Full wwPDB EM Validation Report (i)

Aug 5, 2026 – 05:57 AM EDT

PDB ID	:	7RH5 / pdb_00007rh5
EMDB ID	:	EMD-24455
Title	:	Mycobacterial CIII2CIV2 supercomplex, Inhibitor free
Authors	:	Di Trani, J.M.; Yanofsky, D.J.; Rubinstein, J.L.
Deposited on	:	2021-07-16
Resolution	:	3.00 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 (i) 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 (i)) were used in the production of this report:

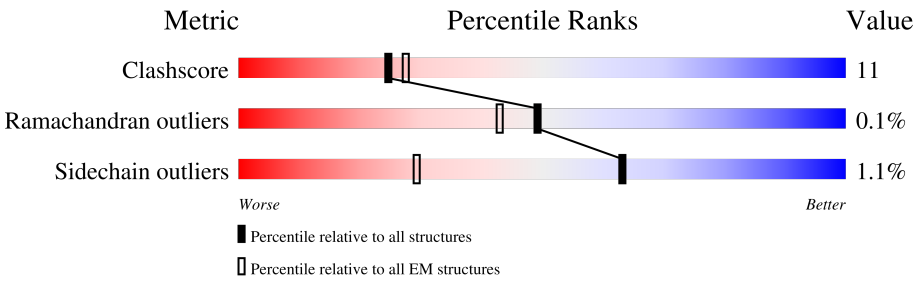
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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)	:	2.50

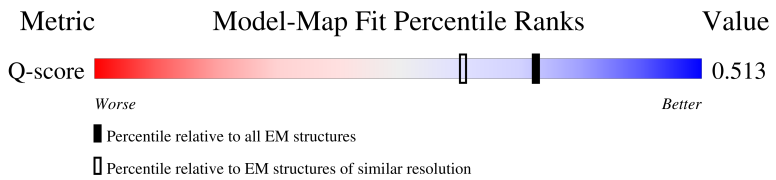
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 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	14081 (2.50 - 3.50)

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	5% 76% 21% •
1	R	566	• 77% 20% • •
2	E	535	5% 81% 18%
2	F	535	• 80% 19%

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Mol	Chain	Length	Quality of chain
3	D	216	91% 97%
3	G	216	91% 99%
4	K	341	31% 76% 15% 9%
4	Q	341	27% 74% 17% 9%
5	S	203	13% 84% 16%
5	X	203	13% 82% 17%
6	T	139	11% 83% 16%
6	Z	139	9% 81% 19%
7	U	79	48% 81% 19%
7	a	79	44% 92% 8%
8	V	145	23% 84% 15%
8	b	145	23% 83% 17%
9	J	100	15% 72% 20% 8%
9	P	100	14% 82% 9% 8%
10	I	223	13% 80% 19%
10	O	223	11% 78% 22%
11	W	159	60% 82% 17%
11	c	159	71% 84% 15%
12	M	382	7% 85% 15%
12	Y	382	6% 84% 16%

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
15	CDL	S	301	-	-	X	-
15	CDL	T	201	-	-	X	-
15	CDL	X	301	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CDL	X	302	-	-	X	-
15	CDL	Z	202	-	-	X	-
15	CDL	Z	203	-	-	X	-
21	HEC	I	302	X	-	-	-
21	HEC	O	302	X	-	-	-

2 Entry composition (i)

There are 23 unique types of molecules in this entry. The entry contains 95903 atoms, of which 46941 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
			Total	C	H	N	O	S		
1	R	552	8716	2937	4346	695	712	26	0	0
1	L	552	8717	2937	4347	695	712	26	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	E	535	8384	2751	4203	711	701	18	0	0
2	F	535	8381	2751	4200	711	701	18	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	D	216	1732	645	640	217	229	1	0	0
3	G	216	1732	645	640	217	229	1	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	Q	312	4857	1592	2392	412	451	10	0	0
4	K	312	4857	1592	2392	412	451	10	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	S	203	3108	1039	1548	253	260	8	0	0
5	X	203	3108	1039	1548	253	260	8	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	T	139	2136	719	1059	167	188	3	0	0
6	Z	139	2135	719	1058	167	188	3	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
7	U	79	1167	381	576	107	101	2	0	0
7	a	79	1167	381	576	107	101	2	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
8	V	145	2093	658	1052	176	205	2	0	0
8	b	145	2093	658	1052	176	205	2	0	0

- Molecule 9 is a protein called Putative conserved transmembrane protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
9	P	92	1453	471	717	136	124	5	0	0
9	J	92	1454	471	718	136	124	5	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
10	O	223	3187	1008	1564	289	314	12	0	0

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Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
10	I	223	3187	1008	1564	289	314	12	0	0

- Molecule 11 is a protein called LpqE protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
11	c	158	2259	708	1110	192	248	1	0	0
11	W	158	2259	708	1110	192	248	1	0	0

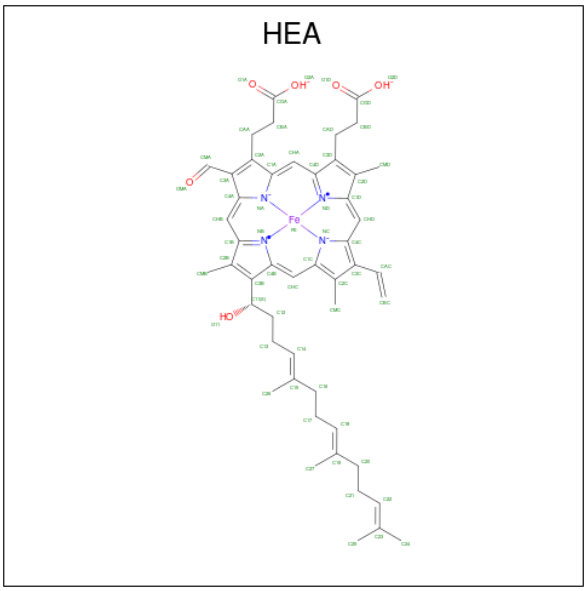
- Molecule 12 is a protein called Cytochrome bc1 complex Rieske iron-sulfur subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
12	Y	382	5961	1924	2984	504	538	11	0	0
12	M	382	5961	1924	2984	504	538	11	0	0

- Molecule 13 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

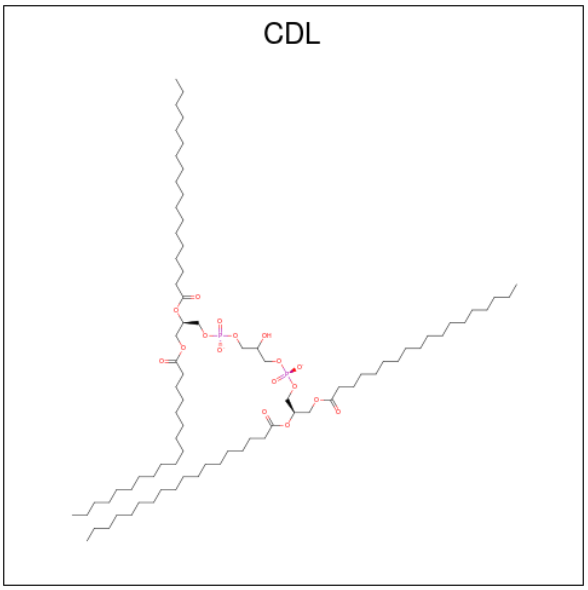
Mol	Chain	Residues	Atoms		AltConf
			Total	Cu	
13	R	1	1	1	0
13	L	1	1	1	0
13	Q	2	2	2	0
13	K	2	2	2	0

- Molecule 14 is HEME-A (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



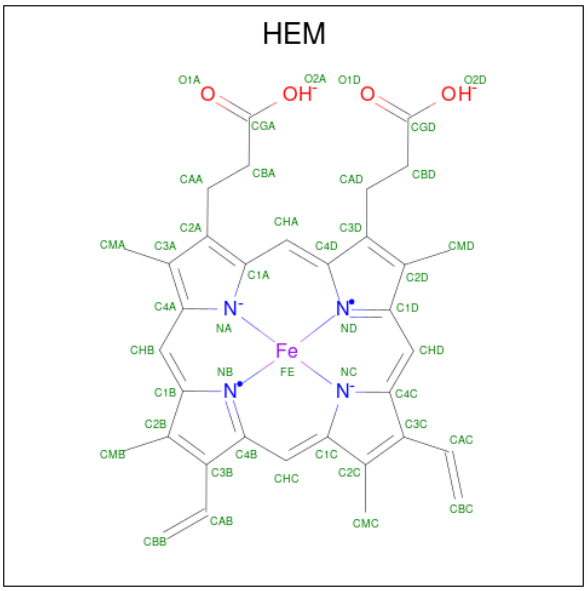
Mol	Chain	Residues	Atoms						AltConf
			Total	C	Fe	H	N	O	
14	R	1	114	49	1	54	4	6	0
			Total	C	Fe	H	N	O	
14	R	1	114	49	1	54	4	6	0
			Total	C	Fe	H	N	O	
14	L	1	114	49	1	54	4	6	0
			Total	C	Fe	H	N	O	
14	L	1	114	49	1	54	4	6	0

- Molecule 15 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



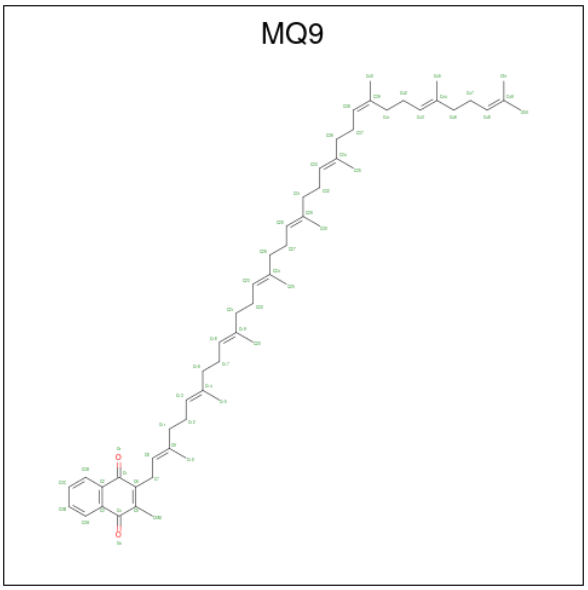
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
15	R	1	76	57	17	2	0
15	E	1	76	57	17	2	0
15	E	1	76	57	17	2	0
15	F	1	76	57	17	2	0
15	F	1	76	57	17	2	0
15	L	1	76	57	17	2	0
15	S	1	76	57	17	2	0
15	T	1	76	57	17	2	0
15	T	1	76	57	17	2	0
15	T	1	76	57	17	2	0
15	P	1	76	57	17	2	0
15	X	1	76	57	17	2	0
15	X	1	76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

- Molecule 16 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



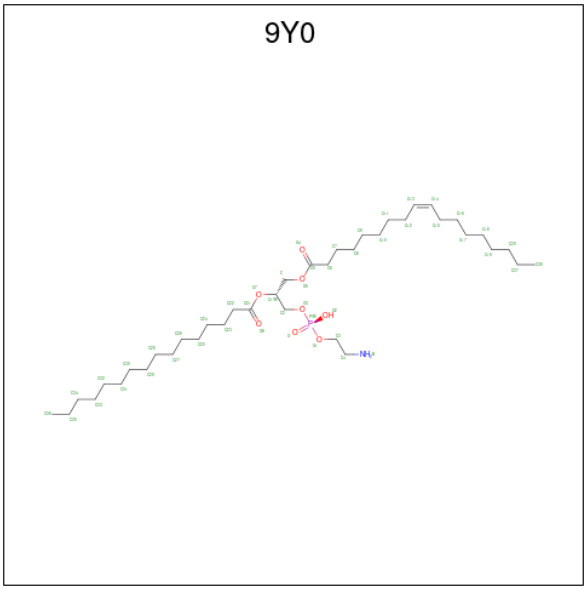
Mol	Chain	Residues	Atoms						AltConf
			Total	C	Fe	H	N	O	
16	E	1	69	33	1	27	4	4	0
			Total	C	Fe	H	N	O	
16	E	1	73	34	1	30	4	4	0
			Total	C	Fe	H	N	O	
16	F	1	69	33	1	27	4	4	0
			Total	C	Fe	H	N	O	
16	F	1	73	34	1	30	4	4	0

- Molecule 17 is MENAQUINONE-9 (CCD ID: MQ9) (formula: $C_{56}H_{80}O_2$).



Mol	Chain	Residues	Atoms				AltConf
17	E	1	Total 138	C 56	H 80	O 2	0
17	E	1	Total 138	C 56	H 80	O 2	0
17	F	1	Total 138	C 56	H 80	O 2	0
17	F	1	Total 138	C 56	H 80	O 2	0
17	F	1	Total 138	C 56	H 80	O 2	0
17	F	1	Total 138	C 56	H 80	O 2	0
17	Z	1	Total 138	C 56	H 80	O 2	0
17	I	1	Total 138	C 56	H 80	O 2	0

- Molecule 18 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
18	F	1	Total 123	C 39	H 74	N 1	O 8	P 1	0
18	S	1	Total 124	C 39	H 75	N 1	O 8	P 1	0
18	P	1	Total 124	C 39	H 75	N 1	O 8	P 1	0

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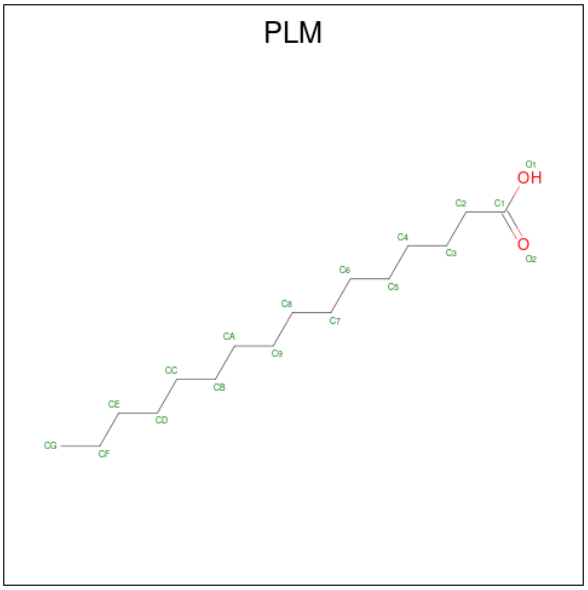
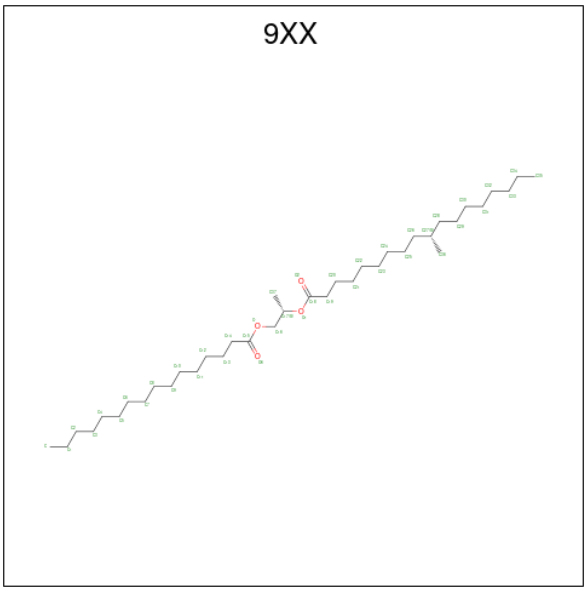
Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
18	X	1	124	39	75	1	8	1	0
18	J	1	124	39	75	1	8	1	0
18	J	1	124	39	75	1	8	1	0

- Molecule 19 is PALMITIC ACID (CCD ID: PLM) (formula: $C_{16}H_{32}O_2$).



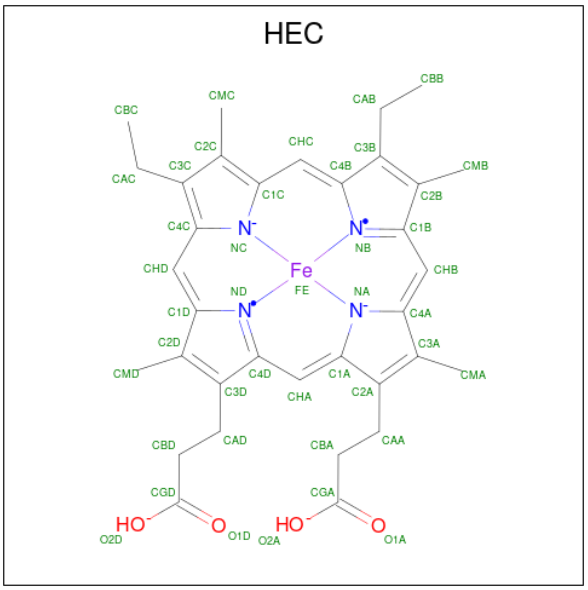
Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
19	D	1	27	10	16	1	0
19	G	1	27	10	16	1	0
19	c	1	48	16	31	1	0
19	W	1	48	16	31	1	0

- Molecule 20 is (2S)-1-(hexadecanoyloxy)propan-2-yl (10S)-10-methyloctadecanoate (CCD ID: 9XX) (formula: $C_{38}H_{74}O_4$).



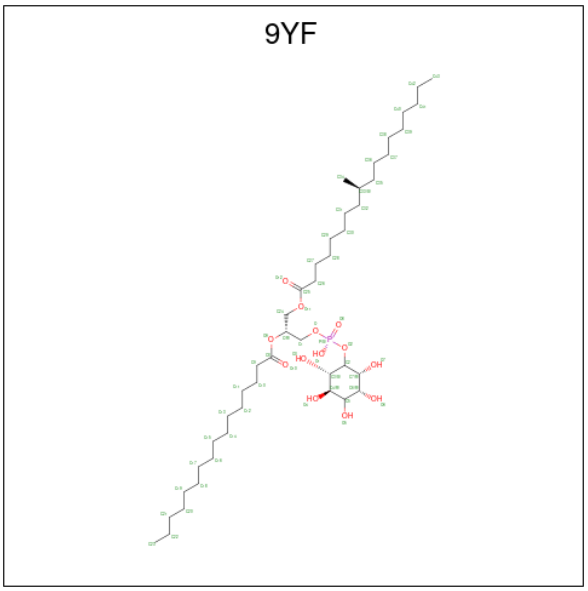
Mol	Chain	Residues	Atoms				AltConf
20	D	1	Total	C	H	O	0
			83	28	51	4	
20	G	1	Total	C	H	O	0
			83	28	51	4	
20	c	1	Total	C	H	O	0
			115	38	73	4	
20	W	1	Total	C	H	O	0
			115	38	73	4	

- Molecule 21 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	Fe	H	N	O	
21	O	1	75	34	1	32	4	4	0
			Total	C	Fe	H	N	O	
21	O	1	75	34	1	32	4	4	0
			Total	C	Fe	H	N	O	
21	I	1	75	34	1	32	4	4	0
			Total	C	Fe	H	N	O	
21	I	1	75	34	1	32	4	4	0

- Molecule 22 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
			Total	C	H	O	P	
22	O	1	142	44	84	13	1	0
			Total	C	H	O	P	
22	c	1	142	44	84	13	1	0
			Total	C	H	O	P	
22	I	1	142	44	84	13	1	0
			Total	C	H	O	P	
22	Y	1	142	44	84	13	1	0
			Total	C	H	O	P	
22	Y	1	142	44	84	13	1	0
			Total	C	H	O	P	
22	W	1	142	44	84	13	1	0
			Total	C	H	O	P	
22	M	1	142	44	84	13	1	0

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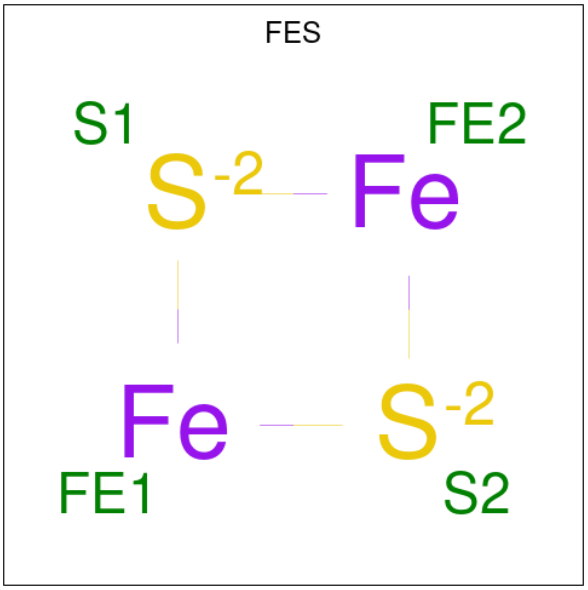
Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	O	P	
22	M	1	142	44	84	13	1	0

- Molecule 23 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



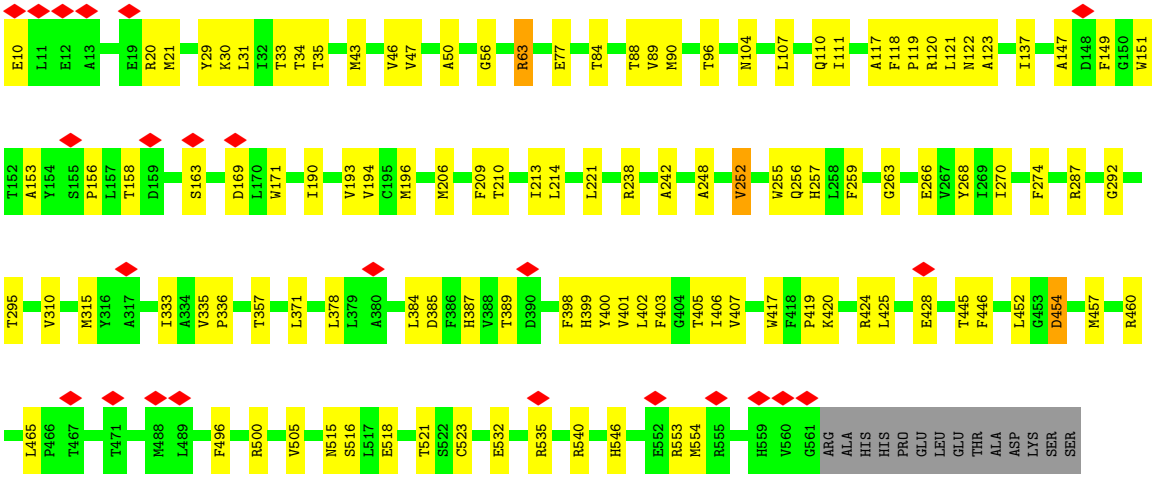
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
23	Y	1	4	2	2	0
23	M	1	4	2	2	0

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.

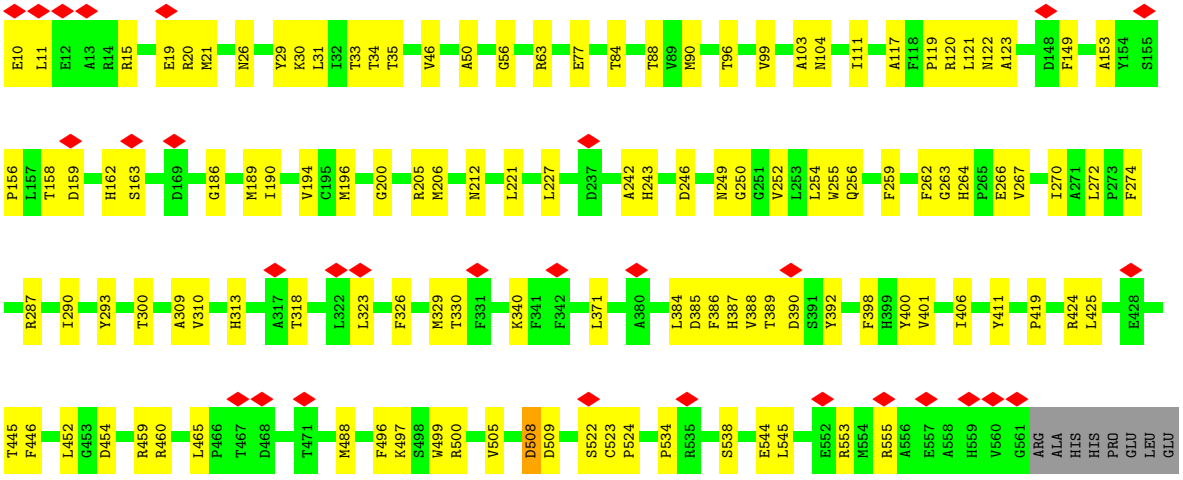
• Molecule 1: Cytochrome c oxidase subunit 1

Chain R:



• Molecule 1: Cytochrome c oxidase subunit 1

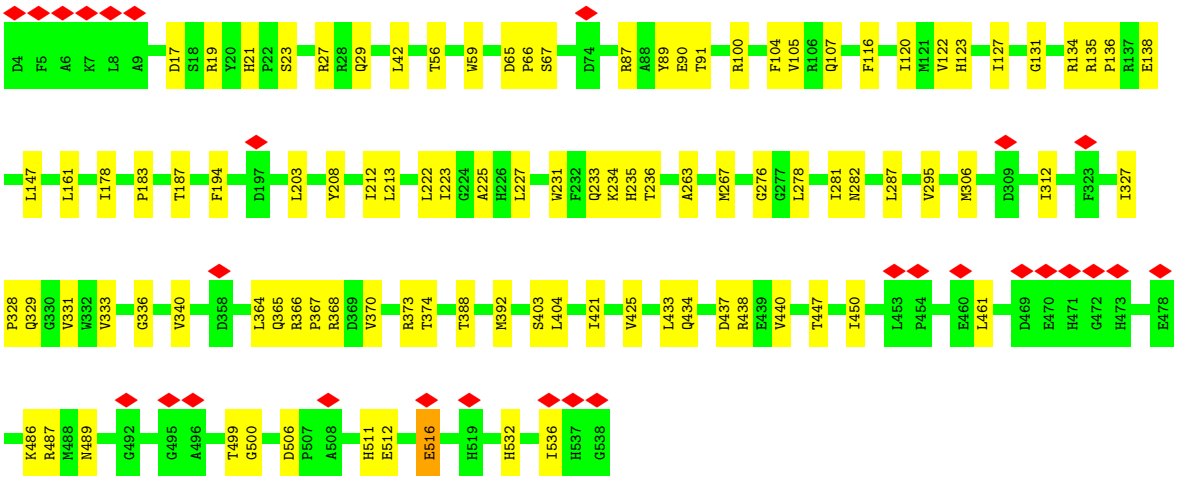
Chain L:



THR
ALA
ASP
LYS
SER
SER

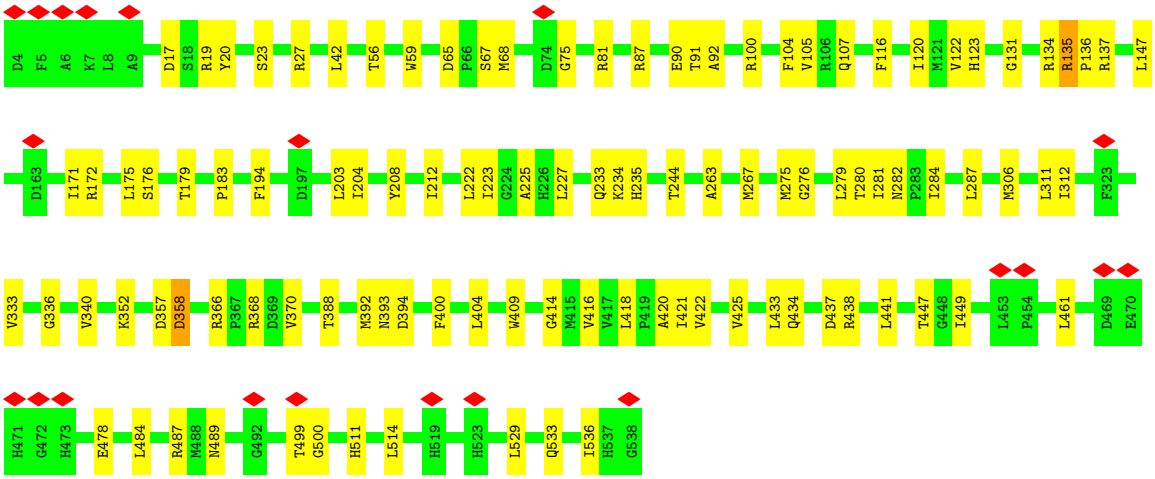
- Molecule 2: Cytochrome bc1 complex cytochrome b subunit

Chain E:



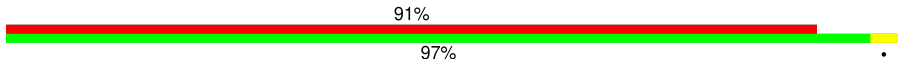
- Molecule 2: Cytochrome bc1 complex cytochrome b subunit

Chain F:



- Molecule 3: Superoxide dismutase [Cu-Zn]

Chain D:



S156 S157 L158 Q159 V160 R161 A162 D163 G164 S165 G166 K167 L168 V169 T170 T171 T172 D173 A174 F175 T176 A177 E178 D179 L180 L181 D182 G183 A184 K185 T186 A187 I188 I189 I190 H191 E192 K193 A194 D195 N196 F197 A198 N199 I200 P201 P202 E203 R204 Y205 Q206 Q207 V208 N209 G210 A211 P212 G213 P214 D215

Q216 T217 T218 M219 A220 T221 G222 D223 A224 G225 S226 R227 V228 A229 C230 G231 V232 I233 S234 A235 G236

• Molecule 3: Superoxide dismutase [Cu-Zn]

Chain G: 91% 99%

C21 S29 S30 E31 P32 P43 S44 P45 A46 A47 P48 S49 G50 E51 D52 H53 G54 G55 G56 H57 G58 A59 G60 A61 A62 G63 A64 G65 E66 T67 L68 T69 A70 E71 L72 K73 T74 A75 D76 G77 T78 S79 V80 A81 T82 A83 D84 F85 Q86 F87 A88 D89 G90 F91 A92 T93 V94 T95

I96 E97 T98 T99 T100 P101 G102 R103 L104 T105 P106 G107 F108 H109 G110 V111 H112 I113 H114 S115 V116 G117 K118 C119 E120 A121 N122 S123 V124 A125 P126 T127 G128 G129 A130 P131 G132 D133 F134 N135 S136 A137 G138 G139 H140 F141 Q142 V143 S144 G145 H146 S147 G148 H149 P150 A151 S152 G153 D154 L155

S156 S157 L158 Q159 V160 R161 A162 D163 G164 S165 G166 K167 L168 V169 T170 T171 T172 D173 A174 F175 T176 A177 E178 D179 L180 L181 D182 G183 A184 K185 T186 A187 I188 I189 I190 H191 E192 K193 A194 D195 N196 F197 A198 N199 I200 P201 P202 E203 R204 Y205 Q206 Q207 V208 N209 G210 A211 P212 G213 P214 D215

Q216 T217 T218 M219 A220 T221 G222 D223 A224 G225 S226 R227 V228 A229 C230 G231 V232 I233 S234 A235 G236

• Molecule 4: Cytochrome aa3 subunit 2

Chain Q: 27% 74% 17% 9%

MET THR PRO ARG GLY PHE ARG VAL VAL ALA LEU SER ILE VAL LEU GLY GLY SER ALA LEU LEU LEU SER GLY CYS SER W27 S28 D29 A30 L31 A32 W35 T40 P41 E42 A43 K44 L45 E48 L49 W50 I55 F58 I63 F69 R76 K77 K78 A79 T80 D81

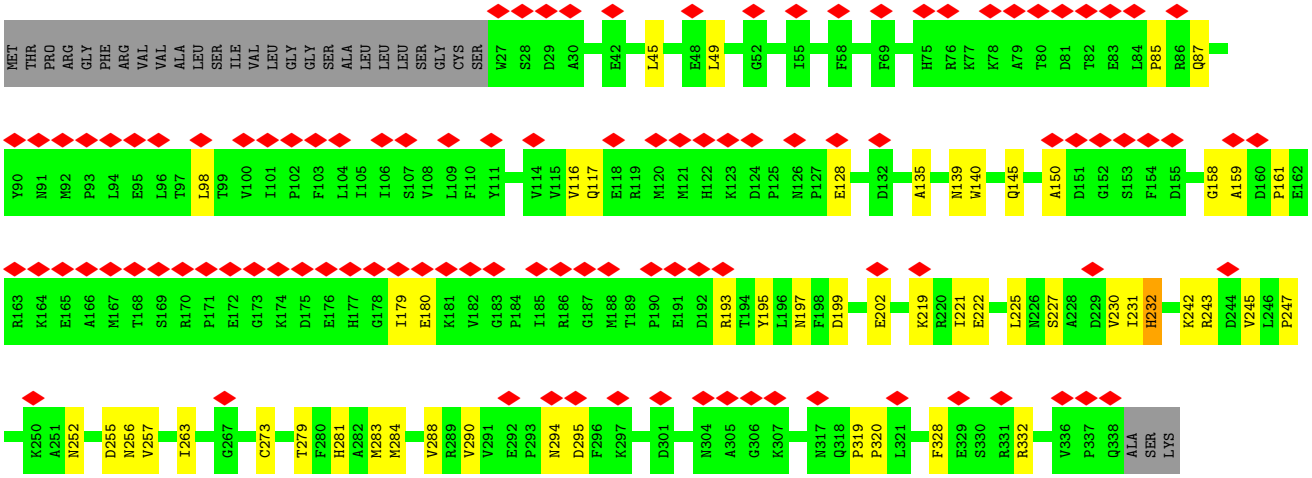
T32 E83 L84 P85 R86 Q87 Y90 N91 M92 P93 L94 E95 L96 T97 L98 T99 V100 I101 P102 F103 L104 I105 I106 S107 V108 L109 F110 Y111 V116 Q117 E118 R119 M120 M121 H122 K123 D124 P125 N126 P127 E128 D132 A135 N139 W140 K146 A150 D151 G152 D155 D160

P161 E162 R163 K164 E165 A166 M167 T168 S169 R170 P171 E172 G173 K174 D175 E176 H177 G178 I179 E180 K181 V182 G183 P184 I185 R186 G187 M188 T189 P190 E191 D192 R193 T194 Y195 E202 T203 L204 G205 E209 R220 T221 E222 L225 D229 V230 I231 H232 V236 F239 K242 R243

D244 V245 L246 P247 N252 D255 N256 V257 I263 Q264 E275 T279 F280 H281 M284 V288 R289 V290 N294 D295 F296 K297 D301 A305 G306 K307 A310 N317 E326 R331 R332 V336 P337 Q338 ALA SER LYS

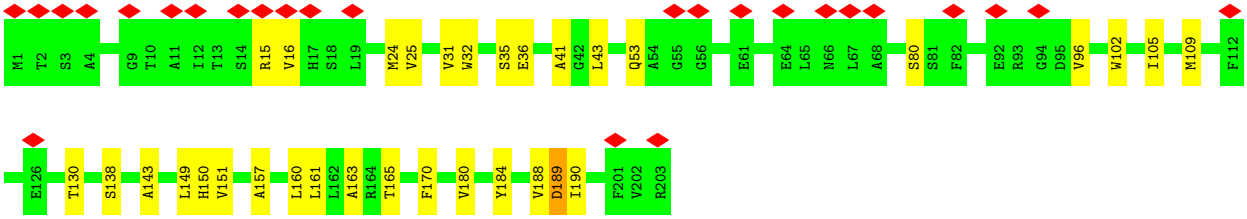
• Molecule 4: Cytochrome aa3 subunit 2

Chain K: 31% 76% 15% 9%



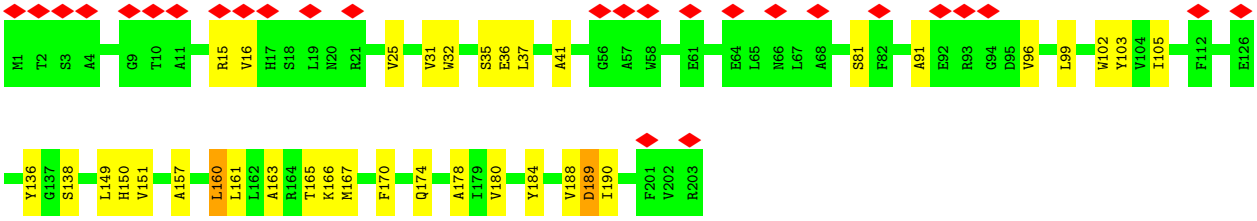
- Molecule 5: Cytochrome aa3 subunit 3

Chain S:



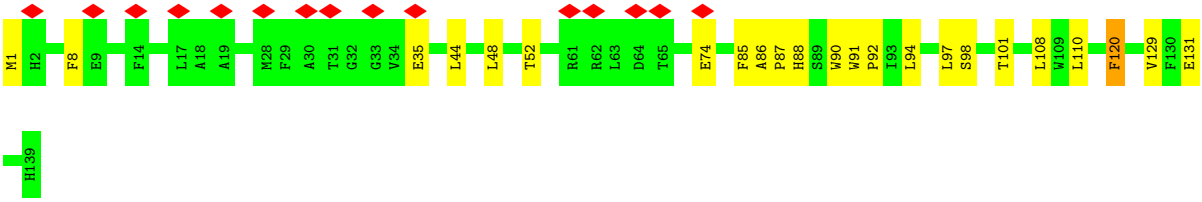
- Molecule 5: Cytochrome aa3 subunit 3

Chain X:



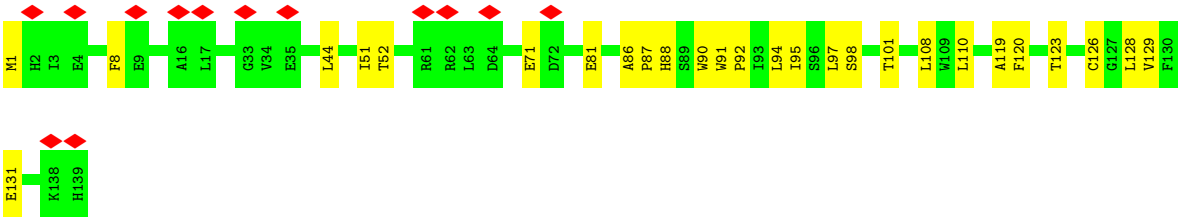
- Molecule 6: Cytochrome c oxidase polypeptide 4

Chain T:



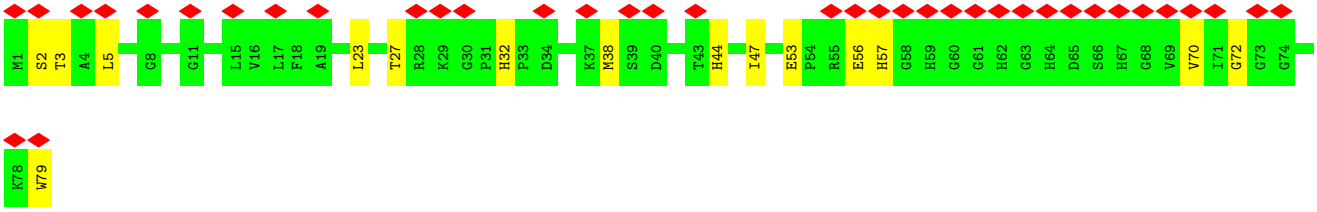
- Molecule 6: Cytochrome c oxidase polypeptide 4

Chain Z:



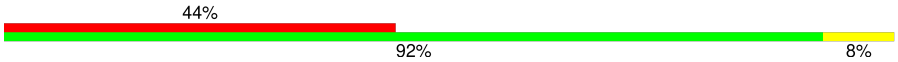
- Molecule 7: Cytochrome c oxidase subunit CtaJ

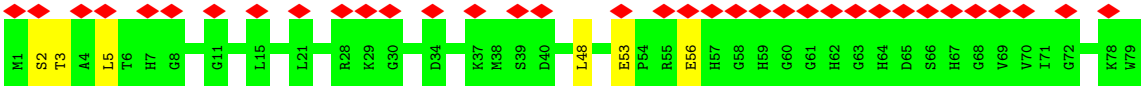
Chain U:



- Molecule 7: Cytochrome c oxidase subunit CtaJ

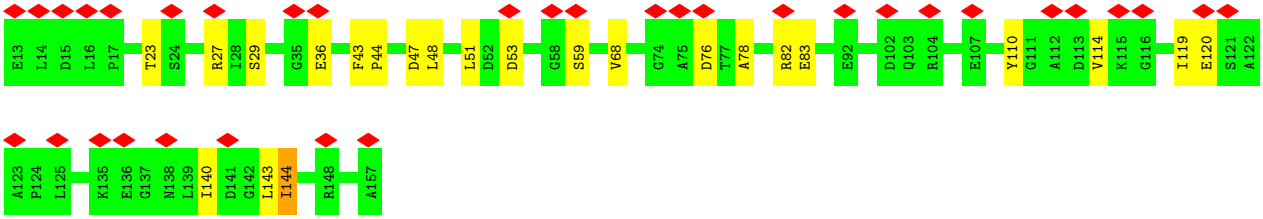
Chain a:





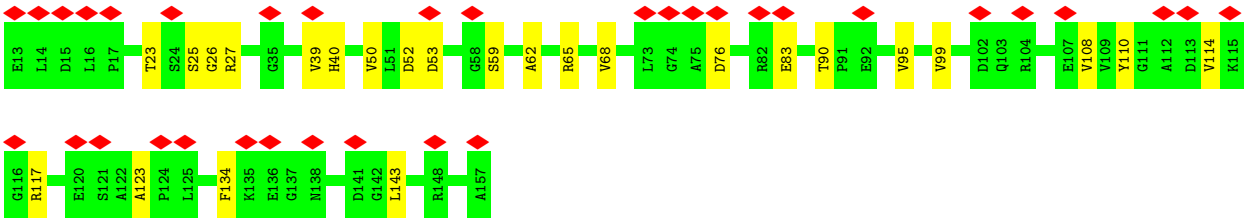
- Molecule 8: Uncharacterized protein MSMEG_4692/MSMEI_4575

Chain V:



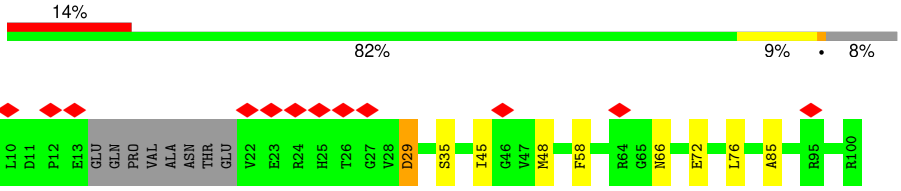
- Molecule 8: Uncharacterized protein MSMEG_4692/MSMEI_4575

Chain b:



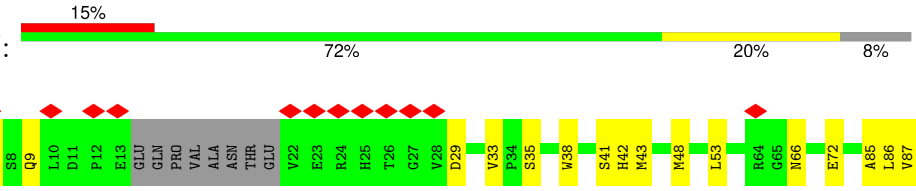
- Molecule 9: Putative conserved transmembrane protein

Chain P:



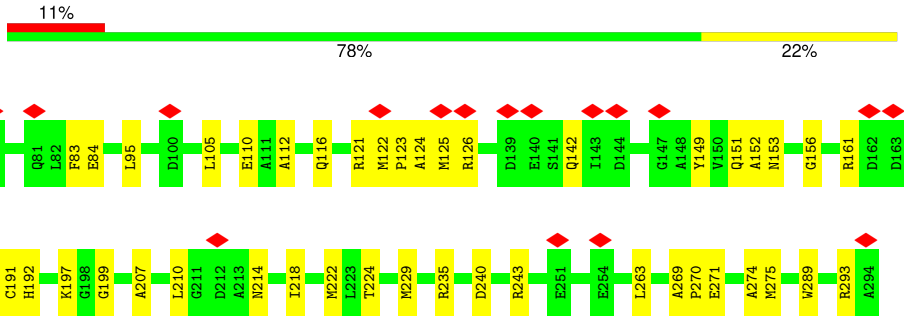
- Molecule 9: Putative conserved transmembrane protein

Chain J:



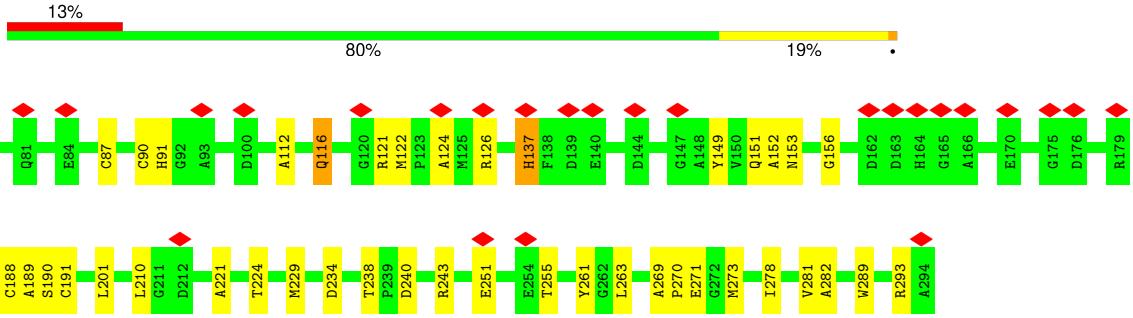
- Molecule 10: Cytochrome bc1 complex cytochrome c subunit

Chain O:



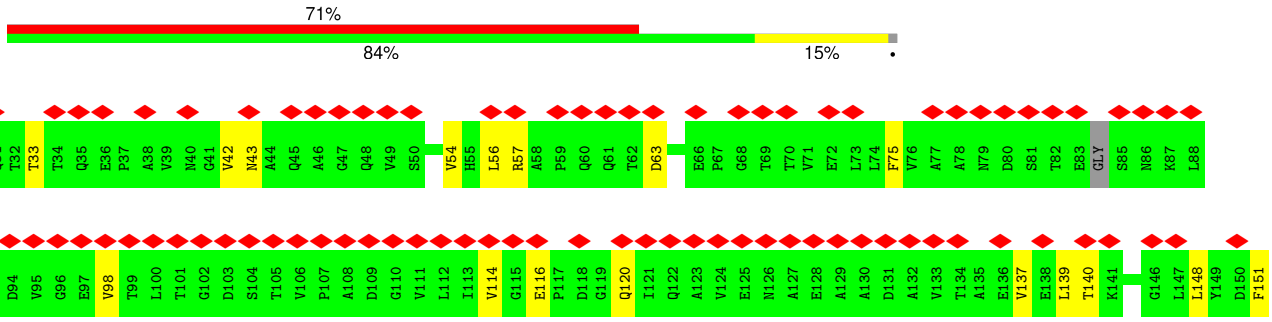
- Molecule 10: Cytochrome bc1 complex cytochrome c subunit

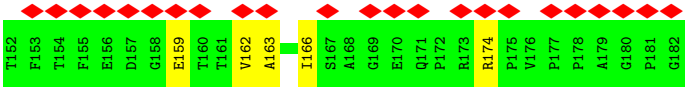
Chain I:



- Molecule 11: LpqE protein

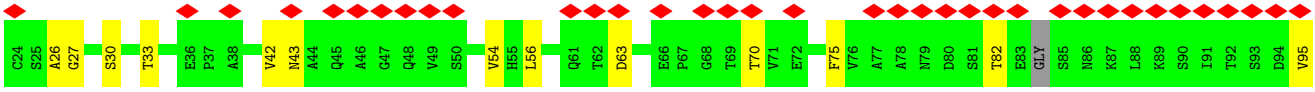
Chain c:

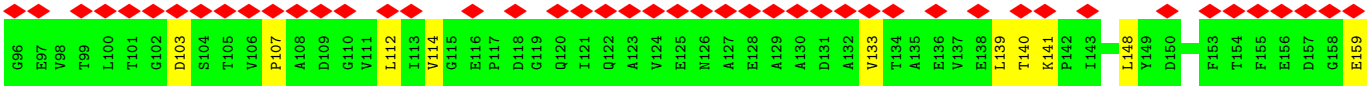


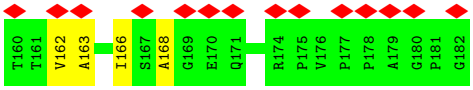


• Molecule 11: LpqE protein

Chain W:

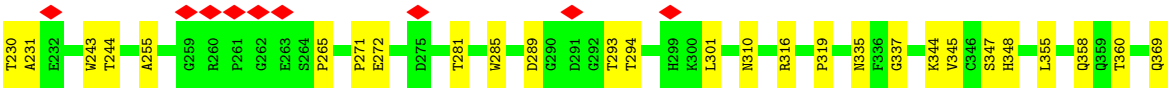


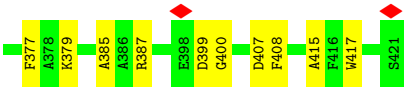




• Molecule 12: Cytochrome bc1 complex Rieske iron-sulfur subunit

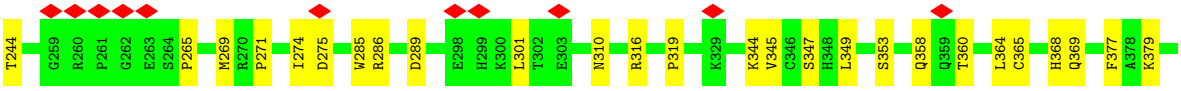
Chain Y:

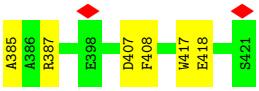




• Molecule 12: Cytochrome bc1 complex Rieske iron-sulfur subunit

Chain M:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	150885	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	43.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	5.732	Depositor
Minimum map value	-3.132	Depositor
Average map value	-0.005	Depositor
Map value standard deviation	0.173	Depositor
Recommended contour level	1.1	Depositor
Map size (Å)	339.9, 339.9, 339.9	wwPDB
Map dimensions	330, 330, 330	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03, 1.03, 1.03	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.17	0/4530	0.34	0/6188
1	R	0.17	0/4530	0.33	0/6188
2	E	0.20	0/4314	0.38	0/5882
2	F	0.22	0/4314	0.40	0/5882
3	D	0.14	0/1099	0.33	0/1519
3	G	0.13	0/1099	0.34	0/1519
4	K	0.18	0/2534	0.37	0/3451
4	Q	0.16	0/2534	0.33	0/3451
5	S	0.17	0/1608	0.32	0/2195
5	X	0.18	0/1608	0.32	0/2195
6	T	0.39	1/1112 (0.1%)	0.64	4/1524 (0.3%)
6	Z	0.17	0/1112	0.31	0/1524
7	U	0.12	0/613	0.27	0/836
7	a	0.12	0/613	0.28	0/836
8	V	0.16	0/1059	0.34	0/1446
8	b	0.15	0/1059	0.35	0/1446
9	J	0.15	0/757	0.29	0/1027
9	P	0.24	0/757	0.33	0/1027
10	I	0.18	0/1660	0.39	0/2250
10	O	0.37	0/1660	0.64	2/2250 (0.1%)
11	W	0.14	0/1166	0.32	0/1599
11	c	0.13	0/1166	0.33	0/1599
12	M	0.26	0/3056	0.47	0/4142
12	Y	0.20	0/3056	0.38	1/4142 (0.0%)
All	All	0.20	1/47016 (0.0%)	0.38	7/64118 (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	-7.60	1.15	1.24

