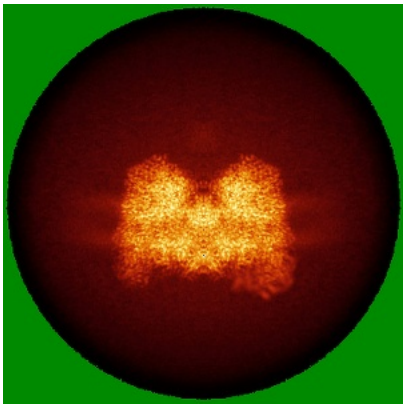


Z Index: 175

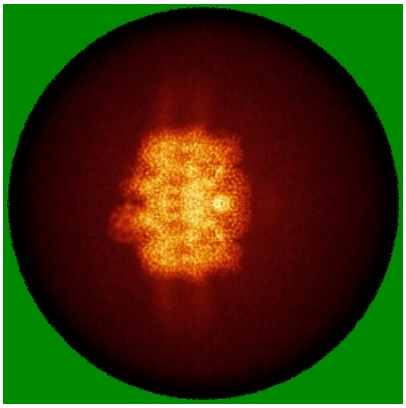
The images above show the largest variance slices of the map in three orthogonal directions.

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

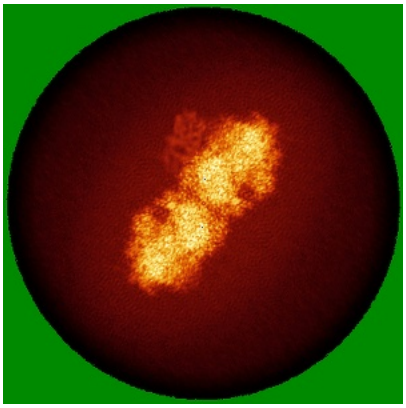
6.4.1 Primary map



X



Y

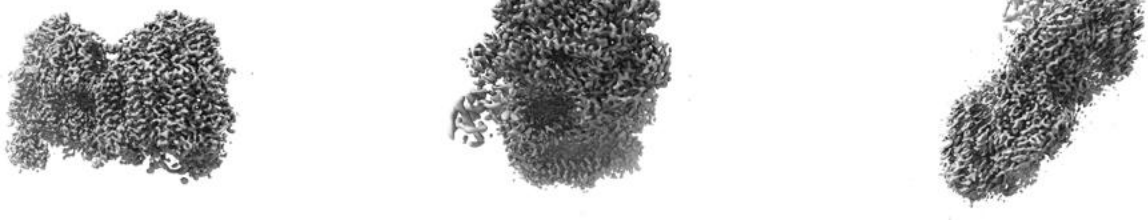


Z

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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.335. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