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	T	120	PHE	CA-C-O	-9.17	111.09	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
10	O	197	LYS	N-CA-C	-5.48	103.39	110.19
10	O	274	ALA	N-CA-C	-5.37	105.50	111.36
6	T	120	PHE	CA-CB-CG	5.37	119.17	113.80
12	Y	112	TRP	CA-C-O	-5.32	115.86	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	4347	4346	99	0
1	R	4370	4346	4345	106	0
2	E	4181	4203	4202	83	0
2	F	4181	4200	4199	86	0
3	D	1092	640	640	3	0
3	G	1092	640	640	1	0
4	K	2465	2392	2392	39	0
4	Q	2465	2392	2392	52	0
5	S	1560	1548	1547	64	0
5	X	1560	1548	1547	82	0
6	T	1077	1059	1058	52	0
6	Z	1077	1058	1058	65	0
7	U	591	576	576	10	0
7	a	591	576	576	5	0
8	V	1041	1052	1052	18	0
8	b	1041	1052	1052	18	0
9	J	736	718	717	14	0
9	P	736	717	717	11	0
10	I	1623	1564	1564	43	0
10	O	1623	1564	1564	46	0
11	W	1149	1110	1110	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	c	1149	1110	1110	20	0
12	M	2977	2984	2984	47	0
12	Y	2977	2984	2984	47	0
13	K	2	0	0	0	0
13	L	1	0	0	0	0
13	Q	2	0	0	0	0
13	R	1	0	0	0	0
14	L	120	108	108	5	0
14	R	120	108	108	4	0
15	E	152	0	192	13	0
15	F	152	0	192	21	0
15	J	76	0	96	11	0
15	L	76	0	96	19	0
15	P	76	0	96	10	0
15	R	76	0	96	19	0
15	S	76	0	96	49	0
15	T	228	0	288	48	0
15	X	152	0	192	96	0
15	Z	152	0	192	81	0
16	E	85	57	57	4	0
16	F	85	57	57	5	0
17	E	116	160	160	4	0
17	F	232	320	320	5	0
17	I	58	80	80	1	0
17	Z	58	80	80	5	0
18	F	49	74	0	0	0
18	J	98	150	0	0	0
18	P	49	75	0	0	0
18	S	49	75	0	0	0
18	X	49	75	0	0	0
19	D	11	16	16	0	0
19	G	11	16	16	0	0
19	W	17	31	31	2	0
19	c	17	31	31	0	0
20	D	32	51	0	0	0
20	G	32	51	0	0	0
20	W	42	73	0	0	0
20	c	42	73	0	0	0
21	I	86	64	64	13	0
21	O	86	64	64	16	0
22	I	58	84	0	5	0
22	M	116	168	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	O	58	84	0	0	0
22	W	58	84	0	1	0
22	Y	116	168	0	5	0
22	c	58	84	0	1	0
23	M	4	0	0	0	0
23	Y	4	0	0	1	0
All	All	48962	46941	47100	1013	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 (1013) 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)
5:X:166:LYS:NZ	15:X:301:CDL:H112	1.28	1.48
15:Z:203:CDL:H631	22:I:304:9YF:C23	1.48	1.41
6:Z:120:PHE:CB	15:Z:202:CDL:H612	1.53	1.38
15:Z:203:CDL:C63	22:I:304:9YF:C23	2.03	1.35
6:Z:120:PHE:HB3	15:Z:202:CDL:C61	1.58	1.31
6:T:94:LEU:HD21	15:T:201:CDL:C32	1.67	1.24
6:Z:94:LEU:HD21	15:Z:202:CDL:C32	1.68	1.23
15:X:301:CDL:H772	15:Z:203:CDL:C55	1.71	1.20
6:Z:90:TRP:CZ2	15:Z:202:CDL:HB4	1.76	1.18
5:X:149:LEU:HD22	15:X:302:CDL:C63	1.74	1.18
15:X:301:CDL:H721	15:Z:203:CDL:C51	1.75	1.17
5:X:166:LYS:NZ	15:X:301:CDL:C11	2.09	1.15
6:T:90:TRP:HZ2	15:T:201:CDL:HB4	1.05	1.15
6:T:90:TRP:CZ2	15:T:201:CDL:HB4	1.82	1.15
5:X:166:LYS:HZ1	15:X:301:CDL:C11	1.60	1.15
6:T:97:LEU:HD11	15:T:201:CDL:H361	1.14	1.13
6:Z:97:LEU:HD11	15:Z:202:CDL:H361	1.18	1.12
15:X:301:CDL:H721	15:Z:203:CDL:H512	1.19	1.12
6:Z:119:ALA:HB1	15:Z:203:CDL:H411	1.23	1.12
6:Z:97:LEU:HD11	15:Z:202:CDL:C36	1.80	1.11
6:T:97:LEU:HD11	15:T:201:CDL:C36	1.80	1.11
5:X:149:LEU:HD22	15:X:302:CDL:H631	1.17	1.09
15:X:301:CDL:H772	15:Z:203:CDL:H551	1.21	1.08
6:Z:94:LEU:HD21	15:Z:202:CDL:H321	1.10	1.08
6:Z:90:TRP:HZ2	15:Z:202:CDL:HB4	1.00	1.08
6:T:94:LEU:HD21	15:T:201:CDL:H321	1.10	1.04
5:S:32:TRP:CZ2	15:S:301:CDL:H382	1.94	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:X:32:TRP:CZ2	15:X:302:CDL:H382	1.93	1.02
5:X:32:TRP:CE2	15:X:302:CDL:H361	1.94	1.02
5:X:32:TRP:CG	15:X:302:CDL:H331	1.95	1.01
5:X:32:TRP:CB	15:X:302:CDL:H331	1.91	1.01
1:R:121:LEU:HD13	15:S:301:CDL:CA3	1.90	1.00
5:S:32:TRP:CE2	15:S:301:CDL:H361	1.98	0.98
1:L:121:LEU:HD13	15:X:302:CDL:CA3	1.95	0.97
5:S:32:TRP:CB	15:S:301:CDL:H331	1.94	0.97
6:Z:120:PHE:CD2	15:Z:202:CDL:H632	2.00	0.96
5:S:32:TRP:CG	15:S:301:CDL:H331	2.02	0.95
5:S:149:LEU:HB3	15:S:301:CDL:H801	1.44	0.95
6:T:97:LEU:CD1	15:T:201:CDL:H361	1.96	0.94
4:Q:231:ILE:HD13	4:Q:246:LEU:HD23	1.49	0.92
15:X:301:CDL:H761	15:Z:203:CDL:H532	1.51	0.92
9:P:66:ASN:ND2	12:M:385:ALA:O	2.03	0.91
15:L:604:CDL:H731	15:L:604:CDL:H512	1.53	0.90
6:T:98:SER:OG	15:T:201:CDL:H621	1.71	0.90
6:Z:97:LEU:CD1	15:Z:202:CDL:H361	2.01	0.90
5:X:157:ALA:HB2	15:X:302:CDL:H532	1.54	0.90
6:Z:98:SER:OG	15:Z:202:CDL:H621	1.72	0.89
1:R:121:LEU:HD13	15:S:301:CDL:HA32	1.52	0.89
1:R:121:LEU:HB2	15:S:301:CDL:OA3	1.73	0.89
1:L:121:LEU:HD13	15:X:302:CDL:HA32	1.53	0.88
6:T:120:PHE:HB3	15:T:201:CDL:H612	1.55	0.87
7:a:53:GLU:OE1	8:b:59:SER:OG	1.93	0.87
5:X:32:TRP:CD2	15:X:302:CDL:H352	2.10	0.87
15:Z:203:CDL:H161	10:I:281:VAL:HG11	1.57	0.86
5:S:32:TRP:NE1	15:S:301:CDL:H361	1.89	0.86
6:T:97:LEU:CD1	15:T:201:CDL:C36	2.52	0.86
6:Z:119:ALA:HB1	15:Z:203:CDL:C41	2.05	0.86
15:L:604:CDL:H542	15:J:201:CDL:H351	1.57	0.86
15:Z:203:CDL:H632	22:I:304:9YF:C23	2.04	0.86
6:T:120:PHE:CB	15:T:201:CDL:H612	2.05	0.86
5:X:32:TRP:NE1	15:X:302:CDL:H361	1.91	0.86
5:X:149:LEU:HD22	15:X:302:CDL:C64	2.05	0.86
1:R:20:ARG:NH2	8:V:53:ASP:OD1	2.09	0.85
1:R:121:LEU:HD13	15:S:301:CDL:HA31	1.58	0.85
5:X:149:LEU:HB3	15:X:302:CDL:H801	1.56	0.85
6:Z:97:LEU:CD1	15:Z:202:CDL:C36	2.54	0.85
5:X:166:LYS:HZ1	15:X:301:CDL:H112	0.71	0.85
6:Z:90:TRP:HZ2	15:Z:202:CDL:CB4	1.89	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:87:ARG:NH1	2:E:90:GLU:OE1	2.10	0.84
4:Q:243:ARG:NH1	4:Q:255:ASP:O	2.11	0.84
1:L:20:ARG:NH2	8:b:53:ASP:OD1	2.10	0.84
15:X:301:CDL:C76	15:Z:203:CDL:H532	2.08	0.83
1:L:121:LEU:HB2	15:X:302:CDL:OA3	1.77	0.83
5:S:32:TRP:CD2	15:S:301:CDL:H352	2.13	0.83
1:R:389:THR:O	4:Q:242:LYS:NZ	2.11	0.82
15:X:301:CDL:H772	15:Z:203:CDL:H552	1.61	0.82
2:E:447:THR:OG1	2:E:461:LEU:O	1.98	0.82
5:X:166:LYS:HZ3	15:X:301:CDL:C11	1.91	0.82
6:Z:94:LEU:HD21	15:Z:202:CDL:H322	1.60	0.82
6:Z:120:PHE:CB	15:Z:202:CDL:C61	2.36	0.81
6:Z:94:LEU:CD2	15:Z:202:CDL:H321	2.04	0.81
1:L:84:THR:OG1	1:L:149:PHE:O	1.98	0.81
11:c:30:SER:HG	11:c:33:THR:HG1	1.16	0.81
2:F:447:THR:OG1	2:F:461:LEU:O	1.97	0.81
8:V:23:THR:OG1	8:V:27:ARG:O	1.99	0.81
17:F:709:MQ9:H501	12:Y:214:ALA:HB1	1.62	0.81
1:L:411:TYR:OH	1:L:488:MET:SD	2.37	0.81
7:U:53:GLU:OE1	8:V:59:SER:OG	1.97	0.81
4:K:243:ARG:NH1	4:K:255:ASP:O	2.14	0.81
4:K:263:ILE:HG21	4:K:290:VAL:HG21	1.62	0.80
5:S:149:LEU:HD23	15:S:301:CDL:H631	1.61	0.80
15:R:604:CDL:HA4	15:P:201:CDL:H312	1.62	0.80
6:T:94:LEU:HD21	15:T:201:CDL:H322	1.59	0.80
10:I:122:MET:O	10:I:124:ALA:N	2.14	0.80
5:S:157:ALA:HB2	15:S:301:CDL:H532	1.65	0.79
15:Z:203:CDL:C64	22:I:304:9YF:C23	2.59	0.79
10:I:251:GLU:O	10:I:255:THR:OG1	2.00	0.79
1:L:300:THR:OG1	1:L:340:LYS:NZ	2.16	0.79
1:R:30:LYS:O	1:R:34:THR:N	2.15	0.79
15:X:301:CDL:C77	15:Z:203:CDL:C55	2.59	0.79
9:J:66:ASN:ND2	12:Y:385:ALA:O	2.16	0.79
15:X:301:CDL:H721	15:Z:203:CDL:H511	1.63	0.78
1:L:497:LYS:NZ	9:J:100:ARG:O	2.17	0.78
15:X:301:CDL:C17	15:Z:203:CDL:H762	2.12	0.78
5:X:184:TYR:OH	15:X:302:CDL:H752	1.84	0.78
11:c:98:VAL:HG22	11:c:137:VAL:HG12	1.65	0.78
1:R:287:ARG:O	4:Q:87:GLN:NE2	2.17	0.77
2:E:489:ASN:ND2	6:Z:131:GLU:O	2.17	0.77
5:X:32:TRP:HB2	15:X:302:CDL:H331	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:32:TRP:HZ2	15:S:301:CDL:H382	1.48	0.77
6:T:94:LEU:CD2	15:T:201:CDL:H321	2.04	0.77
5:X:166:LYS:CE	15:X:301:CDL:H112	2.15	0.77
1:L:30:LYS:O	1:L:34:THR:N	2.17	0.77
1:L:205:ARG:NH1	6:Z:71:GLU:OE2	2.19	0.76
5:X:184:TYR:CZ	15:X:302:CDL:H731	2.19	0.76
1:L:121:LEU:HD13	15:X:302:CDL:HA31	1.65	0.76
4:Q:263:ILE:HG21	4:Q:290:VAL:HG21	1.67	0.76
4:K:227:SER:OG	4:K:230:VAL:O	2.04	0.76
12:Y:285:TRP:NE1	12:Y:289:ASP:O	2.18	0.76
5:X:32:TRP:CZ2	15:X:302:CDL:H361	2.20	0.75
6:Z:97:LEU:CD1	15:Z:202:CDL:C35	2.64	0.75
5:X:32:TRP:HZ2	15:X:302:CDL:H382	1.51	0.75
5:X:166:LYS:HZ3	15:X:301:CDL:CA5	1.98	0.75
5:X:32:TRP:CE2	15:X:302:CDL:C36	2.70	0.75
12:M:285:TRP:NE1	12:M:289:ASP:O	2.20	0.75
15:X:301:CDL:H131	15:Z:203:CDL:OB7	1.87	0.74
8:V:47:ASP:OD1	8:V:48:LEU:N	2.20	0.74
10:O:188:CYS:HB2	21:O:302:HEC:HBB2	1.70	0.74
6:Z:119:ALA:CB	15:Z:203:CDL:H411	2.10	0.74
2:E:365:GLN:NE2	9:J:38:TRP:O	2.21	0.74
6:T:120:PHE:CA	15:T:201:CDL:H612	2.16	0.74
10:O:191:CYS:CB	21:O:302:HEC:HBC2	2.17	0.74
1:R:553:ARG:NH2	4:Q:85:PRO:O	2.21	0.74
5:S:184:TYR:OH	15:S:301:CDL:H752	1.88	0.74
10:O:229:MET:O	12:M:358:GLN:NE2	2.21	0.74
11:c:63:ASP:OD1	12:Y:399:ASP:N	2.22	0.73
2:E:138:GLU:OE2	2:F:19:ARG:NE	2.22	0.73
15:R:604:CDL:C64	19:W:201:PLM:HG1	2.19	0.73
6:T:120:PHE:CD2	15:T:201:CDL:H632	2.23	0.73
5:X:32:TRP:CE2	15:X:302:CDL:H352	2.23	0.73
6:Z:120:PHE:HD2	15:Z:202:CDL:H632	1.54	0.73
15:R:604:CDL:H542	15:P:201:CDL:H351	1.71	0.73
2:F:489:ASN:ND2	6:T:131:GLU:O	2.22	0.72
6:T:90:TRP:HZ2	15:T:201:CDL:CB4	1.93	0.72
5:S:184:TYR:CZ	15:S:301:CDL:H731	2.24	0.72
6:T:97:LEU:CD1	15:T:201:CDL:C35	2.66	0.72
1:L:424:ARG:NH1	1:L:499:TRP:O	2.22	0.72
2:F:75:GLY:O	2:F:81:ARG:NH1	2.21	0.72
6:T:94:LEU:CD2	15:T:201:CDL:C32	2.59	0.72
11:c:148:LEU:HD11	12:Y:319:PRO:HB3	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:L:604:CDL:H521	15:J:201:CDL:H321	1.70	0.72
11:W:148:LEU:HD11	12:M:319:PRO:HB3	1.72	0.72
5:S:149:LEU:CD2	15:S:301:CDL:H631	2.20	0.71
4:Q:275:GLU:O	4:Q:281:HIS:NE2	2.22	0.71
6:Z:94:LEU:CD2	15:Z:202:CDL:C32	2.60	0.71
5:X:157:ALA:HB1	15:X:302:CDL:C51	2.20	0.71
5:S:32:TRP:CE2	15:S:301:CDL:H352	2.25	0.71
5:S:32:TRP:CE2	15:S:301:CDL:C36	2.74	0.71
1:L:385:ASP:O	1:L:389:THR:OG1	2.08	0.71
2:F:42:LEU:HD13	2:F:122:VAL:HG12	1.71	0.71
5:X:149:LEU:CB	15:X:302:CDL:H801	2.20	0.71
1:L:385:ASP:OD1	1:L:389:THR:OG1	2.09	0.70
10:O:151:GLN:OE1	10:O:156:GLY:N	2.24	0.70
2:F:500:GLY:O	12:M:84:ARG:NH2	2.24	0.70
5:X:189:ASP:OD1	5:X:190:ILE:N	2.24	0.70
1:R:10:GLU:N	1:R:10:GLU:OE1	2.25	0.70
5:X:157:ALA:CB	15:X:302:CDL:H511	2.21	0.70
1:R:88:THR:HG21	1:R:171:TRP:HE1	1.57	0.69
2:F:529:LEU:HD21	12:M:159:ILE:HG21	1.74	0.69
1:L:10:GLU:N	1:L:10:GLU:OE1	2.25	0.69
10:O:240:ASP:OD1	10:O:243:ARG:NH2	2.25	0.69
21:I:301:HEC:HBC3	21:I:301:HEC:HHD	1.75	0.69
15:T:203:CDL:H722	15:T:203:CDL:H132	1.75	0.69
4:K:128:GLU:OE1	4:K:150:ALA:N	2.24	0.69
15:X:301:CDL:H111	15:X:301:CDL:HB21	1.75	0.69
1:R:385:ASP:O	1:R:389:THR:OG1	2.10	0.69
2:E:500:GLY:O	12:Y:84:ARG:NH2	2.25	0.69
7:U:44:HIS:ND1	7:U:47:ILE:HD11	2.08	0.69
1:L:270:ILE:HG23	1:L:406:ILE:HG21	1.75	0.69
5:S:32:TRP:HB2	15:S:301:CDL:H331	1.72	0.69
5:X:184:TYR:CE1	15:X:302:CDL:C73	2.76	0.69
6:Z:120:PHE:CA	15:Z:202:CDL:H612	2.22	0.69
10:I:240:ASP:OD1	10:I:243:ARG:NH2	2.26	0.69
2:E:42:LEU:HD13	2:E:122:VAL:HG12	1.73	0.69
8:V:36:GLU:OE1	8:V:36:GLU:N	2.26	0.69
6:Z:120:PHE:CG	15:Z:202:CDL:C61	2.76	0.69
2:E:328:PRO:O	2:E:331:VAL:HG12	1.93	0.68
5:S:32:TRP:CZ2	15:S:301:CDL:H361	2.28	0.68
2:E:235:HIS:O	12:Y:164:ARG:NH2	2.26	0.68
5:S:157:ALA:CB	15:S:301:CDL:H511	2.24	0.68
5:X:150:HIS:HA	15:X:302:CDL:H771	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Z:123:THR:HG23	15:Z:203:CDL:H322	1.75	0.68
15:Z:203:CDL:H572	10:I:282:ALA:HA	1.73	0.68
8:b:23:THR:OG1	8:b:27:ARG:O	2.11	0.68
5:X:149:LEU:CD2	15:X:302:CDL:H631	2.11	0.68
2:E:331:VAL:HG23	22:Y:502:9YF:C42	2.24	0.68
6:Z:97:LEU:CD1	15:Z:202:CDL:H351	2.24	0.68
11:W:54:VAL:HG11	11:W:162:VAL:HG11	1.76	0.68
2:F:235:HIS:O	12:M:164:ARG:NH2	2.27	0.67
5:X:184:TYR:CE1	15:X:302:CDL:H732	2.29	0.67
6:Z:120:PHE:CG	15:Z:202:CDL:H611	2.29	0.67
10:I:90:CYS:SG	21:I:301:HEC:HBC2	2.34	0.67
1:L:249:ASN:O	4:K:252:ASN:ND2	2.28	0.67
4:Q:332:ARG:NH2	11:W:26:ALA:O	2.26	0.67
15:T:202:CDL:HB21	15:T:202:CDL:H111	1.75	0.67
10:I:151:GLN:OE1	10:I:156:GLY:N	2.27	0.67
1:L:553:ARG:NH2	4:K:85:PRO:O	2.28	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
5:X:149:LEU:CD2	15:X:302:CDL:C64	2.71	0.67
6:Z:123:THR:CG2	15:Z:203:CDL:H322	2.25	0.67
15:F:705:CDL:H162	15:F:705:CDL:H771	1.77	0.67
15:X:301:CDL:C13	15:Z:203:CDL:OB7	2.43	0.67
1:R:121:LEU:CD1	15:S:301:CDL:HA32	2.24	0.67
15:X:301:CDL:C77	15:Z:203:CDL:H552	2.22	0.67
4:K:225:LEU:O	4:K:256:ASN:ND2	2.27	0.67
1:R:515:ASN:O	1:R:516:SER:OG	2.06	0.66
5:S:150:HIS:HA	15:S:301:CDL:H771	1.77	0.66
15:X:301:CDL:C72	15:Z:203:CDL:C51	2.66	0.66
12:M:377:PHE:O	12:M:379:LYS:N	2.27	0.66
9:P:72:GLU:HG3	22:W:203:9YF:O10	1.95	0.66
1:R:270:ILE:HG23	1:R:406:ILE:HG21	1.76	0.66
15:R:604:CDL:H521	15:P:201:CDL:H321	1.76	0.66
2:E:329:GLN:OE1	12:Y:348:HIS:NE2	2.28	0.66
2:E:136:PRO:O	2:E:233:GLN:NE2	2.28	0.66
10:O:121:ARG:NE	21:O:302:HEC:O1D	2.28	0.66
8:b:65:ARG:NH1	8:b:90:THR:OG1	2.27	0.66
15:R:604:CDL:H531	15:R:604:CDL:H731	1.76	0.66
21:O:302:HEC:HHD	21:O:302:HEC:HBC3	1.77	0.66
5:X:157:ALA:CB	15:X:302:CDL:C51	2.73	0.66
11:c:98:VAL:HG22	11:c:137:VAL:CG1	2.26	0.66
12:Y:377:PHE:O	12:Y:379:LYS:N	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:184:TYR:CE1	15:S:301:CDL:C73	2.79	0.65
2:F:425:VAL:HG11	15:F:705:CDL:H371	1.77	0.65
15:T:203:CDL:H382	15:T:203:CDL:H772	1.78	0.65
2:F:131:GLY:O	2:F:134:ARG:NH1	2.29	0.65
6:Z:90:TRP:CZ2	15:Z:202:CDL:CB4	2.68	0.65
1:L:96:THR:OG1	1:L:266:GLU:OE2	2.13	0.64
5:S:16:VAL:HG23	5:S:24:MET:HE2	1.80	0.64
1:L:21:MET:HG2	15:L:604:CDL:HA22	1.79	0.64
21:O:301:HEC:HBC3	21:O:301:HEC:HHD	1.77	0.64
15:X:301:CDL:C14	15:Z:203:CDL:OB7	2.44	0.64
16:E:602:HEM:HBB2	16:E:602:HEM:HHC	1.79	0.64
1:L:206:MET:O	1:L:293:TYR:OH	2.12	0.64
2:E:450:ILE:HG21	2:E:461:LEU:HD13	1.79	0.64
6:Z:120:PHE:HB3	15:Z:202:CDL:H612	0.72	0.64
15:X:301:CDL:C77	15:Z:203:CDL:H551	2.14	0.64
15:X:301:CDL:H141	15:Z:203:CDL:OB7	1.97	0.64
15:F:704:CDL:H111	15:F:704:CDL:H311	1.79	0.64
11:c:120:GLN:NE2	10:I:152:ALA:O	2.30	0.64
4:K:256:ASN:OD1	4:K:257:VAL:N	2.31	0.64
15:E:606:CDL:H771	15:E:606:CDL:H162	1.80	0.64
5:S:189:ASP:OD1	5:S:190:ILE:N	2.30	0.64
5:S:157:ALA:HB1	15:S:301:CDL:C51	2.28	0.63
10:O:192:HIS:CE1	10:O:210:LEU:HD21	2.33	0.63
15:E:605:CDL:H111	15:E:605:CDL:H311	1.79	0.63
5:X:157:ALA:HB1	15:X:302:CDL:H511	1.80	0.63
6:T:97:LEU:CD1	15:T:201:CDL:H351	2.29	0.63
5:X:157:ALA:HB1	15:X:302:CDL:H512	1.80	0.63
1:L:190:ILE:HD11	6:Z:8:PHE:HZ	1.63	0.63
1:R:387:HIS:NE2	1:R:454:ASP:O	2.29	0.63
3:G:117:GLY:N	3:G:185:LYS:O	2.31	0.63
5:X:184:TYR:CE2	15:X:302:CDL:H731	2.33	0.63
1:R:120:ARG:HB2	15:S:301:CDL:OA4	1.98	0.63
5:X:184:TYR:CZ	15:X:302:CDL:H752	2.33	0.63
1:R:274:PHE:CD2	1:R:406:ILE:HG22	2.33	0.63
1:R:335:VAL:HG13	1:R:336:PRO:HD3	1.81	0.63
5:S:184:TYR:CE1	15:S:301:CDL:H732	2.34	0.63
1:R:117:ALA:O	5:S:15:ARG:NH2	2.30	0.63
15:R:604:CDL:H731	15:R:604:CDL:H512	1.81	0.63
5:S:43:LEU:HD23	5:S:143:ALA:HA	1.80	0.62
5:S:157:ALA:CB	15:S:301:CDL:C51	2.77	0.62
15:R:604:CDL:H512	15:R:604:CDL:C73	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:O:122:MET:O	10:O:124:ALA:N	2.32	0.62
10:I:269:ALA:HB3	10:I:270:PRO:HD3	1.81	0.62
6:Z:126:CYS:HB2	15:Z:203:CDL:H321	1.82	0.62
4:Q:225:LEU:O	4:Q:256:ASN:ND2	2.32	0.62
4:Q:45:LEU:HD21	4:Q:116:VAL:HG22	1.82	0.62
2:E:161:LEU:HD21	2:E:208:TYR:HA	1.81	0.62
10:I:229:MET:O	12:Y:358:GLN:NE2	2.33	0.62
1:R:454:ASP:OD1	4:Q:35:TRP:NE1	2.33	0.61
1:L:250:GLY:O	1:L:254:LEU:N	2.29	0.61
1:R:401:VAL:O	1:R:405:THR:OG1	2.08	0.61
2:F:263:ALA:HB1	12:M:148:VAL:HG23	1.81	0.61
1:L:252:VAL:HB	4:K:231:ILE:HD11	1.83	0.61
1:L:120:ARG:HB2	15:X:302:CDL:OA4	2.00	0.61
8:V:140:ILE:O	8:V:144:ILE:HD12	2.01	0.61
2:F:87:ARG:NH1	2:F:90:GLU:OE1	2.34	0.61
5:S:102:TRP:CE3	5:S:105:ILE:HD11	2.35	0.61
1:L:274:PHE:CD2	1:L:406:ILE:HG22	2.35	0.61
15:T:203:CDL:H721	15:T:203:CDL:H341	1.81	0.61
5:X:32:TRP:CZ2	15:X:302:CDL:C38	2.78	0.61
22:Y:503:9YF:C14	12:M:108:LEU:HD22	2.31	0.61
5:S:184:TYR:CZ	15:S:301:CDL:H752	2.35	0.60
5:X:32:TRP:CE2	15:X:302:CDL:C35	2.83	0.60
6:Z:97:LEU:HD11	15:Z:202:CDL:C37	2.30	0.60
1:L:227:LEU:HD22	1:L:262:PHE:CZ	2.37	0.60
4:Q:256:ASN:OD1	4:Q:257:VAL:N	2.34	0.60
6:T:90:TRP:CZ2	15:T:201:CDL:CB4	2.73	0.60
2:E:29:GLN:OE1	2:E:231:TRP:NE1	2.32	0.60
2:F:100:ARG:NH1	22:Y:503:9YF:O12	2.34	0.60
5:X:81:SER:OG	5:X:189:ASP:OD2	2.14	0.60
5:X:91:ALA:HB2	5:X:99:LEU:HD12	1.84	0.60
11:c:54:VAL:HG11	11:c:162:VAL:HG11	1.82	0.60
2:F:404:LEU:HD21	12:M:369:GLN:CG	2.32	0.60
17:Z:201:MQ9:H153	22:I:304:9YF:C43	2.32	0.60
2:F:487:ARG:NH1	6:T:131:GLU:O	2.33	0.60
1:L:326:PHE:O	1:L:330:THR:OG1	2.18	0.60
4:Q:279:THR:HG21	10:O:126:ARG:HA	1.81	0.60
6:T:97:LEU:HD11	15:T:201:CDL:C37	2.31	0.60
15:X:301:CDL:H792	15:Z:203:CDL:H581	1.83	0.60
9:P:48:MET:SD	15:P:201:CDL:HB61	2.42	0.59
2:F:533:GLN:OE1	9:P:7:ARG:N	2.36	0.59
4:Q:193:ARG:NH2	10:O:142:GLN:OE1	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:263:ALA:HB1	12:Y:148:VAL:HG23	1.84	0.59
5:X:161:LEU:O	5:X:165:THR:HG23	2.02	0.59
3:D:113:ILE:N	3:D:153:GLY:O	2.34	0.59
11:c:139:LEU:O	11:c:140:THR:OG1	2.16	0.59
15:X:301:CDL:C72	15:Z:203:CDL:H511	2.31	0.59
15:L:604:CDL:H731	15:L:604:CDL:H531	1.84	0.59
1:L:35:THR:HG21	6:Z:86:ALA:O	2.03	0.58
4:K:45:LEU:CD2	4:K:116:VAL:HG22	2.33	0.58
5:X:41:ALA:HA	6:Z:44:LEU:HD22	1.85	0.58
2:E:65:ASP:HB3	2:E:91:THR:HG21	1.84	0.58
2:E:438:ARG:NH2	9:J:35:SER:OG	2.36	0.58
1:R:378:LEU:HD23	4:Q:50:TRP:CZ3	2.38	0.58
1:L:386:PHE:O	4:K:242:LYS:NZ	2.32	0.58
15:T:202:CDL:HB22	15:T:202:CDL:HB4	1.84	0.58
11:W:159:GLU:N	11:W:159:GLU:OE1	2.36	0.58
6:Z:101:THR:HG22	17:Z:201:MQ9:C18	2.33	0.58
5:S:32:TRP:CE2	15:S:301:CDL:C35	2.87	0.58
1:L:84:THR:O	1:L:88:THR:OG1	2.18	0.58
2:E:312:ILE:HD13	2:E:333:VAL:HG21	1.85	0.58
9:P:29:ASP:N	9:P:29:ASP:OD1	2.37	0.58
15:X:301:CDL:HB22	15:X:301:CDL:HB4	1.84	0.58
5:S:184:TYR:CE2	15:S:301:CDL:H731	2.39	0.58
15:Z:203:CDL:C16	10:I:281:VAL:HG11	2.33	0.58
1:R:540:ARG:NH2	1:R:554:MET:SD	2.77	0.58
15:E:605:CDL:H371	15:E:605:CDL:H152	1.86	0.58
1:R:88:THR:HG22	1:R:151:TRP:HD1	1.68	0.57
1:L:200:GLY:O	1:L:205:ARG:NH2	2.36	0.57
6:T:94:LEU:CD2	15:T:201:CDL:H322	2.30	0.57
1:R:268:TYR:OH	1:R:333:ILE:HD12	2.03	0.57
15:F:704:CDL:H371	15:F:704:CDL:H152	1.86	0.57
1:R:274:PHE:CE2	1:R:406:ILE:HG22	2.40	0.57
2:E:66:PRO:O	2:E:67:SER:OG	2.23	0.57
11:c:56:LEU:HD12	11:c:166:ILE:CD1	2.33	0.57
6:T:120:PHE:HA	15:T:201:CDL:H612	1.87	0.57
8:b:68:VAL:HG11	8:b:143:LEU:HD13	1.87	0.57
11:W:139:LEU:O	11:W:140:THR:OG1	2.17	0.57
5:S:157:ALA:HA	15:S:301:CDL:H511	1.87	0.57
5:X:184:TYR:CE1	15:X:302:CDL:H731	2.39	0.57
1:R:465:LEU:HD11	4:Q:326:GLU:O	2.05	0.57
5:S:157:ALA:HB1	15:S:301:CDL:H512	1.87	0.57
2:E:370:VAL:O	2:E:370:VAL:HG13	2.03	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:256:GLN:OE1	1:L:318:THR:HG21	2.05	0.56
1:L:122:ASN:OD1	1:L:123:ALA:N	2.38	0.56
2:E:425:VAL:HG22	15:L:604:CDL:H722	1.87	0.56
1:L:460:ARG:N	14:L:603:HEA:O2A	2.37	0.56
1:L:544:GLU:OE2	1:L:555:ARG:NH2	2.39	0.56
5:S:25:VAL:HG12	5:S:180:VAL:HG11	1.86	0.56
15:T:202:CDL:C17	15:T:203:CDL:H741	2.35	0.56
15:T:203:CDL:HA62	15:T:203:CDL:H712	1.86	0.56
10:O:110:GLU:OE2	10:O:161:ARG:NH2	2.38	0.56
10:O:112:ALA:HB2	10:O:224:THR:HG21	1.87	0.56
2:E:65:ASP:OD1	2:F:67:SER:OG	2.23	0.56
4:K:45:LEU:HD21	4:K:116:VAL:HG22	1.87	0.56
5:X:184:TYR:CD1	15:X:302:CDL:H732	2.41	0.56
1:L:387:HIS:NE2	1:L:454:ASP:O	2.38	0.56
5:S:157:ALA:HB1	15:S:301:CDL:H511	1.88	0.56
1:L:77:GLU:OE1	4:K:332:ARG:NH2	2.39	0.56
4:Q:45:LEU:CD2	4:Q:116:VAL:HG22	2.35	0.56
5:X:149:LEU:CD2	15:X:302:CDL:C63	2.68	0.56
11:W:148:LEU:HD12	11:W:163:ALA:O	2.06	0.56
1:R:357:THR:N	1:R:428:GLU:OE2	2.38	0.56
1:L:274:PHE:CE2	1:L:406:ILE:HG22	2.41	0.56
4:K:279:THR:HG21	10:I:126:ARG:HA	1.87	0.56
2:E:213:LEU:HD21	16:F:703:HEM:CBC	2.36	0.56
2:F:500:GLY:O	12:M:84:ARG:CZ	2.54	0.56
1:L:121:LEU:CD1	15:X:302:CDL:HA32	2.29	0.56
15:T:202:CDL:H572	15:T:202:CDL:H742	1.88	0.56
2:E:89:TYR:OH	2:E:287:LEU:O	2.22	0.55
2:F:422:VAL:HG22	15:F:705:CDL:H402	1.87	0.55
2:E:161:LEU:HD21	2:E:208:TYR:CA	2.37	0.55
2:E:487:ARG:NH1	6:Z:131:GLU:O	2.39	0.55
11:c:42:VAL:HG12	11:c:54:VAL:HG13	1.89	0.55
2:E:17:ASP:OD1	2:E:23:SER:OG	2.18	0.55
1:L:35:THR:HG22	1:L:119:PRO:HB2	1.88	0.55
3:D:74:THR:N	3:D:78:THR:O	2.38	0.55
6:Z:123:THR:HG23	15:Z:203:CDL:H331	1.88	0.55
11:c:148:LEU:HD12	11:c:163:ALA:O	2.07	0.55
1:R:156:PRO:HG3	1:R:252:VAL:HG12	1.88	0.55
2:E:104:PHE:HD2	17:E:604:MQ9:H502	1.72	0.55
2:F:116:PHE:CZ	2:F:120:ILE:HD11	2.41	0.55
15:T:202:CDL:H772	15:T:203:CDL:H582	1.88	0.55
1:R:252:VAL:HG21	4:Q:246:LEU:HD22	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:72:GLY:N	8:V:110:TYR:O	2.39	0.55
1:R:122:ASN:OD1	1:R:123:ALA:N	2.40	0.55
15:R:604:CDL:HB61	15:R:604:CDL:OB4	2.06	0.55
16:F:703:HEM:HHC	16:F:703:HEM:HBB2	1.88	0.55
6:T:120:PHE:HB3	15:T:201:CDL:C61	2.35	0.55
21:O:302:HEC:HHC	21:O:302:HEC:HBB3	1.89	0.55
1:R:209:PHE:CZ	1:R:213:ILE:HD11	2.42	0.55
10:O:191:CYS:HB2	21:O:302:HEC:HBC2	1.89	0.55
2:E:282:ASN:ND2	16:E:602:HEM:O1A	2.38	0.55
5:S:184:TYR:CE1	15:S:301:CDL:H731	2.41	0.55
10:O:116:GLN:CG	10:O:122:MET:HE3	2.37	0.55
15:Z:203:CDL:H161	10:I:281:VAL:CG1	2.33	0.55
4:K:288:VAL:HG23	4:K:288:VAL:O	2.07	0.55
2:F:194:PHE:CE2	2:F:203:LEU:HD22	2.42	0.54
5:X:15:ARG:O	5:X:16:VAL:HG23	2.07	0.54
5:X:32:TRP:CH2	15:X:302:CDL:H382	2.42	0.54
10:O:76:LEU:HD11	10:O:152:ALA:CB	2.38	0.54
15:R:604:CDL:H792	15:F:705:CDL:H391	1.90	0.54
15:X:301:CDL:H572	15:X:301:CDL:H742	1.88	0.54
2:E:19:ARG:O	2:F:233:GLN:NE2	2.37	0.54
6:Z:90:TRP:HH2	15:Z:202:CDL:OB7	1.90	0.54
9:J:29:ASP:OD1	9:J:29:ASP:N	2.40	0.54
11:W:30:SER:HG	11:W:33:THR:HG1	1.55	0.54
1:R:398:PHE:HA	1:R:401:VAL:HG22	1.90	0.54
6:Z:123:THR:HG23	15:Z:203:CDL:C32	2.37	0.54
15:L:604:CDL:HB61	15:L:604:CDL:OB4	2.08	0.54
10:I:87:CYS:SG	21:I:301:HEC:HAB	2.47	0.54
2:E:368:ARG:O	2:E:434:GLN:NE2	2.39	0.54
2:F:404:LEU:HD21	12:M:369:GLN:HG2	1.90	0.54
4:Q:40:THR:HG23	4:Q:43:ALA:H	1.73	0.54
5:X:99:LEU:C	5:X:99:LEU:HD23	2.33	0.54
5:X:81:SER:HG	5:X:189:ASP:CG	2.13	0.54
6:Z:98:SER:OG	15:Z:202:CDL:C62	2.53	0.54
1:R:89:VAL:CG2	1:R:137:ILE:HD11	2.37	0.53
1:L:117:ALA:O	5:X:15:ARG:NH2	2.42	0.53
1:L:259:PHE:O	1:L:263:GLY:N	2.38	0.53
11:c:159:GLU:N	11:c:159:GLU:OE1	2.40	0.53
1:R:46:VAL:CG1	15:P:201:CDL:H371	2.38	0.53
2:F:393:ASN:OD1	2:F:394:ASP:N	2.41	0.53
2:E:278:LEU:O	10:I:261:TYR:N	2.40	0.53
2:F:172:ARG:NH1	2:F:176:SER:OG	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:X:32:TRP:NE1	15:X:302:CDL:C36	2.68	0.53
2:E:116:PHE:CZ	2:E:120:ILE:HD11	2.42	0.53
1:L:194:VAL:HG13	6:Z:1:MET:HE3	1.91	0.53
1:R:21:MET:HG2	15:R:604:CDL:HA22	1.90	0.53
4:Q:294:ASN:OD1	4:Q:295:ASP:N	2.41	0.53
1:R:193:VAL:HG13	1:R:206:MET:HE1	1.90	0.53
1:L:419:PRO:HG3	1:L:425:LEU:HD23	1.90	0.53
17:Z:201:MQ9:H511	22:c:203:9YF:C22	2.39	0.53
10:I:121:ARG:NE	21:I:302:HEC:O1D	2.41	0.53
15:L:604:CDL:H531	15:L:604:CDL:H712	1.91	0.53
1:R:460:ARG:N	14:R:603:HEA:O2A	2.39	0.53
2:E:312:ILE:HA	2:E:333:VAL:HG21	1.90	0.53
6:T:120:PHE:CB	15:T:201:CDL:C61	2.84	0.53
10:O:187:ASN:O	21:O:302:HEC:HMC3	2.09	0.53
15:E:605:CDL:OB7	15:F:704:CDL:H112	2.09	0.53
15:L:604:CDL:H512	15:L:604:CDL:C73	2.33	0.52
4:Q:121:MET:HE1	4:Q:257:VAL:HG13	1.89	0.52
5:S:184:TYR:CD1	15:S:301:CDL:H732	2.44	0.52
2:E:365:GLN:OE1	2:E:373:ARG:NH2	2.42	0.52
2:E:499:THR:HG22	2:E:511:HIS:ND1	2.25	0.52
5:X:157:ALA:HA	15:X:302:CDL:H511	1.90	0.52
4:K:245:VAL:HG23	4:K:245:VAL:O	2.09	0.52
8:b:114:VAL:O	8:b:114:VAL:HG13	2.10	0.52
9:J:93:LEU:O	9:J:98:TRP:N	2.40	0.52
1:R:84:THR:OG1	1:R:149:PHE:O	2.25	0.52
2:E:404:LEU:HD21	12:Y:369:GLN:CG	2.39	0.52
1:L:243:HIS:ND1	1:L:246:ASP:OD2	2.42	0.52
15:T:202:CDL:H741	15:T:202:CDL:H611	1.92	0.52
10:O:76:LEU:HD11	10:O:152:ALA:HB3	1.92	0.52
6:Z:97:LEU:HD12	15:Z:202:CDL:C35	2.38	0.52
2:F:27:ARG:HB2	12:Y:177:VAL:HG22	1.92	0.52
2:E:421:ILE:HG13	15:J:201:CDL:H572	1.92	0.52
4:K:294:ASN:OD1	4:K:295:ASP:N	2.43	0.52
12:M:67:THR:HG23	12:M:67:THR:O	2.10	0.52
1:R:419:PRO:HG3	1:R:425:LEU:HD23	1.91	0.52
1:L:15:ARG:NH1	1:L:19:GLU:OE1	2.43	0.52
4:Q:140:TRP:NE1	4:Q:284:MET:O	2.38	0.52
10:O:214:ASN:O	10:O:218:ILE:HD12	2.10	0.52
5:X:166:LYS:NZ	15:X:301:CDL:CA5	2.62	0.52
15:X:301:CDL:H741	15:X:301:CDL:H611	1.92	0.52
1:R:169:ASP:OD1	1:R:238:ARG:NE	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:94:LEU:HD23	15:T:201:CDL:H352	1.91	0.52
6:T:97:LEU:HD12	15:T:201:CDL:C35	2.39	0.52
11:W:75:PHE:CZ	11:W:114:VAL:HG11	2.45	0.52
1:R:398:PHE:O	1:R:402:LEU:HD12	2.10	0.51
2:F:65:ASP:HB3	2:F:91:THR:HG21	1.91	0.51
5:S:149:LEU:CB	15:S:301:CDL:H801	2.29	0.51
10:I:187:ASN:O	21:I:302:HEC:HMC3	2.09	0.51
1:R:163:SER:OG	1:R:163:SER:O	2.26	0.51
2:E:327:ILE:CG2	2:E:331:VAL:HG11	2.40	0.51
2:E:336:GLY:O	2:E:340:VAL:HG23	2.09	0.51
5:X:32:TRP:CZ2	15:X:302:CDL:C36	2.93	0.51
11:W:56:LEU:HD12	11:W:166:ILE:CD1	2.41	0.51
7:U:56:GLU:N	7:U:56:GLU:OE1	2.43	0.51
5:X:157:ALA:CA	15:X:302:CDL:H511	2.40	0.51
6:Z:94:LEU:CD2	15:Z:202:CDL:H322	2.31	0.51
1:R:158:THR:O	1:R:238:ARG:NH1	2.42	0.51
2:E:236:THR:HG21	2:E:364:LEU:HD21	1.92	0.51
2:F:438:ARG:NH2	9:P:35:SER:OG	2.39	0.51
2:F:368:ARG:O	2:F:434:GLN:NE2	2.38	0.51
1:L:445:THR:HG23	1:L:446:PHE:CD2	2.45	0.51
9:P:45:ILE:HD12	9:P:48:MET:HE3	1.91	0.51
12:M:347:SER:O	12:M:387:ARG:NH1	2.41	0.51
6:T:98:SER:OG	15:T:201:CDL:C62	2.53	0.51
12:Y:407:ASP:OD1	12:Y:408:PHE:N	2.42	0.51
1:R:104:ASN:OD1	1:R:122:ASN:ND2	2.43	0.51
2:E:366:ARG:NH1	2:E:437:ASP:OD2	2.42	0.51
2:F:478:GLU:OE2	9:P:7:ARG:NH1	2.44	0.51
2:F:433:LEU:CD1	15:F:705:CDL:HA61	2.41	0.51
1:L:29:TYR:OH	15:Z:202:CDL:OA4	2.23	0.51
8:V:51:LEU:HB2	8:V:144:ILE:HD11	1.93	0.51
1:R:257:HIS:NE2	6:T:35:GLU:OE1	2.43	0.50
1:L:534:PRO:HB3	1:L:545:LEU:HD12	1.93	0.50
5:S:157:ALA:CA	15:S:301:CDL:H511	2.41	0.50
9:J:87:VAL:HG22	15:J:201:CDL:H511	1.94	0.50
2:E:331:VAL:CG2	22:Y:502:9YF:C42	2.90	0.50
2:F:175:LEU:O	2:F:179:THR:OG1	2.27	0.50
5:S:32:TRP:CZ2	15:S:301:CDL:C38	2.81	0.50
15:T:202:CDL:H732	12:M:145:ILE:HD13	1.92	0.50
8:b:95:VAL:HG13	8:b:110:TYR:CE1	2.46	0.50
1:R:445:THR:HG23	1:R:446:PHE:CD2	2.47	0.50
10:O:76:LEU:HD13	10:O:149:TYR:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:O:124:ALA:O	21:O:301:HEC:HAC	2.10	0.50
6:Z:108:LEU:O	6:Z:110:LEU:N	2.45	0.50
9:J:53:LEU:CD1	9:J:87:VAL:HG11	2.41	0.50
1:R:496:PHE:O	1:R:500:ARG:NH2	2.44	0.50
1:L:35:THR:HG22	1:L:35:THR:O	2.12	0.50
10:O:116:GLN:HG2	10:O:122:MET:HE3	1.92	0.50
5:X:157:ALA:HB2	15:X:302:CDL:C53	2.36	0.50
5:X:189:ASP:OD1	5:X:189:ASP:C	2.54	0.50
4:Q:310:ALA:CB	11:W:82:THR:HG21	2.42	0.50
5:S:32:TRP:NE1	15:S:301:CDL:C36	2.69	0.50
12:M:275:ASP:OD1	12:M:275:ASP:N	2.44	0.50
2:E:433:LEU:CD1	15:E:606:CDL:HA61	2.42	0.50
2:F:135:ARG:HB3	2:F:136:PRO:CD	2.42	0.50
12:M:159:ILE:O	12:M:159:ILE:HG22	2.12	0.50
5:S:15:ARG:HB3	5:S:24:MET:HE3	1.94	0.50
4:K:135:ALA:HB3	4:K:245:VAL:HG21	1.94	0.50
12:Y:265:PRO:CG	12:Y:301:LEU:HD23	2.42	0.50
1:R:35:THR:HG21	6:T:86:ALA:O	2.12	0.49
1:R:406:ILE:HD11	14:R:603:HEA:CBC	2.42	0.49
2:E:227:LEU:HD22	15:E:605:CDL:H782	1.93	0.49
6:T:108:LEU:O	6:T:110:LEU:N	2.45	0.49
6:Z:98:SER:O	6:Z:101:THR:OG1	2.26	0.49
6:Z:101:THR:HG22	17:Z:201:MQ9:H18	1.94	0.49
9:J:86:LEU:HD23	15:J:201:CDL:H162	1.94	0.49
2:F:336:GLY:O	2:F:340:VAL:HG23	2.12	0.49
8:b:25:SER:OG	8:b:26:GLY:N	2.44	0.49
2:F:312:ILE:HG13	2:F:333:VAL:HG21	1.94	0.49
12:M:407:ASP:OD1	12:M:408:PHE:N	2.43	0.49
1:R:515:ASN:N	1:R:515:ASN:OD1	2.44	0.49
2:E:131:GLY:O	2:E:134:ARG:NE	2.41	0.49
1:L:496:PHE:O	1:L:500:ARG:NH2	2.43	0.49
7:a:56:GLU:OE1	7:a:56:GLU:N	2.45	0.49
2:E:127:ILE:HD11	16:E:601:HEM:CAC	2.43	0.49
17:E:604:MQ9:H511	17:E:604:MQ9:H453	1.94	0.49
2:F:65:ASP:CB	2:F:91:THR:HG21	2.43	0.49
15:R:604:CDL:H722	2:F:425:VAL:HG22	1.93	0.49
15:E:605:CDL:H112	15:F:704:CDL:OB7	2.12	0.49
2:F:104:PHE:HD2	17:F:709:MQ9:H502	1.78	0.49
1:L:156:PRO:HG3	1:L:252:VAL:HG12	1.94	0.49
1:L:392:TYR:HD2	1:L:452:LEU:HD23	1.76	0.49
12:M:269:MET:HE1	12:M:274:ILE:HD11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:E:605:CDL:OB7	15:F:704:CDL:C11	2.61	0.49
2:F:281:ILE:HD12	10:O:271:GLU:CG	2.42	0.49
10:O:95:LEU:HD12	10:O:105:LEU:HB2	1.95	0.49
11:c:63:ASP:OD1	12:Y:400:GLY:N	2.46	0.49
7:U:23:LEU:O	7:U:27:THR:OG1	2.24	0.49
15:X:301:CDL:C17	15:Z:203:CDL:H731	2.42	0.49
12:Y:110:TRP:HZ2	12:Y:127:LEU:HD11	1.78	0.49
1:R:34:THR:HG21	1:R:43:MET:CE	2.43	0.49
1:R:89:VAL:HG21	1:R:137:ILE:HD11	1.93	0.49
2:E:27:ARG:HB2	12:M:177:VAL:HG22	1.95	0.49
1:L:401:VAL:HG11	14:L:602:HEA:C2C	2.42	0.49
8:b:76:ASP:OD1	8:b:76:ASP:N	2.46	0.49
2:E:65:ASP:CB	2:E:91:THR:HG21	2.41	0.48
1:L:508:ASP:N	1:L:508:ASP:OD1	2.44	0.48
4:Q:275:GLU:O	4:Q:281:HIS:CE1	2.66	0.48
6:T:90:TRP:HH2	15:T:201:CDL:OB7	1.95	0.48
10:O:192:HIS:ND1	10:O:210:LEU:HD21	2.27	0.48
10:O:235:ARG:NH1	11:W:168:ALA:O	2.46	0.48
15:Z:203:CDL:C57	10:I:282:ALA:HA	2.42	0.48
2:F:227:LEU:HD22	15:F:704:CDL:H782	1.95	0.48
7:U:38:MET:HE3	7:U:79:TRP:CH2	2.48	0.48
10:I:124:ALA:O	21:I:301:HEC:HAC	2.12	0.48
11:W:95:VAL:HG23	11:W:141:LYS:HE2	1.94	0.48
2:F:370:VAL:O	2:F:370:VAL:HG13	2.13	0.48
6:Z:120:PHE:HB3	15:Z:202:CDL:C62	2.38	0.48
1:R:292:GLY:O	1:R:295:THR:OG1	2.25	0.48
15:R:604:CDL:C64	19:W:201:PLM:CG	2.90	0.48
2:E:123:HIS:NE2	16:E:601:HEM:ND	2.62	0.48
1:L:371:LEU:HD23	1:L:400:TYR:CE2	2.48	0.48
4:Q:160:ASP:N	4:Q:161:PRO:CD	2.76	0.48
10:O:184:PHE:O	10:O:188:CYS:N	2.45	0.48
6:Z:94:LEU:HD23	15:Z:202:CDL:H352	1.95	0.48
1:R:107:LEU:HD12	1:R:210:THR:HG22	1.94	0.48
2:E:281:ILE:HD12	10:I:271:GLU:CD	2.39	0.48
15:L:604:CDL:H612	15:J:201:CDL:H402	1.94	0.48
5:S:149:LEU:CG	15:S:301:CDL:H631	2.43	0.48
21:O:301:HEC:HHD	21:O:301:HEC:CBC	2.42	0.48
2:E:388:THR:HG22	2:E:392:MET:HE2	1.95	0.48
5:S:189:ASP:OD1	5:S:189:ASP:C	2.57	0.48
10:O:122:MET:SD	21:O:301:HEC:NA	2.87	0.48
15:X:301:CDL:H732	12:Y:145:ILE:HD13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:335:VAL:HG13	1:R:336:PRO:CD	2.43	0.48
2:F:421:ILE:HG13	15:P:201:CDL:H572	1.94	0.48
1:L:96:THR:O	1:L:99:VAL:HG22	2.14	0.48
1:L:221:LEU:HD22	5:X:35:SER:OG	2.14	0.48
11:W:42:VAL:HG12	11:W:54:VAL:HG13	1.95	0.48
2:F:282:ASN:ND2	16:F:703:HEM:O1A	2.43	0.48
1:R:221:LEU:HD22	5:S:35:SER:OG	2.14	0.47
2:F:306:MET:HE1	10:O:269:ALA:HA	1.95	0.47
1:R:77:GLU:OE2	4:Q:332:ARG:NH1	2.43	0.47
1:R:378:LEU:HD23	4:Q:50:TRP:CH2	2.49	0.47
2:E:107:GLN:NE2	2:E:276:GLY:O	2.46	0.47
2:F:275:MET:HE1	10:O:275:MET:HE1	1.95	0.47
1:L:31:LEU:HD23	15:L:604:CDL:H381	1.96	0.47
11:W:42:VAL:O	11:W:54:VAL:HG12	2.14	0.47
2:F:147:LEU:HD13	2:F:222:LEU:HB2	1.96	0.47
5:S:161:LEU:O	5:S:165:THR:HG23	2.14	0.47
12:M:44:ASP:OD1	12:M:45:ALA:N	2.46	0.47
1:R:194:VAL:CG1	6:T:1:MET:HE3	2.44	0.47
2:F:281:ILE:HD12	10:O:271:GLU:CD	2.39	0.47
1:L:33:THR:HG22	6:Z:90:TRP:HB3	1.97	0.47
1:R:50:ALA:CB	15:P:201:CDL:H401	2.44	0.47
2:E:212:ILE:HD11	2:F:212:ILE:HD11	1.95	0.47
4:Q:222:GLU:OE2	4:Q:257:VAL:HG21	2.14	0.47
1:L:392:TYR:CD2	1:L:452:LEU:HD23	2.49	0.47
4:K:197:ASN:OD1	4:K:197:ASN:N	2.48	0.47
12:Y:293:THR:HG23	12:Y:294:THR:HG23	1.96	0.47
1:R:29:TYR:O	1:R:33:THR:OG1	2.32	0.47
1:R:35:THR:O	1:R:35:THR:HG22	2.15	0.47
1:R:546:HIS:NE2	8:V:29:SER:OG	2.42	0.47
15:E:605:CDL:C11	15:F:704:CDL:OB7	2.63	0.47
2:F:244:THR:HG21	2:F:536:ILE:HG21	1.97	0.47
10:I:210:LEU:HD21	21:I:302:HEC:HHB	1.96	0.47
12:Y:230:THR:HG23	12:Y:244:THR:HG22	1.96	0.47
12:M:230:THR:HG22	12:M:231:ALA:N	2.30	0.47
12:M:265:PRO:CG	12:M:301:LEU:HD23	2.44	0.47
12:M:271:PRO:O	12:M:316:ARG:NH1	2.48	0.47
2:E:147:LEU:HD13	2:E:222:LEU:CB	2.44	0.47
5:X:167:MET:HE2	15:X:301:CDL:HA31	1.95	0.47
6:T:97:LEU:O	6:T:101:THR:HG23	2.15	0.47
5:X:41:ALA:CA	6:Z:44:LEU:HD22	2.45	0.47
10:I:234:ASP:O	10:I:238:THR:HA	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:388:THR:HG22	2:F:392:MET:HE2	1.97	0.47
15:L:604:CDL:HA4	15:J:201:CDL:H312	1.96	0.47
5:X:91:ALA:CB	5:X:99:LEU:HD12	2.45	0.47
1:R:406:ILE:HD11	14:R:603:HEA:HBC2	1.95	0.46
4:K:230:VAL:HG22	4:K:231:ILE:N	2.29	0.46
5:X:184:TYR:CZ	15:X:302:CDL:C73	2.91	0.46
5:X:184:TYR:CD1	15:X:302:CDL:C73	2.99	0.46
2:E:42:LEU:HD13	2:E:122:VAL:CG1	2.43	0.46
5:S:160:LEU:CD2	6:T:129:VAL:HG11	2.46	0.46
8:V:47:ASP:OD1	8:V:47:ASP:C	2.58	0.46
1:R:118:PHE:HB3	15:S:301:CDL:OA3	2.16	0.46
2:E:327:ILE:HG23	2:E:331:VAL:HG11	1.96	0.46
2:E:392:MET:SD	10:I:269:ALA:HB1	2.55	0.46
5:S:184:TYR:CZ	15:S:301:CDL:C73	2.97	0.46
1:R:310:VAL:HG11	1:R:333:ILE:HD13	1.98	0.46
2:E:440:VAL:HG21	2:E:486:LYS:HG2	1.97	0.46
2:F:17:ASP:OD2	2:F:23:SER:OG	2.18	0.46
1:L:46:VAL:CG1	15:J:201:CDL:H371	2.46	0.46
1:L:120:ARG:NH1	6:Z:131:GLU:OE1	2.44	0.46
6:Z:123:THR:HG23	15:Z:203:CDL:C33	2.45	0.46
1:R:35:THR:HG22	1:R:119:PRO:HB2	1.97	0.46
8:b:110:TYR:OH	8:b:123:ALA:HB2	2.16	0.46
1:L:104:ASN:OD1	1:L:122:ASN:ND2	2.48	0.46
1:L:186:GLY:O	1:L:190:ILE:HG22	2.16	0.46
1:R:403:PHE:CZ	1:R:407:VAL:HG11	2.50	0.46
2:E:194:PHE:CE2	2:E:203:LEU:HD22	2.51	0.46
8:V:44:PRO:O	8:V:47:ASP:OD1	2.34	0.46
8:b:99:VAL:HG21	8:b:134:PHE:CE2	2.51	0.46
10:I:112:ALA:HB2	10:I:224:THR:HG21	1.97	0.46
2:F:279:LEU:HD22	10:O:263:LEU:HD21	1.97	0.46
2:F:499:THR:HG22	2:F:511:HIS:ND1	2.30	0.46
7:U:32:HIS:NE2	8:V:43:PHE:O	2.47	0.46
11:c:75:PHE:CZ	11:c:114:VAL:HG11	2.50	0.46
10:I:184:PHE:O	10:I:188:CYS:N	2.46	0.46
21:I:302:HEC:CBB	21:I:302:HEC:HHC	2.45	0.46
12:Y:44:ASP:OD1	12:Y:45:ALA:N	2.48	0.46
12:M:243:TRP:NE1	12:M:310:ASN:O	2.41	0.46
1:R:190:ILE:HD11	6:T:8:PHE:HZ	1.81	0.46
1:R:532:GLU:OE2	8:V:23:THR:OG1	2.33	0.46
15:R:604:CDL:H552	15:R:604:CDL:H522	1.43	0.46
1:L:310:VAL:O	1:L:310:VAL:HG13	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:c:56:LEU:HD12	11:c:166:ILE:HD13	1.95	0.46
2:E:450:ILE:HD12	6:Z:81:GLU:OE2	2.16	0.46
1:L:419:PRO:CG	1:L:425:LEU:HD23	2.46	0.46
6:T:8:PHE:CE1	6:T:52:THR:HG21	2.51	0.46
15:X:301:CDL:H792	15:Z:203:CDL:C58	2.46	0.46
12:M:230:THR:HG23	12:M:244:THR:HG22	1.98	0.46
1:R:266:GLU:OE1	1:R:270:ILE:HD12	2.15	0.45
2:E:213:LEU:HD21	16:F:703:HEM:HBC1	1.98	0.45
6:T:120:PHE:CG	15:T:201:CDL:H632	2.51	0.45
17:Z:201:MQ9:H152	10:I:273:MET:HE3	1.97	0.45
1:R:56:GLY:N	1:R:90:MET:HE2	2.30	0.45
1:R:417:TRP:NE1	1:R:518:GLU:OE2	2.46	0.45
15:X:301:CDL:H622	15:X:301:CDL:H791	1.99	0.45
11:W:63:ASP:OD1	11:W:63:ASP:N	2.48	0.45
2:F:514:LEU:HD11	12:M:81:ALA:HB3	1.99	0.45
1:L:465:LEU:HD21	4:K:328:PHE:CD1	2.51	0.45
12:Y:335:ASN:ND2	12:Y:337:GLY:O	2.49	0.45
1:R:84:THR:O	1:R:88:THR:HG23	2.16	0.45
5:S:41:ALA:HA	6:T:44:LEU:HD22	1.98	0.45
4:K:145:GLN:O	4:K:158:GLY:N	2.49	0.45
5:X:25:VAL:HG12	5:X:180:VAL:HG11	1.99	0.45
12:Y:221:LYS:HG2	22:Y:503:9YF:O6	2.16	0.45
12:M:242:GLY:O	12:M:286:ARG:NH1	2.45	0.45
2:E:116:PHE:CE1	2:E:120:ILE:HD11	2.51	0.45
1:L:264:HIS:O	1:L:267:VAL:HG22	2.16	0.45
1:L:309:ALA:HB3	1:L:329:MET:HE1	1.98	0.45
5:S:163:ALA:HB1	15:T:202:CDL:HA61	1.98	0.45
10:O:122:MET:HA	10:O:122:MET:HE2	1.99	0.45
10:O:149:TYR:O	10:O:153:ASN:ND2	2.50	0.45
8:b:95:VAL:HG13	8:b:110:TYR:HE1	1.82	0.45
12:M:364:LEU:HD12	12:M:365:CYS:H	1.82	0.45
17:F:709:MQ9:H511	17:F:709:MQ9:H453	1.98	0.45
15:L:604:CDL:H711	15:L:604:CDL:C81	2.46	0.45
6:Z:91:TRP:N	6:Z:92:PRO:CD	2.80	0.45
10:I:72:GLN:OE1	10:I:74:ALA:N	2.50	0.45
15:E:605:CDL:H551	15:E:605:CDL:H581	1.70	0.45
2:F:147:LEU:HD13	2:F:222:LEU:CB	2.47	0.45
2:F:414:GLY:O	2:F:418:LEU:N	2.48	0.45
4:Q:32:ALA:HB1	4:Q:35:TRP:HB2	1.98	0.45
5:X:37:LEU:HD22	6:Z:51:ILE:HD12	1.99	0.45
6:Z:97:LEU:HD13	15:Z:202:CDL:H351	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:406:ILE:HD11	14:L:603:HEA:CBC	2.47	0.45
5:S:36:GLU:OE1	5:S:150:HIS:NE2	2.41	0.45
5:S:157:ALA:CB	15:S:301:CDL:H512	2.46	0.45
5:X:157:ALA:CB	15:X:302:CDL:H512	2.43	0.45
11:c:42:VAL:O	11:c:54:VAL:HG12	2.16	0.45
12:Y:230:THR:HG22	12:Y:231:ALA:N	2.32	0.45
1:L:505:VAL:HG13	1:L:505:VAL:O	2.15	0.45
4:Q:231:ILE:HD13	4:Q:246:LEU:CD2	2.35	0.44
4:K:159:ALA:C	4:K:161:PRO:HD3	2.43	0.44
12:Y:355:LEU:N	12:Y:355:LEU:HD12	2.32	0.44
2:E:506:ASP:OD2	12:Y:84:ARG:NH2	2.45	0.44
1:L:212:ASN:ND2	1:L:272:LEU:O	2.45	0.44
15:L:604:CDL:H742	15:L:604:CDL:H771	1.39	0.44
4:Q:195:TYR:CE2	4:Q:247:PRO:O	2.70	0.44
21:I:302:HEC:HBC3	21:I:302:HEC:HHD	1.99	0.44
21:I:302:HEC:HHD	21:I:302:HEC:CBC	2.46	0.44
2:E:56:THR:HG22	17:E:604:MQ9:H451	1.99	0.44
2:E:183:PRO:O	12:Y:417:TRP:CG	2.71	0.44
2:E:404:LEU:HD21	12:Y:369:GLN:HG2	1.99	0.44
2:F:147:LEU:HD21	2:F:223:ILE:HG13	1.99	0.44
2:F:409:TRP:CZ3	9:P:76:LEU:HD11	2.52	0.44
4:Q:230:VAL:O	4:Q:232:HIS:ND1	2.51	0.44
8:V:68:VAL:HG13	8:V:143:LEU:HD22	1.99	0.44
11:W:148:LEU:HD11	12:M:319:PRO:CB	2.46	0.44
1:L:111:ILE:HD12	1:L:196:MET:O	2.16	0.44
1:L:270:ILE:CG2	1:L:406:ILE:HG21	2.47	0.44
12:M:349:LEU:HD12	12:M:368:HIS:CE1	2.52	0.44
2:E:392:MET:HE1	17:I:303:MQ9:C3C	2.47	0.44
15:E:605:CDL:H332	15:E:605:CDL:H362	1.67	0.44
15:F:705:CDL:H542	15:F:705:CDL:H712	2.00	0.44
1:L:20:ARG:NH1	8:b:52:ASP:OD1	2.45	0.44
1:L:538:SER:OG	1:L:544:GLU:OE2	2.35	0.44
14:L:602:HEA:C18	14:L:602:HEA:H261	2.48	0.44
1:R:153:ALA:O	1:R:255:TRP:NE1	2.50	0.44
2:E:306:MET:HE1	10:I:269:ALA:HA	2.00	0.44
1:L:11:LEU:CD1	7:a:48:LEU:HD22	2.47	0.44
5:S:184:TYR:CD1	15:S:301:CDL:C73	3.01	0.44
12:M:172:VAL:HG13	12:M:173:HIS:N	2.33	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
2:F:267:MET:HE2	12:M:148:VAL:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:T:202:CDL:H622	15:T:202:CDL:H791	1.99	0.44
10:O:83:PHE:CZ	10:O:95:LEU:HD13	2.53	0.44
5:X:32:TRP:HB2	15:X:302:CDL:C33	2.44	0.44
9:J:33:VAL:HG11	9:J:41:SER:OG	2.18	0.44
12:M:358:GLN:C	12:M:360:THR:H	2.25	0.44
2:E:500:GLY:O	12:Y:84:ARG:CZ	2.66	0.44
2:E:512:GLU:O	2:E:516:GLU:CD	2.61	0.44
15:L:604:CDL:H381	15:L:604:CDL:H412	1.73	0.44
5:S:151:VAL:HG22	5:S:188:VAL:HG11	2.00	0.44
12:Y:243:TRP:NE1	12:Y:310:ASN:O	2.42	0.44
2:E:235:HIS:ND1	2:E:236:THR:O	2.47	0.44
2:F:135:ARG:NH1	2:F:358:ASP:O	2.51	0.44
1:L:323:LEU:HD23	4:K:117:GLN:CD	2.42	0.44
1:L:385:ASP:O	1:L:389:THR:CB	2.66	0.44
6:Z:8:PHE:CE2	6:Z:52:THR:HG21	2.52	0.44
21:I:302:HEC:HHC	21:I:302:HEC:HBB3	1.99	0.44
1:R:259:PHE:O	1:R:263:GLY:N	2.41	0.43
1:R:535:ARG:NH1	6:T:74:GLU:OE2	2.48	0.43
6:T:91:TRP:N	6:T:92:PRO:CD	2.81	0.43
10:O:72:GLN:OE1	10:O:75:LEU:N	2.49	0.43
10:O:210:LEU:HD22	21:O:302:HEC:C3A	2.48	0.43
1:R:248:ALA:HB3	4:Q:185:ILE:CD1	2.49	0.43
15:E:606:CDL:H722	15:Z:202:CDL:H111	2.00	0.43
4:K:140:TRP:NE1	4:K:284:MET:O	2.47	0.43
1:R:84:THR:HG21	1:R:147:ALA:HB3	2.00	0.43
1:R:252:VAL:HG22	4:Q:252:ASN:CG	2.43	0.43
1:L:50:ALA:CB	15:J:201:CDL:H401	2.48	0.43
8:V:78:ALA:O	8:V:82:ARG:NH1	2.51	0.43
8:V:114:VAL:HG12	8:V:119:ILE:HG21	2.00	0.43
12:Y:41:GLN:NE2	12:Y:46:GLU:OE2	2.51	0.43
1:R:63:ARG:HE	1:R:63:ARG:HA	1.83	0.43
2:F:233:GLN:O	2:F:234:LYS:C	2.60	0.43
4:Q:264:GLN:OE1	4:Q:264:GLN:N	2.50	0.43
4:K:195:TYR:CE1	4:K:247:PRO:O	2.72	0.43
4:K:232:HIS:HB2	4:K:273:CYS:SG	2.58	0.43
11:c:57:ARG:NH1	11:c:116:GLU:O	2.46	0.43
1:R:452:LEU:HD11	1:R:457:MET:SD	2.59	0.43
2:E:233:GLN:O	2:E:234:LYS:C	2.62	0.43
2:F:416:VAL:HG11	9:P:58:PHE:CD2	2.53	0.43
15:F:704:CDL:H621	15:F:704:CDL:H591	1.61	0.43
4:Q:179:ILE:HG23	4:Q:180:GLU:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:O:199:GLY:O	10:O:207:ALA:N	2.52	0.43
12:Y:195:VAL:HG23	12:Y:196:ILE:HD12	2.01	0.43
12:Y:271:PRO:O	12:Y:316:ARG:NH1	2.51	0.43
1:R:110:GLN:OE1	1:R:210:THR:HG23	2.18	0.43
2:E:147:LEU:HD21	2:E:223:ILE:HG13	2.00	0.43
1:L:313:HIS:CD2	1:L:313:HIS:C	2.96	0.43
4:K:193:ARG:NH2	10:I:137:HIS:O	2.52	0.43
11:c:174:ARG:NH1	12:Y:272:GLU:OE2	2.52	0.43
10:I:191:CYS:SG	10:I:201:LEU:HD21	2.59	0.43
2:F:123:HIS:NE2	16:F:702:HEM:ND	2.67	0.43
2:F:171:ILE:HD12	2:F:175:LEU:HD12	2.00	0.43
2:F:284:ILE:O	2:F:287:LEU:O	2.35	0.43
2:F:366:ARG:NH1	2:F:437:ASP:OD2	2.46	0.43
5:X:32:TRP:CG	15:X:302:CDL:C33	2.85	0.43
2:E:134:ARG:O	2:E:135:ARG:C	2.62	0.43
10:O:222:MET:HG3	21:O:302:HEC:HMB2	1.99	0.43
5:X:151:VAL:HG22	5:X:188:VAL:HG11	2.00	0.43
12:M:134:LEU:HD23	12:M:134:LEU:C	2.44	0.43
7:U:2:SER:O	7:U:5:LEU:N	2.51	0.43
10:O:189:ALA:O	10:O:190:SER:C	2.62	0.43
5:X:136:TYR:CD1	5:X:136:TYR:C	2.96	0.43
11:c:56:LEU:HD11	11:c:151:PHE:HE2	1.84	0.43
4:Q:139:ASN:OD1	4:Q:205:GLY:O	2.37	0.43
4:Q:332:ARG:NH2	11:W:27:GLY:O	2.44	0.43
7:a:2:SER:O	7:a:5:LEU:N	2.51	0.43
10:I:189:ALA:O	10:I:190:SER:C	2.62	0.43
12:Y:172:VAL:HG13	12:Y:173:HIS:N	2.33	0.43
11:W:107:PRO:HD3	11:W:112:LEU:HD12	1.99	0.43
1:R:31:LEU:O	1:R:34:THR:HG22	2.19	0.42
1:R:47:VAL:CG2	15:R:604:CDL:H371	2.49	0.42
2:F:225:ALA:HA	15:F:704:CDL:H351	2.01	0.42
2:F:312:ILE:CG1	2:F:333:VAL:HG21	2.48	0.42
1:L:242:ALA:O	5:X:138:SER:CB	2.66	0.42
6:T:120:PHE:HA	15:T:201:CDL:C61	2.48	0.42
10:O:123:PRO:O	10:O:125:MET:HE1	2.19	0.42
4:K:98:LEU:HD12	4:K:98:LEU:C	2.44	0.42
6:Z:95:ILE:CD1	6:Z:128:LEU:HD22	2.48	0.42
10:I:149:TYR:O	10:I:153:ASN:ND2	2.52	0.42
5:S:102:TRP:HE3	5:S:105:ILE:HD11	1.78	0.42
5:X:96:VAL:HG22	5:X:170:PHE:HB2	2.01	0.42
6:Z:123:THR:HG22	15:Z:203:CDL:H322	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Y:348:HIS:O	23:Y:501:FES:S1	2.77	0.42
12:Y:358:GLN:C	12:Y:360:THR:H	2.26	0.42
11:W:56:LEU:HD12	11:W:166:ILE:HD13	2.01	0.42
1:R:384:LEU:CD1	4:Q:49:LEU:HD23	2.48	0.42
15:R:604:CDL:H751	15:R:604:CDL:H562	2.00	0.42
2:F:56:THR:HA	17:F:709:MQ9:H451	2.01	0.42
14:L:603:HEA:H251	15:L:604:CDL:H632	2.00	0.42
4:Q:179:ILE:O	4:Q:180:GLU:C	2.62	0.42
15:T:203:CDL:HA22	10:O:293:ARG:CZ	2.49	0.42
12:Y:347:SER:O	12:Y:387:ARG:NH1	2.44	0.42
11:W:75:PHE:CE2	11:W:114:VAL:HG11	2.54	0.42
4:Q:121:MET:HE2	4:Q:123:LYS:HG3	2.02	0.42
8:V:76:ASP:N	8:V:76:ASP:OD1	2.52	0.42
8:b:62:ALA:O	8:b:117:ARG:NH2	2.52	0.42
1:R:88:THR:HG22	1:R:151:TRP:CD1	2.53	0.42
2:F:311:LEU:HD23	2:F:333:VAL:HG23	2.00	0.42
5:X:160:LEU:CD2	6:Z:129:VAL:HG11	2.49	0.42
15:X:301:CDL:H312	15:X:301:CDL:HA61	1.82	0.42
15:X:301:CDL:C75	15:Z:203:CDL:H532	2.50	0.42
11:W:42:VAL:HG22	11:W:43:ASN:N	2.35	0.42
1:L:290:ILE:HG23	1:L:290:ILE:O	2.18	0.42
15:L:604:CDL:H312	15:L:604:CDL:H342	1.91	0.42
4:Q:186:ARG:NH1	5:S:53:GLN:O	2.45	0.42
5:S:96:VAL:HG22	5:S:170:PHE:CB	2.50	0.42
8:V:119:ILE:HG23	8:V:120:GLU:N	2.35	0.42
1:R:111:ILE:HD12	1:R:196:MET:O	2.19	0.42
1:R:424:ARG:NH1	1:R:500:ARG:O	2.52	0.42
15:F:704:CDL:H551	15:F:704:CDL:H581	1.70	0.42
6:T:97:LEU:HD13	15:T:201:CDL:H351	2.01	0.42
5:X:103:TYR:OH	5:X:178:ALA:O	2.38	0.42
8:b:68:VAL:HG13	8:b:143:LEU:HD22	2.01	0.42
11:W:70:THR:HG23	11:W:70:THR:O	2.20	0.42
12:M:345:VAL:HG23	12:M:345:VAL:O	2.19	0.42
2:E:225:ALA:HA	15:E:605:CDL:H351	2.00	0.42
2:F:422:VAL:CG2	15:F:705:CDL:H402	2.49	0.42
4:Q:96:LEU:HA	4:Q:99:THR:HG22	2.01	0.42
5:S:149:LEU:HG	15:S:301:CDL:H631	2.02	0.42
4:K:281:HIS:O	4:K:281:HIS:ND1	2.53	0.42
8:b:50:VAL:HG22	9:J:99:ILE:HD11	2.00	0.42
12:Y:387:ARG:CZ	12:Y:415:ALA:HB2	2.50	0.42
12:M:42:PRO:O	12:M:43:THR:OG1	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:364:LEU:HD12	12:M:365:CYS:N	2.35	0.42
1:R:454:ASP:OD1	4:Q:35:TRP:CD1	2.73	0.42
15:R:604:CDL:H531	15:R:604:CDL:H712	2.02	0.42
15:R:604:CDL:H612	15:P:201:CDL:H402	2.01	0.42
2:F:68:MET:HE1	2:F:204:ILE:H	1.85	0.42
2:F:404:LEU:HD21	12:M:369:GLN:HG3	2.02	0.42
15:L:604:CDL:H552	15:L:604:CDL:H522	1.68	0.42
4:K:179:ILE:O	4:K:180:GLU:C	2.62	0.42
5:X:36:GLU:OE1	5:X:150:HIS:NE2	2.44	0.42
1:R:399:HIS:O	1:R:403:PHE:N	2.53	0.42
2:F:340:VAL:HG22	17:F:708:MQ9:H401	2.01	0.42
1:L:194:VAL:CG1	6:Z:1:MET:HE3	2.49	0.42
1:L:287:ARG:O	4:K:87:GLN:NE2	2.53	0.42
1:L:522:SER:OG	1:L:524:PRO:O	2.37	0.42
11:c:42:VAL:HG22	11:c:43:ASN:N	2.34	0.42
10:I:190:SER:O	12:Y:355:LEU:HD11	2.20	0.42
1:R:193:VAL:HG11	1:R:214:LEU:HD13	2.01	0.41
2:F:425:VAL:CG1	15:F:705:CDL:H371	2.45	0.41
1:L:26:ASN:OD1	1:L:26:ASN:C	2.63	0.41
4:Q:204:LEU:HD22	10:O:84:GLU:HB3	2.01	0.41
12:Y:190:LEU:O	12:Y:191:LYS:CG	2.68	0.41
12:M:46:GLU:OE1	12:M:46:GLU:N	2.50	0.41
2:E:147:LEU:HD13	2:E:222:LEU:HB2	2.01	0.41
2:E:532:HIS:CD2	2:E:536:ILE:HD11	2.55	0.41
2:F:420:ALA:HB2	15:P:201:CDL:H771	2.01	0.41
4:Q:236:VAL:O	4:Q:239:PHE:N	2.49	0.41
15:T:203:CDL:H381	15:T:203:CDL:H411	1.62	0.41
15:Z:203:CDL:OB4	10:I:289:TRP:HD1	2.03	0.41
15:Z:203:CDL:HB22	10:I:293:ARG:HH12	1.84	0.41
10:I:191:CYS:CB	21:I:302:HEC:HBC2	2.50	0.41
10:I:269:ALA:HB3	10:I:270:PRO:CD	2.47	0.41
12:M:344:LYS:O	12:M:353:SER:N	2.44	0.41
1:R:310:VAL:O	1:R:310:VAL:HG13	2.20	0.41
1:R:420:LYS:NZ	1:R:521:THR:O	2.53	0.41
17:E:603:MQ9:H403	17:E:603:MQ9:H421	1.82	0.41
15:F:705:CDL:H391	15:T:201:CDL:C42	2.50	0.41
4:Q:135:ALA:O	4:Q:232:HIS:NE2	2.53	0.41
10:O:229:MET:HE3	21:O:302:HEC:C4B	2.50	0.41
8:b:108:VAL:HG12	8:b:110:TYR:CE1	2.55	0.41
10:I:122:MET:HE3	10:I:122:MET:HA	2.01	0.41
10:I:263:LEU:HD12	10:I:263:LEU:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Y:159:ILE:O	12:Y:159:ILE:HG22	2.20	0.41
15:R:604:CDL:H512	15:R:604:CDL:H732	2.01	0.41
2:F:449:ILE:HD13	6:T:85:PHE:HD2	1.86	0.41
4:Q:101:ILE:HG22	4:Q:102:PRO:HD3	2.03	0.41
6:T:48:LEU:HD23	6:T:48:LEU:C	2.46	0.41
10:O:289:TRP:O	12:M:152:LYS:NZ	2.46	0.41
1:R:90:MET:HB3	14:R:603:HEA:CAC	2.50	0.41
15:R:604:CDL:H381	15:R:604:CDL:H412	1.39	0.41
6:T:8:PHE:CZ	6:T:52:THR:HG21	2.55	0.41
5:X:102:TRP:CE3	5:X:105:ILE:HD11	2.55	0.41
10:I:210:LEU:HD21	21:I:302:HEC:CHB	2.51	0.41
12:Y:85:THR:HG21	12:Y:153:LYS:HB3	2.01	0.41
12:M:195:VAL:HG23	12:M:196:ILE:HD12	2.02	0.41
1:R:419:PRO:CG	1:R:425:LEU:HD23	2.50	0.41
1:L:56:GLY:HA2	1:L:90:MET:HE2	2.02	0.41
12:M:190:LEU:O	12:M:191:LYS:CG	2.69	0.41
2:F:107:GLN:NE2	2:F:276:GLY:O	2.53	0.41
2:F:183:PRO:O	12:M:417:TRP:CG	2.74	0.41
2:F:400:PHE:HA	6:T:108:LEU:HD13	2.01	0.41
15:F:704:CDL:H332	15:F:704:CDL:H362	1.67	0.41
1:L:163:SER:O	1:L:163:SER:OG	2.36	0.41
1:L:221:LEU:HD13	5:X:31:VAL:HG13	2.03	0.41
5:S:80:SER:HA	5:S:109:MET:HE3	2.02	0.41
4:K:199:ASP:N	4:K:202:GLU:OE2	2.51	0.41
4:K:219:LYS:O	4:K:221:ILE:HD12	2.20	0.41
15:X:301:CDL:H761	15:Z:203:CDL:C53	2.37	0.41
1:R:256:GLN:HB3	1:R:315:MET:SD	2.61	0.41
2:E:267:MET:HE2	12:Y:148:VAL:HG21	2.03	0.41
2:F:441:LEU:HD21	2:F:484:LEU:HD21	2.02	0.41
15:L:604:CDL:H312	15:L:604:CDL:HA61	1.62	0.41
5:S:32:TRP:HB3	15:S:301:CDL:H331	1.95	0.41
15:X:301:CDL:H141	15:X:301:CDL:H712	2.03	0.41
1:R:194:VAL:HG13	6:T:1:MET:HE3	2.03	0.41
2:F:59:TRP:CE3	2:F:105:VAL:HG11	2.56	0.41
1:L:159:ASP:O	1:L:162:HIS:O	2.38	0.41
4:Q:128:GLU:OE1	4:Q:220:ARG:N	2.46	0.41
4:Q:139:ASN:HD22	4:Q:139:ASN:HA	1.63	0.41
4:Q:168:THR:HG23	4:Q:168:THR:O	2.20	0.41
5:X:163:ALA:HB1	15:X:301:CDL:HA61	2.03	0.41
7:a:2:SER:O	7:a:3:THR:C	2.64	0.41
9:J:85:ALA:HB1	15:J:201:CDL:H161	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:116:GLN:HG2	10:I:122:MET:SD	2.61	0.41
11:W:103:ASP:HA	11:W:133:VAL:HG13	2.03	0.41
2:E:367:PRO:O	2:E:374:THR:OG1	2.25	0.41
2:F:208:TYR:CE2	2:F:212:ILE:HD13	2.55	0.41
2:F:392:MET:SD	10:O:269:ALA:HB1	2.61	0.41
15:F:705:CDL:H762	15:F:705:CDL:H792	1.80	0.41
5:X:32:TRP:HZ2	15:X:302:CDL:C38	2.25	0.41
9:J:48:MET:HG2	15:J:201:CDL:HB61	2.03	0.41
2:E:59:TRP:CE3	2:E:105:VAL:HG11	2.56	0.40
1:L:153:ALA:HB1	1:L:158:THR:HG21	2.04	0.40
1:L:252:VAL:HG11	4:K:247:PRO:HD2	2.04	0.40
1:L:384:LEU:CD1	4:K:49:LEU:HD23	2.52	0.40
7:U:2:SER:O	7:U:3:THR:C	2.64	0.40
4:K:319:PRO:HA	4:K:320:PRO:HD3	1.99	0.40
12:Y:345:VAL:HG23	12:Y:345:VAL:O	2.21	0.40
1:R:221:LEU:HD13	5:S:31:VAL:HG13	2.02	0.40
1:R:371:LEU:HD23	1:R:400:TYR:HE2	1.86	0.40
1:R:401:VAL:HG23	1:R:402:LEU:N	2.36	0.40
2:F:92:ALA:HB1	2:F:284:ILE:HD13	2.03	0.40
1:L:103:ALA:HB1	1:L:189:MET:SD	2.61	0.40
1:L:153:ALA:O	1:L:255:TRP:NE1	2.54	0.40
6:T:87:PRO:O	6:T:88:HIS:C	2.64	0.40
9:P:85:ALA:HB1	15:P:201:CDL:H161	2.03	0.40
21:O:301:HEC:CMB	21:O:301:HEC:HBB3	2.51	0.40
4:K:222:GLU:OE2	4:K:257:VAL:HG21	2.21	0.40
9:J:7:ARG:NH1	9:J:9:GLN:OE1	2.55	0.40
10:I:221:ALA:O	10:I:224:THR:O	2.40	0.40
12:Y:281:THR:HG23	12:Y:344:LYS:CD	2.52	0.40
2:E:178:ILE:HD11	2:E:312:ILE:HD11	2.03	0.40
2:F:116:PHE:CE1	2:F:120:ILE:HD11	2.56	0.40
5:S:32:TRP:CZ2	15:S:301:CDL:C36	3.00	0.40
4:K:135:ALA:C	4:K:232:HIS:HE2	2.28	0.40
15:X:301:CDL:C77	15:Z:203:CDL:H532	2.51	0.40
6:Z:87:PRO:O	6:Z:88:HIS:C	2.62	0.40
12:Y:255:ALA:HB2	12:Y:285:TRP:HB3	2.04	0.40
1:L:398:PHE:CD1	1:L:398:PHE:C	2.99	0.40
4:Q:288:VAL:HG13	4:Q:288:VAL:O	2.21	0.40
10:O:191:CYS:HB3	21:O:302:HEC:HBC2	1.98	0.40
15:Z:203:CDL:H611	10:I:278:ILE:HG23	2.02	0.40
8:b:39:VAL:HG23	8:b:40:HIS:N	2.37	0.40
1:R:122:ASN:OD1	1:R:122:ASN:C	2.65	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:41:ALA:HB2	6:T:44:LEU:CB	2.52	0.40
7:U:56:GLU:O	7:U:57:HIS:C	2.63	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	76
3	D	214/216 (99%)	193 (90%)	20 (9%)	1 (0%)	24	60
3	G	214/216 (99%)	187 (87%)	27 (13%)	0	100	100
4	K	310/341 (91%)	282 (91%)	28 (9%)	0	100	100
4	Q	310/341 (91%)	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	38
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
9	J	88/100 (88%)	85 (97%)	3 (3%)	0	100	100
9	P	88/100 (88%)	84 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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	70
All	All	6016/6176 (97%)	5549 (92%)	463 (8%)	4 (0%)	49	80