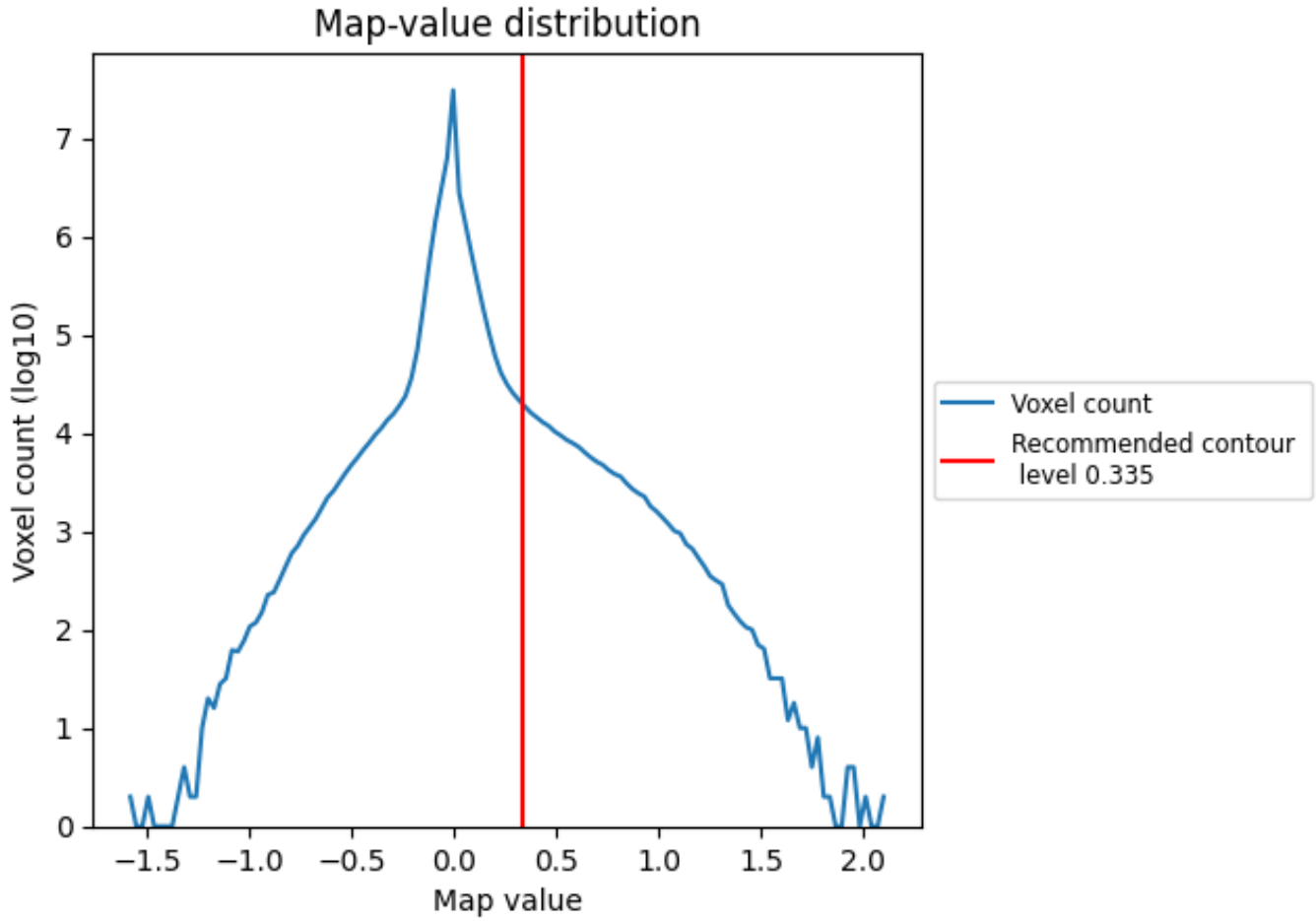
6.6 Mask visualisation (i)

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

7 Map analysis

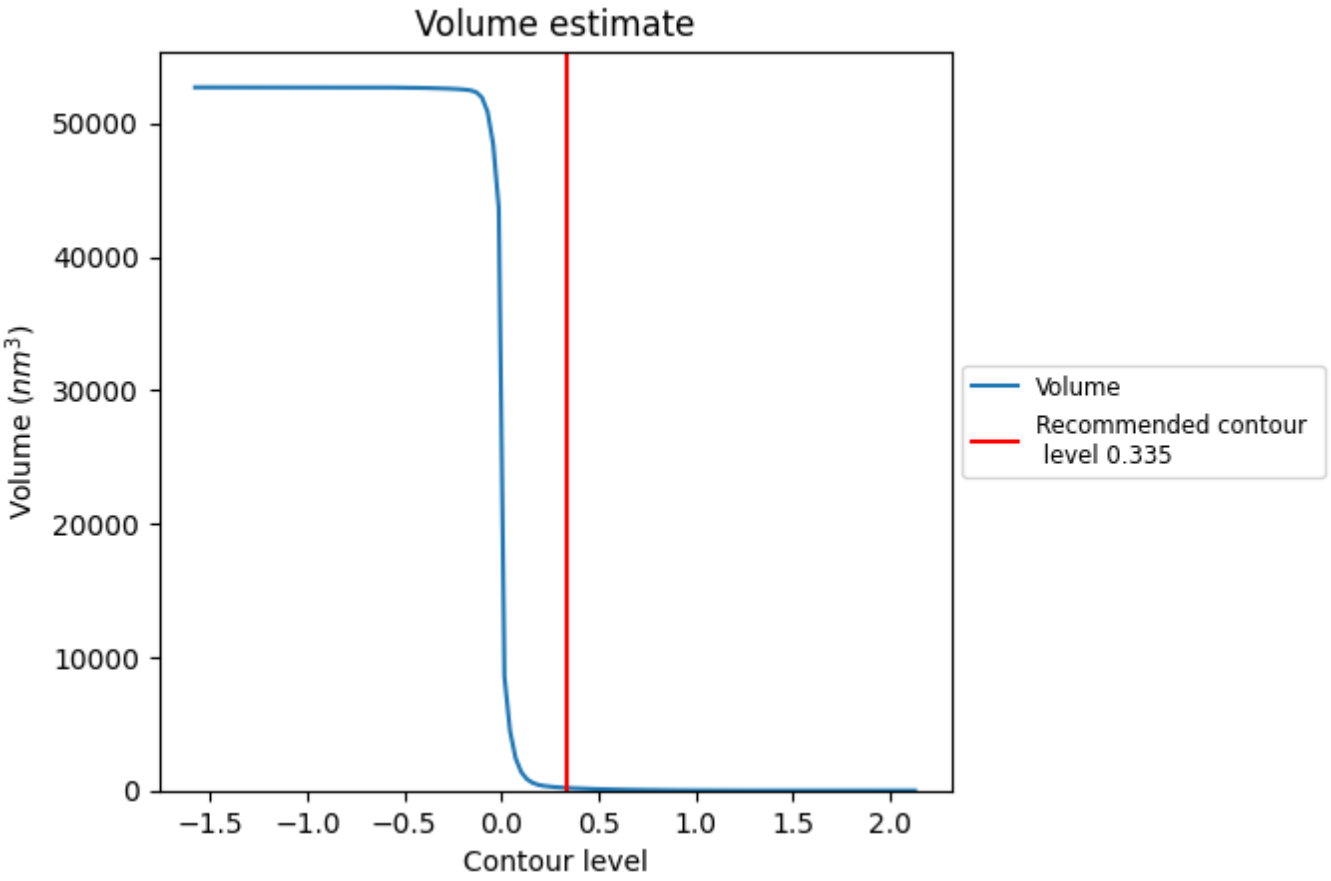
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