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	135	ARG
12	Y	113	GLU
3	D	27	THR
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	80
1	R	452/465 (97%)	447 (99%)	5 (1%)	65	83
2	E	429/429 (100%)	423 (99%)	6 (1%)	59	80
2	F	429/429 (100%)	423 (99%)	6 (1%)	59	80
3	D	20/151 (13%)	20 (100%)	0	100	100
3	G	20/151 (13%)	20 (100%)	0	100	100
4	K	260/288 (90%)	257 (99%)	3 (1%)	63	82
4	Q	260/288 (90%)	258 (99%)	2 (1%)	73	86
5	S	155/161 (96%)	153 (99%)	2 (1%)	61	81
5	X	155/161 (96%)	152 (98%)	3 (2%)	50	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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	76
8	b	107/107 (100%)	106 (99%)	1 (1%)	70	85
9	J	76/83 (92%)	73 (96%)	3 (4%)	28	62
9	P	76/83 (92%)	75 (99%)	1 (1%)	61	81
10	I	163/163 (100%)	160 (98%)	3 (2%)	51	77
10	O	163/163 (100%)	162 (99%)	1 (1%)	78	88
11	W	127/127 (100%)	127 (100%)	0	100	100
11	c	127/127 (100%)	126 (99%)	1 (1%)	73	86
12	M	312/312 (100%)	310 (99%)	2 (1%)	78	88
12	Y	312/312 (100%)	309 (99%)	3 (1%)	68	84
All	All	4532/4902 (92%)	4481 (99%)	51 (1%)	63	83

All (51) 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
2	F	280	THR
2	F	352	LYS
2	F	357	ASP
2	F	358	ASP
1	L	63	ARG

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Mol	Chain	Res	Type
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
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 (21) 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
2	F	532	HIS

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Mol	Chain	Res	Type
1	L	76	ASN
1	L	249	ASN
4	Q	145	GLN
4	Q	265	GLN
7	U	64	HIS
4	K	145	GLN
4	K	265	GLN
5	X	127	HIS
6	Z	139	HIS
7	a	64	HIS
11	c	31	GLN
10	I	81	GLN
10	I	137	HIS
10	I	169	GLN
12	Y	180	ASN
12	M	331	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 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
20	9XX	G	302	3	31,31,41	1.12	3 (9%)	34,34,44	1.47	5 (14%)
17	MQ9	I	303	-	59,59,59	2.39	22 (37%)	73,75,75	1.43	17 (23%)
19	PLM	W	201	11	15,16,17	0.49	0	14,15,17	0.33	0
22	9YF	W	203	-	58,58,58	1.01	5 (8%)	68,71,71	1.13	3 (4%)
15	CDL	L	604	-	75,75,99	0.34	0	81,87,111	0.72	3 (3%)
20	9XX	D	302	-	31,31,41	1.11	3 (9%)	34,34,44	1.44	4 (11%)
15	CDL	T	203	-	75,75,99	0.37	0	81,87,111	0.45	0
18	9Y0	X	303	-	48,48,48	1.16	3 (6%)	51,53,53	0.90	2 (3%)
22	9YF	Y	502	-	58,58,58	1.08	7 (12%)	68,71,71	1.30	7 (10%)
23	FES	Y	501	12	0,4,4	-	-	-		
16	HEM	E	602	2	50,50,50	1.42	7 (14%)	67,82,82	1.14	5 (7%)
16	HEM	F	702	2	49,49,50	1.37	5 (10%)	67,81,82	1.03	2 (2%)
15	CDL	S	301	-	75,75,99	1.33	7 (9%)	81,87,111	1.99	9 (11%)
15	CDL	R	604	-	75,75,99	0.34	0	81,87,111	0.60	2 (2%)
18	9Y0	J	202	-	48,48,48	1.17	3 (6%)	51,53,53	0.90	2 (3%)
16	HEM	E	601	2	49,49,50	1.38	7 (14%)	67,81,82	1.05	2 (2%)
22	9YF	M	501	-	58,58,58	1.08	7 (12%)	68,71,71	1.29	7 (10%)
17	MQ9	F	701	-	59,59,59	2.45	23 (38%)	73,75,75	1.38	15 (20%)
19	PLM	G	301	3	9,10,17	0.54	0	8,9,17	0.43	0
15	CDL	E	606	-	75,75,99	0.36	0	81,87,111	0.42	0
21	HEC	O	302	10	50,50,50	1.72	6 (12%)	68,82,82	1.43	7 (10%)
14	HEA	L	602	1	67,67,67	1.42	11 (16%)	81,103,103	2.38	30 (37%)
21	HEC	I	301	-	50,50,50	1.78	5 (10%)	68,82,82	1.32	5 (7%)
17	MQ9	E	603	-	59,59,59	2.44	23 (38%)	73,75,75	1.38	14 (19%)
20	9XX	W	202	-	41,41,41	1.10	4 (9%)	44,44,44	1.19	3 (6%)
16	HEM	F	703	2	50,50,50	1.40	6 (12%)	67,82,82	1.11	3 (4%)
17	MQ9	E	604	-	59,59,59	2.42	22 (37%)	73,75,75	1.53	16 (21%)
17	MQ9	F	708	-	59,59,59	2.30	22 (37%)	73,75,75	1.42	8 (10%)
15	CDL	Z	203	-	75,75,99	1.32	7 (9%)	81,87,111	2.04	9 (11%)
14	HEA	R	602	1	67,67,67	1.44	10 (14%)	81,103,103	2.33	31 (38%)
17	MQ9	F	709	-	59,59,59	2.43	22 (37%)	73,75,75	1.54	15 (20%)
18	9Y0	J	203	-	48,48,48	1.16	3 (6%)	51,53,53	0.78	2 (3%)
14	HEA	R	603	1	67,67,67	1.37	10 (14%)	81,103,103	2.04	18 (22%)
17	MQ9	Z	201	-	59,59,59	2.36	22 (37%)	73,75,75	1.63	16 (21%)
15	CDL	Z	202	-	75,75,99	1.26	9 (12%)	81,87,111	1.83	15 (18%)
22	9YF	I	304	-	58,58,58	1.05	5 (8%)	68,71,71	1.01	3 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
21	HEC	O	301	10	50,50,50	1.81	5 (10%)	68,82,82	1.28	6 (8%)
18	9Y0	F	706	2	48,48,48	1.17	3 (6%)	51,53,53	0.87	2 (3%)
19	PLM	D	301	3	9,10,17	0.53	0	8,9,17	0.43	0
20	9XX	c	202	11	41,41,41	0.96	3 (7%)	44,44,44	1.18	4 (9%)
22	9YF	Y	503	-	58,58,58	1.09	5 (8%)	68,71,71	1.33	5 (7%)
15	CDL	P	201	-	75,75,99	0.33	0	81,87,111	0.45	0
15	CDL	F	704	-	75,75,99	0.34	0	81,87,111	0.42	0
15	CDL	J	201	-	75,75,99	0.33	0	81,87,111	0.45	0
15	CDL	T	202	-	75,75,99	0.33	0	81,87,111	0.40	0
19	PLM	c	201	11	15,16,17	0.47	0	14,15,17	0.35	0
18	9Y0	S	302	-	48,48,48	1.16	3 (6%)	51,53,53	0.87	2 (3%)
18	9Y0	P	202	-	48,48,48	1.20	3 (6%)	51,53,53	0.95	2 (3%)
15	CDL	E	605	-	75,75,99	0.34	0	81,87,111	0.42	0
15	CDL	X	302	-	75,75,99	1.33	7 (9%)	81,87,111	1.99	9 (11%)
22	9YF	c	203	-	58,58,58	1.01	5 (8%)	68,71,71	1.13	3 (4%)
15	CDL	T	201	-	75,75,99	1.26	9 (12%)	81,87,111	1.83	15 (18%)
22	9YF	M	502	-	58,58,58	1.10	5 (8%)	68,71,71	1.33	5 (7%)
17	MQ9	F	707	-	59,59,59	2.25	21 (35%)	73,75,75	1.73	22 (30%)
23	FES	M	503	12	0,4,4	-	-	-		
15	CDL	F	705	-	75,75,99	0.37	0	81,87,111	0.46	1 (1%)
21	HEC	I	302	10	50,50,50	1.73	6 (12%)	68,82,82	1.65	11 (16%)
22	9YF	O	303	-	58,58,58	1.05	5 (8%)	68,71,71	1.01	3 (4%)
14	HEA	L	603	1	67,67,67	1.37	10 (14%)	81,103,103	1.92	19 (23%)
15	CDL	X	301	-	75,75,99	0.33	0	81,87,111	0.40	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	9XX	G	302	3	-	10/33/33/43	-
17	MQ9	I	303	-	-	8/53/73/73	0/2/2/2
19	PLM	W	201	11	-	4/14/14/15	-
22	9YF	W	203	-	-	22/54/78/78	0/1/1/1
15	CDL	L	604	-	-	48/86/86/110	-
20	9XX	D	302	-	-	9/33/33/43	-
15	CDL	T	203	-	-	47/86/86/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	9Y0	X	303	-	-	17/52/52/52	-
22	9YF	Y	502	-	-	23/54/78/78	0/1/1/1
23	FES	Y	501	12	-	-	0/1/1/1
16	HEM	E	602	2	-	2/14/54/54	-
16	HEM	F	702	2	-	4/12/52/54	-
15	CDL	S	301	-	-	43/86/86/110	-
15	CDL	R	604	-	-	47/86/86/110	-
18	9Y0	J	202	-	-	19/52/52/52	-
16	HEM	E	601	2	-	2/12/52/54	-
22	9YF	M	501	-	-	23/54/78/78	0/1/1/1
17	MQ9	F	701	-	-	6/53/73/73	0/2/2/2
19	PLM	G	301	3	-	2/8/8/15	-
15	CDL	E	606	-	-	40/86/86/110	-
21	HEC	O	302	10	1/1/7/7	6/14/54/54	-
14	HEA	L	602	1	-	12/36/76/76	-
21	HEC	I	301	-	-	6/14/54/54	-
17	MQ9	E	603	-	-	6/53/73/73	0/2/2/2
20	9XX	W	202	-	-	15/43/43/43	-
16	HEM	F	703	2	-	0/14/54/54	-
17	MQ9	E	604	-	-	11/53/73/73	0/2/2/2
17	MQ9	F	708	-	-	11/53/73/73	0/2/2/2
15	CDL	Z	203	-	-	38/86/86/110	-
14	HEA	R	602	1	-	7/36/76/76	-
17	MQ9	F	709	-	-	12/53/73/73	0/2/2/2
18	9Y0	J	203	-	-	25/52/52/52	-
14	HEA	R	603	1	-	3/36/76/76	-
17	MQ9	Z	201	-	-	11/53/73/73	0/2/2/2
15	CDL	Z	202	-	-	34/86/86/110	-
22	9YF	I	304	-	-	27/54/78/78	0/1/1/1
21	HEC	O	301	10	-	6/14/54/54	-
18	9Y0	F	706	2	-	16/52/52/52	-
19	PLM	D	301	3	-	3/8/8/15	-
20	9XX	c	202	11	-	16/43/43/43	-
22	9YF	Y	503	-	-	27/54/78/78	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CDL	P	201	-	-	48/86/86/110	-
15	CDL	F	704	-	-	49/86/86/110	-
15	CDL	J	201	-	-	48/86/86/110	-
15	CDL	T	202	-	-	46/86/86/110	-
19	PLM	c	201	11	-	5/14/14/15	-
18	9Y0	S	302	-	-	19/52/52/52	-
18	9Y0	P	202	-	-	22/52/52/52	-
15	CDL	E	605	-	-	49/86/86/110	-
15	CDL	X	302	-	-	43/86/86/110	-
22	9YF	c	203	-	-	22/54/78/78	0/1/1/1
15	CDL	T	201	-	-	34/86/86/110	-
22	9YF	M	502	-	-	27/54/78/78	0/1/1/1
17	MQ9	F	707	-	-	17/53/73/73	0/2/2/2
23	FES	M	503	12	-	-	0/1/1/1
15	CDL	F	705	-	-	43/86/86/110	-
21	HEC	I	302	10	1/1/7/7	5/14/54/54	-
22	9YF	O	303	-	-	27/54/78/78	0/1/1/1
14	HEA	L	603	1	-	3/36/76/76	-
15	CDL	X	301	-	-	46/86/86/110	-

All (379) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	F	709	MQ9	C6-C5	8.77	1.50	1.35
17	E	604	MQ9	C6-C5	8.77	1.50	1.35
17	F	701	MQ9	C6-C5	8.59	1.50	1.35
17	F	708	MQ9	C6-C5	8.56	1.50	1.35
17	E	603	MQ9	C6-C5	8.53	1.50	1.35
17	I	303	MQ9	C6-C5	8.49	1.50	1.35
17	Z	201	MQ9	C6-C5	8.28	1.50	1.35
17	F	707	MQ9	C6-C5	8.14	1.49	1.35
21	O	301	HEC	C3D-C2D	7.91	1.53	1.36
21	O	302	HEC	C3D-C2D	7.87	1.53	1.36
21	I	301	HEC	C3D-C2D	7.86	1.53	1.36
21	I	302	HEC	C3D-C2D	7.71	1.53	1.36
17	F	709	MQ9	C2-C1	5.05	1.57	1.48
17	F	701	MQ9	C2-C1	5.01	1.57	1.48
17	E	604	MQ9	C2-C1	5.00	1.57	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Z	201	MQ9	C2-C1	4.96	1.57	1.48
17	E	603	MQ9	C2-C1	4.95	1.57	1.48
17	I	303	MQ9	C2-C1	4.93	1.57	1.48
17	I	303	MQ9	C3-C4	4.75	1.57	1.48
17	F	709	MQ9	C3-C4	4.66	1.57	1.48
17	E	603	MQ9	C3-C4	4.65	1.57	1.48
17	F	701	MQ9	C3-C4	4.62	1.57	1.48
17	E	604	MQ9	C3-C4	4.61	1.57	1.48
17	F	709	MQ9	C26-C24	4.61	1.60	1.51
17	F	708	MQ9	C2-C1	4.56	1.57	1.48
17	Z	201	MQ9	C3-C4	4.54	1.57	1.48
17	F	708	MQ9	C3-C4	4.54	1.56	1.48
17	E	604	MQ9	C26-C24	4.52	1.60	1.51
17	E	603	MQ9	C26-C24	4.49	1.60	1.51
17	F	701	MQ9	C26-C24	4.49	1.60	1.51
17	F	707	MQ9	C26-C24	4.46	1.60	1.51
17	I	303	MQ9	C26-C24	4.46	1.60	1.51
17	Z	201	MQ9	C26-C24	4.40	1.60	1.51
17	F	707	MQ9	C11-C9	4.37	1.60	1.51
14	R	602	HEA	C3B-C2B	4.36	1.44	1.34
21	O	301	HEC	FE-ND	4.32	2.08	1.94
21	I	301	HEC	FE-ND	4.30	2.08	1.94
14	R	603	HEA	C3B-C2B	4.30	1.44	1.34
17	F	707	MQ9	C3-C4	4.28	1.56	1.48
14	L	603	HEA	C3B-C2B	4.20	1.44	1.34
14	L	602	HEA	C3B-C2B	4.13	1.44	1.34
17	E	603	MQ9	C31-C29	4.13	1.59	1.51
21	I	301	HEC	FE-NB	4.12	2.07	1.94
17	F	701	MQ9	C31-C29	4.10	1.59	1.51
17	F	707	MQ9	C2-C1	4.08	1.56	1.48
17	F	708	MQ9	C26-C24	4.06	1.59	1.51
17	Z	201	MQ9	C11-C9	4.05	1.59	1.51
17	E	604	MQ9	C11-C9	4.00	1.59	1.51
17	F	709	MQ9	C31-C29	3.98	1.59	1.51
16	E	602	HEM	FE-ND	3.92	2.07	1.94
17	F	709	MQ9	C11-C9	3.92	1.59	1.51
20	G	302	9XX	O1-C17	-3.90	1.40	1.47
20	W	202	9XX	O1-C17	-3.88	1.40	1.47
17	I	303	MQ9	C31-C29	3.88	1.59	1.51
21	I	302	HEC	FE-NB	3.86	2.06	1.94
17	I	303	MQ9	C11-C9	3.86	1.59	1.51
17	E	604	MQ9	C31-C29	3.86	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	O	302	HEC	FE-NB	3.84	2.06	1.94
21	O	302	HEC	FE-ND	3.84	2.06	1.94
20	D	302	9XX	O1-C17	-3.81	1.40	1.47
17	F	701	MQ9	C11-C9	3.80	1.59	1.51
17	Z	201	MQ9	C31-C29	3.80	1.59	1.51
16	F	703	HEM	FE-ND	3.78	2.06	1.94
14	L	602	HEA	C3D-C2D	3.77	1.44	1.36
17	E	603	MQ9	C11-C9	3.75	1.59	1.51
21	O	301	HEC	FE-NB	3.74	2.06	1.94
17	F	708	MQ9	C11-C9	3.74	1.59	1.51
21	O	301	HEC	FE-NA	3.73	2.07	1.95
20	c	202	9XX	O1-C17	-3.72	1.40	1.47
14	L	603	HEA	C3D-C2D	3.67	1.44	1.36
20	W	202	9XX	O-C15	3.67	1.44	1.33
14	R	602	HEA	C3D-C2D	3.64	1.44	1.36
17	F	707	MQ9	C16-C14	3.60	1.58	1.51
16	E	602	HEM	FE-NB	3.59	2.05	1.94
21	I	302	HEC	FE-ND	3.56	2.05	1.94
14	R	602	HEA	C4D-C3D	3.54	1.51	1.45
14	R	603	HEA	C3D-C2D	3.54	1.44	1.36
14	R	602	HEA	C3A-C2A	3.45	1.45	1.37
14	L	602	HEA	C3A-C2A	3.42	1.45	1.37
17	F	708	MQ9	C27-C28	3.40	1.60	1.50
17	F	708	MQ9	C7-C6	3.29	1.57	1.51
17	E	603	MQ9	C22-C23	3.29	1.60	1.50
14	L	602	HEA	C4B-C3B	3.28	1.50	1.44
18	X	303	9Y0	O7-C1	-3.28	1.38	1.46
18	S	302	9Y0	O7-C1	-3.27	1.38	1.46
17	E	604	MQ9	C22-C23	3.26	1.60	1.50
15	T	201	CDL	OA6-CA4	-3.26	1.38	1.46
17	F	709	MQ9	C22-C23	3.26	1.60	1.50
15	Z	202	CDL	OA6-CA4	-3.25	1.38	1.46
17	E	604	MQ9	C21-C19	3.25	1.58	1.51
17	F	701	MQ9	C22-C23	3.23	1.60	1.50
17	F	709	MQ9	C21-C19	3.22	1.57	1.51
16	E	601	HEM	FE-ND	3.22	2.04	1.94
16	E	601	HEM	FE-NB	3.21	2.04	1.94
17	I	303	MQ9	C27-C28	3.21	1.60	1.50
16	F	703	HEM	FE-NB	3.21	2.04	1.94
17	I	303	MQ9	C16-C14	3.20	1.57	1.51
17	I	303	MQ9	C22-C23	3.19	1.60	1.50
18	J	202	9Y0	O7-C1	-3.19	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	E	603	MQ9	C21-C19	3.19	1.57	1.51
18	F	706	9Y0	O7-C1	-3.17	1.39	1.46
17	F	701	MQ9	C21-C19	3.17	1.57	1.51
18	J	203	9Y0	O7-C1	-3.16	1.39	1.46
17	F	707	MQ9	C31-C29	3.15	1.57	1.51
17	E	604	MQ9	C16-C14	3.14	1.57	1.51
17	F	709	MQ9	C16-C14	3.14	1.57	1.51
21	O	301	HEC	FE-NC	3.13	2.05	1.95
17	E	603	MQ9	C41-C39	3.12	1.57	1.51
17	Z	201	MQ9	C21-C19	3.12	1.57	1.51
17	I	303	MQ9	C21-C19	3.11	1.57	1.51
17	Z	201	MQ9	C7-C8	3.11	1.55	1.50
17	F	707	MQ9	C21-C19	3.10	1.57	1.51
17	Z	201	MQ9	C22-C23	3.10	1.59	1.50
17	E	603	MQ9	C27-C28	3.10	1.59	1.50
17	F	708	MQ9	C31-C29	3.10	1.57	1.51
14	R	602	HEA	C4B-C3B	3.09	1.50	1.44
16	F	702	HEM	FE-NA	3.09	2.05	1.95
21	I	301	HEC	FE-NC	3.09	2.05	1.95
16	E	601	HEM	FE-NA	3.09	2.05	1.95
17	F	701	MQ9	C27-C28	3.08	1.59	1.50
17	F	708	MQ9	C22-C23	3.08	1.59	1.50
17	F	701	MQ9	C41-C39	3.08	1.57	1.51
17	Z	201	MQ9	C27-C28	3.08	1.59	1.50
15	Z	203	CDL	OB8-CB7	3.07	1.42	1.33
15	S	301	CDL	OB8-CB7	3.06	1.42	1.33
16	F	702	HEM	FE-NB	3.06	2.04	1.94
18	P	202	9Y0	O7-C1	-3.06	1.39	1.46
15	X	302	CDL	OB8-CB7	3.06	1.42	1.33
14	L	602	HEA	C4D-C3D	3.06	1.50	1.45
14	L	603	HEA	C1C-C2C	3.05	1.50	1.43
17	F	708	MQ9	C21-C19	3.04	1.57	1.51
17	F	709	MQ9	C27-C28	3.04	1.59	1.50
21	I	301	HEC	FE-NA	3.04	2.05	1.95
16	F	702	HEM	FE-ND	3.03	2.04	1.94
17	E	604	MQ9	C27-C28	3.02	1.59	1.50
17	F	701	MQ9	C7-C8	3.02	1.55	1.50
16	E	602	HEM	CAB-C3B	3.00	1.55	1.47
17	E	603	MQ9	C7-C8	2.99	1.55	1.50
17	Z	201	MQ9	C16-C14	2.99	1.57	1.51
17	F	707	MQ9	C7-C8	2.98	1.55	1.50
17	F	708	MQ9	C16-C14	2.97	1.57	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	I	303	MQ9	C7-C8	2.97	1.55	1.50
14	L	603	HEA	C3A-C2A	2.97	1.43	1.37
16	F	702	HEM	FE-NC	2.97	2.04	1.95
18	P	202	9Y0	O5-C5	2.97	1.42	1.33
18	F	706	9Y0	O5-C5	2.96	1.42	1.33
17	F	708	MQ9	C7-C8	2.95	1.55	1.50
17	F	701	MQ9	C16-C14	2.95	1.57	1.51
14	L	603	HEA	C4B-C3B	2.94	1.49	1.44
21	I	302	HEC	FE-NC	2.94	2.04	1.95
18	J	202	9Y0	O5-C5	2.93	1.41	1.33
21	I	302	HEC	FE-NA	2.93	2.04	1.95
14	R	603	HEA	C1C-C2C	2.92	1.50	1.43
17	F	707	MQ9	C22-C23	2.92	1.59	1.50
16	F	703	HEM	CAB-C3B	2.91	1.55	1.47
15	S	301	CDL	OA6-CA5	2.91	1.42	1.34
17	E	603	MQ9	C16-C14	2.91	1.57	1.51
15	Z	203	CDL	OA6-CA5	2.91	1.42	1.34
17	E	604	MQ9	C7-C8	2.90	1.55	1.50
15	X	302	CDL	OA6-CA5	2.90	1.42	1.34
22	W	203	9YF	O9-C	-2.90	1.39	1.46
17	F	709	MQ9	C7-C8	2.89	1.55	1.50
22	Y	502	9YF	O9-C8	2.89	1.42	1.34
16	E	601	HEM	FE-NC	2.89	2.04	1.95
15	X	302	CDL	CB6-CB4	2.89	1.59	1.50
15	S	301	CDL	CB6-CB4	2.89	1.59	1.50
16	F	702	HEM	CAB-C3B	2.88	1.55	1.47
15	X	302	CDL	OB6-CB5	2.88	1.42	1.34
15	S	301	CDL	OB6-CB5	2.88	1.42	1.34
22	M	501	9YF	O9-C8	2.88	1.42	1.34
16	E	601	HEM	CAB-C3B	2.87	1.55	1.47
18	J	203	9Y0	O5-C5	2.87	1.41	1.33
17	F	701	MQ9	C7-C6	2.86	1.56	1.51
15	Z	203	CDL	OB6-CB5	2.86	1.42	1.34
17	E	603	MQ9	C7-C6	2.86	1.56	1.51
17	E	604	MQ9	C7-C6	2.85	1.56	1.51
22	c	203	9YF	O9-C	-2.85	1.39	1.46
17	F	709	MQ9	C7-C6	2.85	1.56	1.51
14	R	603	HEA	C3A-C2A	2.84	1.43	1.37
14	R	602	HEA	C1C-C2C	2.83	1.49	1.43
17	F	701	MQ9	C5M-C5	2.83	1.56	1.50
14	L	602	HEA	C1C-C2C	2.83	1.49	1.43
17	F	709	MQ9	C20-C19	2.82	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	E	603	MQ9	C5M-C5	2.82	1.56	1.50
17	F	707	MQ9	C20-C19	2.82	1.57	1.50
22	Y	502	9YF	O11-C25	2.81	1.41	1.33
15	Z	203	CDL	OA8-CA7	2.81	1.41	1.33
15	S	301	CDL	OA8-CA7	2.81	1.41	1.33
17	F	708	MQ9	C5M-C5	2.80	1.56	1.50
15	X	302	CDL	OA8-CA7	2.80	1.41	1.33
17	E	604	MQ9	C5M-C5	2.80	1.56	1.50
18	X	303	9Y0	O5-C5	2.80	1.41	1.33
17	E	604	MQ9	C20-C19	2.79	1.57	1.50
22	M	501	9YF	O11-C25	2.79	1.41	1.33
15	X	302	CDL	CB3-CB4	2.79	1.59	1.50
17	I	303	MQ9	C7-C6	2.78	1.56	1.51
15	S	301	CDL	CB3-CB4	2.78	1.59	1.50
16	F	703	HEM	CAC-C3C	2.77	1.54	1.47
18	J	202	9Y0	O7-C21	2.77	1.42	1.34
17	F	709	MQ9	C5M-C5	2.77	1.56	1.50
22	Y	503	9YF	O9-C	-2.77	1.40	1.46
15	Z	203	CDL	CB6-CB4	2.76	1.59	1.50
18	S	302	9Y0	O5-C5	2.76	1.41	1.33
18	J	203	9Y0	O7-C21	2.76	1.42	1.34
17	I	303	MQ9	C20-C19	2.76	1.57	1.50
17	Z	201	MQ9	C7-C6	2.76	1.56	1.51
22	M	502	9YF	O9-C	-2.75	1.40	1.46
15	Z	202	CDL	CB6-CB4	2.74	1.59	1.50
15	T	201	CDL	CB6-CB4	2.74	1.59	1.50
17	E	603	MQ9	C20-C19	2.74	1.57	1.50
18	F	706	9Y0	O7-C21	2.74	1.42	1.34
17	F	701	MQ9	C20-C19	2.73	1.57	1.50
15	Z	203	CDL	CB3-CB4	2.73	1.59	1.50
17	Z	201	MQ9	C20-C19	2.73	1.57	1.50
18	P	202	9Y0	O7-C21	2.72	1.42	1.34
15	Z	202	CDL	OB8-CB7	2.72	1.41	1.33
18	S	302	9Y0	O7-C21	2.71	1.41	1.34
18	X	303	9Y0	O7-C21	2.71	1.41	1.34
22	M	502	9YF	O9-C8	2.70	1.41	1.34
15	T	201	CDL	OB8-CB7	2.69	1.41	1.33
16	E	602	HEM	CAC-C3C	2.68	1.54	1.47
22	Y	503	9YF	O9-C8	2.68	1.41	1.34
15	X	302	CDL	OA6-CA4	-2.66	1.40	1.46
17	F	707	MQ9	C27-C28	2.66	1.58	1.50
16	F	703	HEM	FE-NA	2.65	2.03	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	S	301	CDL	OA6-CA4	-2.64	1.40	1.46
15	Z	203	CDL	OA6-CA4	-2.64	1.40	1.46
17	I	303	MQ9	C5M-C5	2.64	1.56	1.50
14	R	603	HEA	C4B-C3B	2.63	1.49	1.44
17	F	701	MQ9	C42-C43	2.62	1.58	1.50
17	F	708	MQ9	C20-C19	2.62	1.57	1.50
17	F	708	MQ9	O4-C4	-2.61	1.17	1.23
17	F	707	MQ9	C7-C6	2.61	1.56	1.51
17	E	603	MQ9	C42-C43	2.60	1.58	1.50
22	O	303	9YF	O9-C8	2.59	1.41	1.34
15	T	201	CDL	OB6-CB5	2.57	1.41	1.34
17	F	707	MQ9	O4-C4	-2.57	1.17	1.23
15	Z	202	CDL	OB6-CB5	2.57	1.41	1.34
20	c	202	9XX	O-C15	2.56	1.40	1.33
22	W	203	9YF	O11-C24	-2.56	1.39	1.45
22	I	304	9YF	O9-C8	2.56	1.41	1.34
22	c	203	9YF	O11-C24	-2.56	1.39	1.45
17	I	303	MQ9	C42-C43	2.56	1.58	1.50
17	E	604	MQ9	C46-C44	2.56	1.56	1.51
21	O	302	HEC	FE-NA	2.56	2.03	1.95
17	F	709	MQ9	C41-C39	2.55	1.56	1.51
22	W	203	9YF	O9-C8	2.55	1.41	1.34
22	c	203	9YF	O9-C8	2.51	1.41	1.34
16	E	602	HEM	FE-NA	2.50	2.03	1.95
17	F	709	MQ9	C46-C44	2.50	1.56	1.51
17	I	303	MQ9	C41-C39	2.49	1.56	1.51
20	D	302	9XX	O-C15	2.49	1.40	1.33
17	F	701	MQ9	C46-C44	2.49	1.56	1.51
22	c	203	9YF	P-O2	2.48	1.66	1.59
17	E	603	MQ9	C46-C44	2.47	1.56	1.51
17	E	604	MQ9	C41-C39	2.47	1.56	1.51
22	W	203	9YF	P-O2	2.47	1.66	1.59
17	Z	201	MQ9	C5M-C5	2.46	1.55	1.50
17	F	708	MQ9	C41-C39	2.46	1.56	1.51
22	I	304	9YF	O11-C25	2.46	1.40	1.33
22	O	303	9YF	O11-C25	2.45	1.40	1.33
22	Y	503	9YF	O11-C24	-2.45	1.39	1.45
17	E	603	MQ9	C12-C13	2.43	1.57	1.50
17	F	701	MQ9	C12-C13	2.43	1.57	1.50
22	M	502	9YF	O11-C24	-2.43	1.39	1.45
20	G	302	9XX	O-C15	2.43	1.40	1.33
22	O	303	9YF	O11-C24	-2.42	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	F	707	MQ9	C5M-C5	2.42	1.55	1.50
22	M	502	9YF	O11-C25	2.41	1.40	1.33
22	I	304	9YF	O11-C24	-2.41	1.39	1.45
14	R	603	HEA	C1D-ND	-2.40	1.36	1.40
22	Y	503	9YF	O11-C25	2.40	1.40	1.33
17	F	709	MQ9	C42-C43	2.39	1.57	1.50
14	R	602	HEA	C1A-C2A	2.39	1.49	1.45
17	Z	201	MQ9	C46-C44	2.38	1.56	1.51
17	Z	201	MQ9	C42-C43	2.37	1.57	1.50
17	F	707	MQ9	O1-C1	-2.37	1.18	1.23
14	R	602	HEA	C1B-C2B	2.37	1.49	1.44
17	F	701	MQ9	C43-C44	2.37	1.38	1.33
17	F	709	MQ9	C12-C13	2.36	1.57	1.50
17	I	303	MQ9	C12-C13	2.36	1.57	1.50
14	L	602	HEA	C1B-C2B	2.36	1.49	1.44
21	O	302	HEC	FE-NC	2.35	2.02	1.95
17	E	604	MQ9	C12-C13	2.35	1.57	1.50
14	R	602	HEA	C3C-C4C	2.35	1.49	1.42
14	L	603	HEA	C1D-ND	-2.34	1.36	1.40
17	F	701	MQ9	C28-C29	2.34	1.38	1.33
17	E	603	MQ9	C43-C44	2.33	1.38	1.33
22	O	303	9YF	O9-C	-2.33	1.41	1.46
17	E	604	MQ9	C42-C43	2.33	1.57	1.50
22	I	304	9YF	O9-C	-2.32	1.41	1.46
17	F	708	MQ9	C42-C43	2.32	1.57	1.50
17	E	603	MQ9	C28-C29	2.32	1.38	1.33
17	Z	201	MQ9	C41-C39	2.32	1.56	1.51
17	I	303	MQ9	C43-C44	2.31	1.38	1.33
17	F	709	MQ9	O4-C4	-2.31	1.18	1.23
14	L	602	HEA	C3C-C4C	2.31	1.49	1.42
17	Z	201	MQ9	O4-C4	-2.30	1.18	1.23
17	Z	201	MQ9	C12-C13	2.29	1.57	1.50
17	E	604	MQ9	O4-C4	-2.29	1.18	1.23
20	G	302	9XX	O1-C18	2.29	1.40	1.34
17	I	303	MQ9	C28-C29	2.28	1.38	1.33
17	E	603	MQ9	O4-C4	-2.27	1.18	1.23
17	I	303	MQ9	O4-C4	-2.27	1.18	1.23
16	F	703	HEM	FE-NC	2.27	2.02	1.95
20	D	302	9XX	O1-C18	2.26	1.40	1.34
17	F	707	MQ9	C46-C44	2.26	1.56	1.51
17	F	701	MQ9	O4-C4	-2.26	1.18	1.23
17	F	709	MQ9	C43-C44	2.26	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	L	602	HEA	C1A-C2A	2.26	1.49	1.45
22	Y	502	9YF	P-O2	2.25	1.66	1.59
14	R	603	HEA	C3C-C4C	2.25	1.49	1.42
15	T	201	CDL	PA1-OA4	-2.25	1.44	1.55
17	E	604	MQ9	C43-C44	2.25	1.38	1.33
15	Z	202	CDL	PA1-OA4	-2.24	1.44	1.55
17	F	707	MQ9	C12-C13	2.24	1.57	1.50
20	W	202	9XX	C14-C15	2.24	1.57	1.50
22	M	501	9YF	P-O2	2.24	1.66	1.59
22	W	203	9YF	O11-C25	2.24	1.39	1.33
15	T	201	CDL	CB3-CB4	2.23	1.57	1.50
15	Z	202	CDL	CB3-CB4	2.23	1.57	1.50
22	c	203	9YF	O11-C25	2.22	1.39	1.33
20	W	202	9XX	O1-C18	2.21	1.40	1.34
14	R	602	HEA	C1D-ND	-2.20	1.36	1.40
22	M	501	9YF	O4-C4	-2.20	1.37	1.43
14	L	602	HEA	C1D-ND	-2.20	1.36	1.40
14	R	603	HEA	C4D-C3D	2.19	1.48	1.45
17	F	708	MQ9	C43-C44	2.19	1.38	1.33
22	Y	502	9YF	O4-C4	-2.19	1.37	1.43
17	E	604	MQ9	C28-C29	2.18	1.38	1.33
17	I	303	MQ9	C46-C44	2.18	1.55	1.51
14	R	603	HEA	C1B-C2B	2.17	1.48	1.44
17	F	708	MQ9	C28-C29	2.16	1.38	1.33
14	L	603	HEA	C3C-C4C	2.16	1.49	1.42
17	F	707	MQ9	C41-C39	2.15	1.55	1.51
22	Y	502	9YF	O11-C24	-2.15	1.40	1.45
17	Z	201	MQ9	C28-C29	2.14	1.38	1.33
17	E	603	MQ9	C3C-C3B	2.14	1.42	1.38
17	Z	201	MQ9	C43-C44	2.12	1.38	1.33
17	F	708	MQ9	C51-C49	2.12	1.56	1.50
22	M	501	9YF	O11-C24	-2.12	1.40	1.45
17	E	604	MQ9	C3C-C3B	2.12	1.42	1.38
17	F	701	MQ9	C3C-C3B	2.12	1.42	1.38
17	F	708	MQ9	C6-C1	2.12	1.52	1.47
22	Y	503	9YF	O4-C4	-2.10	1.37	1.43
14	L	603	HEA	C1B-C2B	2.10	1.48	1.44
22	M	502	9YF	O4-C4	-2.10	1.37	1.43
17	F	709	MQ9	C28-C29	2.10	1.37	1.33
16	E	602	HEM	FE-NC	2.09	2.02	1.95
22	O	303	9YF	P-O2	2.09	1.65	1.59
17	Z	201	MQ9	C3C-C3B	2.08	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	Y	502	9YF	O9-C	-2.08	1.41	1.46
17	F	709	MQ9	C3C-C3B	2.07	1.42	1.38
22	I	304	9YF	P-O2	2.07	1.65	1.59
17	F	708	MQ9	C12-C13	2.07	1.56	1.50
16	E	602	HEM	CMB-C2B	2.07	1.55	1.50
15	Z	202	CDL	OA8-CA7	2.07	1.39	1.33
17	E	603	MQ9	C5-C4	2.06	1.52	1.47
14	R	603	HEA	C1D-C2D	2.06	1.48	1.44
15	T	201	CDL	OA8-CA7	2.05	1.39	1.33
21	I	302	HEC	CMC-C2C	2.04	1.55	1.50
15	T	201	CDL	OA6-CA5	2.04	1.40	1.34
16	E	601	HEM	CMD-C2D	2.04	1.55	1.50
14	L	602	HEA	C1D-C2D	2.04	1.48	1.44
22	M	501	9YF	O9-C	-2.04	1.41	1.46
15	Z	202	CDL	OA6-CA5	2.04	1.40	1.34
20	c	202	9XX	O1-C18	2.04	1.40	1.34
17	F	707	MQ9	C18-C19	2.03	1.37	1.33
16	E	601	HEM	CMB-C2B	2.02	1.54	1.50
21	O	302	HEC	CMC-C2C	2.02	1.54	1.50
22	Y	502	9YF	P-O	2.02	1.67	1.59
17	F	701	MQ9	C5-C4	2.02	1.52	1.47
17	F	707	MQ9	C42-C43	2.02	1.56	1.50
15	T	201	CDL	PB2-OB5	2.02	1.67	1.59
22	M	501	9YF	P-O	2.02	1.67	1.59
15	Z	202	CDL	PB2-OB5	2.02	1.67	1.59
14	L	603	HEA	C1D-C2D	2.02	1.48	1.44
17	I	303	MQ9	C3C-C3B	2.01	1.42	1.38
14	L	603	HEA	C4D-C3D	2.00	1.48	1.45

All (389) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	Z	203	CDL	CB6-CB4-CB3	-9.90	88.70	111.78
15	X	302	CDL	CB6-CB4-CB3	-9.67	89.23	111.78
15	S	301	CDL	CB6-CB4-CB3	-9.66	89.26	111.78
15	T	201	CDL	OB6-CB4-CB6	9.23	141.46	108.34
15	Z	202	CDL	OB6-CB4-CB6	9.23	141.46	108.34
15	Z	203	CDL	OB6-CB4-CB3	-8.35	78.39	108.34
14	L	602	HEA	C12-C11-C3B	8.17	124.90	112.12
14	R	602	HEA	CAD-C3D-C4D	8.13	138.87	124.70
15	X	302	CDL	OB6-CB4-CB3	-8.00	79.66	108.34
15	S	301	CDL	OB6-CB4-CB3	-7.99	79.68	108.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	S	301	CDL	OB6-CB4-CB6	7.22	134.25	108.34
15	X	302	CDL	OB6-CB4-CB6	7.22	134.24	108.34
15	Z	203	CDL	OB6-CB4-CB6	6.87	132.98	108.34
14	L	602	HEA	C3A-C2A-C1A	-6.20	101.18	107.05
14	L	602	HEA	CAD-C3D-C4D	5.95	135.07	124.70
14	R	602	HEA	C3A-C2A-C1A	-5.94	101.42	107.05
22	Y	503	9YF	O6-C6-C7	5.92	124.33	110.38
22	M	502	9YF	O6-C6-C7	5.92	124.33	110.38
14	R	603	HEA	C3A-C2A-C1A	-5.57	101.77	107.05
14	L	603	HEA	C3A-C2A-C1A	-5.52	101.82	107.05
21	O	302	HEC	C1D-ND-C4D	5.51	111.73	105.21
21	I	302	HEC	C1D-ND-C4D	5.50	111.72	105.21
14	R	602	HEA	C12-C11-C3B	5.48	120.68	112.12
22	Y	502	9YF	O9-C8-C9	5.37	123.10	111.48
21	I	301	HEC	C1D-ND-C4D	5.37	111.56	105.21
22	M	501	9YF	O9-C8-C9	5.36	123.07	111.48
21	O	301	HEC	C1D-ND-C4D	5.14	111.30	105.21
21	I	302	HEC	CAB-C3B-C4B	5.13	131.47	124.79
20	G	302	9XX	O1-C18-C19	4.91	122.10	111.48
14	R	603	HEA	C3D-C4D-ND	4.71	114.91	110.35
14	L	602	HEA	O11-C11-C3B	-4.67	102.70	111.26
15	T	201	CDL	OB6-CB4-CB3	-4.65	91.66	108.34
17	Z	201	MQ9	C7-C8-C9	-4.65	118.83	126.83
15	Z	202	CDL	OB6-CB4-CB3	-4.64	91.69	108.34
20	D	302	9XX	O1-C18-C19	4.64	121.52	111.48
22	c	203	9YF	O9-C8-C9	4.55	121.32	111.48
22	W	203	9YF	O9-C8-C9	4.52	121.27	111.48
15	Z	203	CDL	OA6-CA5-C11	4.52	121.25	111.48
15	T	201	CDL	OB6-CB5-C51	4.49	121.20	111.48
15	Z	202	CDL	OB6-CB5-C51	4.48	121.18	111.48
17	F	707	MQ9	C15-C14-C16	4.46	122.98	115.23
14	L	603	HEA	C3D-C4D-ND	4.44	114.64	110.35
14	L	602	HEA	CMC-C2C-C3C	4.38	136.85	126.55
15	Z	202	CDL	OA6-CA5-C11	4.37	120.94	111.48
15	T	201	CDL	OA6-CA5-C11	4.37	120.93	111.48
14	L	603	HEA	C2A-C1A-NA	4.31	114.48	110.32
14	L	602	HEA	C2A-C1A-NA	4.29	114.46	110.32
14	R	603	HEA	C2A-C1A-NA	4.27	114.44	110.32
14	R	602	HEA	CAD-C3D-C2D	-4.24	119.92	127.87
20	W	202	9XX	O1-C18-C19	4.22	120.61	111.48
18	J	202	9Y0	O7-C21-C22	4.18	120.52	111.48
14	R	603	HEA	CMC-C2C-C3C	4.15	136.32	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	S	301	CDL	OB6-CB5-C51	4.13	120.42	111.48
15	X	302	CDL	OB6-CB5-C51	4.12	120.40	111.48
14	R	603	HEA	CHA-C1A-C2A	-4.11	118.38	124.86
14	R	602	HEA	CMC-C2C-C3C	4.08	136.15	126.55
14	R	603	HEA	CHA-C4D-C3D	-4.05	118.86	124.77
22	Y	503	9YF	O9-C8-C9	4.01	120.15	111.48
14	L	602	HEA	C3D-C4D-ND	4.00	114.21	110.35
22	M	502	9YF	O9-C8-C9	3.99	120.12	111.48
14	R	603	HEA	C12-C11-C3B	-3.98	105.91	112.12
18	X	303	9Y0	O7-C21-C22	3.94	120.01	111.48
14	L	602	HEA	CMC-C2C-C1C	-3.92	119.45	125.42
14	R	602	HEA	C4D-C3D-C2D	-3.91	101.20	106.89
14	L	603	HEA	CHA-C4D-C3D	-3.90	119.09	124.77
18	F	706	9Y0	O7-C21-C22	3.89	119.90	111.48
14	L	603	HEA	CHA-C1A-C2A	-3.89	118.72	124.86
14	R	602	HEA	C2A-C1A-NA	3.87	114.06	110.32
18	S	302	9Y0	O7-C21-C22	3.83	119.76	111.48
15	Z	203	CDL	OB6-CB5-C51	3.78	119.65	111.48
17	F	707	MQ9	C45-C44-C46	3.78	121.78	115.23
22	I	304	9YF	O9-C8-C9	3.78	119.65	111.48
22	O	303	9YF	O9-C8-C9	3.77	119.63	111.48
14	L	602	HEA	CHA-C1A-C2A	-3.74	118.96	124.86
22	Y	503	9YF	O11-C25-C26	3.73	123.22	111.83
22	M	502	9YF	O11-C25-C26	3.73	123.20	111.83
15	X	302	CDL	OA6-CA5-C11	3.71	119.52	111.48
14	L	602	HEA	C4D-C3D-C2D	-3.70	101.50	106.89
15	S	301	CDL	OA6-CA5-C11	3.70	119.49	111.48
14	R	602	HEA	CHA-C1A-C2A	-3.68	119.05	124.86
14	R	603	HEA	CMC-C2C-C1C	-3.66	119.85	125.42
20	c	202	9XX	O1-C18-C19	3.65	119.39	111.48
14	R	602	HEA	C3D-C4D-ND	3.64	113.87	110.35
14	R	603	HEA	CAD-C3D-C4D	3.60	130.97	124.70
17	F	707	MQ9	C11-C9-C8	3.57	129.18	121.17
14	R	603	HEA	C4D-C3D-C2D	-3.56	101.71	106.89
14	R	602	HEA	C26-C15-C14	-3.55	114.50	123.63
17	F	708	MQ9	C50-C49-C48	-3.55	112.01	122.66
21	I	302	HEC	CAB-C3B-C2B	-3.50	121.12	127.56
14	L	602	HEA	C26-C15-C16	3.47	121.24	115.23
18	P	202	9Y0	O7-C21-C22	3.46	118.97	111.48
17	E	604	MQ9	C12-C13-C14	-3.45	119.72	127.62
14	L	602	HEA	OMA-CMA-C3A	-3.43	117.88	125.62
17	F	709	MQ9	C12-C13-C14	-3.41	119.81	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	F	708	MQ9	C8-C7-C6	3.41	120.48	112.08
21	I	302	HEC	CAC-C3C-C4C	3.38	129.57	124.91
17	F	709	MQ9	C30-C29-C31	3.36	121.06	115.23
14	L	603	HEA	C4D-C3D-C2D	-3.35	102.01	106.89
14	R	602	HEA	OMA-CMA-C3A	-3.34	118.08	125.62
17	F	709	MQ9	C17-C18-C19	-3.30	120.07	127.62
15	Z	202	CDL	CB6-CB4-CB3	-3.30	104.09	111.78
14	R	603	HEA	CAA-C2A-C1A	3.30	131.56	124.85
14	R	602	HEA	CMC-C2C-C1C	-3.30	120.40	125.42
17	E	604	MQ9	C17-C18-C19	-3.29	120.08	127.62
17	Z	201	MQ9	C40-C39-C41	-3.29	109.52	115.23
17	F	708	MQ9	C15-C14-C16	3.29	120.94	115.23
15	T	201	CDL	CB6-CB4-CB3	-3.29	104.12	111.78
14	R	602	HEA	C26-C15-C16	3.28	120.93	115.23
15	T	201	CDL	CA4-OA6-CA5	-3.27	109.96	117.80
22	M	501	9YF	O11-C25-C26	3.27	121.80	111.83
15	Z	202	CDL	CA4-OA6-CA5	-3.26	109.99	117.80
22	Y	502	9YF	O11-C25-C26	3.26	121.76	111.83
17	F	708	MQ9	C51-C49-C50	3.25	122.07	114.59
22	O	303	9YF	O11-C25-C26	3.20	121.59	111.83
22	I	304	9YF	O11-C25-C26	3.19	121.57	111.83
14	L	603	HEA	CAA-C2A-C1A	3.18	131.33	124.85
17	F	707	MQ9	C8-C7-C6	3.18	119.92	112.08
17	E	604	MQ9	C32-C33-C34	-3.18	120.34	127.62
17	Z	201	MQ9	C42-C43-C44	-3.17	120.36	127.62
14	L	602	HEA	C26-C15-C14	-3.17	115.48	123.63
17	E	603	MQ9	C17-C18-C19	-3.17	120.37	127.62
14	R	602	HEA	C3C-C2C-C1C	-3.15	103.46	107.17
14	L	603	HEA	CMC-C2C-C3C	3.15	133.96	126.55
14	L	603	HEA	CAD-C3D-C4D	3.15	130.19	124.70
17	F	709	MQ9	C32-C33-C34	-3.14	120.43	127.62
15	L	604	CDL	OA5-PA1-OA3	-3.14	96.50	108.94
18	J	203	9Y0	O7-C21-C22	3.14	118.27	111.48
17	F	701	MQ9	C17-C18-C19	-3.13	120.45	127.62
15	L	604	CDL	OA2-PA1-OA3	3.11	121.25	108.94
18	P	202	9Y0	C29-C28-C27	3.10	130.05	114.37
17	F	709	MQ9	C35-C34-C36	3.05	120.52	115.23
20	G	302	9XX	O-C15-C14	3.05	121.13	111.83
14	R	603	HEA	CAA-CBA-CGA	-3.05	105.59	113.67
14	L	603	HEA	C3C-C2C-C1C	-3.04	103.58	107.17
17	E	604	MQ9	C30-C29-C31	3.04	120.50	115.23
17	Z	201	MQ9	C17-C18-C19	-3.03	120.68	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	D	302	9XX	O-C15-C14	3.00	120.97	111.83
17	Z	201	MQ9	C12-C13-C14	-2.96	120.85	127.62
14	L	602	HEA	C3C-C2C-C1C	-2.95	103.69	107.17
17	F	707	MQ9	O1-C1-C2	-2.95	116.85	121.57
17	F	707	MQ9	C20-C19-C21	2.92	120.30	115.23
15	T	201	CDL	OB8-CB7-C71	2.91	120.71	111.83
21	I	302	HEC	CAC-C3C-C2C	-2.91	122.29	126.89
15	Z	202	CDL	OB8-CB7-C71	2.90	120.69	111.83
17	Z	201	MQ9	C5M-C5-C6	-2.89	119.70	124.45
17	E	604	MQ9	C35-C34-C36	2.88	120.22	115.23
14	L	603	HEA	CMD-C2D-C1D	-2.86	120.56	125.03
15	Z	203	CDL	OB8-CB7-C71	2.86	120.55	111.83
17	F	701	MQ9	C42-C43-C44	-2.84	121.11	127.62
17	E	604	MQ9	C15-C14-C16	2.84	120.16	115.23
21	O	302	HEC	CAB-C3B-C4B	2.84	128.49	124.79
14	L	602	HEA	C17-C18-C19	-2.84	121.12	127.62
18	X	303	9Y0	O5-C5-C6	2.84	120.50	111.83
17	F	709	MQ9	C27-C28-C29	-2.84	121.12	127.62
17	F	708	MQ9	C42-C41-C39	2.84	122.59	113.19
17	F	709	MQ9	C15-C14-C16	2.84	120.15	115.23
17	E	604	MQ9	C27-C28-C29	-2.83	121.14	127.62
14	R	603	HEA	C3C-C2C-C1C	-2.83	103.83	107.17
14	L	602	HEA	CHA-C4D-C3D	-2.83	120.65	124.77
14	R	602	HEA	C3B-C4B-NB	2.82	113.08	109.84
14	R	603	HEA	C3C-C4C-NC	2.82	112.17	109.80
17	I	303	MQ9	C7-C8-C9	-2.82	121.98	126.83
17	Z	201	MQ9	C22-C23-C24	-2.81	121.18	127.62
17	F	708	MQ9	C42-C43-C44	-2.80	121.21	127.62
17	E	603	MQ9	C42-C43-C44	-2.80	121.22	127.62
15	T	201	CDL	OA8-CA7-C31	2.80	120.37	111.83
18	J	202	9Y0	O5-C5-C6	2.79	120.34	111.83
17	E	604	MQ9	C7-C8-C9	-2.79	122.03	126.83
15	Z	202	CDL	OA8-CA7-C31	2.78	120.31	111.83
17	F	707	MQ9	C22-C23-C24	-2.78	121.27	127.62
15	X	302	CDL	OB8-CB7-C71	2.78	120.30	111.83
16	E	602	HEM	C3B-C2B-C1B	2.77	108.49	106.41
18	F	706	9Y0	O5-C5-C6	2.77	120.27	111.83
16	F	703	HEM	C3B-C2B-C1B	2.76	108.49	106.41
15	T	201	CDL	OA6-CA5-OA7	-2.76	117.24	123.70
15	S	301	CDL	OB8-CB7-C71	2.76	120.27	111.83
15	Z	202	CDL	OA6-CA5-OA7	-2.76	117.24	123.70
17	Z	201	MQ9	C32-C33-C34	-2.76	121.30	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	I	303	MQ9	C5M-C5-C6	-2.76	119.92	124.45
17	F	709	MQ9	C7-C8-C9	-2.74	122.11	126.83
15	Z	203	CDL	OA8-CA7-C31	2.74	120.19	111.83
17	Z	201	MQ9	C7-C6-C5	-2.74	120.20	124.89
21	O	301	HEC	CAC-C3C-C4C	2.73	128.66	124.91
14	L	603	HEA	C3C-C4C-NC	2.73	112.09	109.80
21	I	301	HEC	C4B-NB-C1B	2.72	108.43	105.21
18	S	302	9Y0	O5-C5-C6	2.71	120.10	111.83
17	E	603	MQ9	C20-C19-C21	2.71	119.93	115.23
14	L	603	HEA	CAA-CBA-CGA	-2.70	106.50	113.67
17	F	701	MQ9	C20-C19-C21	2.70	119.91	115.23
17	F	707	MQ9	C35-C34-C36	2.70	119.91	115.23
17	F	708	MQ9	C27-C26-C24	2.70	122.12	113.19
14	L	602	HEA	C3C-C4C-NC	2.69	112.07	109.80
14	R	602	HEA	CAA-C2A-C1A	2.69	130.32	124.85
15	X	302	CDL	OA8-CA7-C31	2.68	120.01	111.83
20	c	202	9XX	O-C15-C14	2.67	119.99	111.83
15	S	301	CDL	OA8-CA7-C31	2.67	119.97	111.83
14	R	602	HEA	C3C-C4C-NC	2.66	112.04	109.80
14	L	602	HEA	CAA-C2A-C1A	2.66	130.27	124.85
18	J	203	9Y0	O5-C5-C6	2.66	119.95	111.83
14	L	603	HEA	CMD-C2D-C3D	2.66	133.34	126.15
17	F	707	MQ9	C31-C29-C28	-2.63	115.25	121.17
22	c	203	9YF	O11-C25-C26	2.63	119.86	111.83
14	L	602	HEA	C27-C19-C20	2.63	119.80	115.23
22	W	203	9YF	O11-C25-C26	2.63	119.85	111.83
17	Z	201	MQ9	C35-C34-C36	2.61	119.76	115.23
17	F	707	MQ9	C5M-C5-C6	-2.60	120.18	124.45
17	Z	201	MQ9	C30-C29-C31	2.59	119.73	115.23
21	O	302	HEC	C3C-C4C-NC	-2.58	107.29	110.15
17	F	707	MQ9	C7-C6-C5	-2.57	120.48	124.89
17	I	303	MQ9	C12-C13-C14	-2.57	121.74	127.62
15	X	302	CDL	OB4-PB2-OB3	-2.57	100.49	112.44
15	S	301	CDL	OB4-PB2-OB3	-2.57	100.50	112.44
14	R	602	HEA	CMD-C2D-C1D	-2.56	121.03	125.03
21	I	302	HEC	C3C-C4C-NC	-2.56	107.31	110.15
14	R	602	HEA	C27-C19-C20	2.55	119.66	115.23
14	L	602	HEA	CAD-CBD-CGD	-2.55	106.91	113.67
14	L	602	HEA	C3B-C4B-NB	2.55	112.77	109.84
17	E	604	MQ9	C20-C19-C21	2.54	119.64	115.23
15	Z	203	CDL	OA4-PA1-OA3	-2.54	100.62	112.44
17	Z	201	MQ9	C25-C24-C26	2.54	119.64	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	E	602	HEM	CHD-C4C-NC	2.53	127.21	124.45
20	G	302	9XX	C17-O1-C18	-2.53	114.13	117.78
17	F	707	MQ9	C7-C8-C9	-2.52	122.48	126.83
17	I	303	MQ9	C32-C33-C34	-2.52	121.85	127.62
17	F	709	MQ9	C20-C19-C21	2.52	119.60	115.23
14	L	602	HEA	CMD-C2D-C1D	-2.52	121.10	125.03
15	T	201	CDL	OB6-CB5-OB7	-2.52	117.82	123.70
15	Z	202	CDL	OB6-CB5-OB7	-2.52	117.82	123.70
17	Z	201	MQ9	C11-C9-C8	2.51	126.81	121.17
17	E	604	MQ9	C40-C39-C41	-2.51	110.87	115.23
15	T	201	CDL	OA8-CA7-OA9	-2.51	117.35	123.63
14	R	603	HEA	CHA-C1A-NA	2.50	127.18	124.45
17	I	303	MQ9	C30-C29-C28	-2.50	117.20	123.63
15	Z	202	CDL	OA8-CA7-OA9	-2.50	117.37	123.63
14	R	603	HEA	CMD-C2D-C1D	-2.50	121.13	125.03
17	F	701	MQ9	C27-C28-C29	-2.50	121.91	127.62
17	F	701	MQ9	C5M-C5-C6	-2.48	120.37	124.45
17	E	603	MQ9	C27-C28-C29	-2.48	121.95	127.62
15	T	201	CDL	OA4-PA1-OA3	-2.47	100.95	112.44
14	R	602	HEA	C17-C18-C19	-2.47	121.97	127.62
15	Z	202	CDL	OA4-PA1-OA3	-2.47	100.95	112.44
21	I	301	HEC	C2A-C1A-NA	-2.47	107.94	110.32
21	I	302	HEC	C4B-NB-C1B	2.47	108.13	105.21
22	Y	503	9YF	O3-C3-C4	-2.47	104.56	110.38
14	R	602	HEA	C4B-C3B-C2B	-2.46	103.30	107.44
17	E	604	MQ9	C45-C44-C43	-2.46	117.30	123.63
17	E	603	MQ9	C5M-C5-C6	-2.46	120.41	124.45
17	E	603	MQ9	C7-C6-C5	-2.46	120.67	124.89
17	F	707	MQ9	C10-C9-C11	-2.46	110.96	115.23
15	Z	203	CDL	OB4-PB2-OB3	-2.46	101.01	112.44
21	O	302	HEC	C2A-C1A-NA	-2.45	107.96	110.32
17	F	707	MQ9	C40-C39-C41	-2.44	110.99	115.23
22	M	502	9YF	O3-C3-C4	-2.44	104.62	110.38
17	E	603	MQ9	C22-C23-C24	-2.44	122.03	127.62
17	Z	201	MQ9	C45-C44-C46	2.43	119.45	115.23
17	F	701	MQ9	C7-C6-C5	-2.43	120.73	124.89
17	I	303	MQ9	C20-C19-C21	2.43	119.44	115.23
16	F	703	HEM	C3B-C4B-NB	-2.42	107.73	109.47
21	I	301	HEC	C3B-C4B-NB	-2.42	107.52	110.17
17	F	701	MQ9	C32-C33-C34	-2.41	122.10	127.62
16	F	703	HEM	C1B-NB-C4B	2.41	108.06	105.21
20	W	202	9XX	O-C15-O6	2.41	129.65	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	F	701	MQ9	C22-C23-C24	-2.40	122.13	127.62
17	Z	201	MQ9	C15-C14-C16	2.39	119.37	115.23
22	Y	502	9YF	C7-C2-C3	-2.39	107.55	110.86
21	I	302	HEC	C3B-C4B-NB	-2.39	107.56	110.17
22	M	501	9YF	C7-C2-C3	-2.38	107.55	110.86
16	E	602	HEM	C1B-NB-C4B	2.38	108.03	105.21
14	R	603	HEA	CMD-C2D-C3D	2.38	132.58	126.15
14	L	602	HEA	CAD-C3D-C2D	-2.38	123.42	127.87
14	L	602	HEA	C4B-C3B-C2B	-2.38	103.44	107.44
22	Y	502	9YF	C30-C31-C32	2.37	122.56	113.62
22	M	501	9YF	C30-C31-C32	2.37	122.55	113.62
17	I	303	MQ9	C22-C23-C24	-2.37	122.20	127.62
17	E	603	MQ9	C32-C33-C34	-2.36	122.22	127.62
17	E	603	MQ9	C7-C8-C9	-2.35	122.77	126.83
17	F	709	MQ9	C22-C23-C24	-2.34	122.27	127.62
17	F	707	MQ9	C46-C44-C43	-2.34	115.92	121.17
17	I	303	MQ9	C51-C49-C50	2.34	119.97	114.59
22	Y	502	9YF	O4-C4-C3	-2.33	104.89	110.38
21	O	301	HEC	C3C-C4C-NC	-2.33	107.57	110.15
15	S	301	CDL	OA4-PA1-OA3	-2.33	101.62	112.44
17	E	604	MQ9	C22-C23-C24	-2.32	122.30	127.62
17	F	707	MQ9	C16-C14-C13	-2.32	115.95	121.17
15	X	302	CDL	OA4-PA1-OA3	-2.32	101.63	112.44
17	I	303	MQ9	C15-C14-C16	2.32	119.26	115.23
17	F	701	MQ9	C25-C24-C26	2.32	119.25	115.23
17	F	708	MQ9	O1-C1-C2	-2.32	117.86	121.57
22	M	501	9YF	O4-C4-C3	-2.32	104.91	110.38
14	R	602	HEA	CHD-C1D-ND	2.32	127.23	124.37
17	F	709	MQ9	C45-C44-C43	-2.31	117.68	123.63
21	I	302	HEC	C2A-C1A-NA	-2.31	108.09	110.32
15	T	201	CDL	OB4-PB2-OB3	-2.31	101.71	112.44
15	Z	202	CDL	OB4-PB2-OB3	-2.30	101.75	112.44
16	E	602	HEM	C3B-C4B-NB	-2.30	107.82	109.47
17	F	701	MQ9	C7-C8-C9	-2.29	122.89	126.83
14	L	603	HEA	C25-C23-C24	2.28	119.84	114.59
17	I	303	MQ9	C7-C6-C5	-2.28	120.98	124.89
20	D	302	9XX	C17-O1-C18	-2.28	114.50	117.78
21	O	301	HEC	CAC-C3C-C2C	-2.27	123.29	126.89
14	R	602	HEA	CBD-CAD-C3D	2.27	118.81	112.53
22	O	303	9YF	O5-C5-C4	-2.27	105.02	110.38
17	E	603	MQ9	C25-C24-C26	2.27	119.16	115.23
21	I	302	HEC	CHC-C4B-C3B	2.26	129.40	125.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	I	302	HEC	CHB-C1B-NB	2.26	126.86	124.42
14	R	602	HEA	CAA-CBA-CGA	-2.26	107.66	113.67
17	F	707	MQ9	C12-C11-C9	2.26	120.68	113.19
22	Y	502	9YF	O9-C8-O10	-2.26	118.42	123.70
17	F	701	MQ9	C15-C14-C16	2.26	119.15	115.23
17	I	303	MQ9	C35-C34-C36	2.25	119.13	115.23
20	c	202	9XX	O1-C17-C37	2.25	112.99	107.96
22	I	304	9YF	O5-C5-C4	-2.24	105.09	110.38
17	F	709	MQ9	C40-C39-C41	-2.24	111.34	115.23
14	R	602	HEA	CHA-C1A-NA	2.24	126.89	124.45
22	M	501	9YF	O9-C8-O10	-2.23	118.49	123.70
17	F	707	MQ9	C7-C6-C1	2.22	120.92	118.58
21	O	301	HEC	C4B-NB-C1B	2.22	107.83	105.21
14	R	602	HEA	CHB-C4A-NA	2.21	126.86	124.45
17	E	603	MQ9	C15-C14-C16	2.21	119.06	115.23
14	R	603	HEA	C25-C23-C24	2.21	119.67	114.59
21	O	302	HEC	C4B-NB-C1B	2.21	107.82	105.21
16	F	702	HEM	C4D-ND-C1D	2.21	107.82	105.21
17	Z	201	MQ9	C20-C19-C21	2.20	119.04	115.23
17	E	604	MQ9	C42-C43-C44	-2.19	122.60	127.62
22	W	203	9YF	C7-C2-C3	-2.19	107.82	110.86
22	c	203	9YF	C7-C2-C3	-2.19	107.82	110.86
16	E	601	HEM	C4D-ND-C1D	2.19	107.80	105.21
21	O	301	HEC	C2A-C1A-NA	-2.18	108.22	110.32
16	E	601	HEM	C3D-C4D-ND	-2.18	107.78	110.17
22	Y	502	9YF	O11-C24-C	2.17	114.66	108.40
22	M	501	9YF	O11-C24-C	2.17	114.65	108.40
17	I	303	MQ9	C32-C31-C29	-2.17	106.00	113.19
17	I	303	MQ9	C42-C43-C44	-2.17	122.66	127.62
17	I	303	MQ9	C25-C24-C26	2.17	118.99	115.23
14	R	602	HEA	C25-C23-C24	2.16	119.56	114.59
14	L	603	HEA	CHA-C1A-NA	2.15	126.80	124.45
17	F	701	MQ9	C12-C13-C14	-2.15	122.70	127.62
14	L	602	HEA	CMD-C2D-C3D	2.14	131.95	126.15
20	D	302	9XX	O1-C17-C16	2.14	111.12	106.21
17	I	303	MQ9	C40-C39-C41	-2.13	111.53	115.23
17	I	303	MQ9	C10-C9-C11	2.13	118.93	115.23
14	L	602	HEA	CAA-CBA-CGA	-2.13	108.01	113.67
14	L	602	HEA	C25-C23-C24	2.13	119.49	114.59
16	F	702	HEM	C3D-C4D-ND	-2.13	107.84	110.17
14	L	602	HEA	CBD-CAD-C3D	2.13	118.41	112.53
14	L	603	HEA	C12-C11-C3B	-2.12	108.80	112.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	M	502	9YF	C7-C6-C5	2.12	114.56	110.83
20	G	302	9XX	O1-C17-C16	2.12	111.08	106.21
17	F	707	MQ9	C32-C31-C29	-2.11	106.19	113.19
22	Y	503	9YF	C7-C6-C5	2.11	114.53	110.83
20	W	202	9XX	O6-C15-C14	-2.11	115.54	123.78
17	E	603	MQ9	C12-C13-C14	-2.11	122.80	127.62
17	F	709	MQ9	C7-C6-C5	-2.10	121.30	124.89
15	R	604	CDL	OB4-PB2-OB5	-2.09	98.08	107.57
21	O	302	HEC	CHC-C4B-C3B	2.09	129.07	125.23
17	I	303	MQ9	C17-C18-C19	-2.09	122.85	127.62
14	R	602	HEA	CHC-C1C-C2C	-2.08	121.39	127.43
14	L	602	HEA	CHC-C1C-C2C	-2.07	121.40	127.43
15	R	604	CDL	OA5-PA1-OA3	-2.07	100.72	108.94
14	R	602	HEA	CHD-C1D-C2D	-2.07	121.08	126.95
17	F	707	MQ9	C25-C24-C26	2.06	118.81	115.23
20	c	202	9XX	C25-C26-C27	-2.06	109.12	115.97
21	O	302	HEC	CAC-C3C-C4C	2.06	127.74	124.91
14	L	602	HEA	CHB-C4A-NA	2.06	126.69	124.45
16	E	602	HEM	CHC-C1C-NC	2.05	126.69	124.45
15	Z	202	CDL	C58-C57-C56	-2.05	103.99	114.37
17	F	709	MQ9	C10-C9-C11	2.05	118.79	115.23
17	F	701	MQ9	C35-C34-C36	2.05	118.79	115.23
17	E	604	MQ9	C10-C9-C11	2.05	118.79	115.23
14	R	602	HEA	CHB-C1B-C2B	-2.05	121.79	125.03
15	T	201	CDL	C58-C57-C56	-2.05	104.02	114.37
14	L	603	HEA	CHB-C1B-C2B	-2.04	121.80	125.03
17	F	701	MQ9	C30-C29-C31	2.04	118.77	115.23
17	E	603	MQ9	C30-C29-C28	-2.04	118.39	123.63
15	L	604	CDL	OB4-PB2-OB5	-2.04	98.34	107.57
15	T	201	CDL	C56-C55-C54	-2.03	104.10	114.37
15	Z	202	CDL	C56-C55-C54	-2.03	104.10	114.37
14	L	603	HEA	OMA-CMA-C3A	-2.03	121.04	125.62
17	E	604	MQ9	C7-C6-C5	-2.03	121.42	124.89
21	I	301	HEC	C3C-C4C-NC	-2.03	107.90	110.15
17	E	604	MQ9	C5M-C5-C6	-2.02	121.13	124.45
17	F	701	MQ9	C30-C29-C28	-2.02	118.45	123.63
14	R	602	HEA	O11-C11-C3B	-2.02	107.56	111.26
17	F	707	MQ9	C21-C19-C18	-2.01	116.65	121.17
17	F	707	MQ9	C36-C34-C33	-2.01	116.66	121.17
17	E	603	MQ9	C35-C34-C36	2.01	118.72	115.23
17	F	709	MQ9	C42-C43-C44	-2.01	123.03	127.62
20	G	302	9XX	O1-C18-O2	-2.01	119.01	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	F	705	CDL	OA6-CA5-C11	2.00	115.81	111.48

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
21	O	302	HEC	NA
21	I	302	HEC	NA

All (1221) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
15	F	704	CDL	CA3-OA5-PA1-OA2
15	F	704	CDL	C1-CB2-OB2-PB2
15	F	704	CDL	CB2-OB2-PB2-OB3
15	F	704	CDL	CB2-OB2-PB2-OB4
15	F	704	CDL	CB2-OB2-PB2-OB5
15	F	704	CDL	CB3-OB5-PB2-OB2
15	F	704	CDL	CB3-OB5-PB2-OB3
15	F	704	CDL	CB4-CB3-OB5-PB2
15	F	705	CDL	CA2-OA2-PA1-OA3
15	F	705	CDL	CA2-OA2-PA1-OA4
15	F	705	CDL	CA2-OA2-PA1-OA5
15	F	705	CDL	CA3-OA5-PA1-OA2
15	F	705	CDL	CA3-OA5-PA1-OA4
15	F	705	CDL	CB3-OB5-PB2-OB2
15	F	705	CDL	CB3-OB5-PB2-OB3
15	F	705	CDL	CB3-OB5-PB2-OB4
15	L	604	CDL	CA3-OA5-PA1-OA2
15	L	604	CDL	CA3-OA5-PA1-OA4
15	L	604	CDL	C11-CA5-OA6-CA4
15	L	604	CDL	C31-CA7-OA8-CA6
15	L	604	CDL	CB2-OB2-PB2-OB3
15	L	604	CDL	CB2-OB2-PB2-OB5
15	L	604	CDL	OB7-CB5-OB6-CB4
15	S	301	CDL	CA3-OA5-PA1-OA2
15	S	301	CDL	CA3-OA5-PA1-OA3
15	S	301	CDL	CB2-OB2-PB2-OB3
15	S	301	CDL	CB2-OB2-PB2-OB4
15	S	301	CDL	CB2-OB2-PB2-OB5
15	S	301	CDL	CB3-OB5-PB2-OB2
15	S	301	CDL	CB3-OB5-PB2-OB3
15	S	301	CDL	CB3-OB5-PB2-OB4
15	S	301	CDL	OB7-CB5-OB6-CB4
15	T	201	CDL	CA3-OA5-PA1-OA2
15	T	201	CDL	CA3-OA5-PA1-OA3
15	T	201	CDL	OA6-CA4-CA6-OA8
15	T	201	CDL	C11-CA5-OA6-CA4
15	T	201	CDL	C51-CB5-OB6-CB4
15	T	202	CDL	CA2-OA2-PA1-OA4
15	T	202	CDL	CA2-OA2-PA1-OA5
15	T	202	CDL	OA6-CA4-CA6-OA8
15	T	202	CDL	CB3-OB5-PB2-OB2
15	T	202	CDL	CB3-OB5-PB2-OB4

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Mol	Chain	Res	Type	Atoms
15	T	202	CDL	C51-CB5-OB6-CB4
15	T	203	CDL	O1-C1-CA2-OA2
15	T	203	CDL	CA2-C1-CB2-OB2
15	T	203	CDL	OA7-CA5-OA6-CA4
15	T	203	CDL	C11-CA5-OA6-CA4
15	T	203	CDL	CB3-OB5-PB2-OB2
15	T	203	CDL	CB3-OB5-PB2-OB3
15	P	201	CDL	CA2-OA2-PA1-OA3
15	P	201	CDL	CA2-OA2-PA1-OA4
15	P	201	CDL	CA2-OA2-PA1-OA5
15	P	201	CDL	CB2-OB2-PB2-OB3
15	P	201	CDL	CB2-OB2-PB2-OB4
15	P	201	CDL	CB2-OB2-PB2-OB5
15	X	301	CDL	CA2-OA2-PA1-OA4
15	X	301	CDL	CA2-OA2-PA1-OA5
15	X	301	CDL	OA6-CA4-CA6-OA8
15	X	301	CDL	CB3-OB5-PB2-OB2
15	X	301	CDL	CB3-OB5-PB2-OB4
15	X	301	CDL	C51-CB5-OB6-CB4
15	X	302	CDL	CA3-OA5-PA1-OA2
15	X	302	CDL	CA3-OA5-PA1-OA3
15	X	302	CDL	CB2-OB2-PB2-OB3
15	X	302	CDL	CB2-OB2-PB2-OB4
15	X	302	CDL	CB2-OB2-PB2-OB5
15	X	302	CDL	CB3-OB5-PB2-OB2
15	X	302	CDL	CB3-OB5-PB2-OB3
15	X	302	CDL	CB3-OB5-PB2-OB4
15	X	302	CDL	OB7-CB5-OB6-CB4
15	Z	202	CDL	CA3-OA5-PA1-OA2
15	Z	202	CDL	CA3-OA5-PA1-OA3
15	Z	202	CDL	OA6-CA4-CA6-OA8
15	Z	202	CDL	C11-CA5-OA6-CA4
15	Z	202	CDL	C51-CB5-OB6-CB4
15	Z	203	CDL	O1-C1-CB2-OB2
15	Z	203	CDL	CA2-OA2-PA1-OA3
15	Z	203	CDL	CA2-OA2-PA1-OA4
15	Z	203	CDL	CA2-OA2-PA1-OA5
15	Z	203	CDL	OA7-CA5-OA6-CA4
15	Z	203	CDL	C11-CA5-OA6-CA4
15	J	201	CDL	CA2-OA2-PA1-OA3
15	J	201	CDL	CA2-OA2-PA1-OA4
15	J	201	CDL	CA2-OA2-PA1-OA5

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Mol	Chain	Res	Type	Atoms
15	J	201	CDL	CB2-OB2-PB2-OB3
15	J	201	CDL	CB2-OB2-PB2-OB4
15	J	201	CDL	CB2-OB2-PB2-OB5
17	E	603	MQ9	C9-C11-C12-C13
18	F	706	9Y0	C22-C21-O7-C1
18	F	706	9Y0	O6-C21-O7-C1
18	S	302	9Y0	O1-C3-C4-N
18	P	202	9Y0	C22-C21-O7-C1
18	P	202	9Y0	O1-C3-C4-N
18	P	202	9Y0	C3-O1-P-O
18	X	303	9Y0	O1-C3-C4-N
18	J	202	9Y0	C22-C21-O7-C1
18	J	202	9Y0	O6-C21-O7-C1
18	J	202	9Y0	C2-O3-P-O
18	J	202	9Y0	C2-O3-P-O1
18	J	202	9Y0	C2-O3-P-O2
18	J	203	9Y0	O1-C3-C4-N
20	D	302	9XX	C19-C18-O1-C17
20	G	302	9XX	C19-C18-O1-C17
20	c	202	9XX	O-C16-C17-O1
20	c	202	9XX	C37-C17-O1-C18
20	c	202	9XX	C19-C18-O1-C17
20	c	202	9XX	O2-C18-O1-C17
20	W	202	9XX	O-C16-C17-O1
21	I	302	HEC	C2B-C3B-CAB-CBB
21	I	302	HEC	C4B-C3B-CAB-CBB
22	O	303	9YF	C-C1-O-P
22	O	303	9YF	C9-C8-O9-C
22	c	203	9YF	C2-O2-P-O
22	c	203	9YF	C2-O2-P-O8
22	c	203	9YF	C1-O-P-O1
22	c	203	9YF	C1-O-P-O2
22	c	203	9YF	C1-O-P-O8
22	c	203	9YF	C9-C8-O9-C
22	I	304	9YF	C-C1-O-P
22	I	304	9YF	C9-C8-O9-C
22	Y	502	9YF	C1-O-P-O1
22	Y	502	9YF	C1-O-P-O2
22	Y	502	9YF	C9-C8-O9-C
22	Y	503	9YF	C1-O-P-O8
22	Y	503	9YF	C9-C8-O9-C
22	W	203	9YF	C2-O2-P-O

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Mol	Chain	Res	Type	Atoms
22	W	203	9YF	C2-O2-P-O8
22	W	203	9YF	C1-O-P-O1
22	W	203	9YF	C1-O-P-O2
22	W	203	9YF	C1-O-P-O8
22	W	203	9YF	C9-C8-O9-C
22	M	501	9YF	C1-O-P-O1
22	M	501	9YF	C1-O-P-O2
22	M	501	9YF	C9-C8-O9-C
22	M	502	9YF	C1-O-P-O8
22	M	502	9YF	C9-C8-O9-C
21	I	302	HEC	C4C-C3C-CAC-CBC
15	R	604	CDL	OA9-CA7-OA8-CA6
15	L	604	CDL	OA9-CA7-OA8-CA6
20	W	202	9XX	O6-C15-O-C16
21	I	302	HEC	C2C-C3C-CAC-CBC
15	R	604	CDL	C31-CA7-OA8-CA6
15	T	201	CDL	OA9-CA7-OA8-CA6
15	T	202	CDL	OA9-CA7-OA8-CA6
15	T	203	CDL	OA9-CA7-OA8-CA6
15	T	203	CDL	OB9-CB7-OB8-CB6
15	X	301	CDL	OA9-CA7-OA8-CA6
15	Z	202	CDL	OA9-CA7-OA8-CA6
15	Z	203	CDL	OA9-CA7-OA8-CA6
15	Z	203	CDL	OB9-CB7-OB8-CB6
22	O	303	9YF	O12-C25-O11-C24
22	I	304	9YF	O12-C25-O11-C24
22	Y	502	9YF	O12-C25-O11-C24
22	M	501	9YF	O12-C25-O11-C24
21	O	302	HEC	C2B-C3B-CAB-CBB
15	R	604	CDL	OA7-CA5-OA6-CA4
15	R	604	CDL	OB7-CB5-OB6-CB4
15	E	605	CDL	OB7-CB5-OB6-CB4
15	E	606	CDL	OB7-CB5-OB6-CB4
15	F	704	CDL	OB7-CB5-OB6-CB4
15	F	705	CDL	OA7-CA5-OA6-CA4
15	L	604	CDL	OA7-CA5-OA6-CA4
15	T	201	CDL	OA7-CA5-OA6-CA4
15	T	201	CDL	OB7-CB5-OB6-CB4
15	T	202	CDL	OB7-CB5-OB6-CB4
15	X	301	CDL	OB7-CB5-OB6-CB4
15	Z	202	CDL	OA7-CA5-OA6-CA4
15	Z	202	CDL	OB7-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
18	P	202	9Y0	O6-C21-O7-C1
20	D	302	9XX	O2-C18-O1-C17
20	G	302	9XX	O2-C18-O1-C17
22	O	303	9YF	O10-C8-O9-C
22	c	203	9YF	O10-C8-O9-C
22	I	304	9YF	O10-C8-O9-C
22	Y	502	9YF	O10-C8-O9-C
22	Y	503	9YF	O10-C8-O9-C
22	W	203	9YF	O10-C8-O9-C
22	M	501	9YF	O10-C8-O9-C
22	M	502	9YF	O10-C8-O9-C
21	O	301	HEC	C2C-C3C-CAC-CBC
15	T	202	CDL	C31-CA7-OA8-CA6
15	T	203	CDL	C31-CA7-OA8-CA6
15	X	301	CDL	C31-CA7-OA8-CA6
15	Z	203	CDL	C71-CB7-OB8-CB6
18	X	303	9Y0	C6-C5-O5-C
18	J	202	9Y0	C6-C5-O5-C
20	W	202	9XX	C14-C15-O-C16
22	O	303	9YF	C26-C25-O11-C24
22	I	304	9YF	C26-C25-O11-C24
22	Y	502	9YF	C26-C25-O11-C24
22	M	501	9YF	C26-C25-O11-C24
15	E	605	CDL	C51-CB5-OB6-CB4
15	F	704	CDL	C51-CB5-OB6-CB4
15	F	705	CDL	C11-CA5-OA6-CA4
15	L	604	CDL	C51-CB5-OB6-CB4
15	S	301	CDL	C51-CB5-OB6-CB4
15	X	302	CDL	C51-CB5-OB6-CB4
21	O	301	HEC	C4C-C3C-CAC-CBC
21	O	301	HEC	C2B-C3B-CAB-CBB
14	L	602	HEA	C26-C15-C16-C17
17	F	707	MQ9	C15-C14-C16-C17
14	L	602	HEA	C14-C15-C16-C17
17	F	707	MQ9	C13-C14-C16-C17
22	Y	503	9YF	O12-C25-O11-C24
22	M	502	9YF	O12-C25-O11-C24
15	T	201	CDL	C31-CA7-OA8-CA6
15	T	203	CDL	C71-CB7-OB8-CB6
15	Z	202	CDL	C31-CA7-OA8-CA6
15	Z	203	CDL	C31-CA7-OA8-CA6
18	F	706	9Y0	C6-C5-O5-C