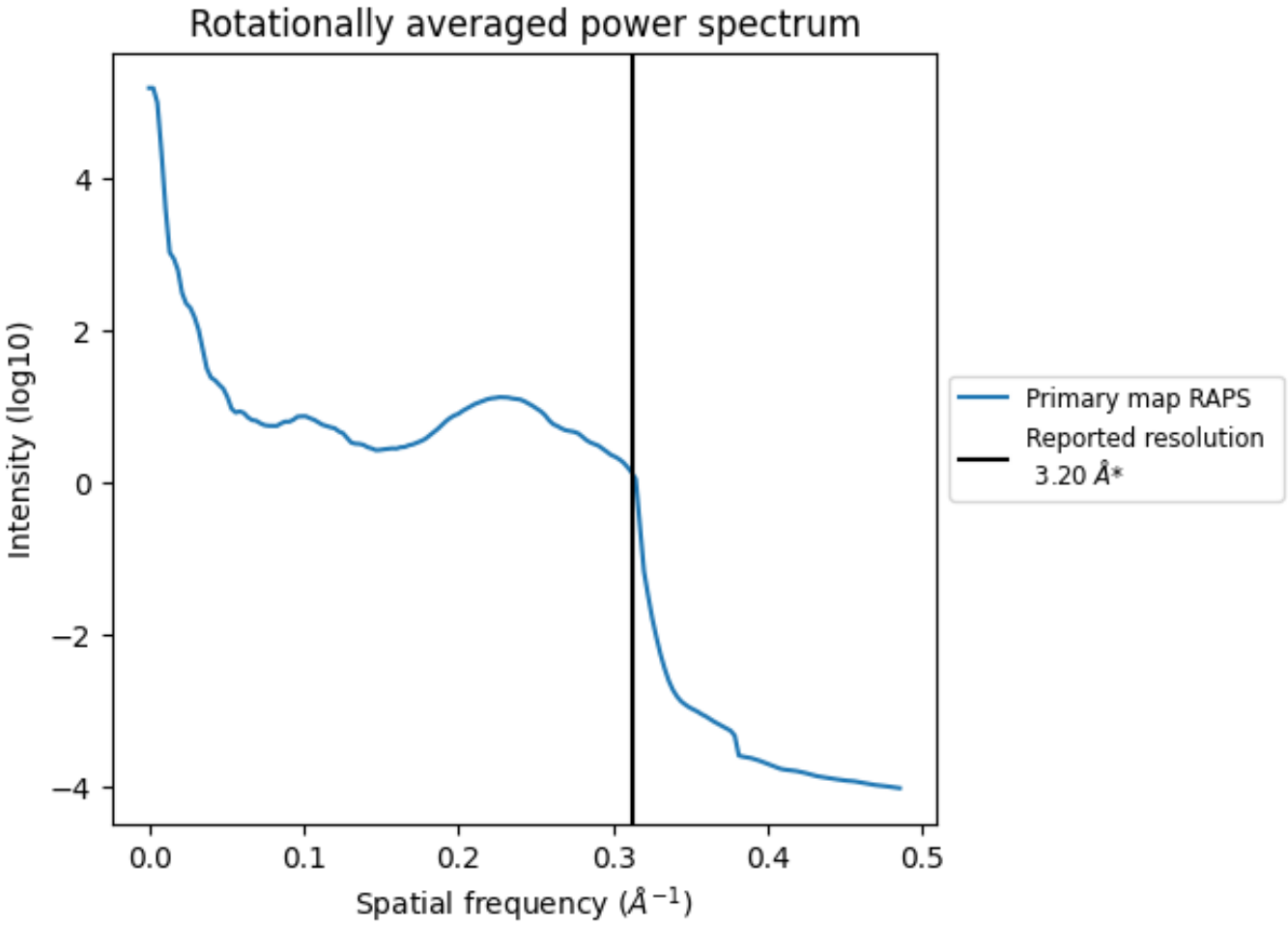
7.2 Volume estimate



The volume at the recommended contour level is 200 nm^3; this corresponds to an approximate mass of 181 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 (i)



*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

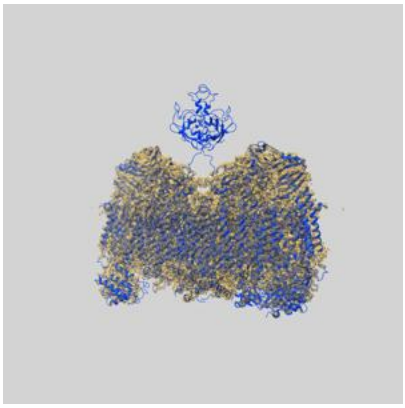
8 Fourier-Shell correlation

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

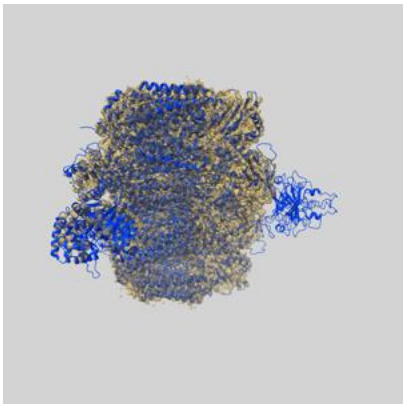
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-46995 and PDB model 9DM1. Per-residue inclusion information can be found in section 3 on page 17.