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Mol	Chain	Res	Type	Atoms
18	S	302	9Y0	C6-C5-O5-C
22	Y	503	9YF	C26-C25-O11-C24
22	M	502	9YF	C26-C25-O11-C24
18	F	706	9Y0	O4-C5-O5-C
18	X	303	9Y0	O4-C5-O5-C
18	J	202	9Y0	O4-C5-O5-C
18	S	302	9Y0	O6-C21-O7-C1
21	O	302	HEC	C4B-C3B-CAB-CBB
15	E	606	CDL	O1-C1-CB2-OB2
15	T	201	CDL	O1-C1-CB2-OB2
15	T	203	CDL	O1-C1-CB2-OB2
15	P	201	CDL	O1-C1-CA2-OA2
15	P	201	CDL	O1-C1-CB2-OB2
15	Z	202	CDL	O1-C1-CB2-OB2
15	J	201	CDL	O1-C1-CA2-OA2
15	J	201	CDL	O1-C1-CB2-OB2
22	c	203	9YF	C26-C25-O11-C24
22	W	203	9YF	C26-C25-O11-C24
18	S	302	9Y0	O4-C5-O5-C
15	E	606	CDL	C51-CB5-OB6-CB4
15	T	202	CDL	C11-CA5-OA6-CA4
15	X	301	CDL	C11-CA5-OA6-CA4
18	S	302	9Y0	C22-C21-O7-C1
18	X	303	9Y0	C22-C21-O7-C1
21	O	301	HEC	C4B-C3B-CAB-CBB
15	T	202	CDL	OA7-CA5-OA6-CA4
15	X	301	CDL	OA7-CA5-OA6-CA4
14	R	603	HEA	C15-C16-C17-C18
14	L	603	HEA	C15-C16-C17-C18
17	E	603	MQ9	C44-C46-C47-C48
17	E	604	MQ9	C29-C31-C32-C33
17	E	604	MQ9	C39-C41-C42-C43
17	F	701	MQ9	C9-C11-C12-C13
17	F	701	MQ9	C44-C46-C47-C48
17	F	707	MQ9	C9-C11-C12-C13
17	F	707	MQ9	C14-C16-C17-C18
17	F	708	MQ9	C14-C16-C17-C18
17	F	709	MQ9	C29-C31-C32-C33
17	F	709	MQ9	C39-C41-C42-C43
17	Z	201	MQ9	C9-C11-C12-C13
17	Z	201	MQ9	C14-C16-C17-C18
17	Z	201	MQ9	C29-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
17	Z	201	MQ9	C44-C46-C47-C48
17	I	303	MQ9	C14-C16-C17-C18
15	T	203	CDL	C38-C39-C40-C41
15	P	201	CDL	C1-CA2-OA2-PA1
15	J	201	CDL	C1-CA2-OA2-PA1
14	L	602	HEA	C3D-CAD-CBD-CGD
15	F	705	CDL	C76-C77-C78-C79
18	J	202	9Y0	C22-C23-C24-C25
15	E	605	CDL	C31-CA7-OA8-CA6
15	F	704	CDL	C31-CA7-OA8-CA6
15	L	604	CDL	C74-C75-C76-C77
22	c	203	9YF	O12-C25-O11-C24
22	W	203	9YF	O12-C25-O11-C24
15	R	604	CDL	C38-C39-C40-C41
15	E	605	CDL	C59-C60-C61-C62
15	F	704	CDL	C59-C60-C61-C62
15	E	606	CDL	C76-C77-C78-C79
15	E	605	CDL	OA9-CA7-OA8-CA6
15	F	704	CDL	OA9-CA7-OA8-CA6
18	X	303	9Y0	O6-C21-O7-C1
15	T	201	CDL	CA2-C1-CB2-OB2
15	P	201	CDL	CA2-C1-CB2-OB2
15	Z	202	CDL	CA2-C1-CB2-OB2
15	Z	203	CDL	CA2-C1-CB2-OB2
15	J	201	CDL	CA2-C1-CB2-OB2
15	R	604	CDL	C71-CB7-OB8-CB6
15	L	604	CDL	C71-CB7-OB8-CB6
15	S	301	CDL	C31-CA7-OA8-CA6
15	X	302	CDL	C31-CA7-OA8-CA6
18	J	203	9Y0	C6-C5-O5-C
15	R	604	CDL	C52-C53-C54-C55
15	P	201	CDL	C55-C56-C57-C58
15	J	201	CDL	C55-C56-C57-C58
15	E	606	CDL	C58-C59-C60-C61
18	P	202	9Y0	C23-C24-C25-C26
21	O	302	HEC	C4C-C3C-CAC-CBC
21	I	301	HEC	C4C-C3C-CAC-CBC
15	F	705	CDL	C57-C58-C59-C60
15	T	201	CDL	O1-C1-CA2-OA2
15	Z	202	CDL	O1-C1-CA2-OA2
15	E	605	CDL	C33-C34-C35-C36
15	F	704	CDL	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
18	P	202	9Y0	C27-C28-C29-C30
15	E	606	CDL	C11-CA5-OA6-CA4
15	P	201	CDL	C51-CB5-OB6-CB4
15	J	201	CDL	C51-CB5-OB6-CB4
21	I	301	HEC	C2C-C3C-CAC-CBC
15	T	201	CDL	OB6-CB4-CB6-OB8
15	P	201	CDL	OB6-CB4-CB6-OB8
15	Z	202	CDL	OB6-CB4-CB6-OB8
15	J	201	CDL	OB6-CB4-CB6-OB8
15	Z	203	CDL	CB7-C71-C72-C73
22	Y	502	9YF	C11-C10-C9-C8
22	M	501	9YF	C11-C10-C9-C8
21	O	302	HEC	C2C-C3C-CAC-CBC
17	E	603	MQ9	C40-C39-C41-C42
18	P	202	9Y0	C29-C30-C31-C32
15	S	301	CDL	CB7-C71-C72-C73
15	X	302	CDL	CB7-C71-C72-C73
14	L	602	HEA	C4D-C3D-CAD-CBD
17	E	604	MQ9	C9-C11-C12-C13
17	E	604	MQ9	C44-C46-C47-C48
17	F	707	MQ9	C24-C26-C27-C28
17	F	707	MQ9	C29-C31-C32-C33
17	F	707	MQ9	C39-C41-C42-C43
17	F	707	MQ9	C44-C46-C47-C48
17	F	708	MQ9	C29-C31-C32-C33
17	F	709	MQ9	C9-C11-C12-C13
17	F	709	MQ9	C44-C46-C47-C48
17	Z	201	MQ9	C39-C41-C42-C43
15	L	604	CDL	C31-C32-C33-C34
15	R	604	CDL	CB7-C71-C72-C73
15	L	604	CDL	CA5-C11-C12-C13
15	T	201	CDL	CA5-C11-C12-C13
15	Z	202	CDL	CA5-C11-C12-C13
18	J	203	9Y0	C21-C22-C23-C24
20	W	202	9XX	C12-C13-C14-C15
22	Y	503	9YF	C25-C26-C27-C28
22	M	502	9YF	C25-C26-C27-C28
15	R	604	CDL	OB9-CB7-OB8-CB6
15	L	604	CDL	OB9-CB7-OB8-CB6
15	S	301	CDL	OA9-CA7-OA8-CA6
15	X	302	CDL	OA9-CA7-OA8-CA6
22	c	203	9YF	C33-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
22	W	203	9YF	C33-C35-C36-C37
15	L	604	CDL	CB7-C71-C72-C73
15	S	301	CDL	CA5-C11-C12-C13
15	T	202	CDL	CB7-C71-C72-C73
15	X	301	CDL	CB7-C71-C72-C73
15	X	302	CDL	CA5-C11-C12-C13
18	J	203	9Y0	O4-C5-O5-C
15	R	604	CDL	C31-C32-C33-C34
15	R	604	CDL	C58-C59-C60-C61
15	E	606	CDL	OA7-CA5-OA6-CA4
15	L	604	CDL	C61-C62-C63-C64
15	P	201	CDL	OB7-CB5-OB6-CB4
15	J	201	CDL	OB7-CB5-OB6-CB4
15	T	203	CDL	CB2-C1-CA2-OA2
15	P	201	CDL	CB2-C1-CA2-OA2
15	J	201	CDL	CB2-C1-CA2-OA2
15	L	604	CDL	C38-C39-C40-C41
15	Z	203	CDL	CB5-C51-C52-C53
20	W	202	9XX	C19-C18-O1-C17
15	F	705	CDL	C78-C79-C80-C81
20	W	202	9XX	O2-C18-O1-C17
17	I	303	MQ9	C34-C36-C37-C38
22	Y	503	9YF	C9-C10-C11-C12
22	M	502	9YF	C9-C10-C11-C12
14	L	602	HEA	C2D-C3D-CAD-CBD
18	X	303	9Y0	C21-C22-C23-C24
15	T	201	CDL	CB6-CB4-OB6-CB5
15	Z	202	CDL	CB6-CB4-OB6-CB5
15	E	606	CDL	C78-C79-C80-C81
18	F	706	9Y0	C22-C23-C24-C25
15	E	605	CDL	C11-CA5-OA6-CA4
15	F	704	CDL	C11-CA5-OA6-CA4
17	E	603	MQ9	C38-C39-C41-C42
15	E	605	CDL	C55-C56-C57-C58
15	F	704	CDL	C55-C56-C57-C58
20	G	302	9XX	C17-C16-O-C15
15	T	201	CDL	C12-C13-C14-C15
15	Z	202	CDL	C12-C13-C14-C15
18	J	203	9Y0	C9-C10-C11-C12
20	W	202	9XX	C28-C29-C30-C31
22	Y	503	9YF	C26-C27-C28-C29
22	M	502	9YF	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
15	R	604	CDL	C35-C36-C37-C38
15	R	604	CDL	C55-C56-C57-C58
15	L	604	CDL	C75-C76-C77-C78
22	Y	503	9YF	C35-C36-C37-C38
22	Y	503	9YF	C37-C38-C39-C40
22	M	502	9YF	C35-C36-C37-C38
22	M	502	9YF	C37-C38-C39-C40
15	P	201	CDL	C60-C61-C62-C63
15	J	201	CDL	C60-C61-C62-C63
20	c	202	9XX	C31-C32-C33-C34
15	S	301	CDL	C71-CB7-OB8-CB6
15	X	302	CDL	C71-CB7-OB8-CB6
15	E	605	CDL	OA7-CA5-OA6-CA4
15	F	704	CDL	OA7-CA5-OA6-CA4
15	R	604	CDL	C75-C76-C77-C78
15	T	203	CDL	C73-C74-C75-C76
15	E	605	CDL	C56-C57-C58-C59
15	T	203	CDL	C56-C57-C58-C59
15	Z	203	CDL	C37-C38-C39-C40
15	F	704	CDL	C56-C57-C58-C59
15	F	705	CDL	C51-CB5-OB6-CB4
15	P	201	CDL	C11-CA5-OA6-CA4
15	J	201	CDL	C11-CA5-OA6-CA4
15	Z	203	CDL	C52-C53-C54-C55
18	S	302	9Y0	C21-C22-C23-C24
15	E	605	CDL	C75-C76-C77-C78
15	F	704	CDL	C75-C76-C77-C78
15	S	301	CDL	C35-C36-C37-C38
15	T	202	CDL	C59-C60-C61-C62
15	P	201	CDL	C75-C76-C77-C78
15	X	301	CDL	C59-C60-C61-C62
15	X	302	CDL	C35-C36-C37-C38
15	Z	203	CDL	C31-C32-C33-C34
15	J	201	CDL	C75-C76-C77-C78
18	J	203	9Y0	C6-C7-C8-C9
15	T	203	CDL	C32-C33-C34-C35
15	R	604	CDL	C53-C54-C55-C56
15	P	201	CDL	C32-C33-C34-C35
15	J	201	CDL	C32-C33-C34-C35
18	J	202	9Y0	C16-C17-C18-C19
15	S	301	CDL	C74-C75-C76-C77
15	X	302	CDL	C74-C75-C76-C77

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Mol	Chain	Res	Type	Atoms
18	F	706	9Y0	C15-C16-C17-C18
22	Y	502	9YF	C10-C11-C12-C13
22	M	501	9YF	C10-C11-C12-C13
20	D	302	9XX	C14-C15-O-C16
15	E	605	CDL	CA3-CA4-CA6-OA8
15	F	704	CDL	CA3-CA4-CA6-OA8
15	F	705	CDL	C34-C35-C36-C37
15	T	203	CDL	C74-C75-C76-C77
18	P	202	9Y0	C21-C22-C23-C24
15	L	604	CDL	C55-C56-C57-C58
15	T	201	CDL	C51-C52-C53-C54
15	P	201	CDL	C31-C32-C33-C34
15	Z	202	CDL	C51-C52-C53-C54
15	Z	203	CDL	C32-C33-C34-C35
15	J	201	CDL	C31-C32-C33-C34
18	P	202	9Y0	C9-C10-C11-C12
18	J	202	9Y0	C15-C16-C17-C18
20	W	202	9XX	C31-C32-C33-C34
15	F	705	CDL	C52-C53-C54-C55
15	Z	203	CDL	C35-C36-C37-C38
15	L	604	CDL	C76-C77-C78-C79
15	S	301	CDL	C31-C32-C33-C34
15	X	302	CDL	C31-C32-C33-C34
15	P	201	CDL	CB7-C71-C72-C73
15	J	201	CDL	CB7-C71-C72-C73
18	P	202	9Y0	C5-C6-C7-C8
15	E	606	CDL	C34-C35-C36-C37
15	F	705	CDL	C37-C38-C39-C40
15	L	604	CDL	C37-C38-C39-C40
15	S	301	CDL	C72-C73-C74-C75
15	T	203	CDL	C53-C54-C55-C56
15	X	302	CDL	C72-C73-C74-C75
16	E	602	HEM	C3D-CAD-CBD-CGD
15	L	604	CDL	C52-C53-C54-C55
15	P	201	CDL	C54-C55-C56-C57
15	P	201	CDL	C56-C57-C58-C59
15	J	201	CDL	C56-C57-C58-C59
22	O	303	9YF	C35-C36-C37-C38
22	I	304	9YF	C35-C36-C37-C38
15	R	604	CDL	C32-C33-C34-C35
15	E	606	CDL	C52-C53-C54-C55
15	F	705	CDL	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
15	Z	203	CDL	C11-C12-C13-C14
15	Z	203	CDL	C59-C60-C61-C62
15	J	201	CDL	C54-C55-C56-C57
15	S	301	CDL	OB9-CB7-OB8-CB6
15	X	302	CDL	OB9-CB7-OB8-CB6
15	P	201	CDL	OA7-CA5-OA6-CA4
15	J	201	CDL	OA7-CA5-OA6-CA4
17	F	701	MQ9	C40-C39-C41-C42
15	R	604	CDL	C37-C38-C39-C40
15	E	606	CDL	C37-C38-C39-C40
15	E	606	CDL	C53-C54-C55-C56
15	T	201	CDL	C76-C77-C78-C79
15	F	705	CDL	C31-CA7-OA8-CA6
15	L	604	CDL	C11-C12-C13-C14
15	Z	202	CDL	C76-C77-C78-C79
22	O	303	9YF	C26-C27-C28-C29
22	I	304	9YF	C26-C27-C28-C29
22	Y	503	9YF	C27-C28-C29-C30
22	M	502	9YF	C27-C28-C29-C30
15	S	301	CDL	C11-C12-C13-C14
15	X	302	CDL	C11-C12-C13-C14
22	Y	502	9YF	C28-C29-C30-C31
22	M	501	9YF	C28-C29-C30-C31
15	T	202	CDL	C11-C12-C13-C14
15	X	301	CDL	C11-C12-C13-C14
22	Y	503	9YF	C11-C12-C13-C14
22	M	502	9YF	C11-C12-C13-C14
15	T	203	CDL	C11-C12-C13-C14
15	X	301	CDL	C52-C53-C54-C55
18	F	706	9Y0	C29-C30-C31-C32
15	T	202	CDL	C52-C53-C54-C55
18	J	203	9Y0	C22-C23-C24-C25
22	Y	503	9YF	C19-C20-C21-C22
22	M	502	9YF	C19-C20-C21-C22
15	E	606	CDL	CB5-C51-C52-C53
15	J	201	CDL	CA7-C31-C32-C33
15	L	604	CDL	C32-C33-C34-C35
18	J	203	9Y0	C24-C25-C26-C27
15	F	705	CDL	OB7-CB5-OB6-CB4
18	F	706	9Y0	C16-C17-C18-C19
15	E	605	CDL	CA7-C31-C32-C33
15	F	704	CDL	CA7-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
15	P	201	CDL	CA7-C31-C32-C33
22	O	303	9YF	C11-C10-C9-C8
22	I	304	9YF	C11-C10-C9-C8
15	L	604	CDL	C53-C54-C55-C56
15	S	301	CDL	C60-C61-C62-C63
15	X	302	CDL	C60-C61-C62-C63
15	Z	203	CDL	C73-C74-C75-C76
22	c	203	9YF	C17-C18-C19-C20
22	W	203	9YF	C17-C18-C19-C20
15	T	201	CDL	C31-C32-C33-C34
15	Z	202	CDL	C31-C32-C33-C34
15	F	705	CDL	C59-C60-C61-C62
18	P	202	9Y0	C6-C7-C8-C9
19	c	201	PLM	C5-C6-C7-C8
22	Y	502	9YF	C33-C35-C36-C37
22	M	501	9YF	C33-C35-C36-C37
15	E	605	CDL	CB7-C71-C72-C73
15	L	604	CDL	CB5-C51-C52-C53
22	c	203	9YF	C15-C16-C17-C18
22	W	203	9YF	C15-C16-C17-C18
18	S	302	9Y0	C18-C19-C20-C37
17	E	603	MQ9	C39-C41-C42-C43
17	F	708	MQ9	C39-C41-C42-C43
15	P	201	CDL	C52-C53-C54-C55
15	F	704	CDL	CB7-C71-C72-C73
15	J	201	CDL	C52-C53-C54-C55
15	S	301	CDL	OA6-CA4-CA6-OA8
15	X	302	CDL	OA6-CA4-CA6-OA8
15	E	605	CDL	C12-C13-C14-C15
15	F	704	CDL	C12-C13-C14-C15
15	L	604	CDL	C12-C13-C14-C15
15	P	201	CDL	C57-C58-C59-C60
15	Z	203	CDL	C56-C57-C58-C59
15	J	201	CDL	C57-C58-C59-C60
15	F	705	CDL	C56-C57-C58-C59
18	J	202	9Y0	C6-C7-C8-C9
15	E	605	CDL	C34-C35-C36-C37
15	F	704	CDL	C34-C35-C36-C37
15	T	202	CDL	C55-C56-C57-C58
15	X	301	CDL	C55-C56-C57-C58
19	W	201	PLM	C2-C3-C4-C5
15	P	201	CDL	C74-C75-C76-C77

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Mol	Chain	Res	Type	Atoms
15	J	201	CDL	C74-C75-C76-C77
15	E	606	CDL	CA2-C1-CB2-OB2
15	F	705	CDL	OA9-CA7-OA8-CA6
20	c	202	9XX	C1-C2-C3-C4
15	T	201	CDL	C59-C60-C61-C62
15	Z	202	CDL	C59-C60-C61-C62
15	T	202	CDL	C75-C76-C77-C78
15	X	301	CDL	C75-C76-C77-C78
18	F	706	9Y0	C6-C7-C8-C9
18	P	202	9Y0	C14-C15-C16-C17
15	E	605	CDL	OB5-CB3-CB4-CB6
15	F	704	CDL	OB5-CB3-CB4-CB6
22	O	303	9YF	C24-C-C1-O
22	I	304	9YF	C24-C-C1-O
15	F	704	CDL	C32-C33-C34-C35
15	P	201	CDL	C73-C74-C75-C76
15	X	301	CDL	C38-C39-C40-C41
15	J	201	CDL	C73-C74-C75-C76
22	Y	503	9YF	C31-C32-C33-C35
22	Y	503	9YF	C32-C33-C35-C36
22	M	502	9YF	C31-C32-C33-C35
22	M	502	9YF	C32-C33-C35-C36
15	E	605	CDL	C32-C33-C34-C35
15	T	202	CDL	C38-C39-C40-C41
18	J	202	9Y0	C29-C30-C31-C32
20	D	302	9XX	O6-C15-O-C16
15	T	202	CDL	CA5-C11-C12-C13
15	X	301	CDL	CA5-C11-C12-C13
15	S	301	CDL	C76-C77-C78-C79
15	X	302	CDL	C76-C77-C78-C79
18	J	203	9Y0	C16-C17-C18-C19
15	F	704	CDL	C71-C72-C73-C74
21	O	301	HEC	C4D-C3D-CAD-CBD
15	E	605	CDL	C71-C72-C73-C74
15	T	203	CDL	C31-C32-C33-C34
15	E	605	CDL	CB3-CB4-CB6-OB8
15	F	704	CDL	CB3-CB4-CB6-OB8
15	S	301	CDL	CB3-CB4-CB6-OB8
15	T	202	CDL	CA3-CA4-CA6-OA8
15	P	201	CDL	CA3-CA4-CA6-OA8
15	P	201	CDL	CB3-CB4-CB6-OB8
15	X	301	CDL	CA3-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
15	X	302	CDL	CB3-CB4-CB6-OB8
15	J	201	CDL	CA3-CA4-CA6-OA8
15	J	201	CDL	CB3-CB4-CB6-OB8
17	F	708	MQ9	C34-C36-C37-C38
18	X	303	9Y0	O5-C-C1-C2
22	c	203	9YF	C1-C-C24-O11
22	W	203	9YF	C1-C-C24-O11
15	R	604	CDL	C72-C73-C74-C75
20	G	302	9XX	C14-C15-O-C16
15	Z	203	CDL	C72-C73-C74-C75
15	P	201	CDL	C76-C77-C78-C79
15	J	201	CDL	C76-C77-C78-C79
22	Y	502	9YF	C26-C27-C28-C29
22	M	501	9YF	C26-C27-C28-C29
15	T	201	CDL	CB5-C51-C52-C53
15	Z	202	CDL	CB5-C51-C52-C53
15	Z	203	CDL	CA7-C31-C32-C33
18	P	202	9Y0	C26-C27-C28-C29
17	F	701	MQ9	C38-C39-C41-C42
17	Z	201	MQ9	C12-C11-C9-C8
15	T	203	CDL	C57-C58-C59-C60
15	E	605	CDL	C72-C73-C74-C75
15	F	704	CDL	C72-C73-C74-C75
15	X	302	CDL	C34-C35-C36-C37
15	S	301	CDL	C34-C35-C36-C37
15	T	202	CDL	C72-C73-C74-C75
15	X	301	CDL	C72-C73-C74-C75
21	O	301	HEC	C2D-C3D-CAD-CBD
22	Y	502	9YF	C12-C13-C14-C15
22	M	501	9YF	C12-C13-C14-C15
15	E	605	CDL	CB6-CB4-OB6-CB5
15	F	704	CDL	CB6-CB4-OB6-CB5
20	c	202	9XX	C28-C29-C30-C31
20	c	202	9XX	C24-C25-C26-C27
18	X	303	9Y0	C14-C15-C16-C17
20	W	202	9XX	C20-C21-C22-C23
15	E	605	CDL	OA5-CA3-CA4-OA6
15	E	606	CDL	OA5-CA3-CA4-OA6
15	F	704	CDL	OA5-CA3-CA4-OA6
15	S	301	CDL	OA5-CA3-CA4-OA6
15	X	302	CDL	OA5-CA3-CA4-OA6
18	F	706	9Y0	O7-C1-C2-O3

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Mol	Chain	Res	Type	Atoms
15	E	606	CDL	C54-C55-C56-C57
20	c	202	9XX	C7-C8-C9-C10
15	X	302	CDL	C77-C78-C79-C80
15	J	201	CDL	C59-C60-C61-C62
15	R	604	CDL	C59-C60-C61-C62
15	S	301	CDL	C77-C78-C79-C80
15	T	202	CDL	C36-C37-C38-C39
15	P	201	CDL	C34-C35-C36-C37
15	P	201	CDL	C59-C60-C61-C62
15	X	301	CDL	C36-C37-C38-C39
15	J	201	CDL	C34-C35-C36-C37
22	c	203	9YF	C27-C28-C29-C30
22	W	203	9YF	C27-C28-C29-C30
15	L	604	CDL	C33-C34-C35-C36
15	T	203	CDL	C71-C72-C73-C74
15	F	705	CDL	OB6-CB4-CB6-OB8
15	Z	203	CDL	OB6-CB4-CB6-OB8
18	X	303	9Y0	O5-C-C1-O7
18	J	203	9Y0	O5-C-C1-O7
15	R	604	CDL	C11-C12-C13-C14
21	I	301	HEC	C2B-C3B-CAB-CBB
18	J	203	9Y0	C32-C33-C34-C35
15	X	301	CDL	C14-C15-C16-C17
15	T	203	CDL	C77-C78-C79-C80
19	G	301	PLM	C4-C5-C6-C7
15	L	604	CDL	C78-C79-C80-C81
15	T	202	CDL	C14-C15-C16-C17
15	T	202	CDL	C54-C55-C56-C57
15	X	301	CDL	C54-C55-C56-C57
15	P	201	CDL	C61-C62-C63-C64
15	J	201	CDL	C61-C62-C63-C64
22	Y	503	9YF	C40-C41-C42-C43
22	M	502	9YF	C40-C41-C42-C43
18	X	303	9Y0	C6-C7-C8-C9
15	R	604	CDL	C39-C40-C41-C42
22	c	203	9YF	C20-C21-C22-C23
17	I	303	MQ9	C15-C14-C16-C17
22	W	203	9YF	C20-C21-C22-C23
22	Y	502	9YF	C18-C19-C20-C21
22	M	501	9YF	C18-C19-C20-C21
22	Y	503	9YF	C31-C32-C33-C34
22	Y	503	9YF	C34-C33-C35-C36

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Mol	Chain	Res	Type	Atoms
22	M	502	9YF	C31-C32-C33-C34
22	M	502	9YF	C34-C33-C35-C36
15	T	201	CDL	CB4-CB3-OB5-PB2
15	T	202	CDL	C1-CB2-OB2-PB2
15	X	301	CDL	C1-CB2-OB2-PB2
15	Z	202	CDL	CB4-CB3-OB5-PB2
22	Y	502	9YF	C-C1-O-P
22	M	501	9YF	C-C1-O-P
15	R	604	CDL	C54-C55-C56-C57
15	T	203	CDL	C54-C55-C56-C57
18	X	303	9Y0	C18-C19-C20-C37
18	J	203	9Y0	C26-C27-C28-C29
19	W	201	PLM	C9-CA-CB-CC
15	Z	202	CDL	C33-C34-C35-C36
15	E	606	CDL	C39-C40-C41-C42
15	F	705	CDL	C58-C59-C60-C61
15	T	201	CDL	C33-C34-C35-C36
18	S	302	9Y0	C6-C7-C8-C9
18	X	303	9Y0	C27-C28-C29-C30
15	X	301	CDL	C76-C77-C78-C79
15	R	604	CDL	C78-C79-C80-C81
15	S	301	CDL	C39-C40-C41-C42
15	X	302	CDL	C39-C40-C41-C42
15	E	606	CDL	OA5-CA3-CA4-CA6
15	T	202	CDL	OB5-CB3-CB4-CB6
15	X	301	CDL	OB5-CB3-CB4-CB6
15	R	604	CDL	C60-C61-C62-C63
15	T	202	CDL	C76-C77-C78-C79
20	c	202	9XX	O1-C18-C19-C20
20	G	302	9XX	C26-C27-C28-C29
15	E	605	CDL	C78-C79-C80-C81
15	F	704	CDL	C78-C79-C80-C81
22	O	303	9YF	C20-C21-C22-C23
22	I	304	9YF	C20-C21-C22-C23
15	T	201	CDL	C36-C37-C38-C39
15	Z	202	CDL	C36-C37-C38-C39
15	T	203	CDL	C52-C53-C54-C55
22	M	502	9YF	C16-C17-C18-C19
15	T	203	CDL	C61-C62-C63-C64
15	Z	203	CDL	C38-C39-C40-C41
22	Y	503	9YF	C16-C17-C18-C19
17	Z	201	MQ9	C12-C11-C9-C10

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Mol	Chain	Res	Type	Atoms
15	R	604	CDL	C72-C71-CB7-OB8
20	c	202	9XX	O-C16-C17-C37
20	W	202	9XX	O-C16-C17-C37
15	R	604	CDL	C77-C78-C79-C80
14	R	602	HEA	C15-C16-C17-C18
15	L	604	CDL	CB3-CB4-CB6-OB8
15	S	301	CDL	CA3-CA4-CA6-OA8
15	X	302	CDL	CA3-CA4-CA6-OA8
17	F	701	MQ9	C39-C41-C42-C43
18	S	302	9Y0	O5-C-C1-C2
18	J	203	9Y0	O5-C-C1-C2
22	O	303	9YF	C1-C-C24-O11
22	I	304	9YF	C1-C-C24-O11
15	F	704	CDL	C53-C54-C55-C56
15	E	606	CDL	CA5-C11-C12-C13
15	T	202	CDL	CA7-C31-C32-C33
15	X	301	CDL	CA7-C31-C32-C33
15	F	704	CDL	C76-C77-C78-C79
15	E	605	CDL	C53-C54-C55-C56
15	S	301	CDL	C59-C60-C61-C62
15	X	302	CDL	C59-C60-C61-C62
15	E	605	CDL	C76-C77-C78-C79
15	R	604	CDL	CB5-C51-C52-C53
15	R	604	CDL	OA5-CA3-CA4-OA6
15	F	705	CDL	OA5-CA3-CA4-OA6
15	T	203	CDL	OB5-CB3-CB4-OB6
18	S	302	9Y0	C14-C15-C16-C17
15	S	301	CDL	C61-C62-C63-C64
15	X	302	CDL	C61-C62-C63-C64
15	L	604	CDL	C72-C71-CB7-OB8
15	T	201	CDL	CB7-C71-C72-C73
15	Z	202	CDL	CB7-C71-C72-C73
15	E	606	CDL	OB6-CB4-CB6-OB8
15	L	604	CDL	OB6-CB4-CB6-OB8
18	S	302	9Y0	O5-C-C1-O7
15	E	605	CDL	C31-C32-C33-C34
15	F	704	CDL	C31-C32-C33-C34
15	L	604	CDL	C35-C36-C37-C38
18	X	303	9Y0	C29-C30-C31-C32
22	M	502	9YF	C15-C16-C17-C18
22	Y	503	9YF	C15-C16-C17-C18
15	R	604	CDL	C73-C74-C75-C76

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Mol	Chain	Res	Type	Atoms
17	I	303	MQ9	C13-C14-C16-C17
19	c	201	PLM	CA-CB-CC-CD
15	R	604	CDL	C51-C52-C53-C54
20	G	302	9XX	O6-C15-O-C16
22	Y	503	9YF	C14-C15-C16-C17
22	M	502	9YF	C14-C15-C16-C17
15	E	605	CDL	C61-C62-C63-C64
15	F	704	CDL	C61-C62-C63-C64
15	F	705	CDL	C61-C62-C63-C64
17	F	708	MQ9	C9-C11-C12-C13
17	F	708	MQ9	C19-C21-C22-C23
18	S	302	9Y0	C29-C30-C31-C32
15	E	606	CDL	C57-C58-C59-C60
18	S	302	9Y0	C27-C28-C29-C30
22	c	203	9YF	C9-C10-C11-C12
22	W	203	9YF	C9-C10-C11-C12
15	T	201	CDL	CB2-C1-CA2-OA2
15	Z	202	CDL	CB2-C1-CA2-OA2
22	O	303	9YF	C27-C28-C29-C30
22	I	304	9YF	C27-C28-C29-C30
15	P	201	CDL	C36-C37-C38-C39
15	T	203	CDL	OB5-CB3-CB4-CB6
15	L	604	CDL	C56-C57-C58-C59
15	J	201	CDL	C36-C37-C38-C39
15	R	604	CDL	C12-C13-C14-C15
15	S	301	CDL	C71-C72-C73-C74
15	X	302	CDL	C71-C72-C73-C74
22	O	303	9YF	C39-C40-C41-C42
22	I	304	9YF	C39-C40-C41-C42
15	F	705	CDL	C52-C51-CB5-OB6
15	P	201	CDL	C12-C13-C14-C15
15	Z	203	CDL	C54-C55-C56-C57
17	Z	201	MQ9	C20-C19-C21-C22
15	L	604	CDL	C73-C74-C75-C76
15	J	201	CDL	C12-C13-C14-C15
19	D	301	PLM	C4-C5-C6-C7
15	T	202	CDL	OB5-CB3-CB4-OB6
15	T	203	CDL	OA5-CA3-CA4-OA6
15	X	301	CDL	OB5-CB3-CB4-OB6
15	F	705	CDL	C39-C40-C41-C42
15	R	604	CDL	CB3-CB4-CB6-OB8
15	F	705	CDL	CB3-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
15	T	201	CDL	CA3-CA4-CA6-OA8
15	T	201	CDL	CB3-CB4-CB6-OB8
15	Z	202	CDL	CA3-CA4-CA6-OA8
15	Z	202	CDL	CB3-CB4-CB6-OB8
17	F	707	MQ9	C19-C21-C22-C23
16	E	602	HEM	C4B-C3B-CAB-CBB
20	W	202	9XX	C1-C2-C3-C4
18	J	202	9Y0	C19-C20-C37-C38
15	E	605	CDL	OB6-CB4-CB6-OB8
15	F	704	CDL	OB6-CB4-CB6-OB8
15	Z	203	CDL	C78-C79-C80-C81
15	X	301	CDL	C73-C74-C75-C76
15	T	202	CDL	C73-C74-C75-C76
18	J	202	9Y0	C5-C6-C7-C8
20	c	202	9XX	C19-C20-C21-C22
20	G	302	9XX	C5-C6-C7-C8
15	F	705	CDL	O1-C1-CB2-OB2
15	S	301	CDL	C33-C34-C35-C36
15	X	302	CDL	C33-C34-C35-C36
15	E	606	CDL	C51-C52-C53-C54
15	T	203	CDL	C58-C59-C60-C61
20	D	302	9XX	C17-C16-O-C15
17	F	707	MQ9	C20-C19-C21-C22
15	E	605	CDL	OA5-CA3-CA4-CA6
15	F	704	CDL	OA5-CA3-CA4-CA6
15	S	301	CDL	OA5-CA3-CA4-CA6
15	X	302	CDL	OA5-CA3-CA4-CA6
22	Y	502	9YF	C19-C20-C21-C22
22	Y	503	9YF	C12-C13-C14-C15
22	M	502	9YF	C12-C13-C14-C15
20	D	302	9XX	C26-C27-C28-C29
15	L	604	CDL	C39-C40-C41-C42
22	M	501	9YF	C19-C20-C21-C22
18	J	203	9Y0	C30-C31-C32-C33
20	c	202	9XX	C6-C7-C8-C9
15	T	202	CDL	CB4-CB3-OB5-PB2
15	X	301	CDL	CB4-CB3-OB5-PB2
15	E	606	CDL	C77-C78-C79-C80
15	T	203	CDL	C59-C60-C61-C62
15	E	606	CDL	C59-C60-C61-C62
15	E	605	CDL	OB5-CB3-CB4-OB6
15	F	704	CDL	OB5-CB3-CB4-OB6

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Mol	Chain	Res	Type	Atoms
22	O	303	9YF	O9-C-C1-O
22	I	304	9YF	O9-C-C1-O
22	Y	502	9YF	O9-C-C1-O
22	M	501	9YF	O9-C-C1-O
18	P	202	9Y0	C18-C19-C20-C37
20	D	302	9XX	C20-C21-C22-C23
22	Y	503	9YF	C33-C35-C36-C37
22	M	502	9YF	C33-C35-C36-C37
15	R	604	CDL	OB6-CB4-CB6-OB8
15	E	605	CDL	OA6-CA4-CA6-OA8
15	F	704	CDL	OA6-CA4-CA6-OA8
15	S	301	CDL	OB6-CB4-CB6-OB8
15	P	201	CDL	OA6-CA4-CA6-OA8
15	X	302	CDL	OB6-CB4-CB6-OB8
15	J	201	CDL	OA6-CA4-CA6-OA8
22	O	303	9YF	O9-C-C24-O11
22	I	304	9YF	O9-C-C24-O11
15	T	202	CDL	C33-C34-C35-C36
15	X	301	CDL	C33-C34-C35-C36
19	G	301	PLM	C7-C8-C9-CA
15	E	606	CDL	C61-C62-C63-C64
22	O	303	9YF	C33-C35-C36-C37
22	I	304	9YF	C33-C35-C36-C37
22	c	203	9YF	C39-C40-C41-C42
15	L	604	CDL	C60-C61-C62-C63
22	W	203	9YF	C39-C40-C41-C42
15	R	604	CDL	CB2-OB2-PB2-OB5
15	E	605	CDL	CB3-OB5-PB2-OB4
15	E	606	CDL	CA2-OA2-PA1-OA3
15	F	704	CDL	CB3-OB5-PB2-OB4
15	F	705	CDL	CB2-OB2-PB2-OB4
15	S	301	CDL	CA3-OA5-PA1-OA4
15	T	201	CDL	CA2-OA2-PA1-OA3
15	T	201	CDL	CB2-OB2-PB2-OB3
15	T	202	CDL	CB2-OB2-PB2-OB3
15	T	202	CDL	CB2-OB2-PB2-OB4
15	T	202	CDL	CB2-OB2-PB2-OB5
15	T	202	CDL	CB3-OB5-PB2-OB3
15	T	203	CDL	CA3-OA5-PA1-OA2
15	T	203	CDL	CA3-OA5-PA1-OA3
15	T	203	CDL	CA3-OA5-PA1-OA4
15	T	203	CDL	CB3-OB5-PB2-OB4

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Mol	Chain	Res	Type	Atoms
15	X	301	CDL	CB2-OB2-PB2-OB3
15	X	301	CDL	CB2-OB2-PB2-OB4
15	X	301	CDL	CB2-OB2-PB2-OB5
15	X	301	CDL	CB3-OB5-PB2-OB3
15	X	302	CDL	CA3-OA5-PA1-OA4
15	Z	202	CDL	CA2-OA2-PA1-OA3
15	Z	202	CDL	CB2-OB2-PB2-OB3
15	Z	203	CDL	CA3-OA5-PA1-OA2
15	Z	203	CDL	CA3-OA5-PA1-OA3
15	Z	203	CDL	CA3-OA5-PA1-OA4
18	P	202	9Y0	C2-O3-P-O1
18	P	202	9Y0	C2-O3-P-O2
18	J	203	9Y0	C2-O3-P-O
22	O	303	9YF	C1-O-P-O1
22	I	304	9YF	C1-O-P-O1
17	F	707	MQ9	C12-C11-C9-C8
17	Z	201	MQ9	C18-C19-C21-C22
15	R	604	CDL	C1-CA2-OA2-PA1
15	E	606	CDL	C1-CA2-OA2-PA1
15	E	606	CDL	C1-CB2-OB2-PB2
15	F	705	CDL	C1-CA2-OA2-PA1
15	S	301	CDL	C1-CA2-OA2-PA1
15	S	301	CDL	C1-CB2-OB2-PB2
15	X	302	CDL	C1-CA2-OA2-PA1
15	X	302	CDL	C1-CB2-OB2-PB2
15	Z	203	CDL	C1-CA2-OA2-PA1
18	F	706	9Y0	C30-C31-C32-C33
19	c	201	PLM	CC-CD-CE-CF
14	L	602	HEA	C12-C11-C3B-C4B
15	F	705	CDL	C73-C74-C75-C76
22	I	304	9YF	C29-C30-C31-C32
15	E	605	CDL	C60-C61-C62-C63
15	F	704	CDL	C60-C61-C62-C63
18	P	202	9Y0	C25-C26-C27-C28
22	O	303	9YF	C29-C30-C31-C32
22	Y	502	9YF	C25-C26-C27-C28
18	S	302	9Y0	C22-C23-C24-C25
18	S	302	9Y0	C13-C14-C15-C16
22	M	501	9YF	C25-C26-C27-C28
15	T	202	CDL	C35-C36-C37-C38
22	I	304	9YF	C18-C19-C20-C21
15	T	203	CDL	CA6-CA4-OA6-CA5

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Mol	Chain	Res	Type	Atoms
15	X	301	CDL	C35-C36-C37-C38
22	O	303	9YF	C18-C19-C20-C21
15	R	604	CDL	OA5-CA3-CA4-CA6
18	F	706	9Y0	C-C1-C2-O3
20	G	302	9XX	C36-C27-C28-C29
22	M	501	9YF	C16-C17-C18-C19
22	Y	502	9YF	C16-C17-C18-C19
18	P	202	9Y0	C11-C12-C13-C14
18	X	303	9Y0	C13-C14-C15-C16
18	J	203	9Y0	C11-C12-C13-C14
22	Y	503	9YF	O9-C-C1-O
22	M	502	9YF	O9-C-C1-O
15	L	604	CDL	C77-C78-C79-C80
17	F	707	MQ9	C12-C11-C9-C10
15	F	705	CDL	C1-CB2-OB2-PB2
22	c	203	9YF	O9-C-C24-O11
22	W	203	9YF	O9-C-C24-O11
15	T	203	CDL	C55-C56-C57-C58
19	D	301	PLM	C7-C8-C9-CA
22	Y	502	9YF	C40-C41-C42-C43
22	M	501	9YF	C40-C41-C42-C43
21	I	301	HEC	C4B-C3B-CAB-CBB
17	F	707	MQ9	C16-C17-C18-C19
17	F	709	MQ9	C35-C34-C36-C37
17	I	303	MQ9	C29-C31-C32-C33
15	R	604	CDL	C71-C72-C73-C74
18	F	706	9Y0	C19-C20-C37-C38
15	F	705	CDL	C54-C55-C56-C57
20	G	302	9XX	C20-C21-C22-C23
15	F	705	CDL	C38-C39-C40-C41
17	F	709	MQ9	C40-C39-C41-C42
17	F	707	MQ9	C18-C19-C21-C22
15	X	301	CDL	C53-C54-C55-C56
15	T	202	CDL	C53-C54-C55-C56
20	D	302	9XX	C36-C27-C28-C29
15	P	201	CDL	C37-C38-C39-C40
22	Y	502	9YF	C35-C36-C37-C38
22	M	501	9YF	C35-C36-C37-C38
15	J	201	CDL	C37-C38-C39-C40
18	J	203	9Y0	C14-C15-C16-C17
17	F	708	MQ9	C15-C14-C16-C17
15	P	201	CDL	C12-C11-CA5-OA6

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Mol	Chain	Res	Type	Atoms
15	J	201	CDL	C12-C11-CA5-OA6
15	T	201	CDL	OB5-CB3-CB4-OB6
15	Z	202	CDL	OB5-CB3-CB4-OB6
18	X	303	9Y0	C22-C23-C24-C25
15	Z	203	CDL	C57-C58-C59-C60
18	J	202	9Y0	C7-C8-C9-C10
17	F	708	MQ9	C40-C39-C41-C42
17	F	709	MQ9	C33-C34-C36-C37
18	S	302	9Y0	C5-C6-C7-C8
15	S	301	CDL	C57-C58-C59-C60
15	P	201	CDL	C38-C39-C40-C41
15	X	302	CDL	C57-C58-C59-C60
15	J	201	CDL	C38-C39-C40-C41
18	P	202	9Y0	C16-C17-C18-C19
22	I	304	9YF	C37-C38-C39-C40
22	O	303	9YF	C37-C38-C39-C40
22	Y	502	9YF	C37-C38-C39-C40
22	M	501	9YF	C37-C38-C39-C40
15	X	301	CDL	C13-C14-C15-C16
15	T	202	CDL	C13-C14-C15-C16
22	M	502	9YF	C29-C30-C31-C32
22	Y	503	9YF	C29-C30-C31-C32
15	R	604	CDL	C33-C34-C35-C36
15	F	705	CDL	C77-C78-C79-C80
14	R	602	HEA	CAA-CBA-CGA-O1A
15	T	203	CDL	C14-C15-C16-C17
17	F	709	MQ9	C38-C39-C41-C42
18	P	202	9Y0	C24-C25-C26-C27
14	L	602	HEA	CAD-CBD-CGD-O1D
14	L	603	HEA	CAA-CBA-CGA-O1A
18	J	202	9Y0	O7-C1-C2-O3
15	E	605	CDL	CB5-C51-C52-C53
15	F	704	CDL	CB5-C51-C52-C53
14	R	602	HEA	CAD-CBD-CGD-O1D
20	c	202	9XX	O2-C18-C19-C20
17	E	604	MQ9	C40-C39-C41-C42
15	T	202	CDL	OA5-CA3-CA4-CA6
15	X	301	CDL	OA5-CA3-CA4-CA6
18	F	706	9Y0	C7-C8-C9-C10
14	R	602	HEA	CAA-CBA-CGA-O2A
14	L	602	HEA	CAA-CBA-CGA-O1A
22	c	203	9YF	C31-C32-C33-C35

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Mol	Chain	Res	Type	Atoms
22	W	203	9YF	C31-C32-C33-C35
15	P	201	CDL	C11-C12-C13-C14
15	J	201	CDL	C11-C12-C13-C14
15	T	203	CDL	C39-C40-C41-C42
15	F	704	CDL	C11-C12-C13-C14
15	E	605	CDL	C11-C12-C13-C14
18	S	302	9Y0	C7-C8-C9-C10
14	R	603	HEA	CAA-CBA-CGA-O1A
17	F	701	MQ9	C15-C14-C16-C17
17	Z	201	MQ9	C30-C29-C31-C32
17	F	708	MQ9	C13-C14-C16-C17
19	D	301	PLM	C2-C3-C4-C5
19	c	201	PLM	C7-C8-C9-CA
22	I	304	9YF	C30-C31-C32-C33
15	Z	203	CDL	C14-C15-C16-C17
15	X	302	CDL	C55-C56-C57-C58
15	L	604	CDL	C59-C60-C61-C62
15	S	301	CDL	C55-C56-C57-C58
18	J	203	9Y0	C7-C8-C9-C10
19	c	201	PLM	C8-C9-CA-CB
14	L	602	HEA	CAD-CBD-CGD-O2D
22	O	303	9YF	C30-C31-C32-C33
17	E	604	MQ9	C35-C34-C36-C37
14	R	602	HEA	CAD-CBD-CGD-O2D
14	L	602	HEA	CAA-CBA-CGA-O2A
15	L	604	CDL	C1-CB2-OB2-PB2
15	L	604	CDL	CB4-CB3-OB5-PB2
14	L	603	HEA	CAA-CBA-CGA-O2A
15	F	705	CDL	CB7-C71-C72-C73
21	I	301	HEC	C2D-C3D-CAD-CBD
15	T	203	CDL	C13-C14-C15-C16
15	E	606	CDL	CB3-CB4-CB6-OB8
17	I	303	MQ9	C9-C11-C12-C13
14	R	603	HEA	CAA-CBA-CGA-O2A
19	W	201	PLM	CC-CD-CE-CF
15	T	202	CDL	OA5-CA3-CA4-OA6
15	X	301	CDL	OA5-CA3-CA4-OA6
17	F	709	MQ9	C30-C29-C31-C32
15	R	604	CDL	C72-C71-CB7-OB9
15	X	301	CDL	C56-C57-C58-C59
18	F	706	9Y0	C11-C12-C13-C14
15	F	705	CDL	C60-C61-C62-C63

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Mol	Chain	Res	Type	Atoms
15	T	202	CDL	C56-C57-C58-C59
20	W	202	9XX	O1-C18-C19-C20
15	Z	203	CDL	C13-C14-C15-C16
16	F	702	HEM	CAD-CBD-CGD-O2D
15	T	203	CDL	CA7-C31-C32-C33
15	F	705	CDL	OA5-CA3-CA4-CA6
15	T	203	CDL	OA5-CA3-CA4-CA6
17	F	708	MQ9	C38-C39-C41-C42
17	Z	201	MQ9	C28-C29-C31-C32
15	R	604	CDL	CB4-CB3-OB5-PB2
15	E	605	CDL	C1-CA2-OA2-PA1
15	F	704	CDL	C1-CA2-OA2-PA1
15	L	604	CDL	C1-CA2-OA2-PA1
15	P	201	CDL	CA4-CA3-OA5-PA1
15	J	201	CDL	CA4-CA3-OA5-PA1
15	Z	202	CDL	C78-C79-C80-C81
15	T	203	CDL	C35-C36-C37-C38
18	J	202	9Y0	C24-C25-C26-C27
20	W	202	9XX	C3-C4-C5-C6
15	T	201	CDL	C78-C79-C80-C81
22	W	203	9YF	C13-C14-C15-C16
22	c	203	9YF	C13-C14-C15-C16
15	P	201	CDL	C14-C15-C16-C17
15	J	201	CDL	C14-C15-C16-C17
18	S	302	9Y0	C10-C11-C12-C13
15	F	705	CDL	C33-C34-C35-C36
19	W	201	PLM	C7-C8-C9-CA
15	T	203	CDL	C75-C76-C77-C78
17	E	604	MQ9	C20-C19-C21-C22
15	E	606	CDL	C72-C73-C74-C75
15	T	203	CDL	C52-C51-CB5-OB6
18	P	202	9Y0	C-C1-O7-C21
15	L	604	CDL	C57-C58-C59-C60
15	T	201	CDL	C32-C33-C34-C35
15	Z	202	CDL	C32-C33-C34-C35
17	I	303	MQ9	C12-C11-C9-C10
18	J	203	9Y0	O7-C1-C2-O3
17	F	709	MQ9	C24-C26-C27-C28
15	L	604	CDL	C72-C71-CB7-OB9
17	F	707	MQ9	C45-C44-C46-C47
17	F	709	MQ9	C20-C19-C21-C22
20	W	202	9XX	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
16	F	702	HEM	CAD-CBD-CGD-O1D
22	Y	503	9YF	O11-C25-C26-C27
22	M	502	9YF	O11-C25-C26-C27
18	J	202	9Y0	C11-C12-C13-C14
17	F	707	MQ9	C25-C24-C26-C27
18	J	203	9Y0	C13-C14-C15-C16
18	J	203	9Y0	C23-C24-C25-C26
17	E	604	MQ9	C24-C26-C27-C28
22	c	203	9YF	C2-O2-P-O1
22	W	203	9YF	C2-O2-P-O1
15	Z	203	CDL	C58-C59-C60-C61
15	X	301	CDL	O1-C1-CB2-OB2
15	E	606	CDL	OA9-CA7-OA8-CA6
15	Z	203	CDL	C71-C72-C73-C74
15	S	301	CDL	C12-C11-CA5-OA6
15	X	302	CDL	C12-C11-CA5-OA6
22	O	303	9YF	O11-C25-C26-C27
22	O	303	9YF	O9-C8-C9-C10
22	I	304	9YF	O11-C25-C26-C27
22	I	304	9YF	O9-C8-C9-C10
22	Y	502	9YF	O9-C8-C9-C10
22	M	501	9YF	O9-C8-C9-C10
17	E	603	MQ9	C15-C14-C16-C17
21	I	302	HEC	C3A-C2A-CAA-CBA
15	T	201	CDL	C74-C75-C76-C77
15	Z	202	CDL	C74-C75-C76-C77
16	E	601	HEM	CAA-CBA-CGA-O2A
22	c	203	9YF	C31-C32-C33-C34
22	W	203	9YF	C31-C32-C33-C34
15	T	202	CDL	O1-C1-CB2-OB2
15	T	203	CDL	CB3-CB4-CB6-OB8
18	F	706	9Y0	C31-C32-C33-C34
22	Y	503	9YF	C18-C19-C20-C21
17	E	604	MQ9	C12-C11-C9-C10
16	E	601	HEM	CAA-CBA-CGA-O1A
20	W	202	9XX	C24-C25-C26-C27
22	M	502	9YF	C18-C19-C20-C21
16	F	702	HEM	CAA-CBA-CGA-O1A
15	L	604	CDL	C12-C11-CA5-OA6
15	P	201	CDL	C32-C31-CA7-OA8
15	J	201	CDL	C32-C31-CA7-OA8
18	J	203	9Y0	C18-C19-C20-C37

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Mol	Chain	Res	Type	Atoms
20	c	202	9XX	C10-C11-C12-C13
15	T	202	CDL	CA2-C1-CB2-OB2
15	X	301	CDL	CA2-C1-CB2-OB2
17	F	708	MQ9	C31-C32-C33-C34
20	c	202	9XX	C26-C27-C28-C29
15	T	202	CDL	CB3-CB4-OB6-CB5
15	T	202	CDL	CB6-CB4-OB6-CB5
15	T	203	CDL	CA3-CA4-OA6-CA5
15	X	301	CDL	CB3-CB4-OB6-CB5
15	X	301	CDL	CB6-CB4-OB6-CB5
18	P	202	9Y0	C2-C1-O7-C21
15	E	606	CDL	C31-CA7-OA8-CA6
15	R	604	CDL	C57-C58-C59-C60
17	F	707	MQ9	C30-C29-C31-C32
17	F	709	MQ9	C12-C11-C9-C10
15	S	301	CDL	C12-C11-CA5-OA7
15	X	302	CDL	C12-C11-CA5-OA7
15	P	201	CDL	C32-C31-CA7-OA9
15	J	201	CDL	C32-C31-CA7-OA9
15	P	201	CDL	C52-C51-CB5-OB6
15	J	201	CDL	C52-C51-CB5-OB6
18	X	303	9Y0	C32-C33-C34-C35
15	Z	203	CDL	CB4-CB6-OB8-CB7
18	J	203	9Y0	O5-C5-C6-C7
21	I	301	HEC	C4D-C3D-CAD-CBD
16	F	702	HEM	CAA-CBA-CGA-O2A
15	E	606	CDL	C36-C37-C38-C39
22	I	304	9YF	O12-C25-C26-C27
21	O	302	HEC	CAA-CBA-CGA-O2A
15	L	604	CDL	C12-C11-CA5-OA7
22	O	303	9YF	O12-C25-C26-C27
22	M	501	9YF	O10-C8-C9-C10
17	E	604	MQ9	C11-C12-C13-C14
17	I	303	MQ9	C31-C32-C33-C34
18	J	203	9Y0	C1-C2-O3-P
17	E	604	MQ9	C33-C34-C36-C37
22	Y	502	9YF	O10-C8-C9-C10
22	I	304	9YF	C12-C13-C14-C15
14	L	602	HEA	O11-C11-C3B-C4B
22	O	303	9YF	C11-C12-C13-C14
18	S	302	9Y0	O7-C21-C22-C23
22	I	304	9YF	O10-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
15	F	705	CDL	O1-C1-CA2-OA2
20	D	302	9XX	C11-C12-C13-C14
22	I	304	9YF	C11-C12-C13-C14
22	O	303	9YF	O10-C8-C9-C10
22	O	303	9YF	C12-C13-C14-C15
18	J	202	9Y0	C11-C10-C9-C8
21	O	302	HEC	CAA-CBA-CGA-O1A
18	J	203	9Y0	O4-C5-C6-C7
20	G	302	9XX	C12-C13-C14-C15
15	E	606	CDL	C52-C51-CB5-OB6
18	X	303	9Y0	O7-C21-C22-C23
15	L	604	CDL	C51-C52-C53-C54
15	P	201	CDL	C52-C51-CB5-OB7
15	J	201	CDL	C52-C51-CB5-OB7

There are no ring outliers.