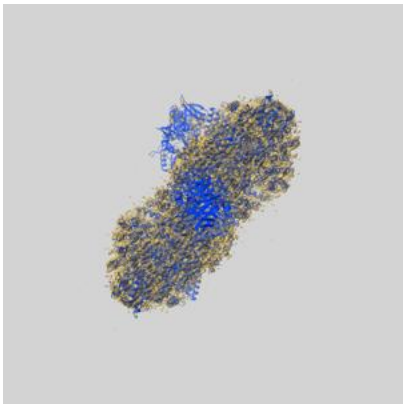
9.1 Map-model overlay



X



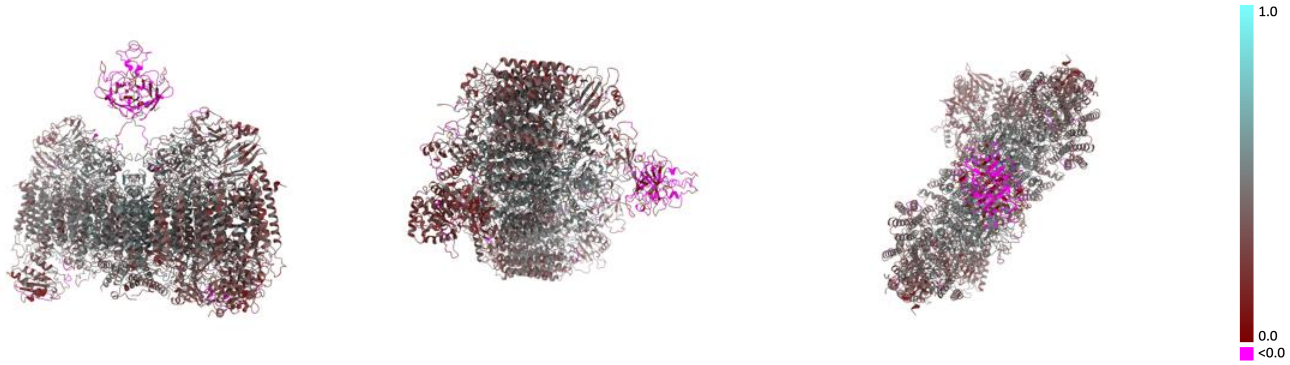
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.335 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.

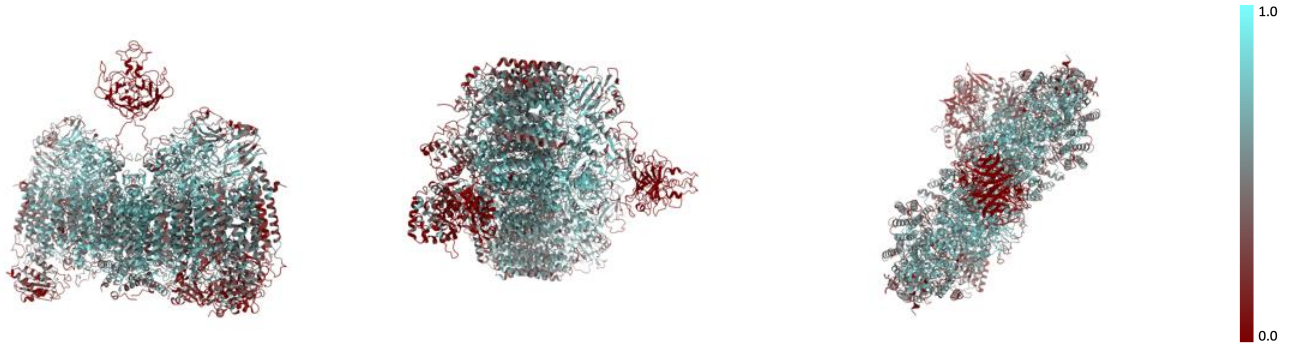
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

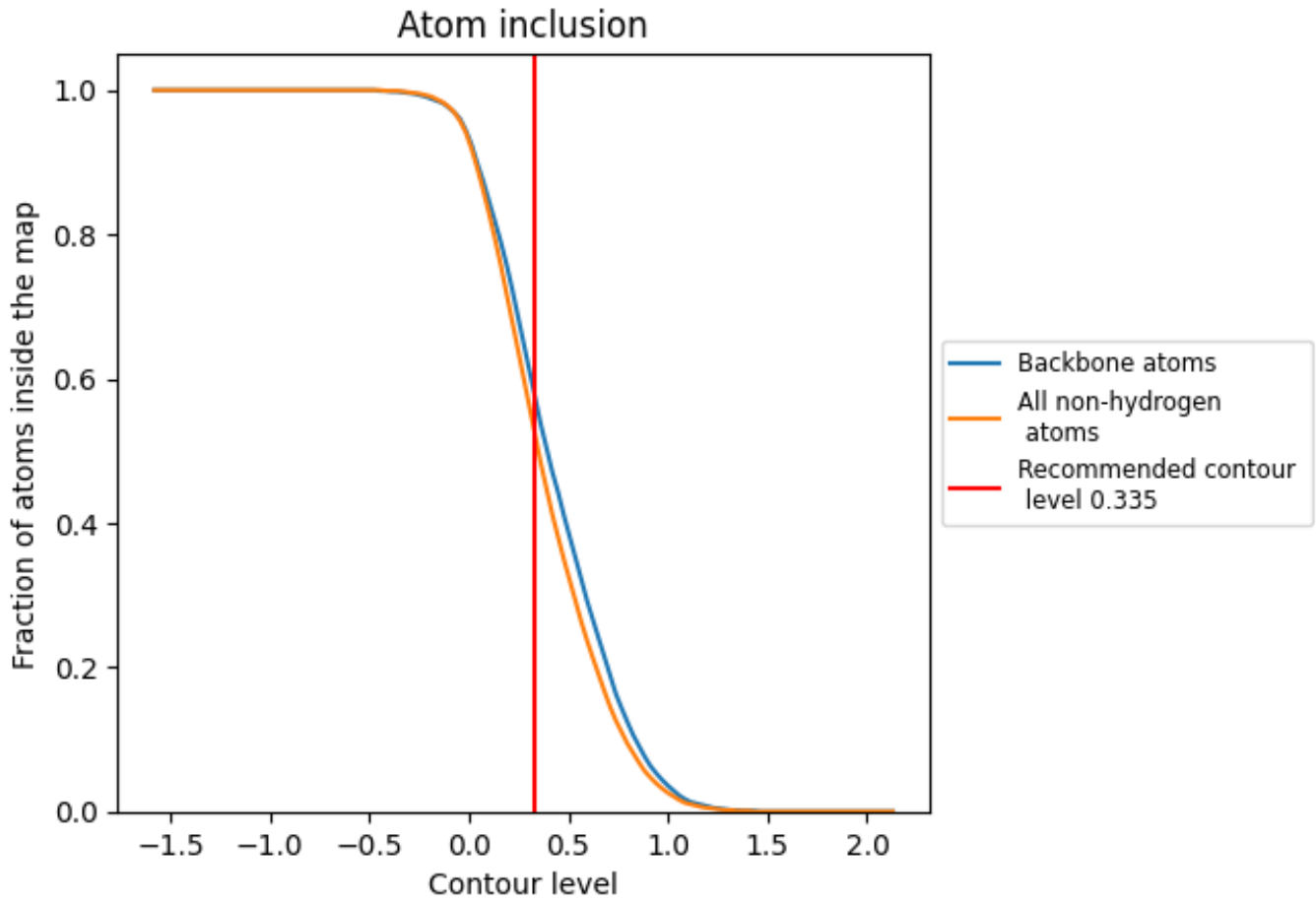
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.335).

9.4 Atom inclusion (i)



At the recommended contour level, 57% of all backbone atoms, 52% 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 (0.335) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5180	0.3800
A	0.1360	0.2590
D	0.0790	0.0750
E	0.6770	0.4710
F	0.6650	0.4700
G	0.0860	0.0680
I	0.6890	0.4580
J	0.5010	0.3780
K	0.4450	0.3360
L	0.6040	0.4050
M	0.6340	0.4430
O	0.6830	0.4550
P	0.5030	0.3780
Q	0.4460	0.3330
R	0.6010	0.4050
S	0.5180	0.3590
T	0.4840	0.3780
U	0.2070	0.2670
V	0.2750	0.2860
W	0.4470	0.3430
X	0.5010	0.3510
Y	0.6330	0.4410
Z	0.4860	0.3760
a	0.2040	0.2620
b	0.2730	0.2940
c	0.4510	0.3510