40 monomers are involved in 396 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	I	303	MQ9	1	0
19	W	201	PLM	2	0
22	W	203	9YF	1	0
15	L	604	CDL	19	0
15	T	203	CDL	8	0
22	Y	502	9YF	2	0
23	Y	501	FES	1	0
16	E	602	HEM	2	0
16	F	702	HEM	1	0
15	S	301	CDL	49	0
15	R	604	CDL	19	0
16	E	601	HEM	2	0
15	E	606	CDL	3	0
21	O	302	HEC	11	0
14	L	602	HEA	2	0
21	I	301	HEC	4	0
17	E	603	MQ9	1	0
16	F	703	HEM	4	0
17	E	604	MQ9	3	0
17	F	708	MQ9	1	0
15	Z	203	CDL	46	0
17	F	709	MQ9	4	0
14	R	603	HEA	4	0

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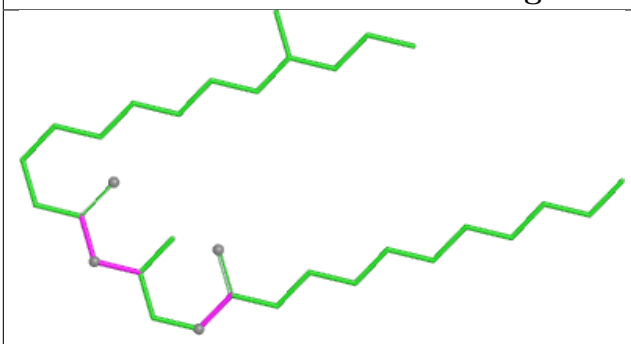
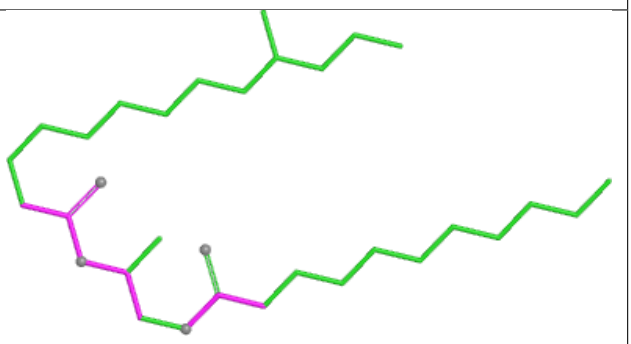
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	Z	201	MQ9	5	0
15	Z	202	CDL	35	0
22	I	304	9YF	5	0
21	O	301	HEC	5	0
22	Y	503	9YF	3	0
15	P	201	CDL	10	0
15	F	704	CDL	11	0
15	J	201	CDL	11	0
15	T	202	CDL	9	0
15	E	605	CDL	10	0
15	X	302	CDL	54	0
22	c	203	9YF	1	0
15	T	201	CDL	33	0
15	F	705	CDL	10	0
21	I	302	HEC	9	0
14	L	603	HEA	3	0
15	X	301	CDL	42	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.

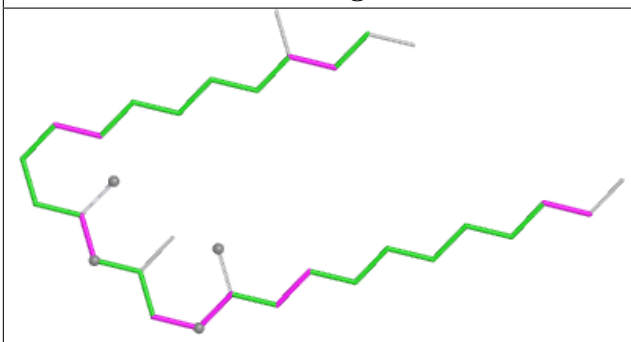
Ligand 9XX G 302



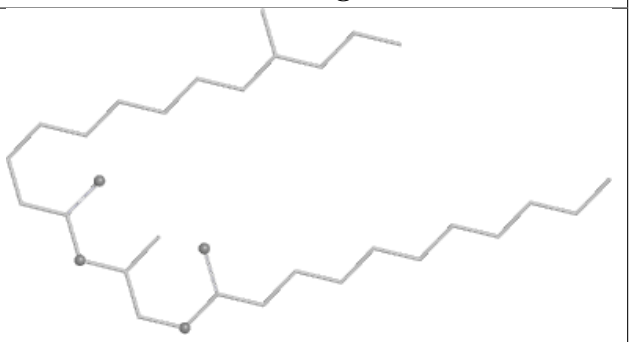
Bond lengths



Bond angles

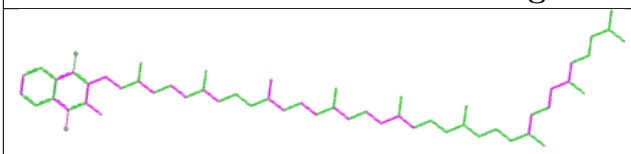


Torsions

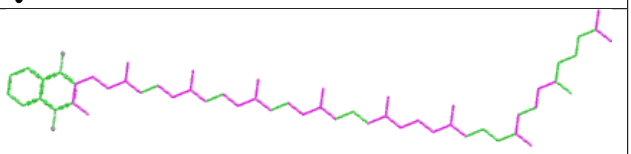


Rings

Ligand MQ9 I 303



Bond lengths



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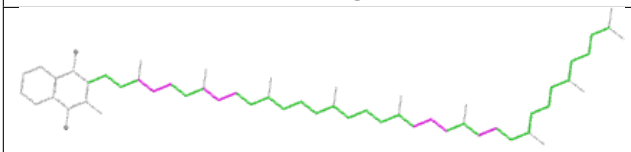

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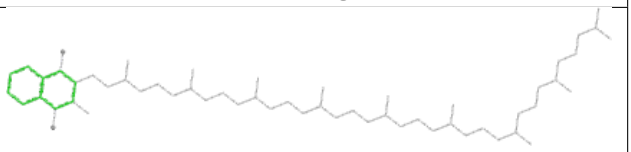
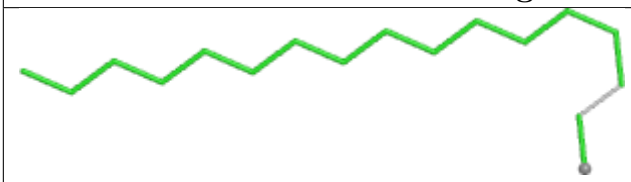
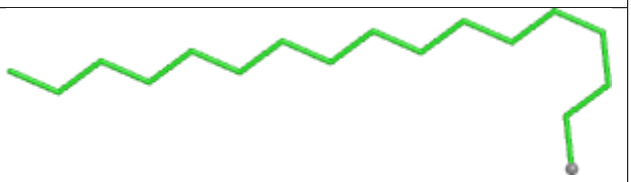


Rings

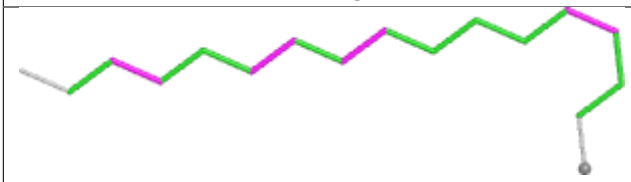
Ligand PLM W 201



Bond lengths



Bond angles



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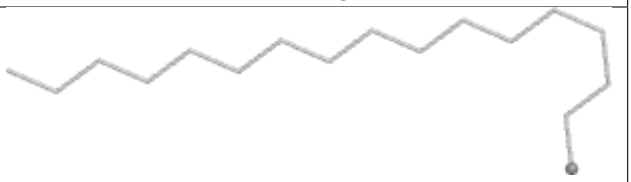
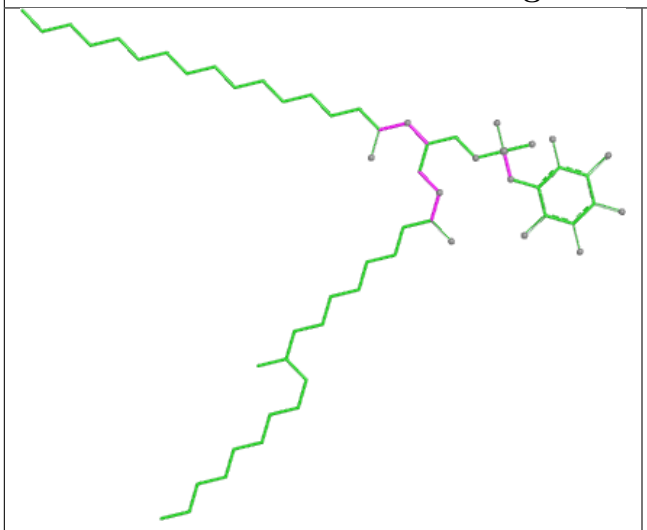


Rings

Ligand 9YF W 203



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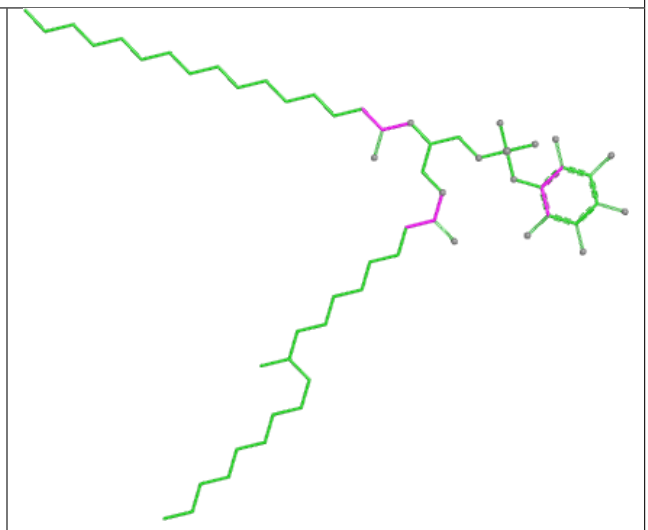
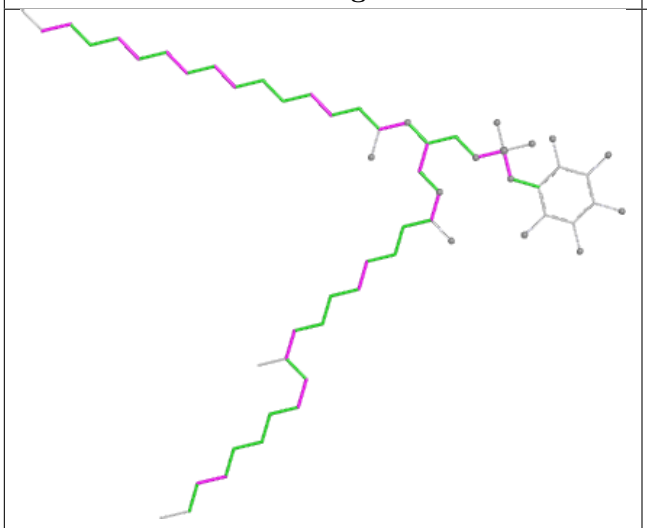
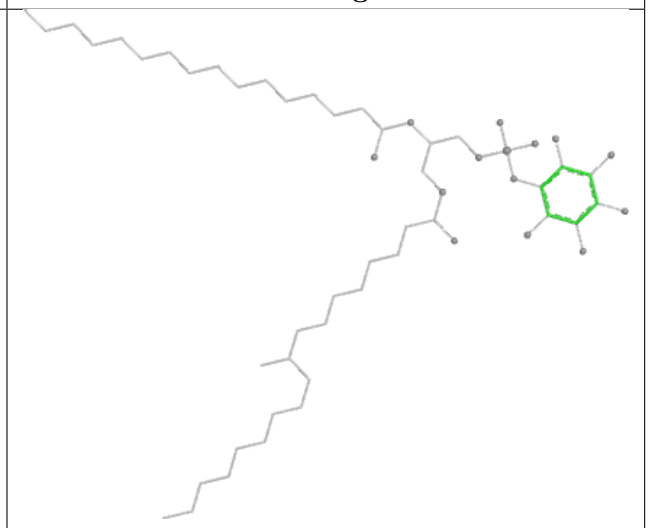


Bond angles

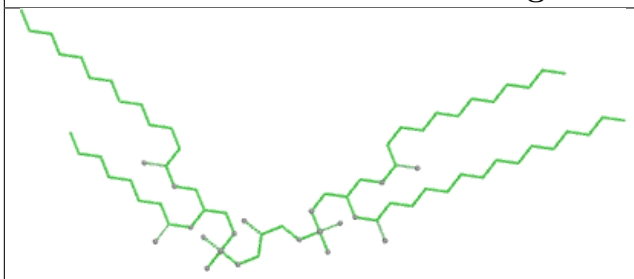


Torsions



Rings

Ligand CDL L 604



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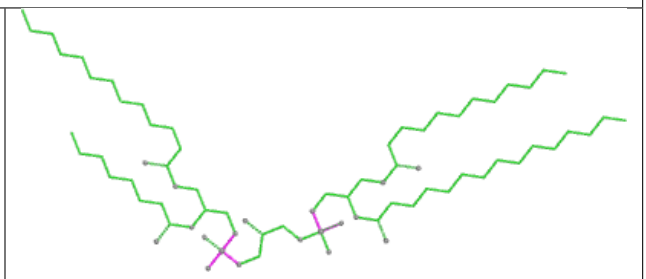

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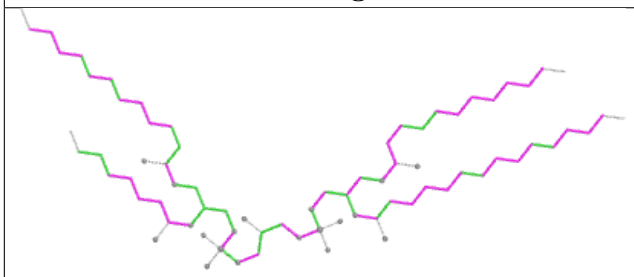

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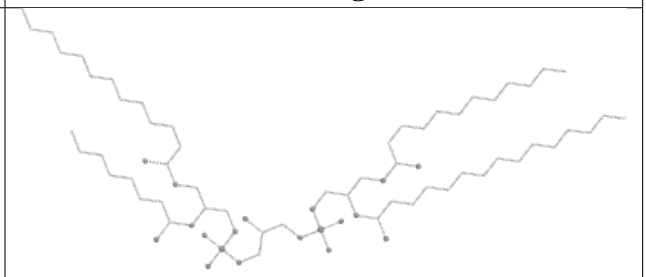
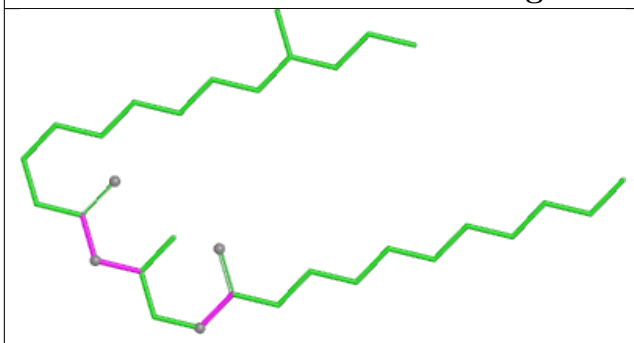


Rings

Ligand 9XX D 302



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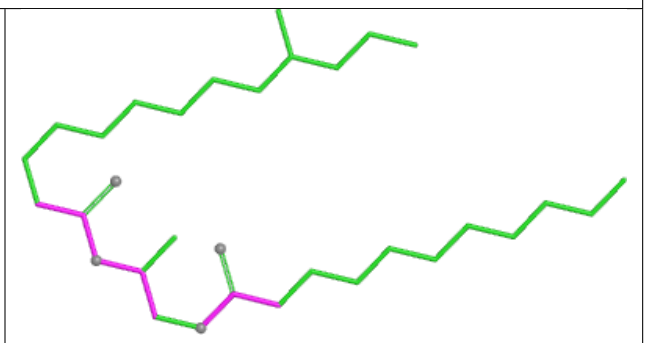
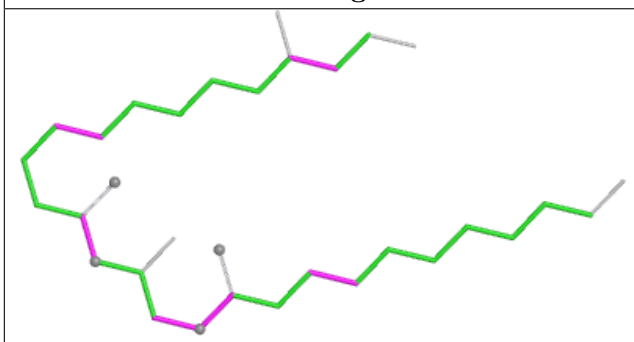


Bond angles



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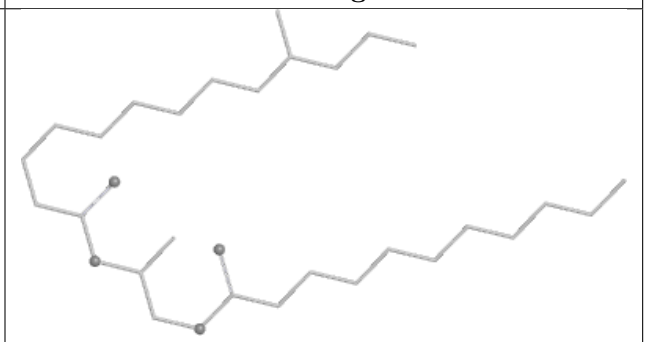
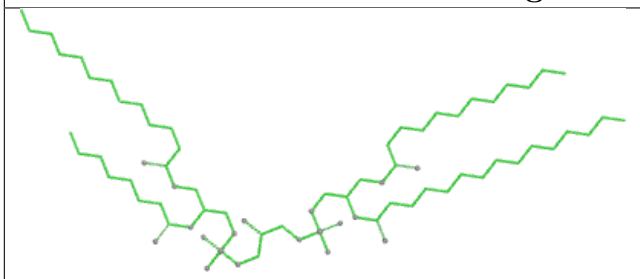
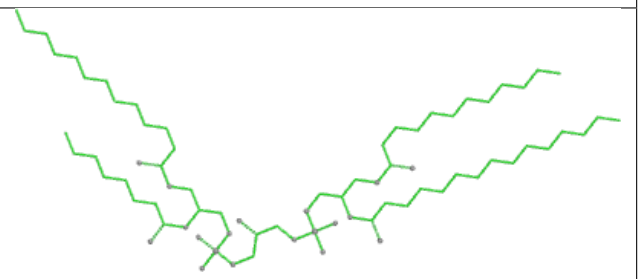
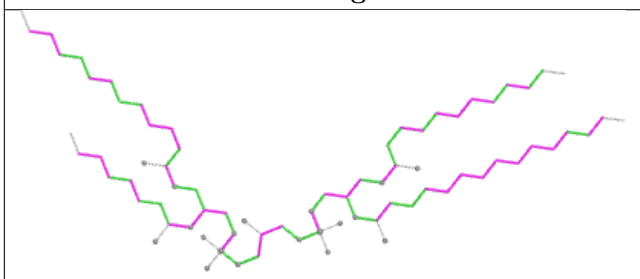
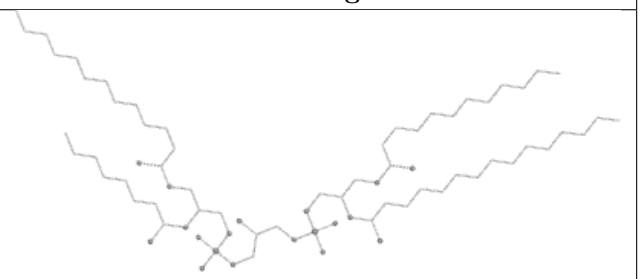
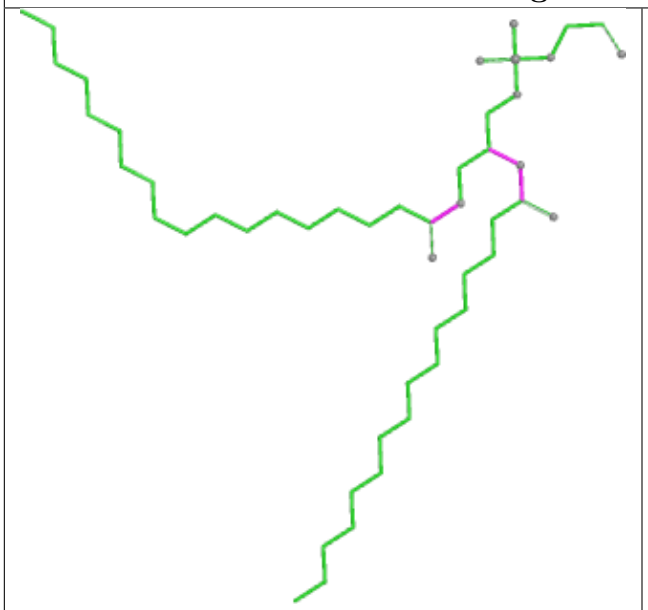


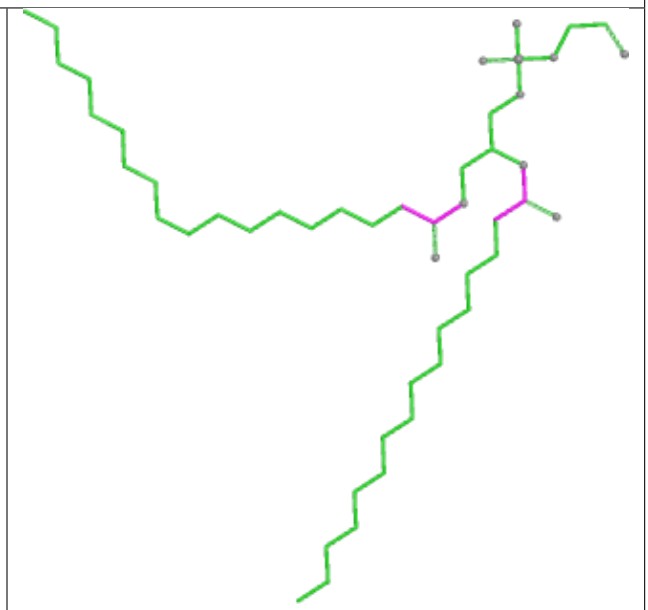
Rings

Ligand CDL T 203	
 Bond lengths	 Bond angles
 Torsions	 Rings

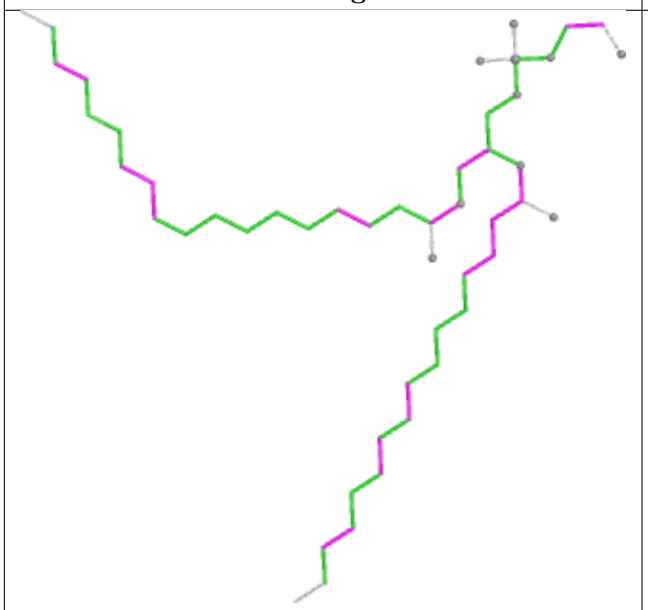
Ligand 9Y0 X 303



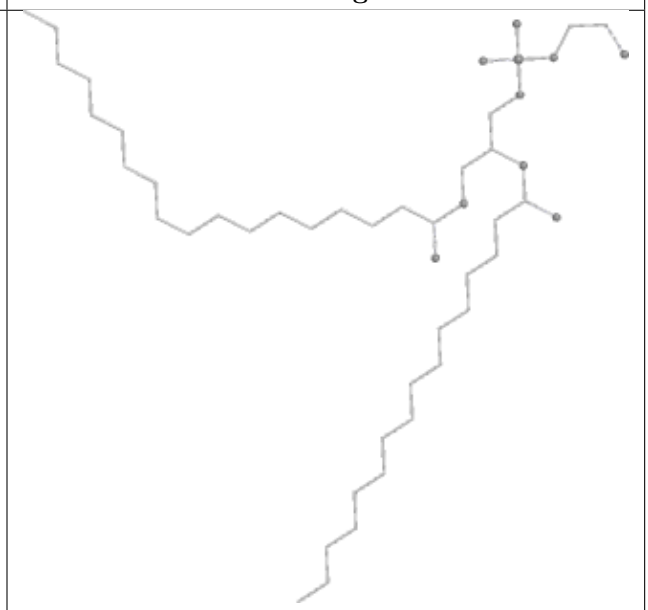
Bond lengths



Bond angles

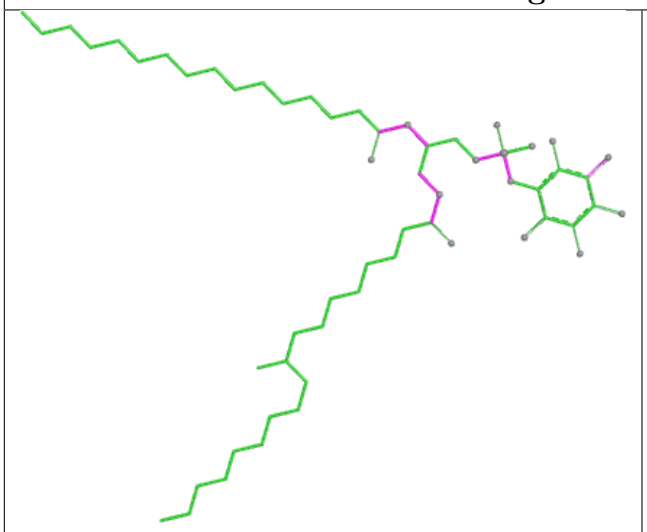


Torsions

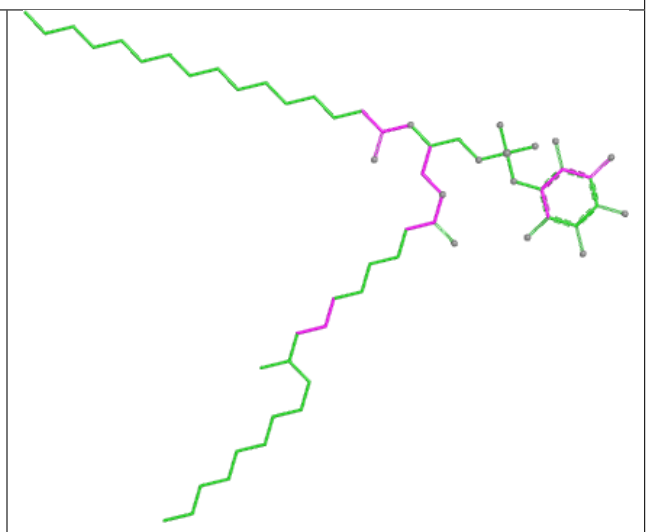


Rings

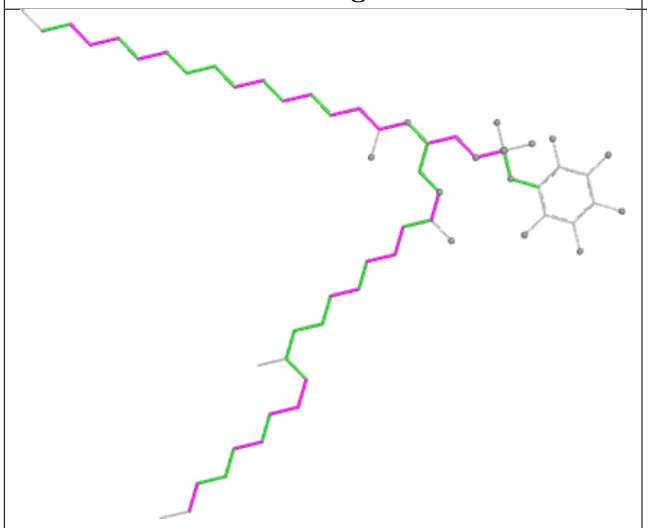
Ligand 9YF Y 502



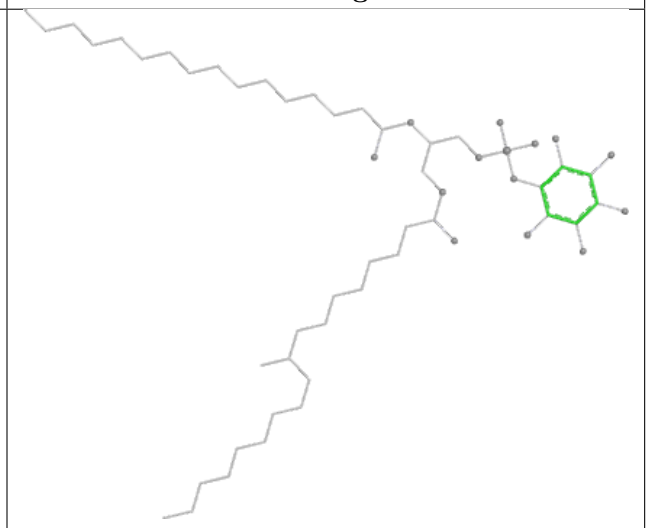
Bond lengths



Bond angles

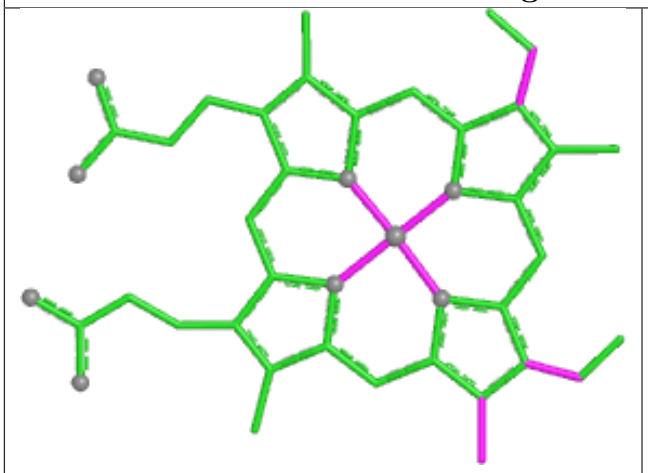


Torsions



Rings

Ligand HEM E 602



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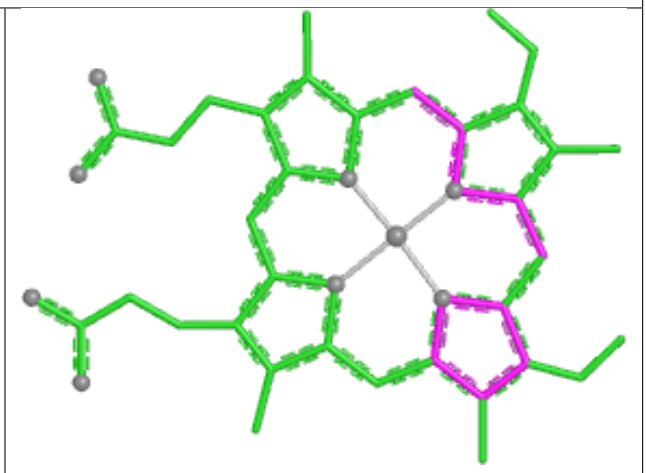

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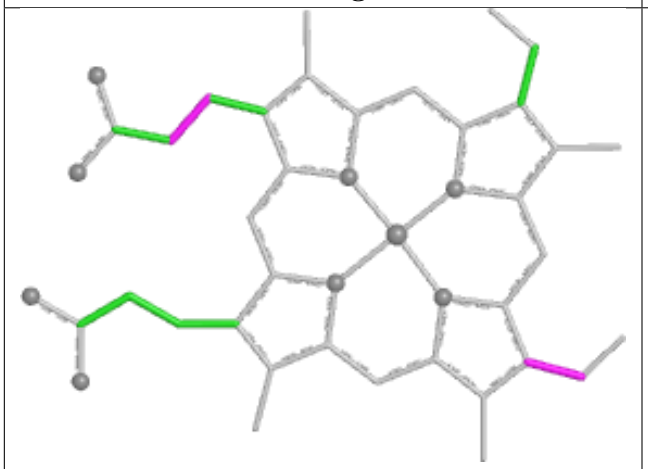

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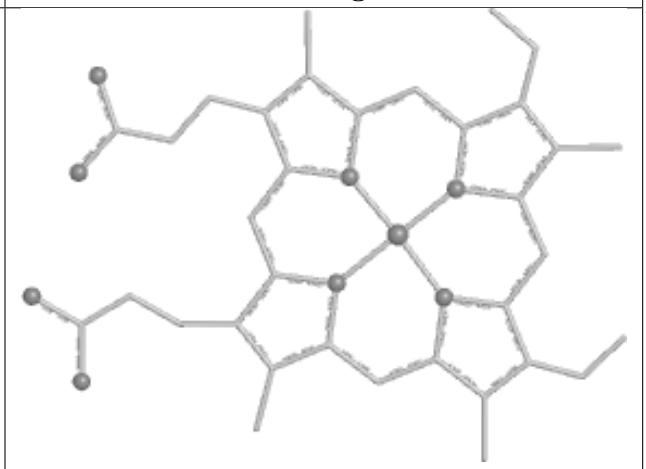
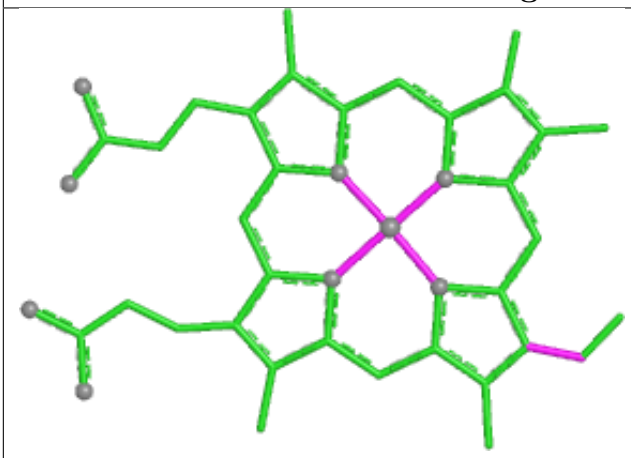


Rings

Ligand HEM F 702



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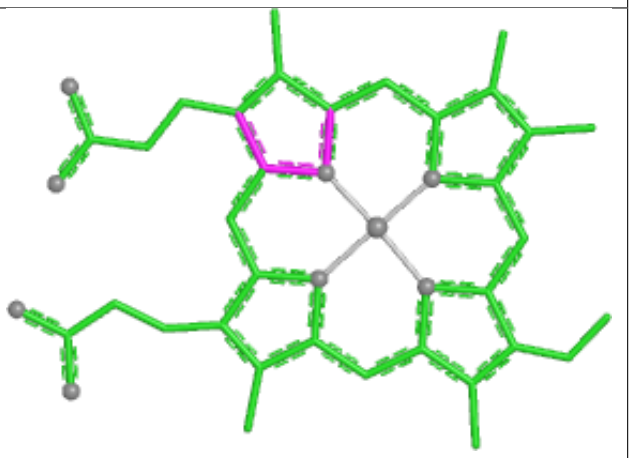

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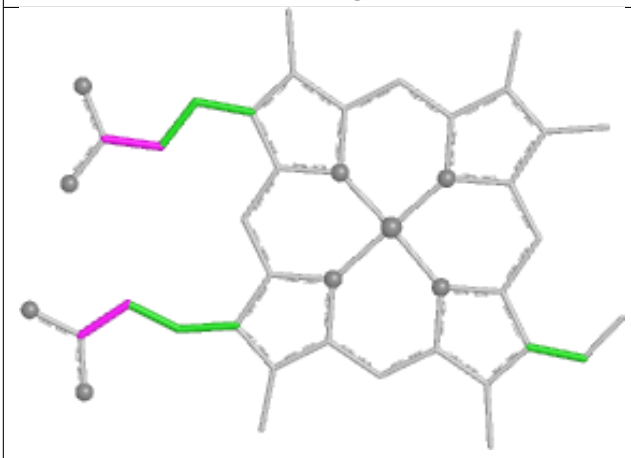

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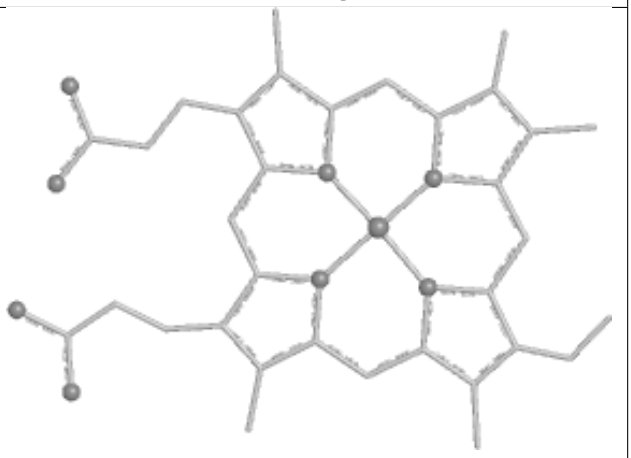
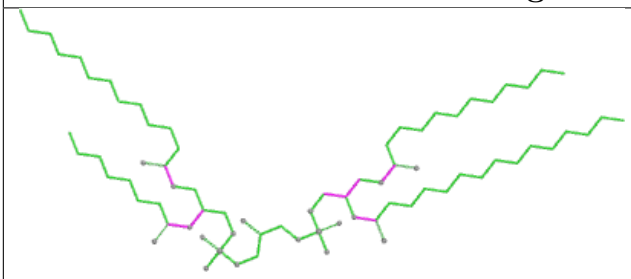


Rings

Ligand CDL S 301



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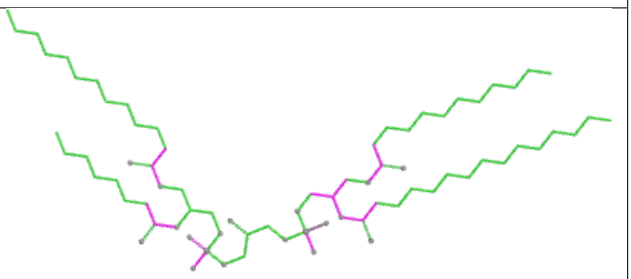

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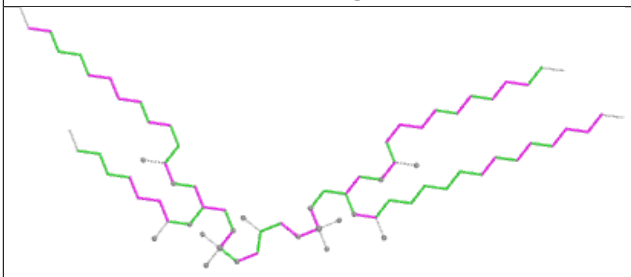

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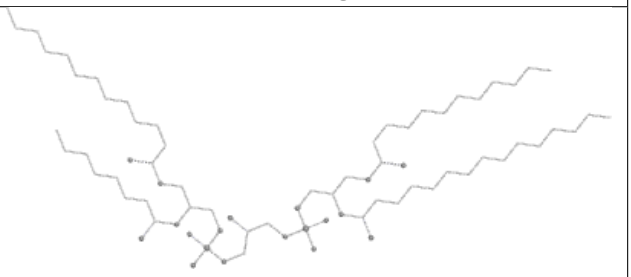
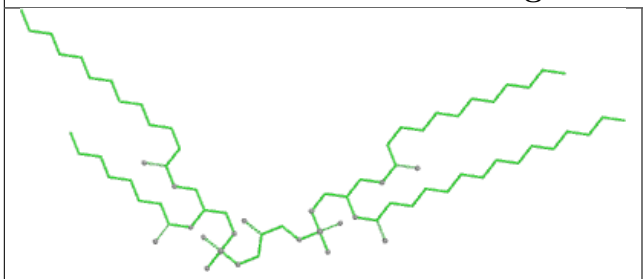
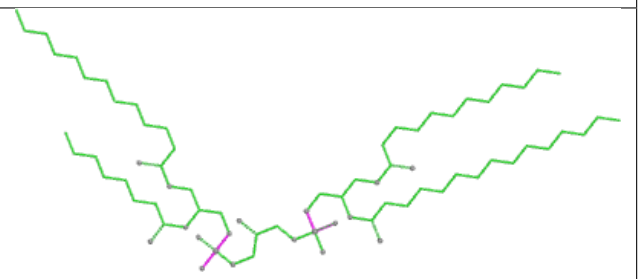
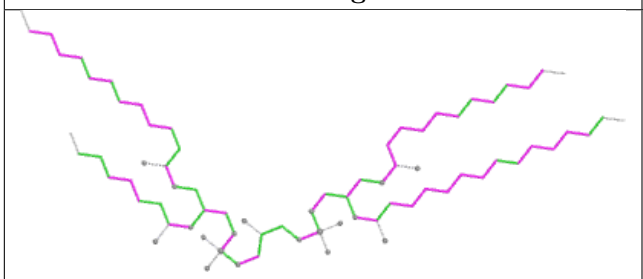
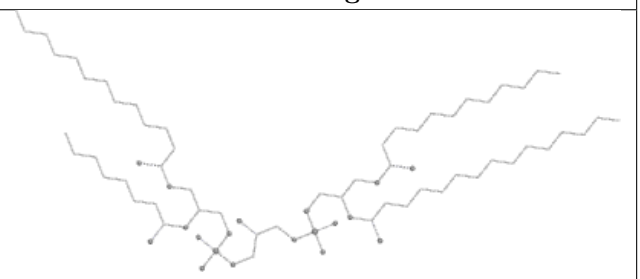
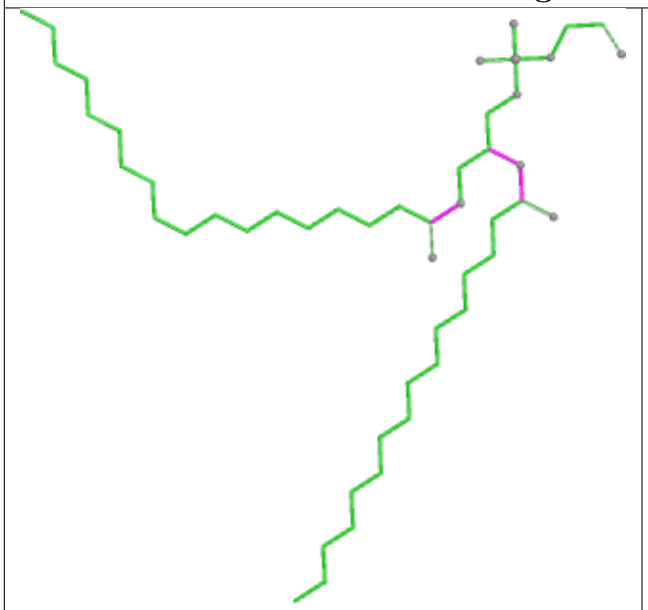


Rings

Ligand CDL R 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 9Y0 J 202



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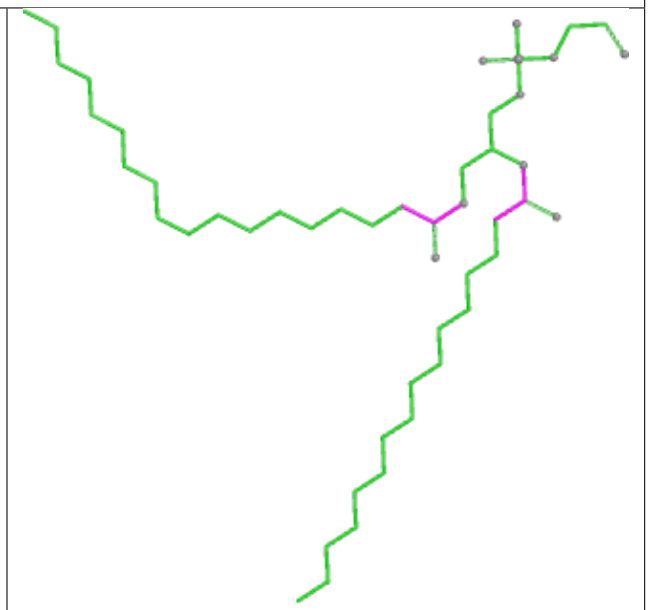
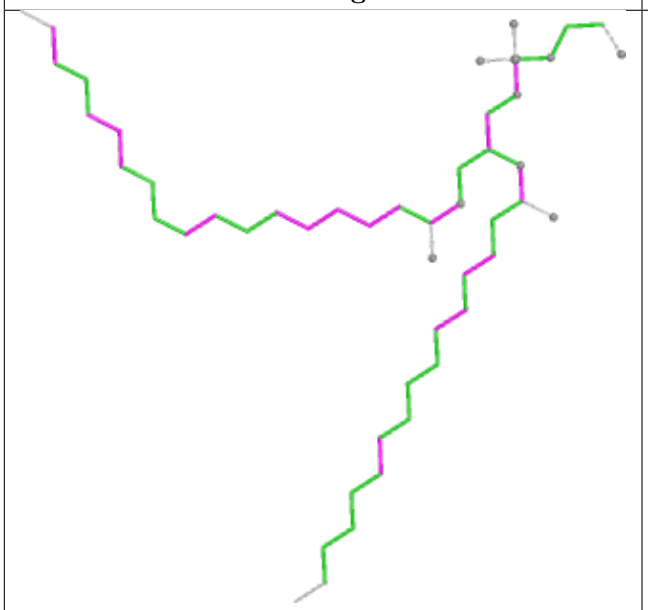


Bond angles



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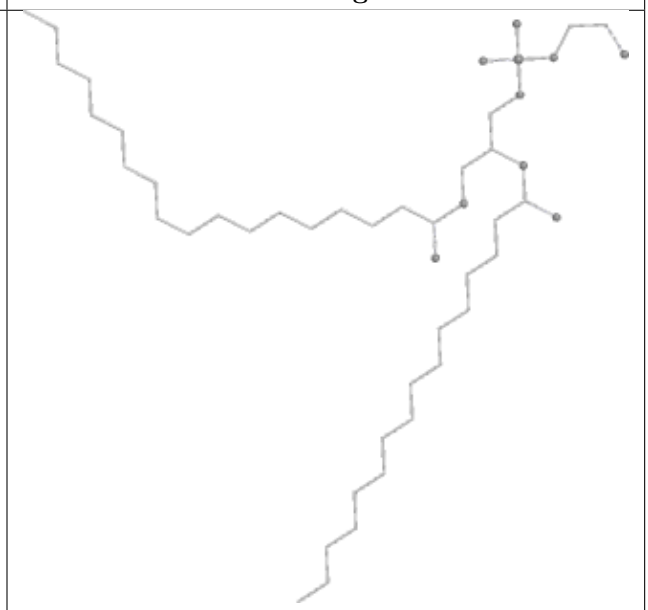
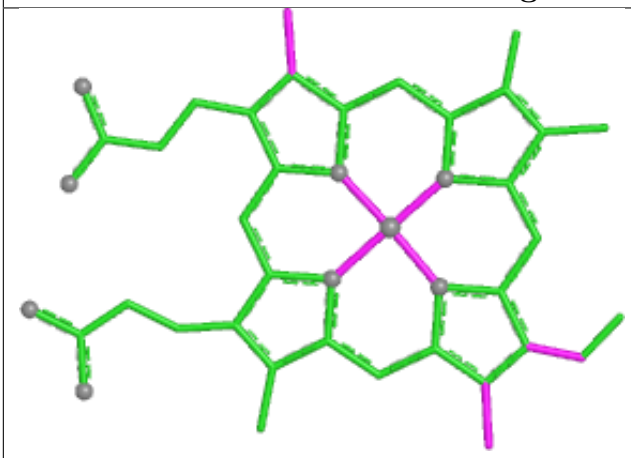


Rings

Ligand HEM E 601



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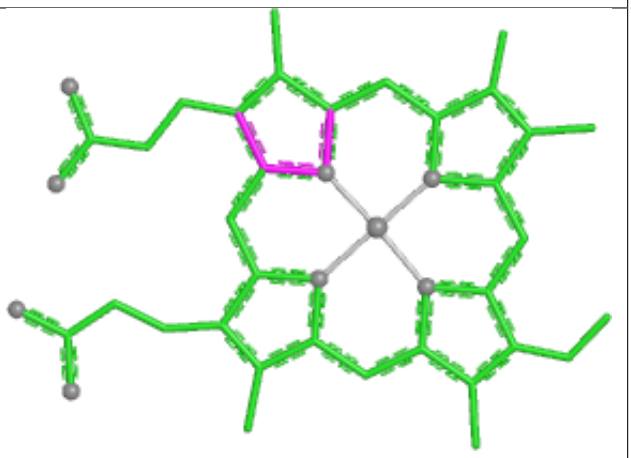
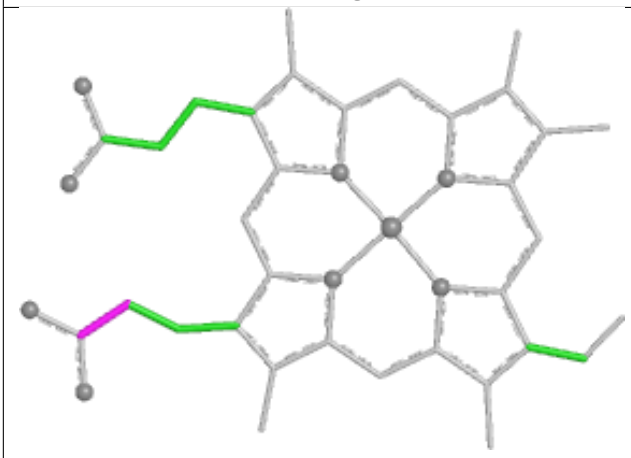


Bond angles



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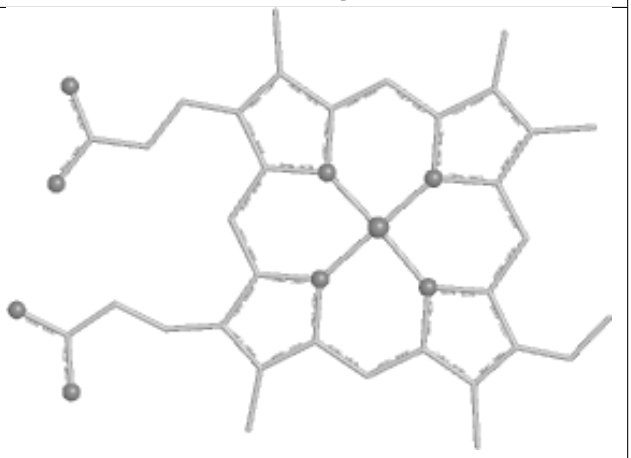
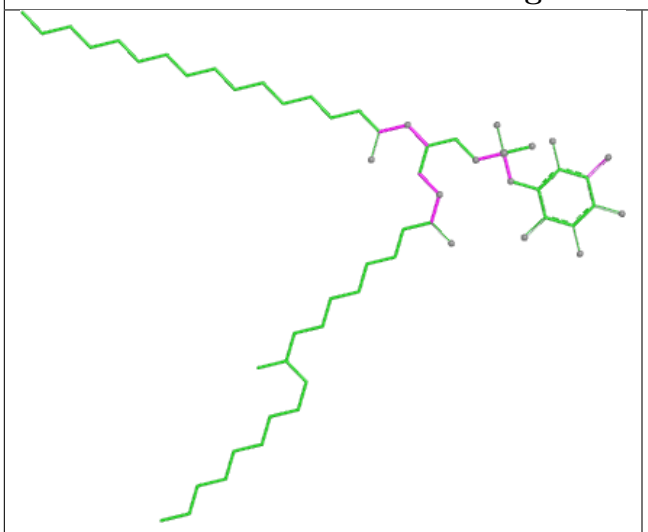


Rings

Ligand 9YF M 501



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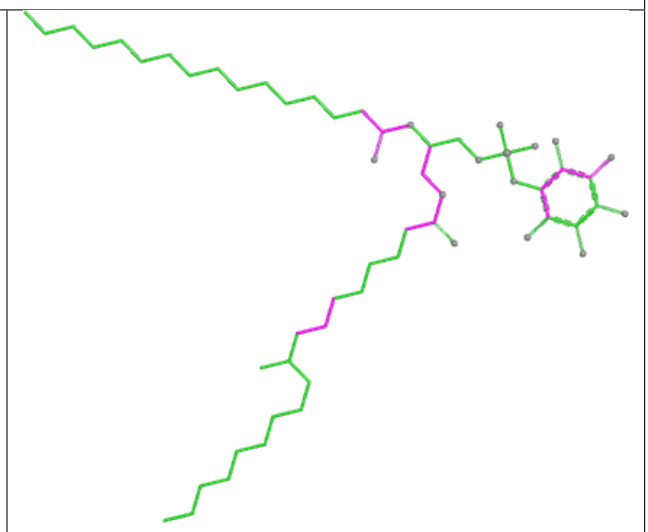

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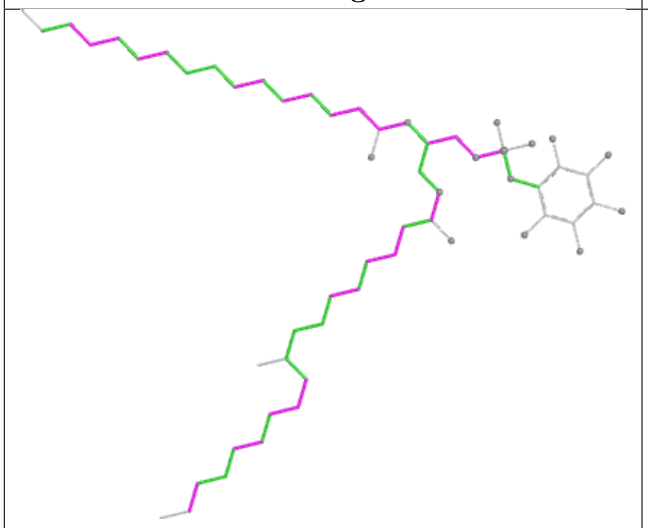

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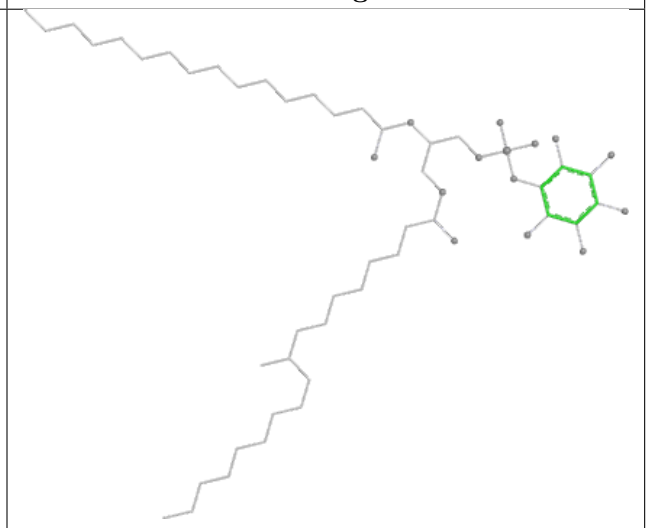
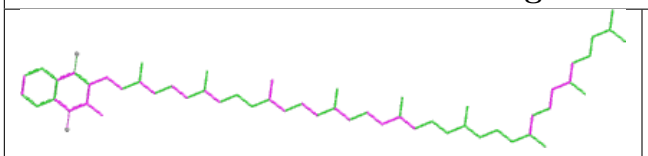


Rings

Ligand MQ9 F 701



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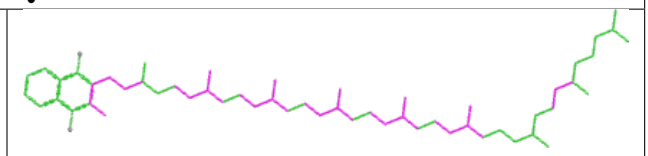
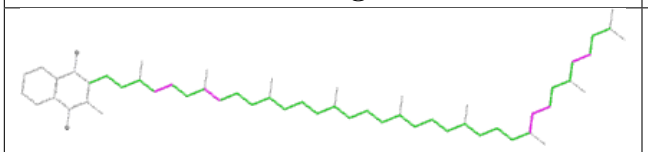


Bond angles



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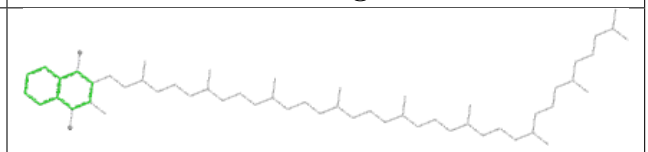
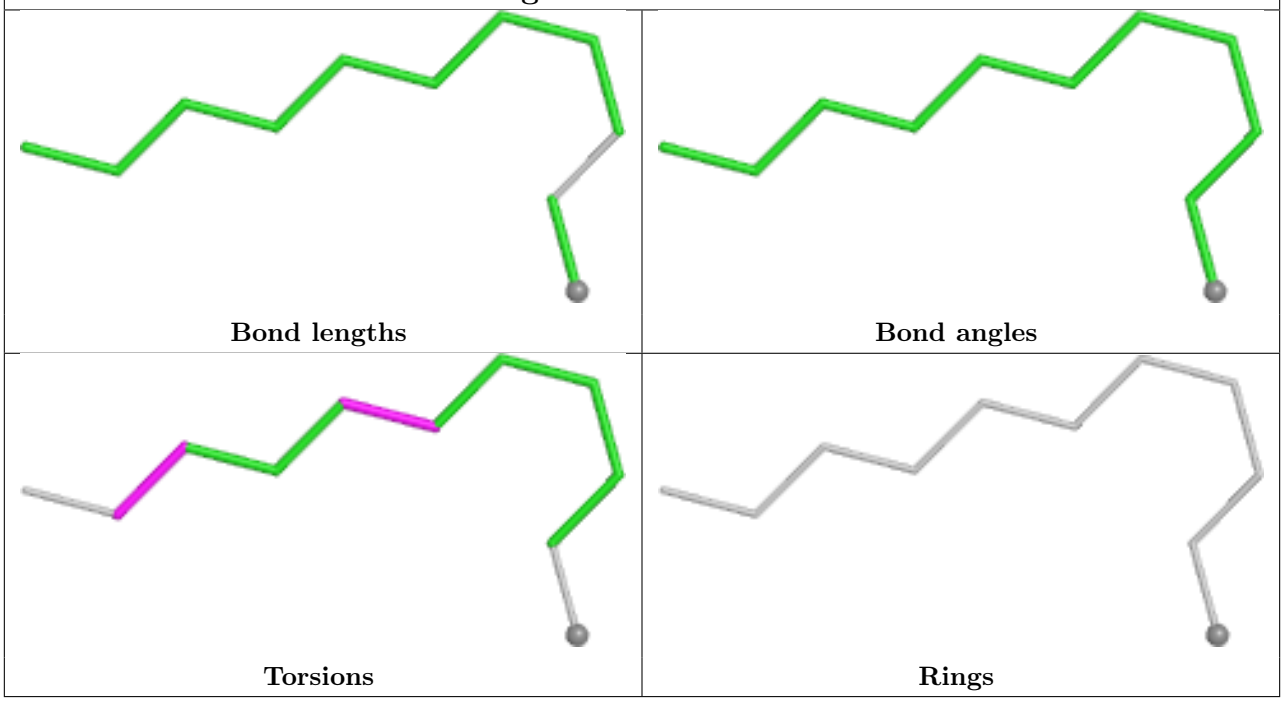
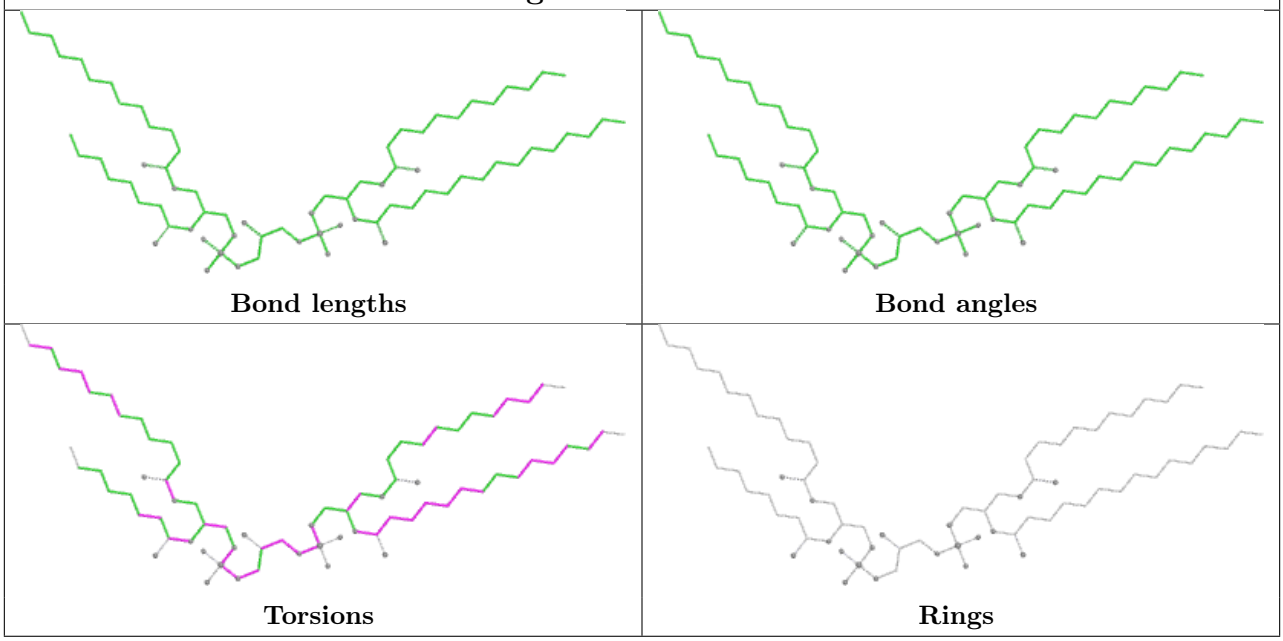


Rings

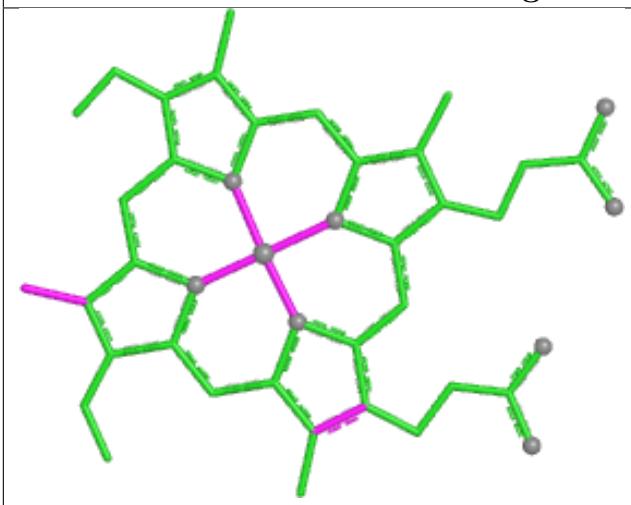
Ligand PLM G 301



Ligand CDL E 606



Ligand HEC O 302



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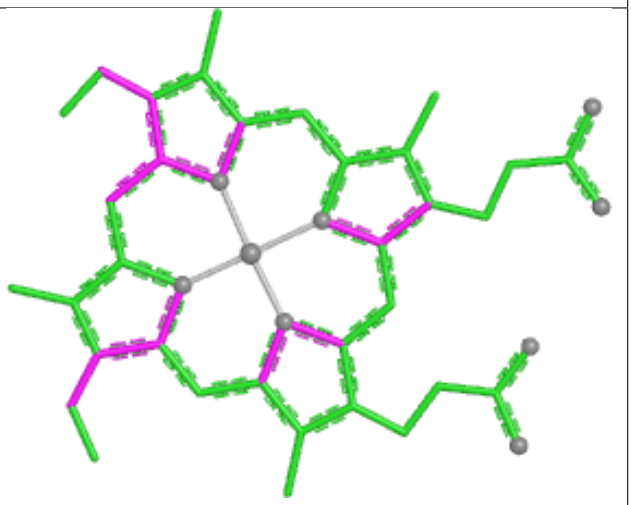
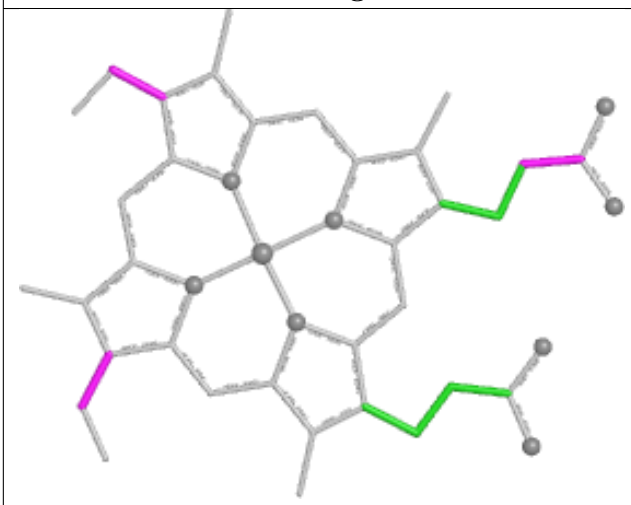


Bond angles



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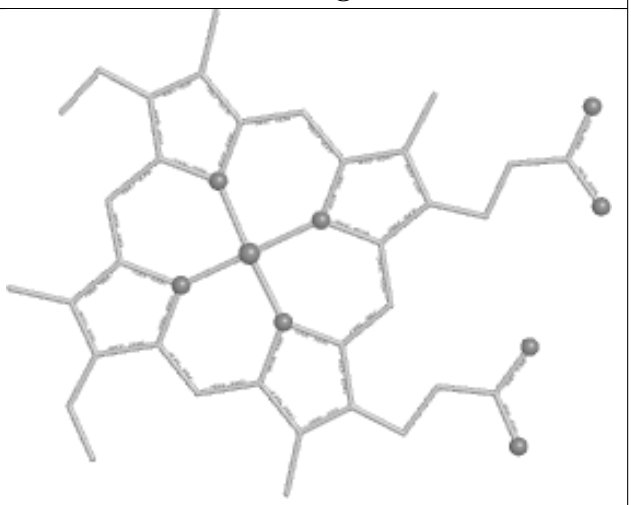
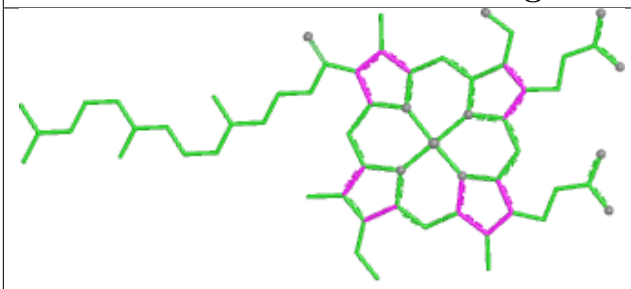
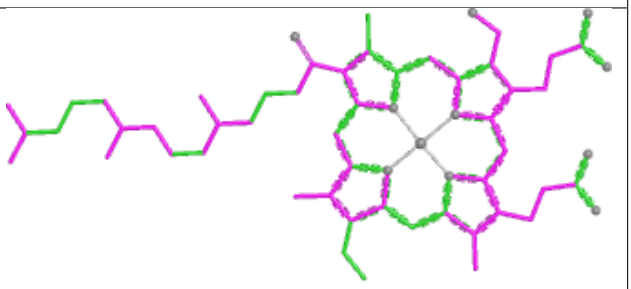
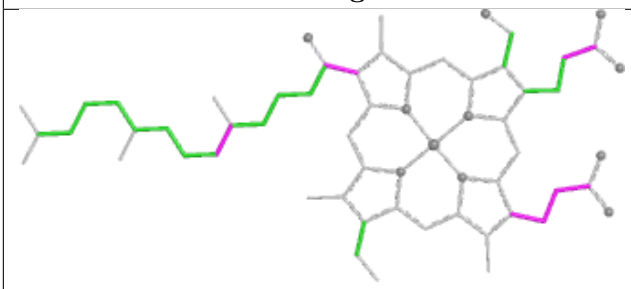
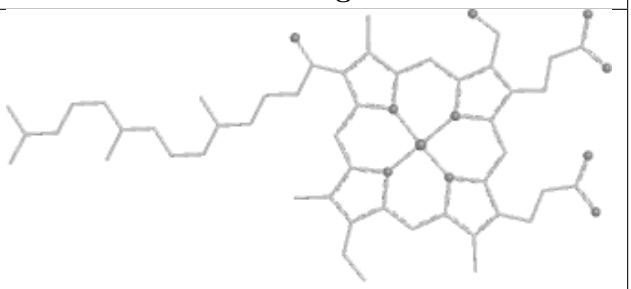
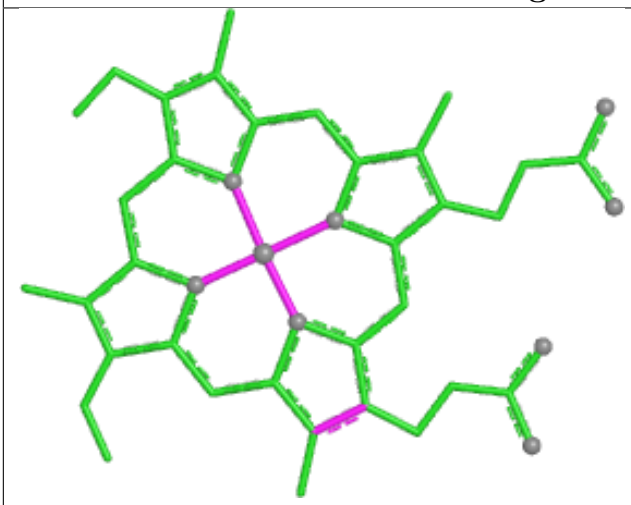


Rings

Ligand HEA L 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand HEC I 301



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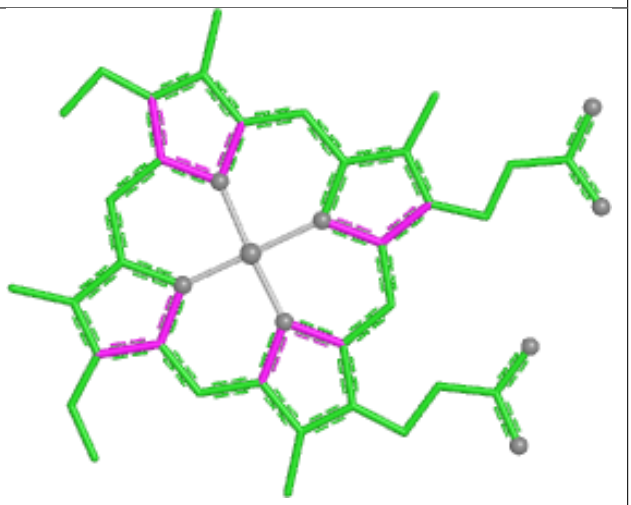
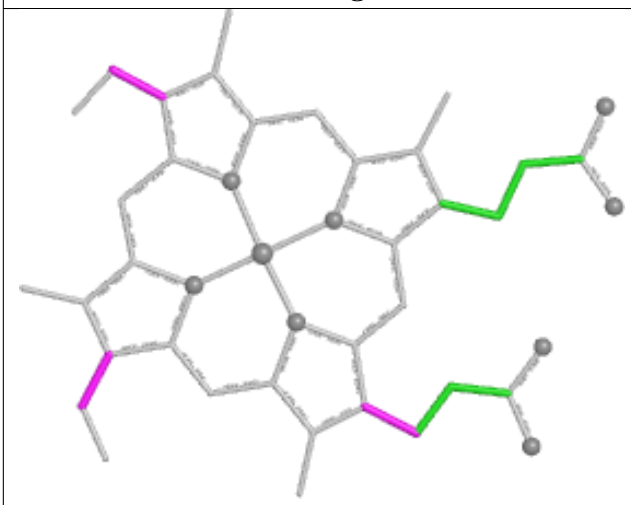


Bond angles



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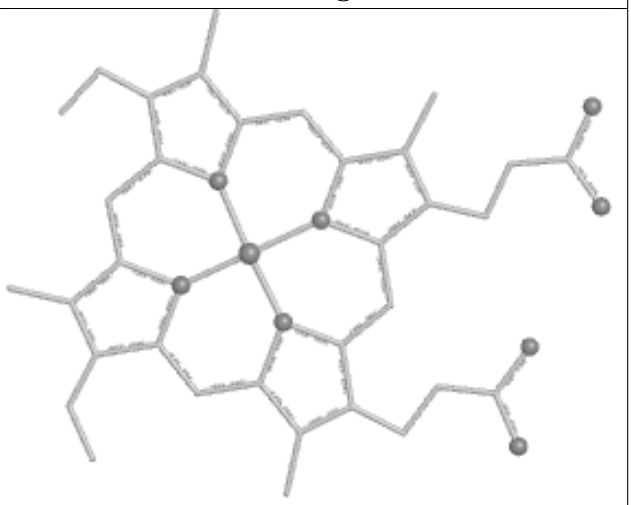
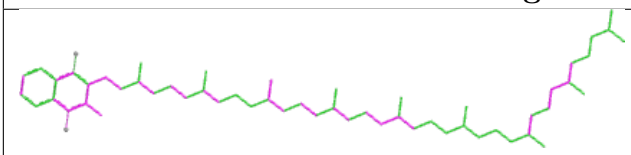


Rings

Ligand MQ9 E 603



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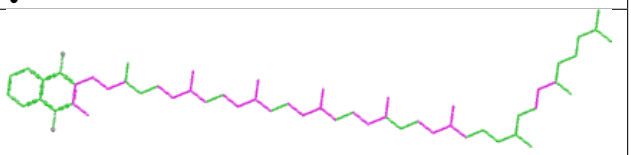
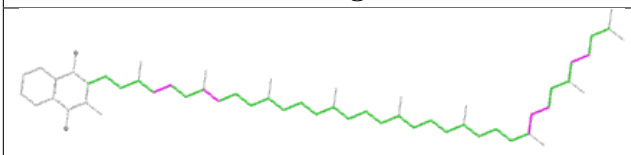


Bond angles



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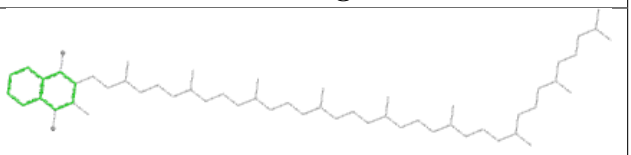
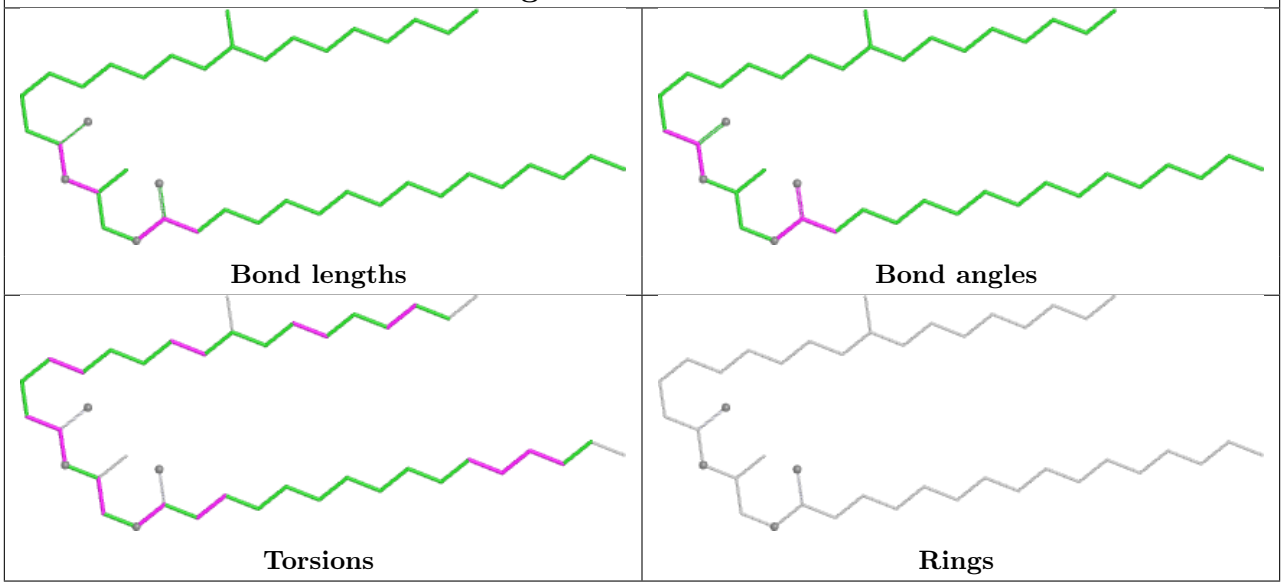
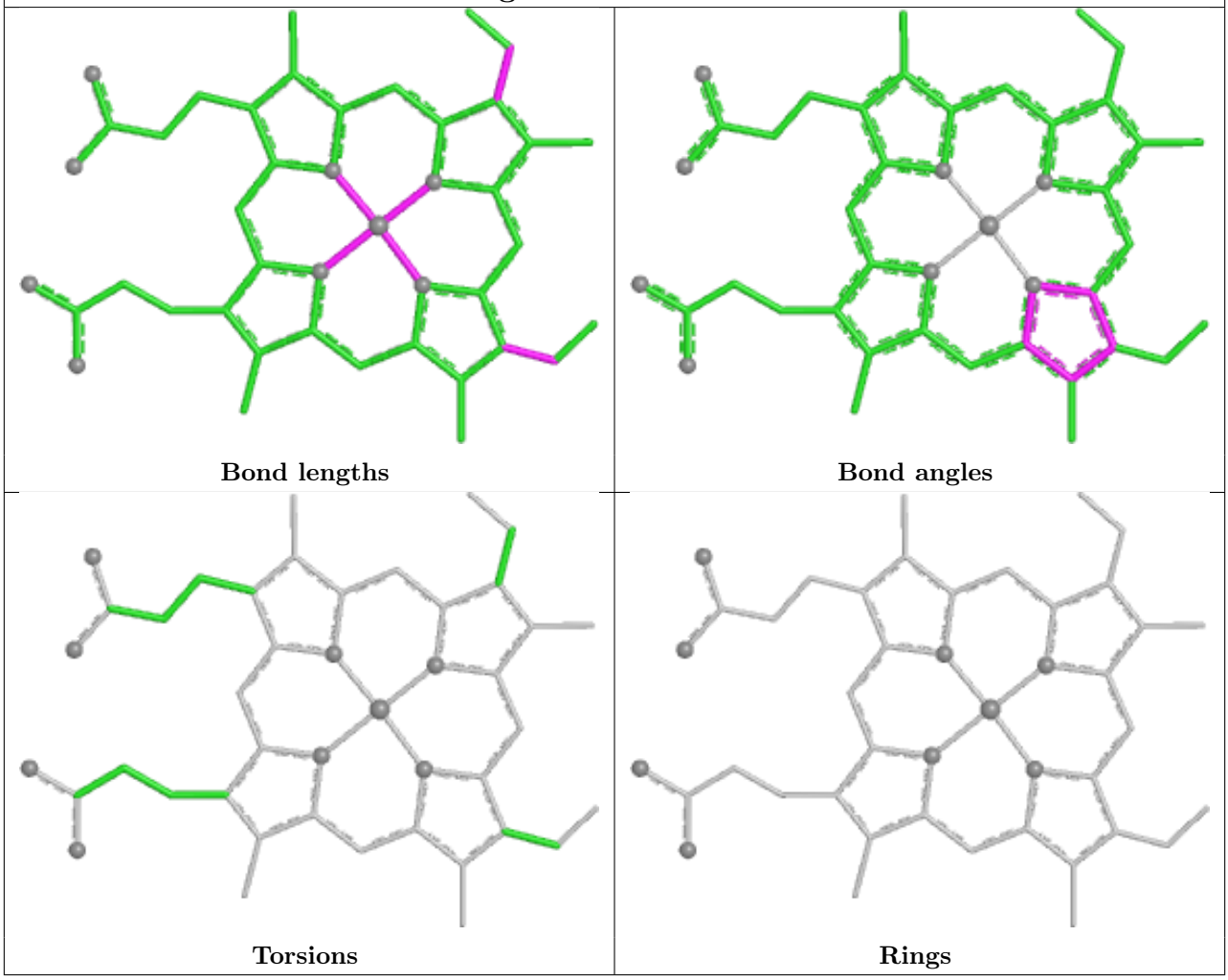


Rings

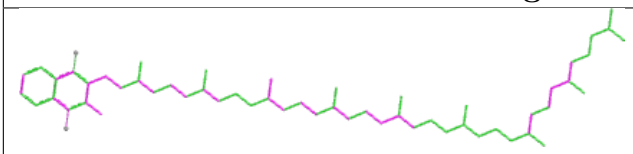
Ligand 9XX W 202



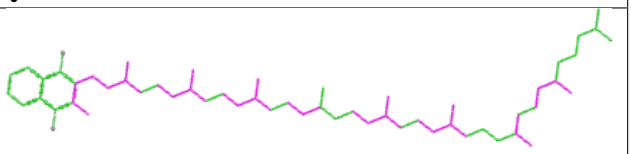
Ligand HEM F 703



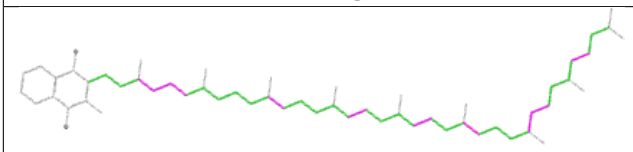
Ligand MQ9 E 604



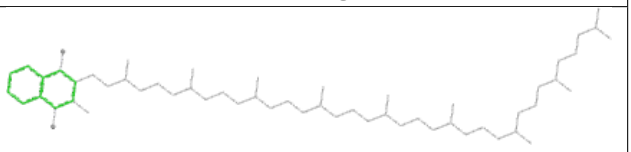
Bond lengths



Bond angles

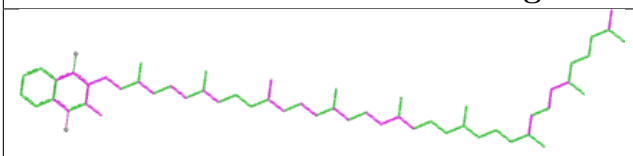


Torsions



Rings

Ligand MQ9 F 708



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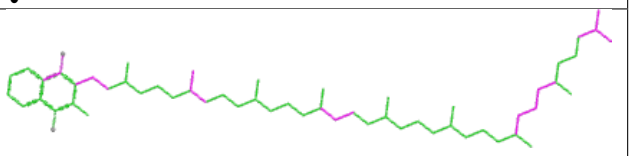
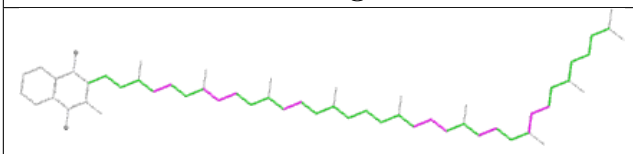


Bond angles



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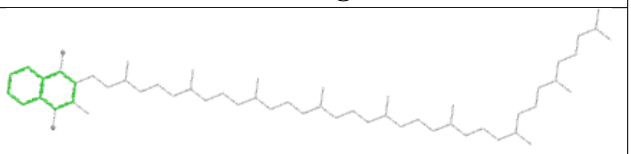
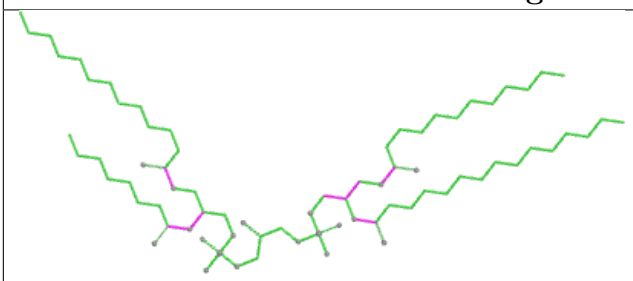


Rings

Ligand CDL Z 203



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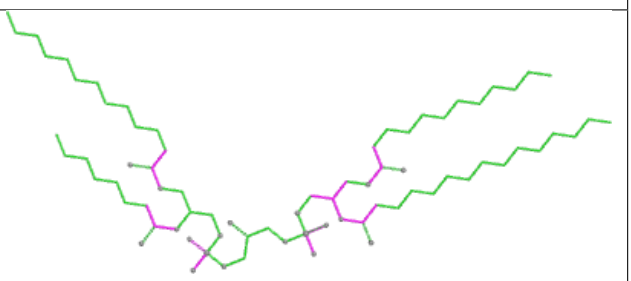
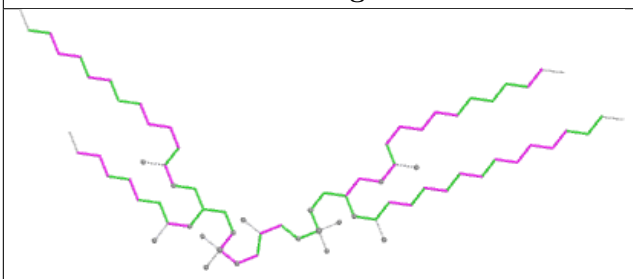


Bond angles



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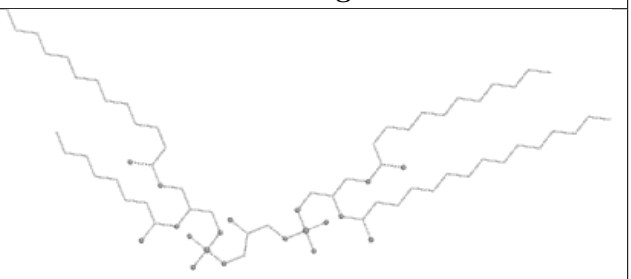
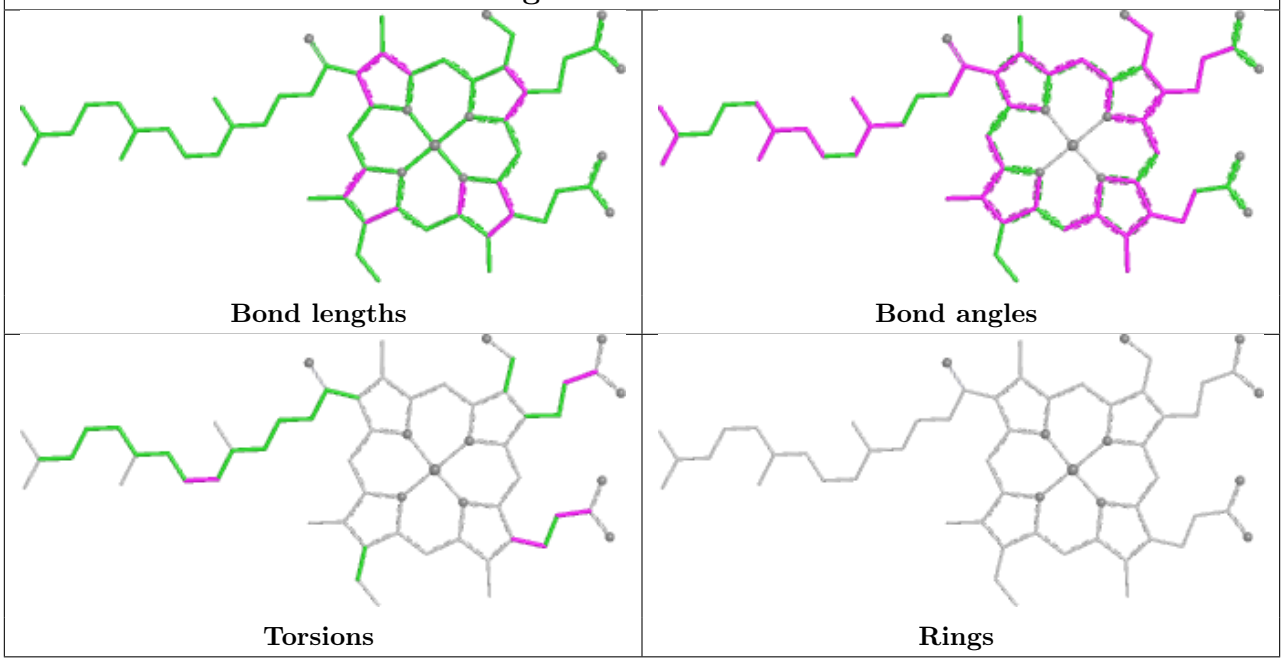
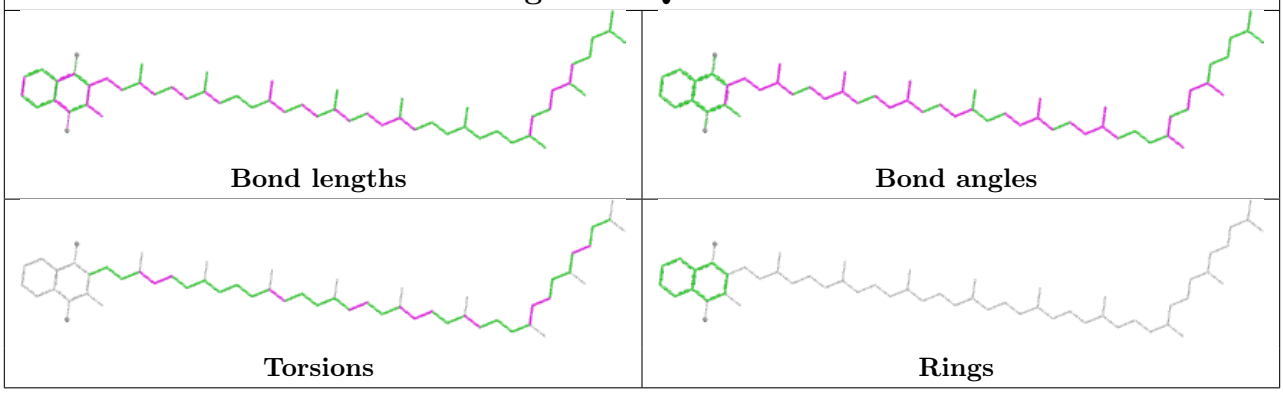


Rings

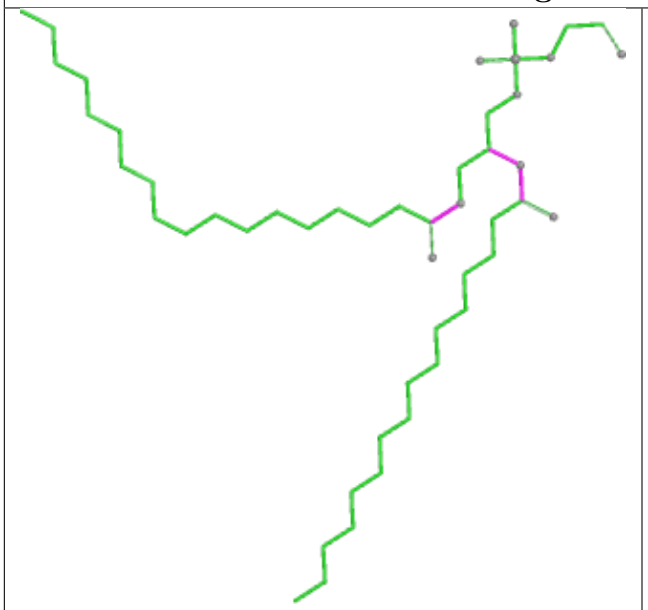
Ligand HEA R 602



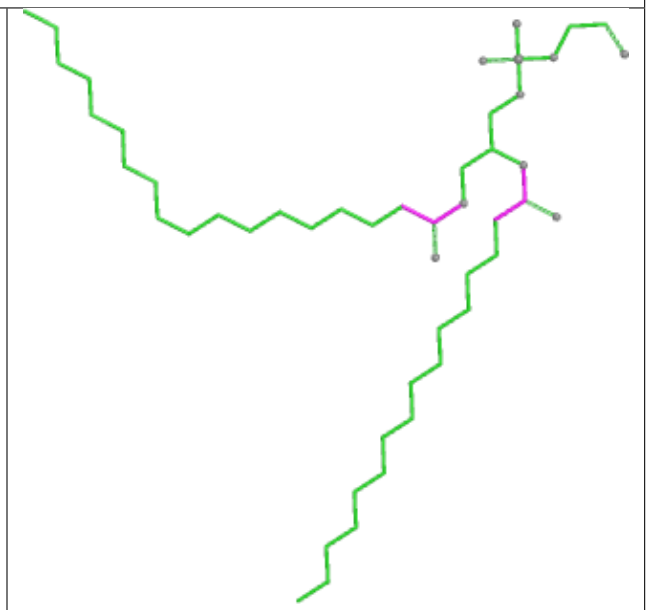
Ligand MQ9 F 709



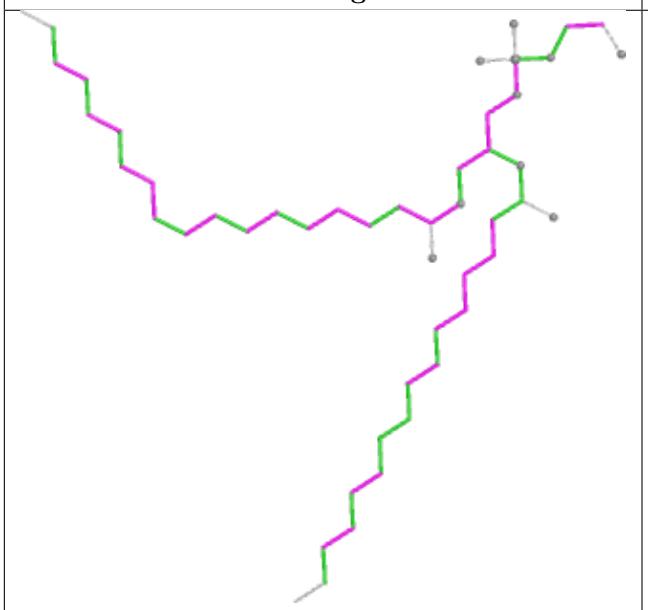
Ligand 9Y0 J 203



Bond lengths



Bond angles



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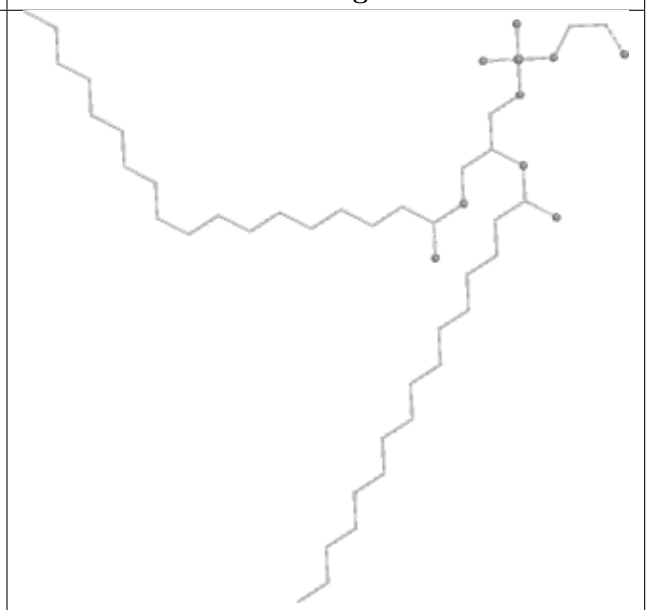
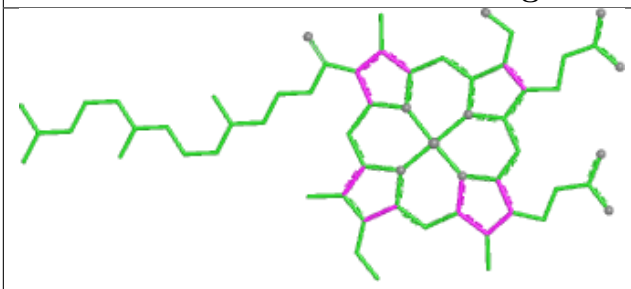
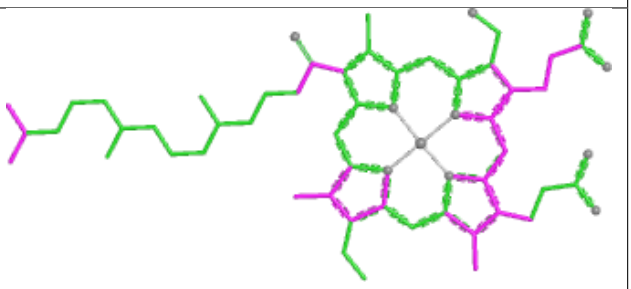
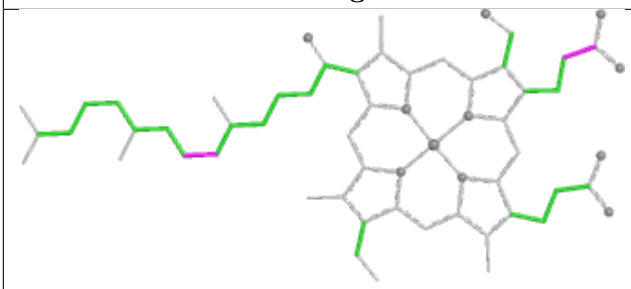
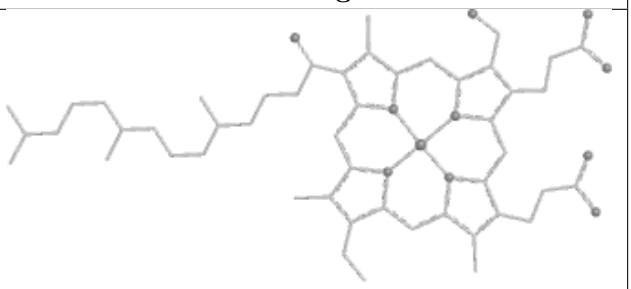
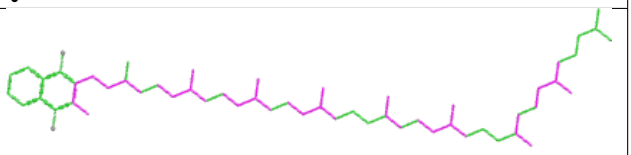
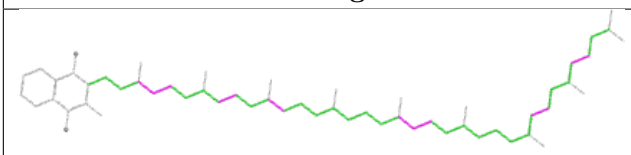
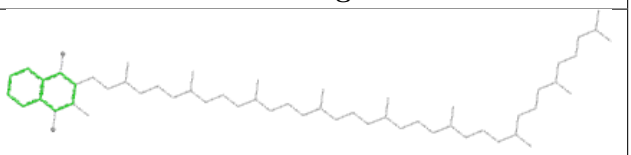
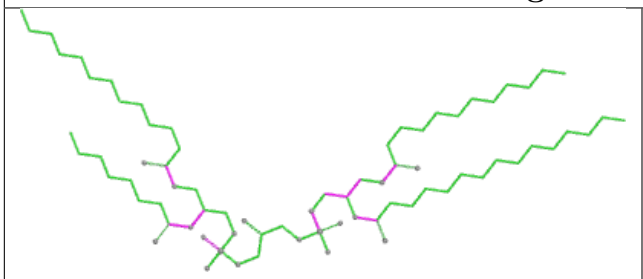
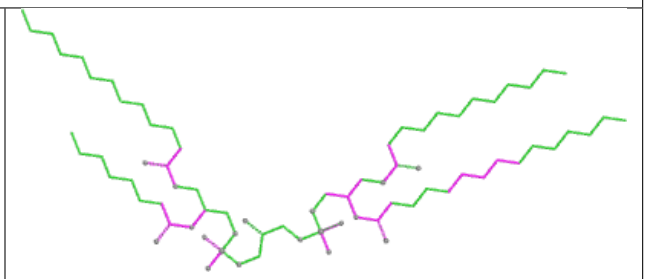
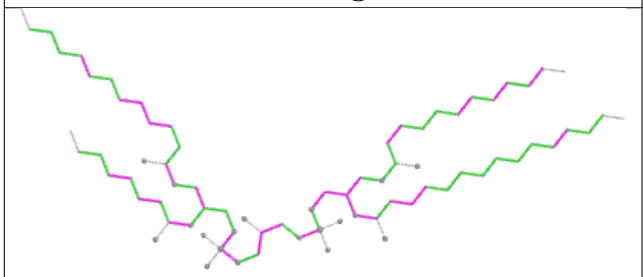
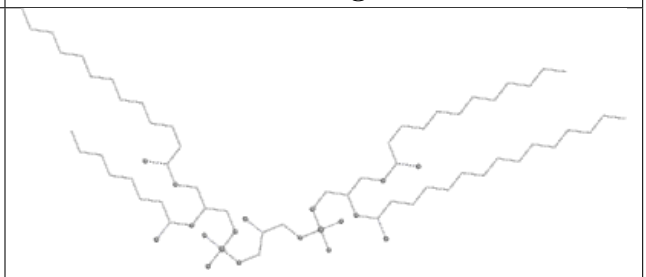


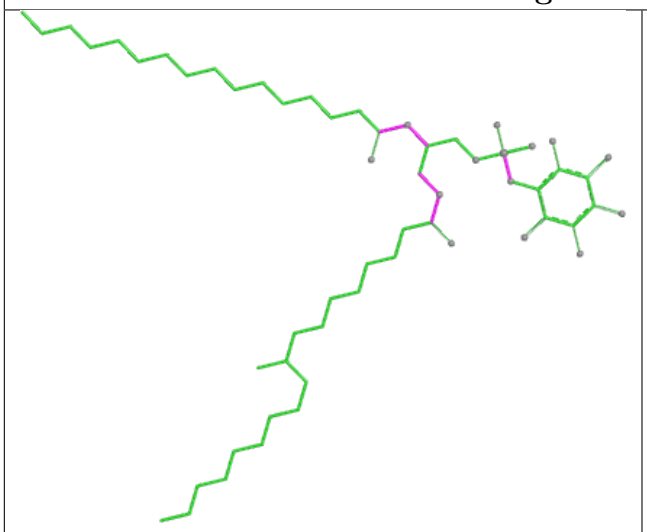
Rings

Ligand HEA R 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

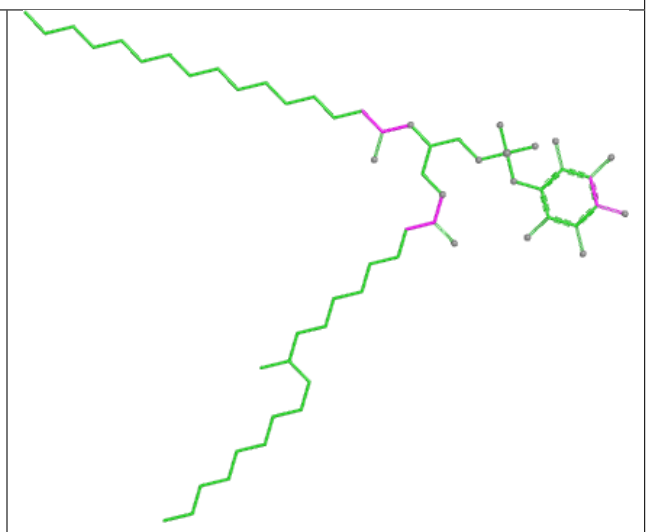
Ligand MQ9 Z 201	
Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CDL Z 202	
 Bond lengths	 Bond angles
 Torsions	 Rings

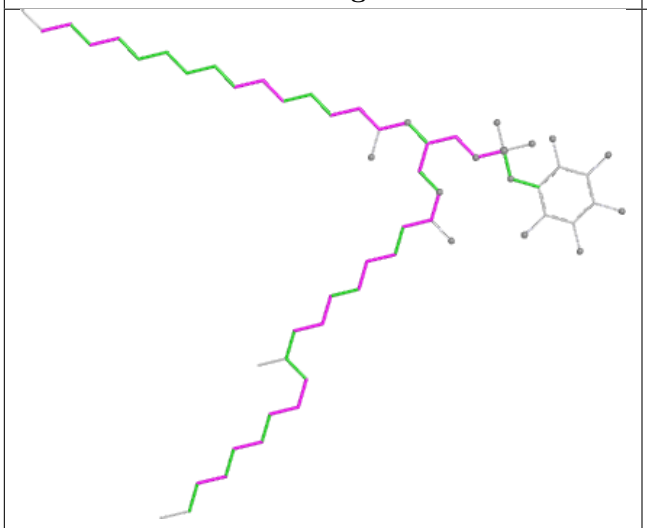
Ligand 9YF I 304



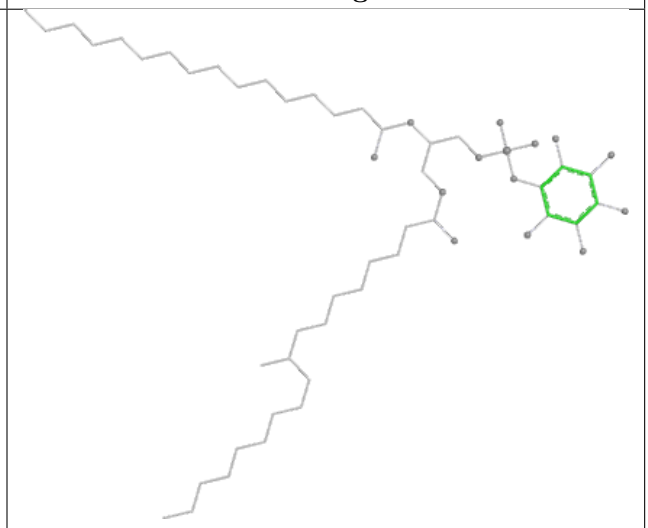
Bond lengths



Bond angles

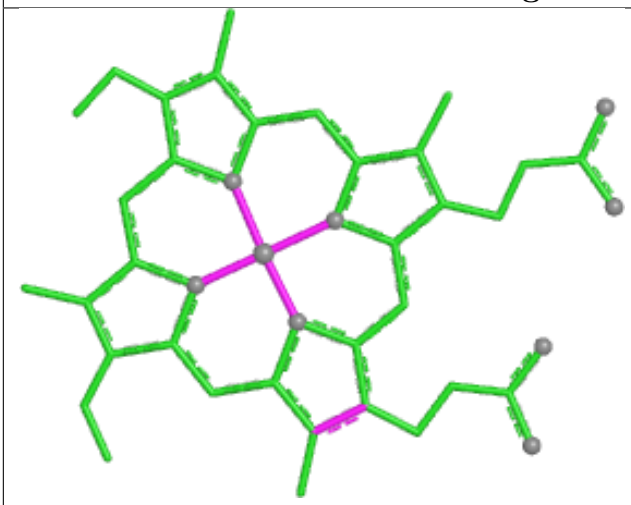


Torsions



Rings

Ligand HEC O 301



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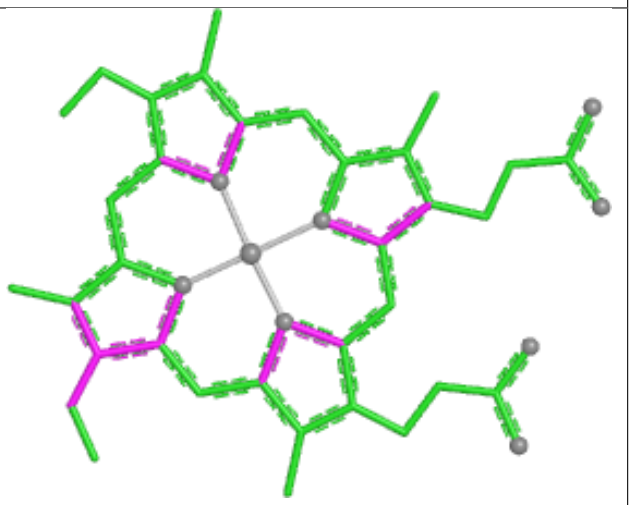
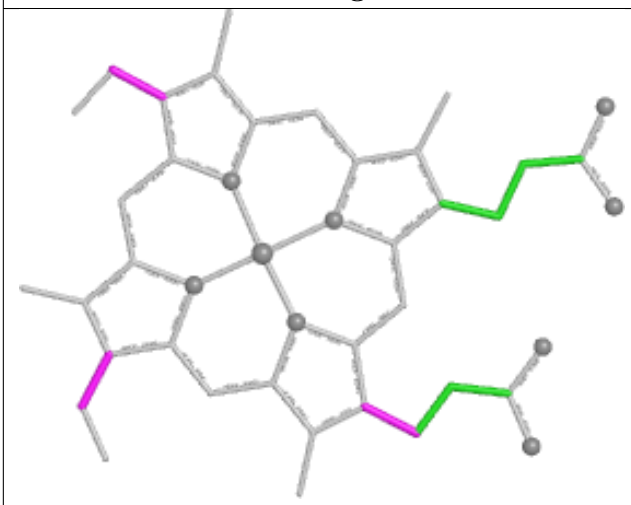


Bond angles



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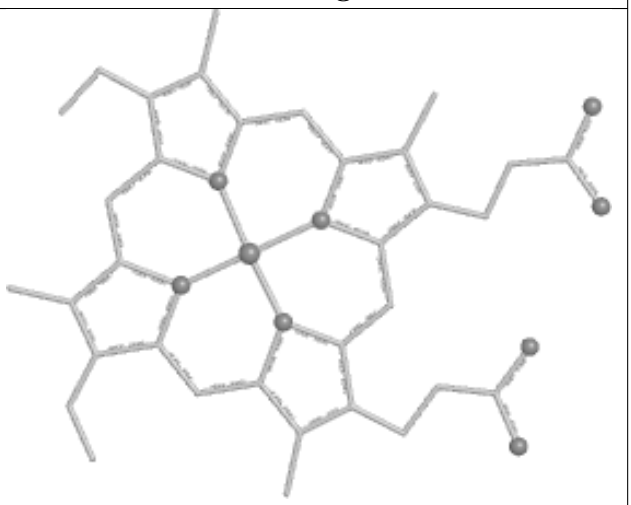
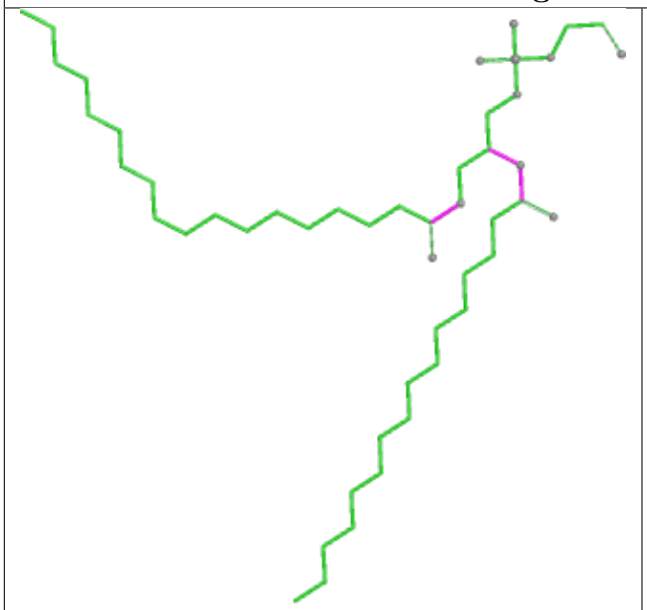


Rings

Ligand 9Y0 F 706



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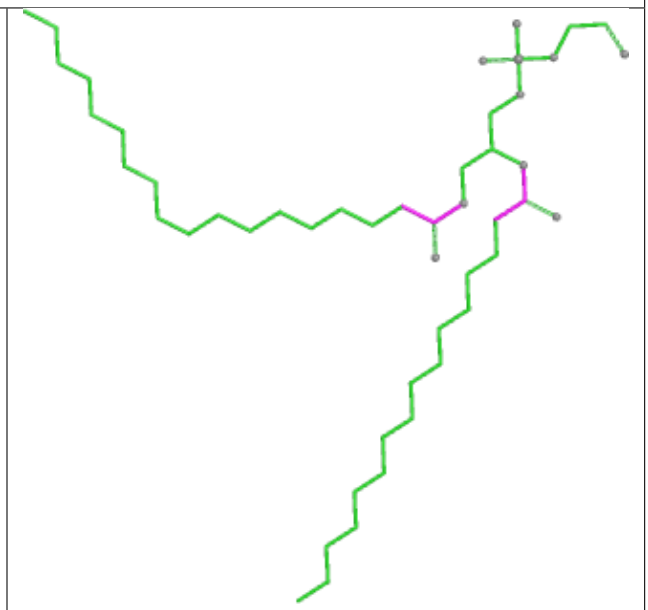
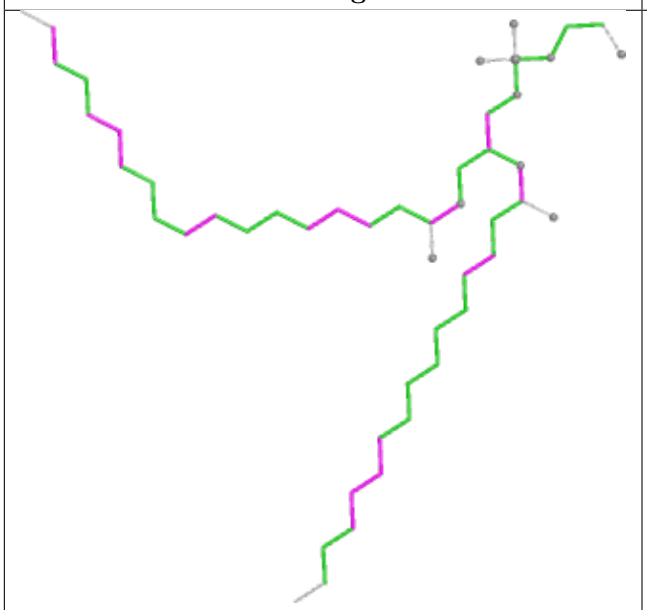


Bond angles



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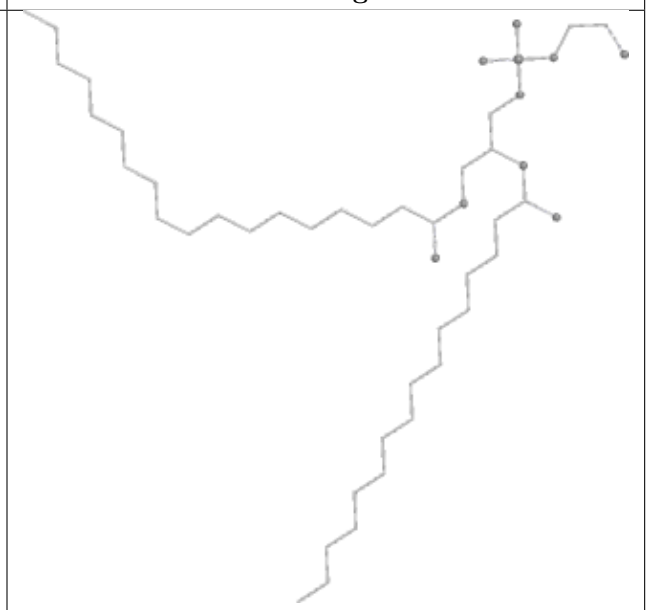
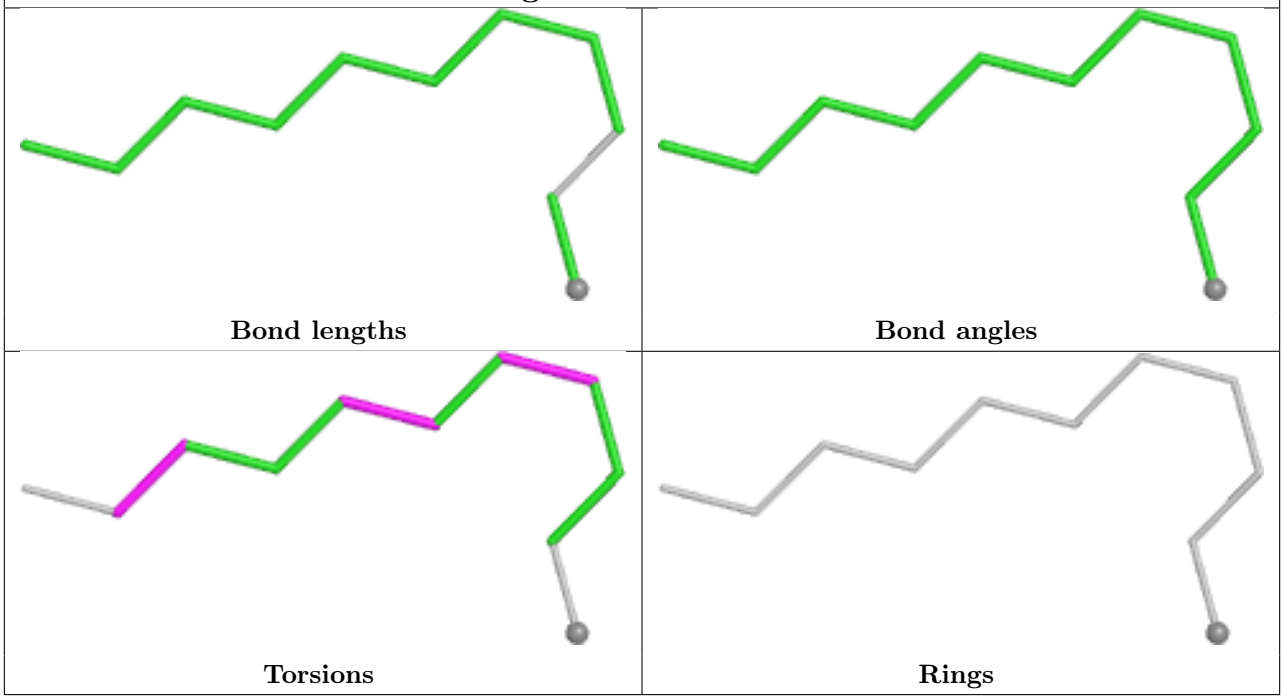
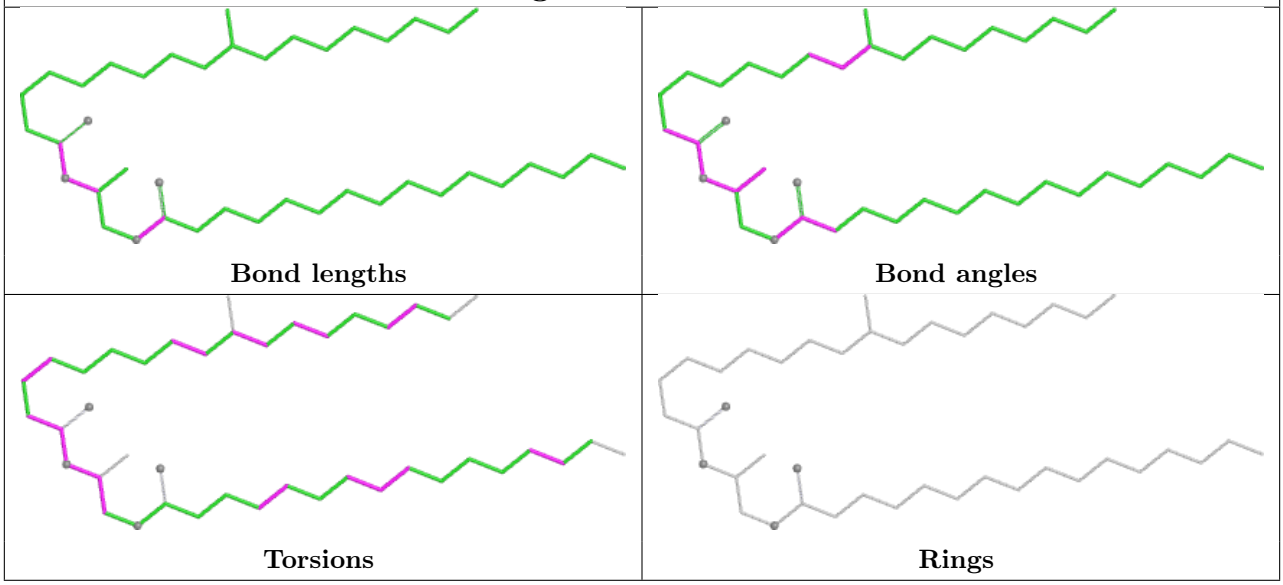


Rings

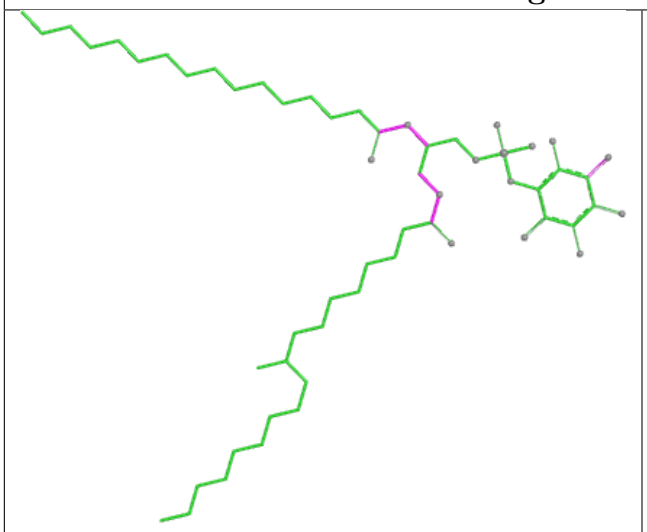
Ligand PLM D 301



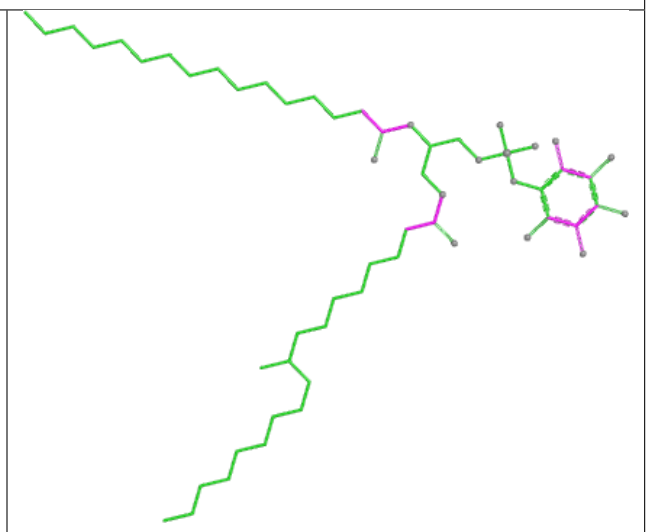
Ligand 9XX c 202



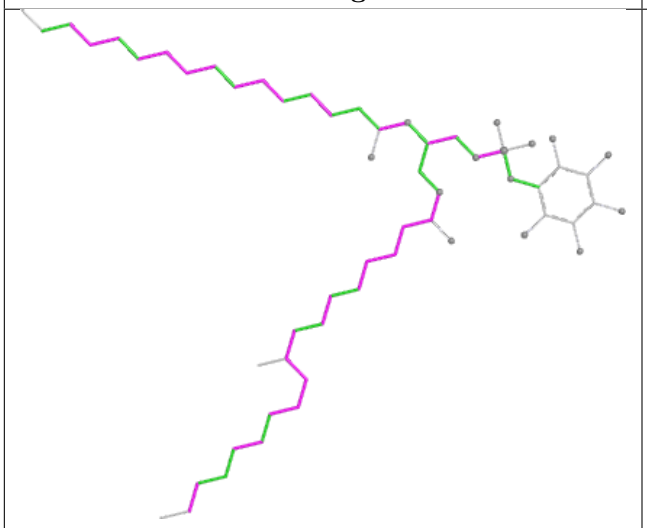
Ligand 9YF Y 503



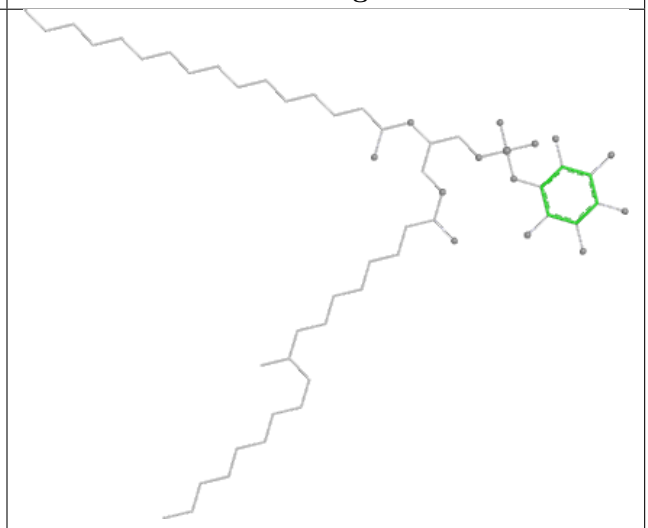
Bond lengths



Bond angles

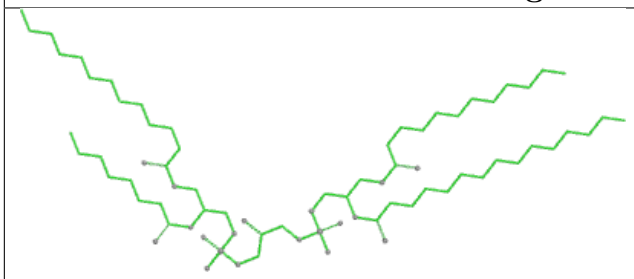


Torsions

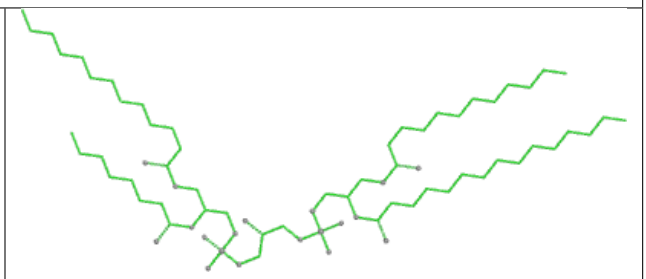


Rings

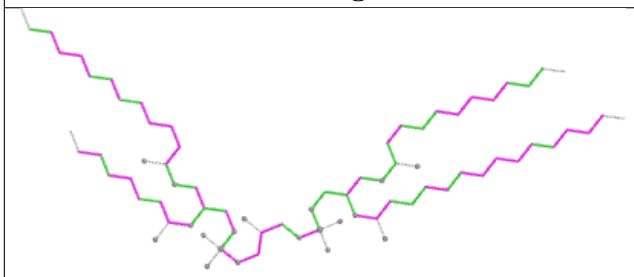
Ligand CDL P 201



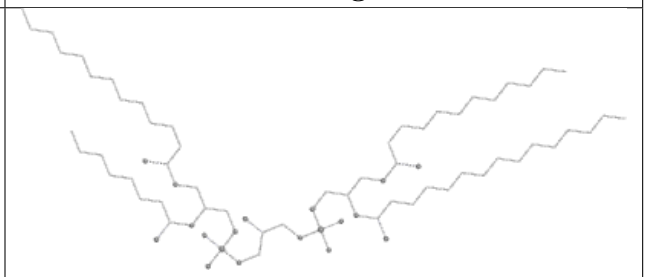
Bond lengths



Bond angles

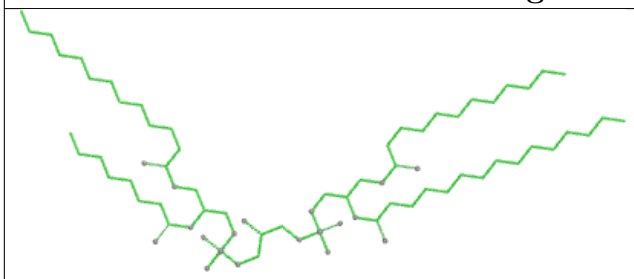


Torsions

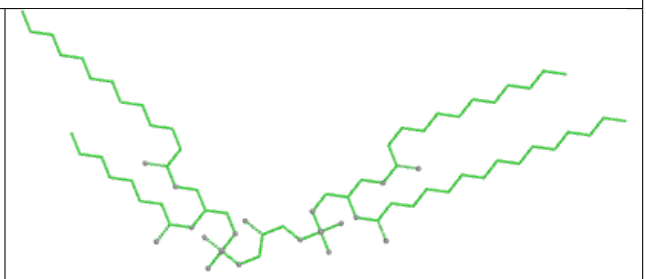


Rings

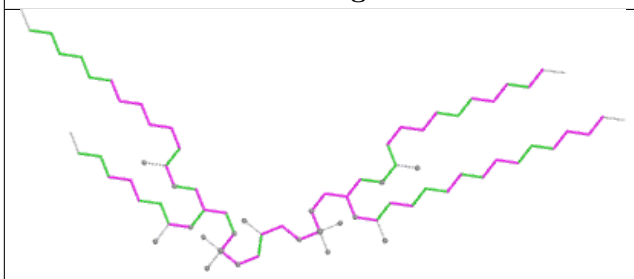
Ligand CDL F 704



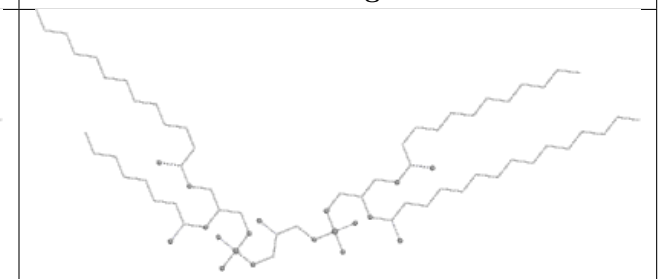
Bond lengths



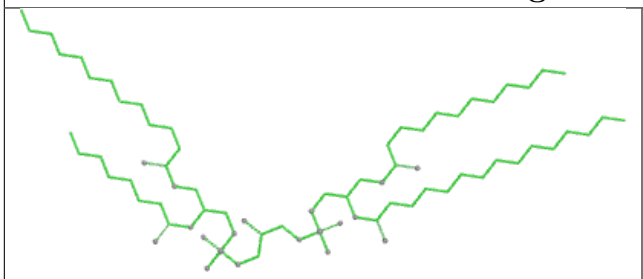
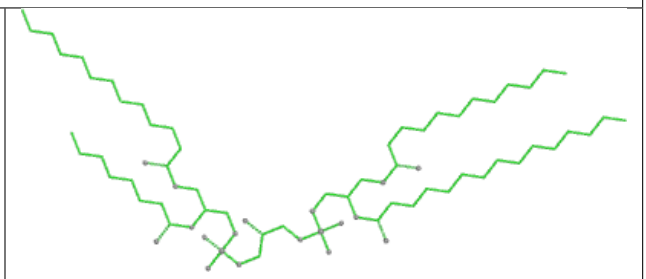
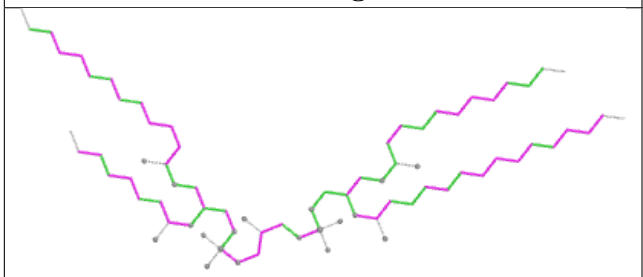
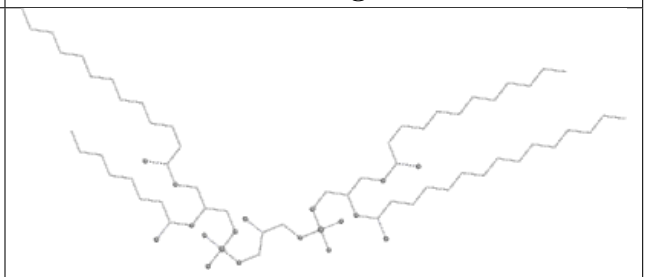
Bond angles



Torsions



Rings

Ligand CDL J 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

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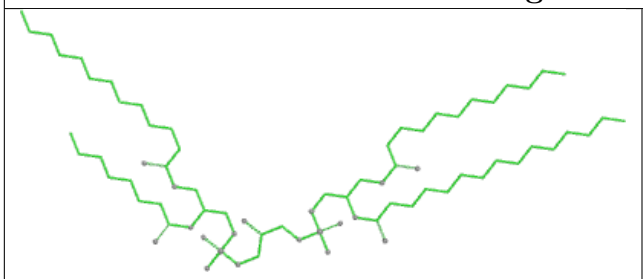
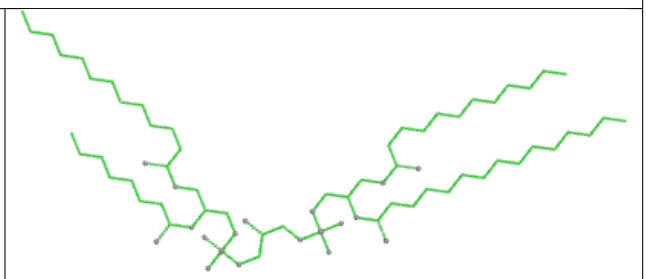
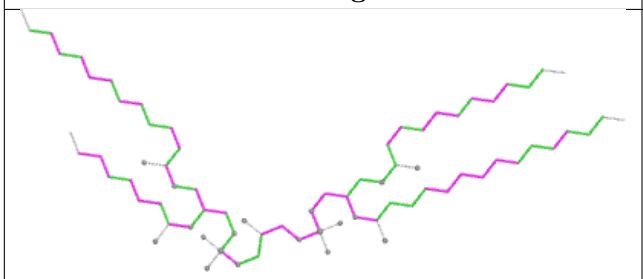
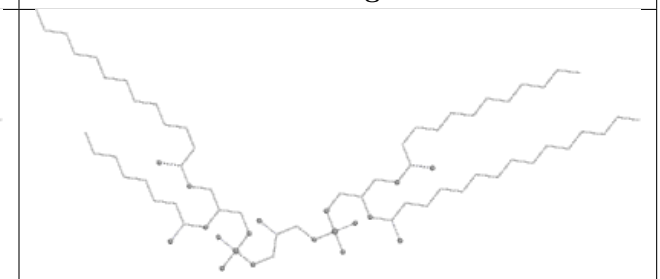
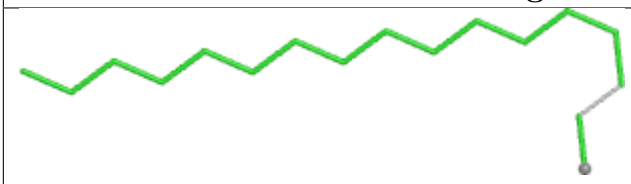
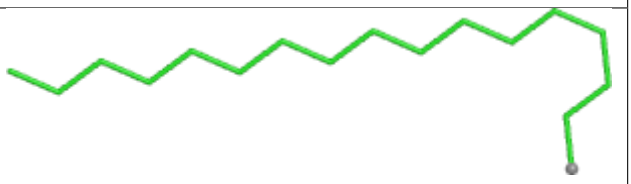
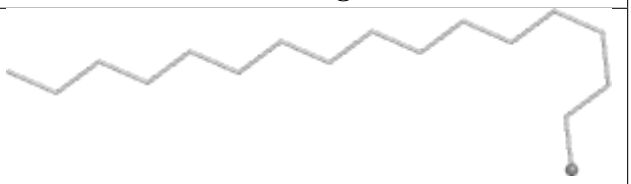
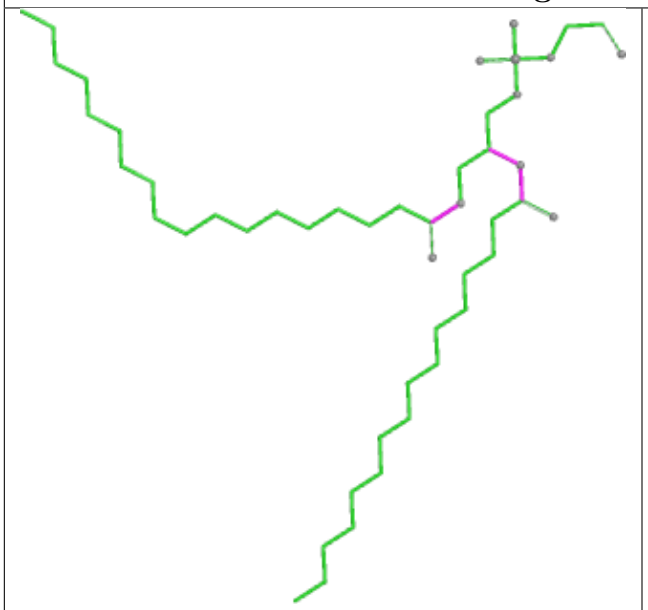
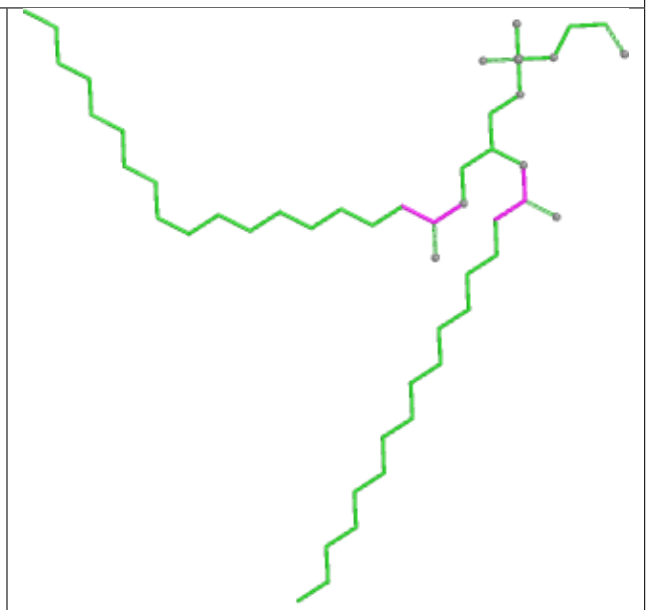
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PLM c 201	
 Bond lengths	 Bond angles
Torsions	 Rings

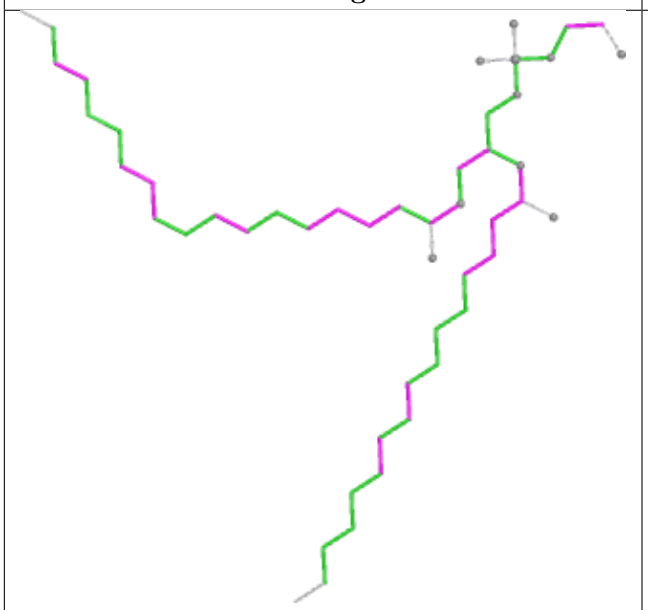
Ligand 9Y0 S 302



Bond lengths



Bond angles



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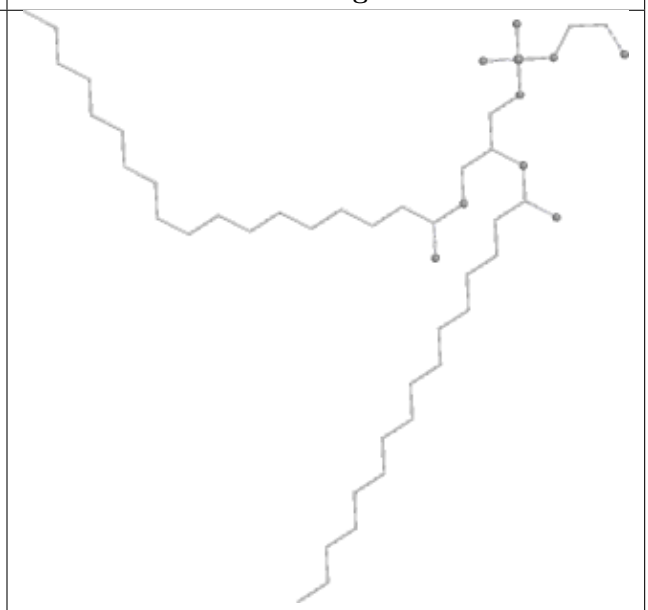
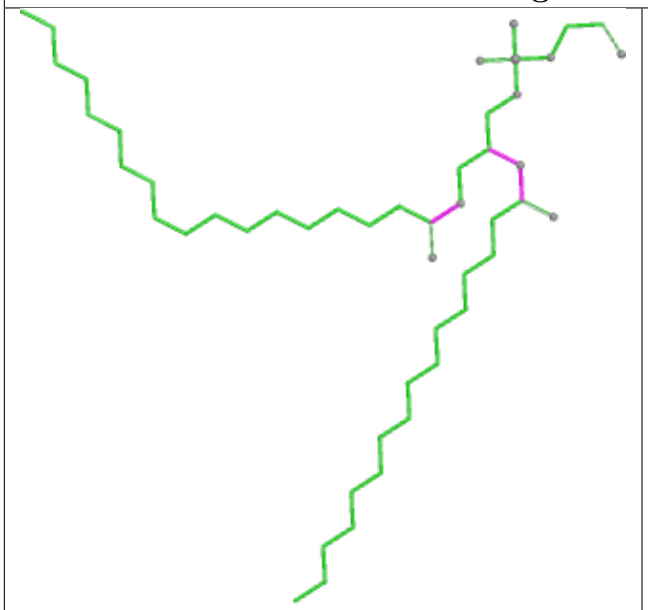


Rings

Ligand 9Y0 P 202



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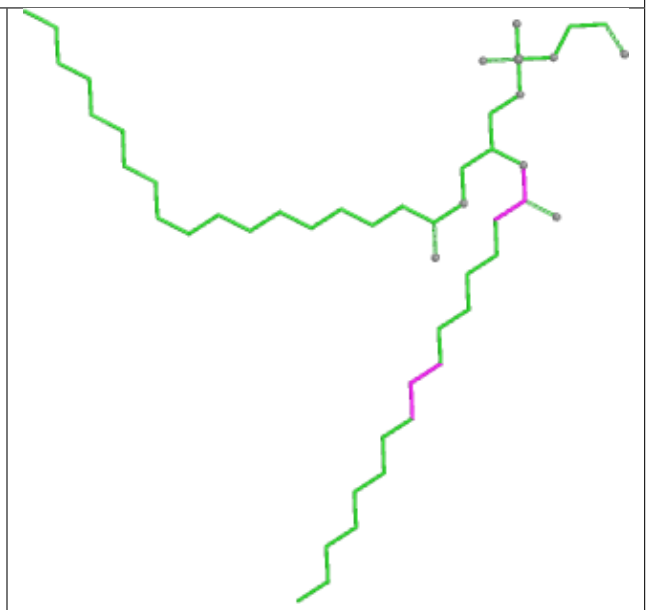

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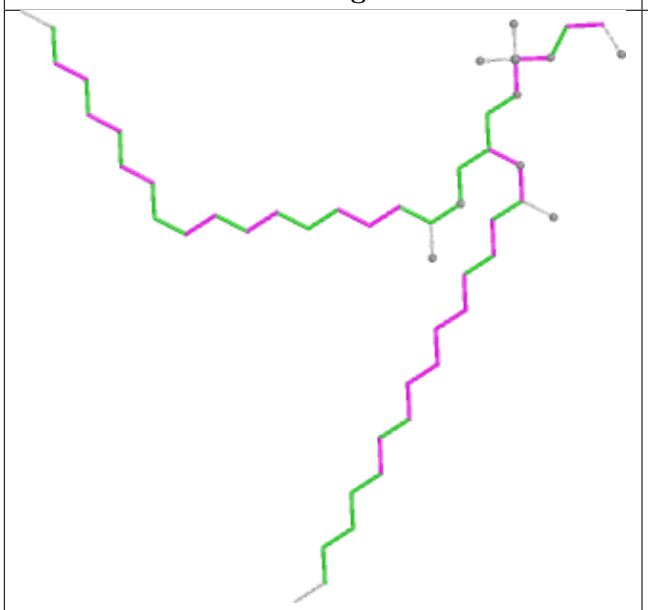

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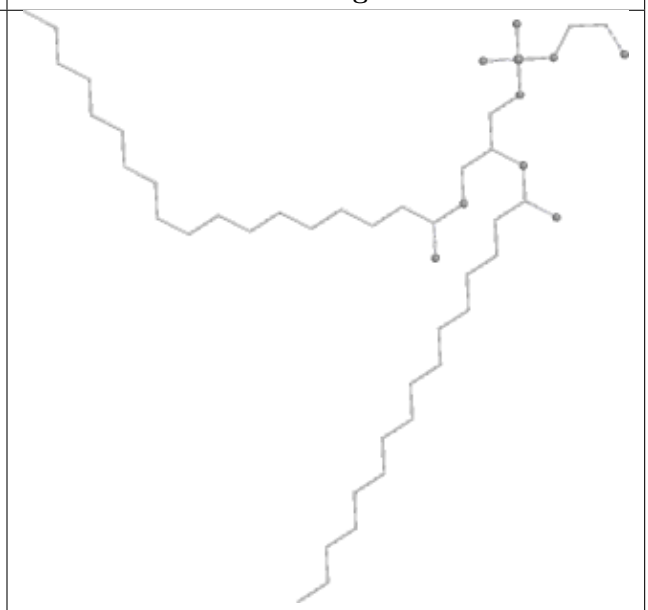
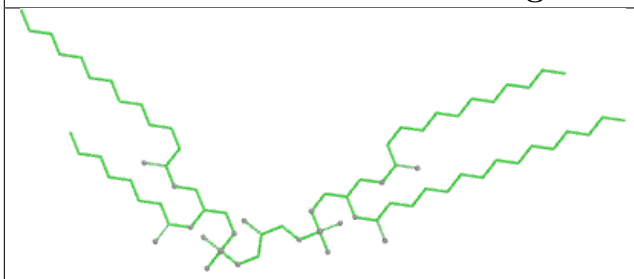


Rings

Ligand CDL E 605



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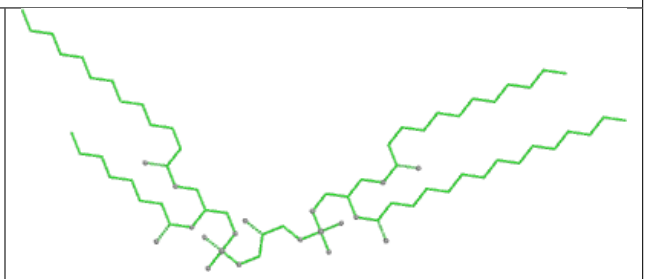
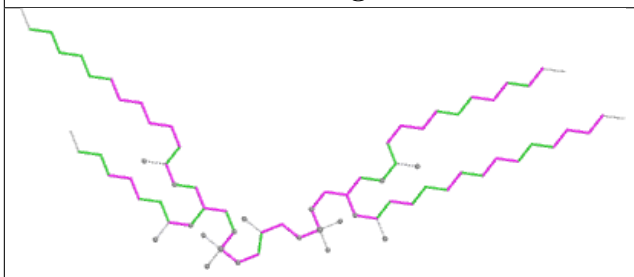


Bond angles



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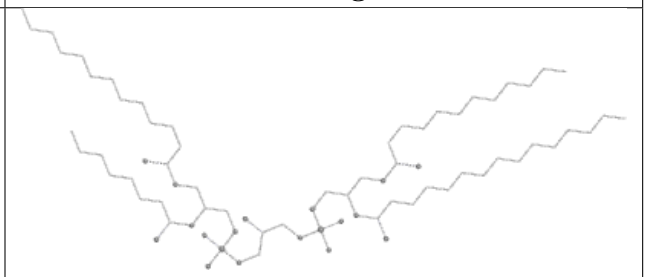
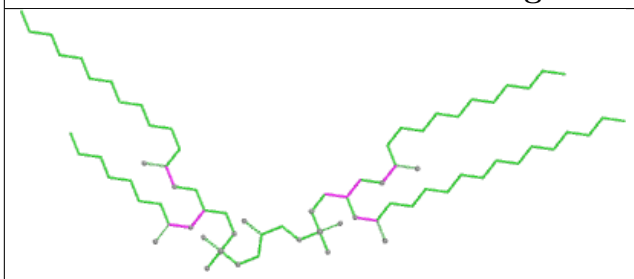


Rings

Ligand CDL X 302



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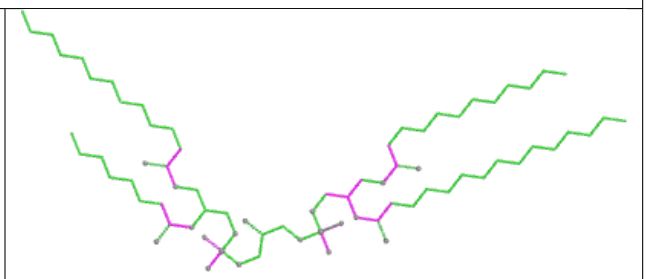

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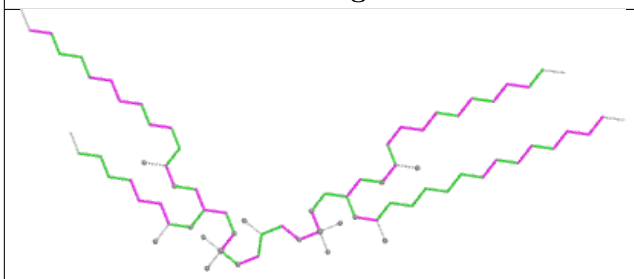

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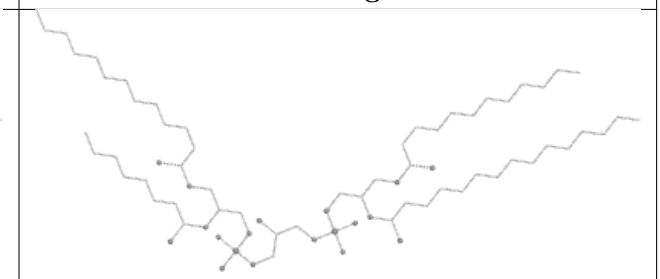
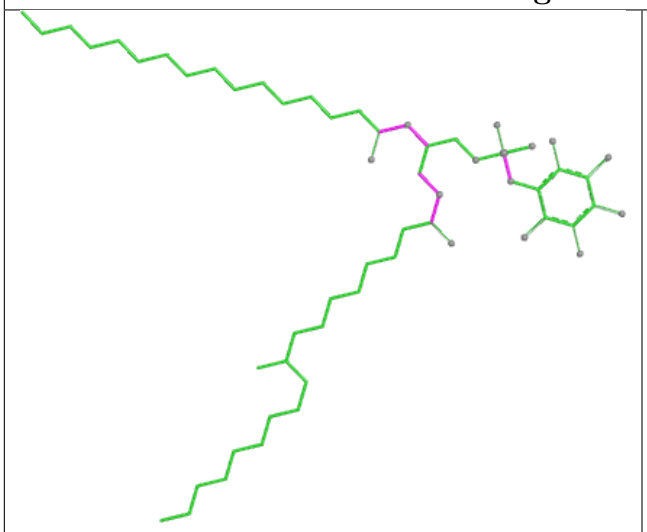


Rings

Ligand 9YF c 203



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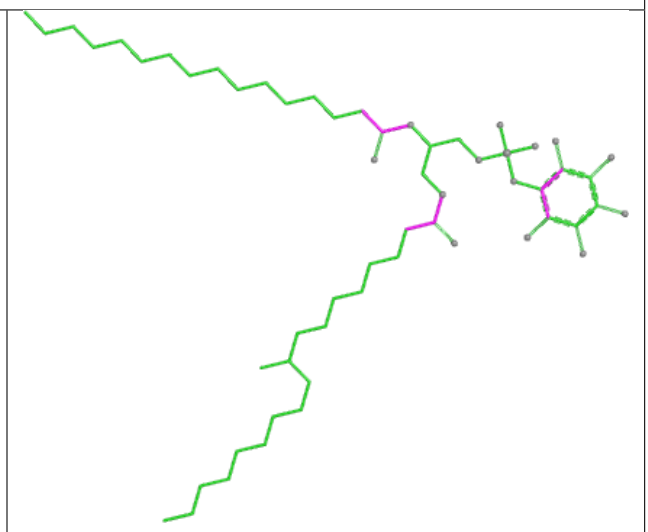
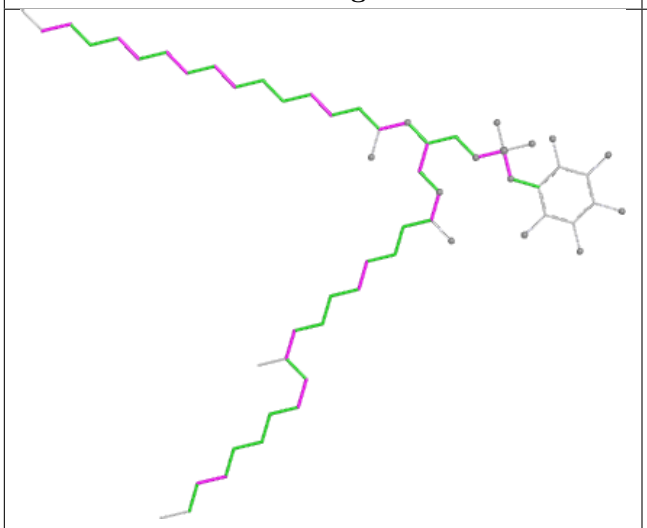


Bond angles



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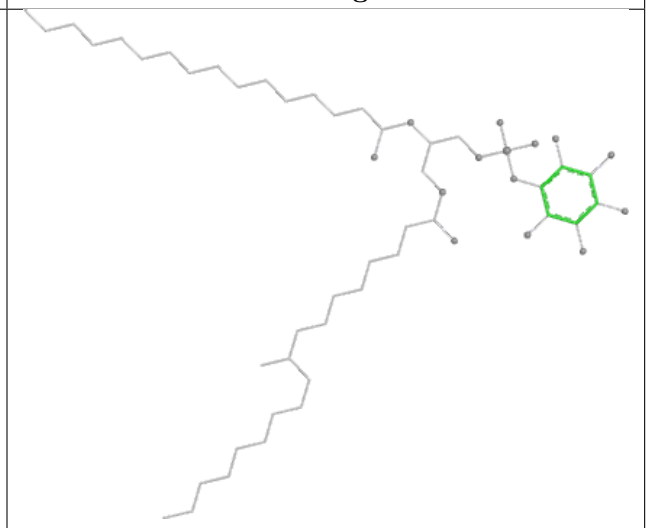
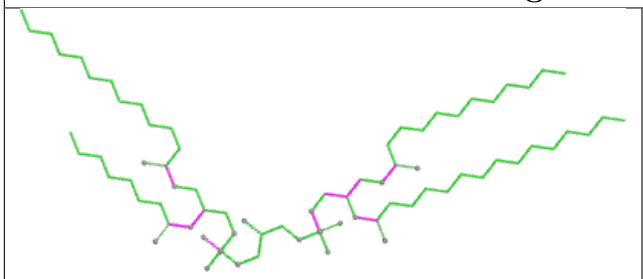
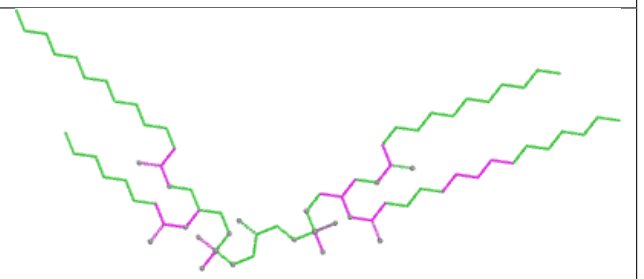
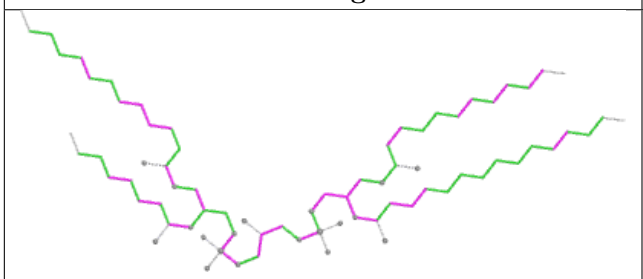
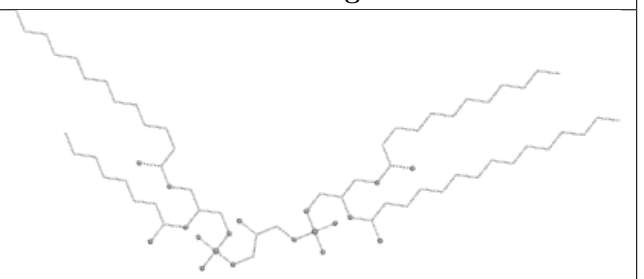
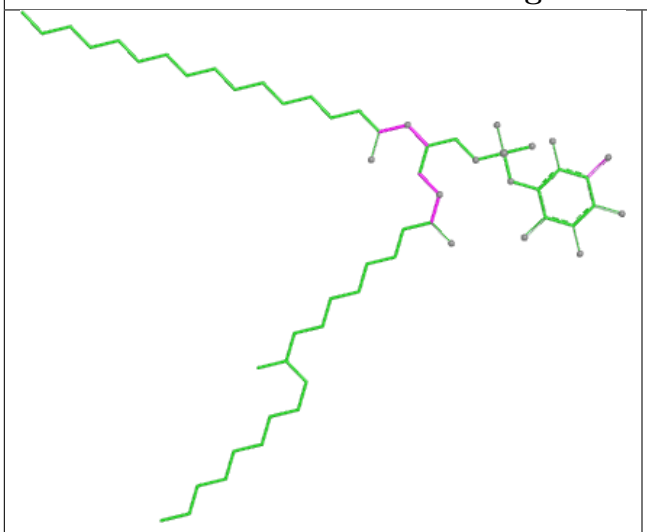


Rings

Ligand CDL T 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 9YF M 502



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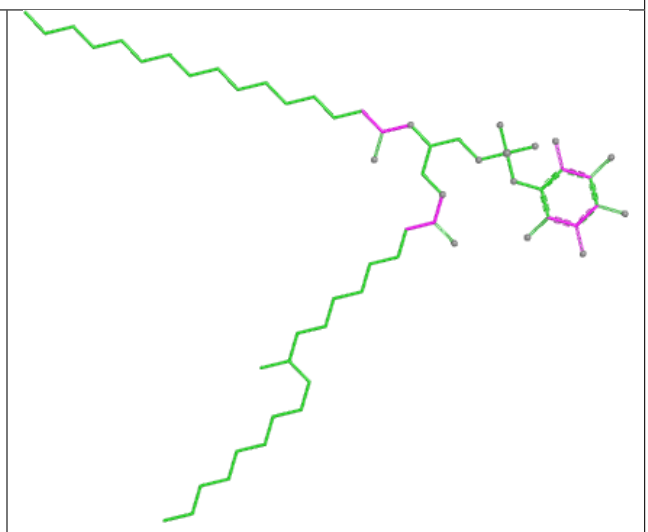
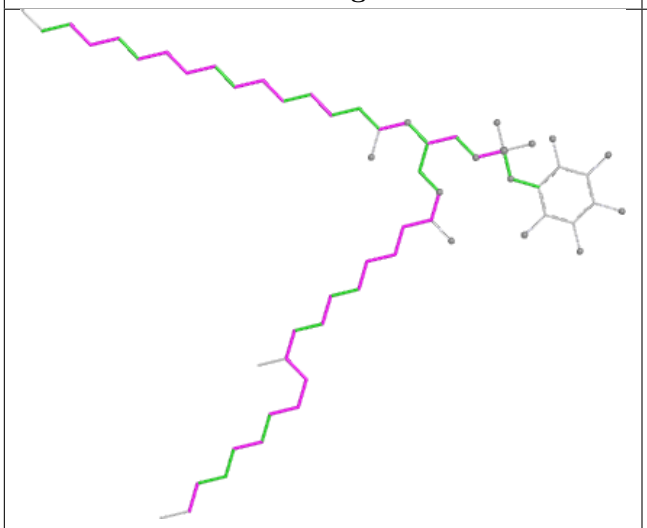
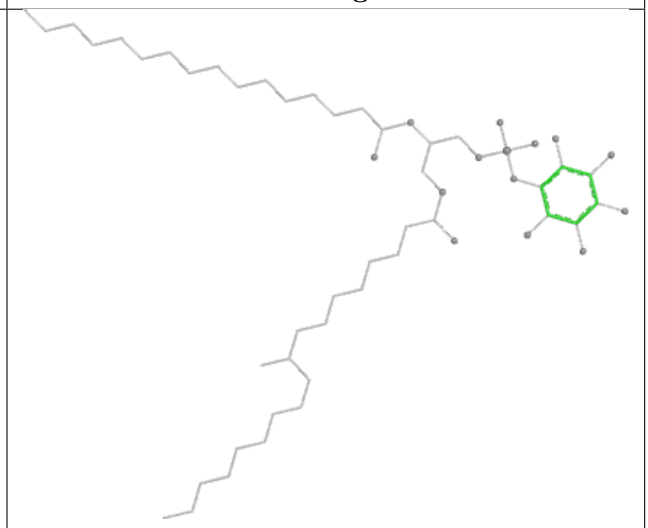


Bond angles

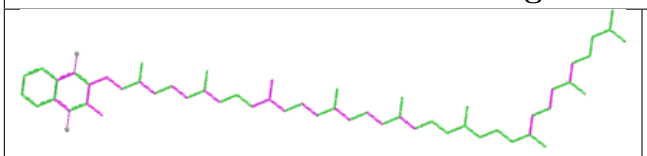


Torsions



Rings

Ligand MQ9 F 707



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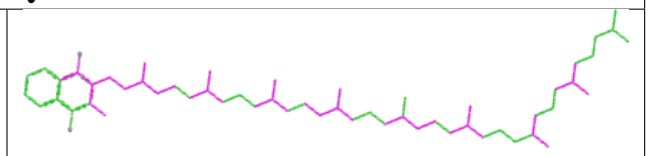
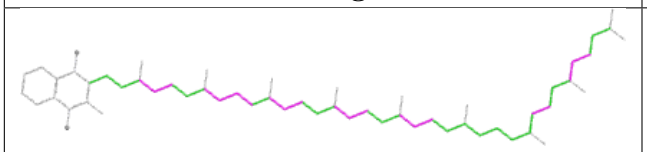


Bond angles



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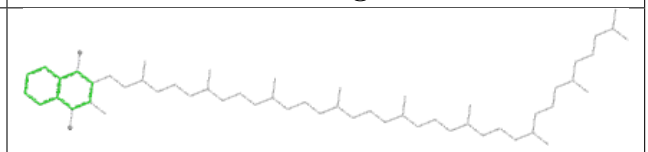
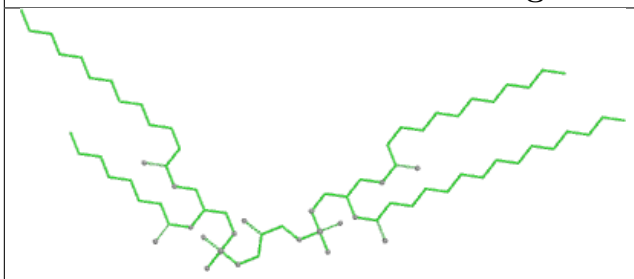


Rings

Ligand CDL F 705



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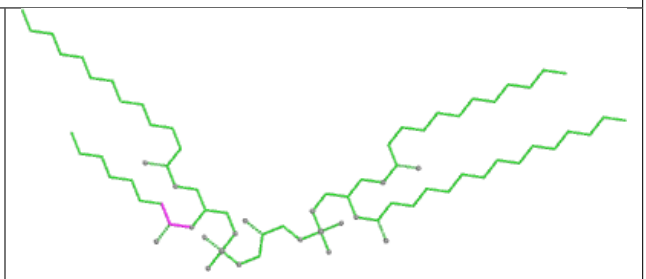

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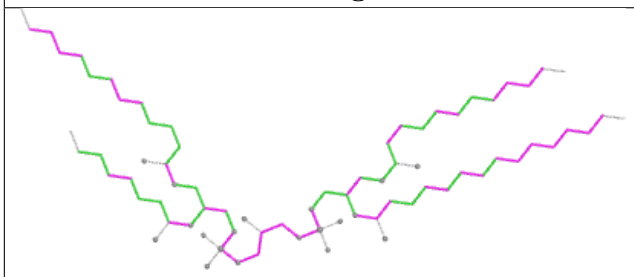

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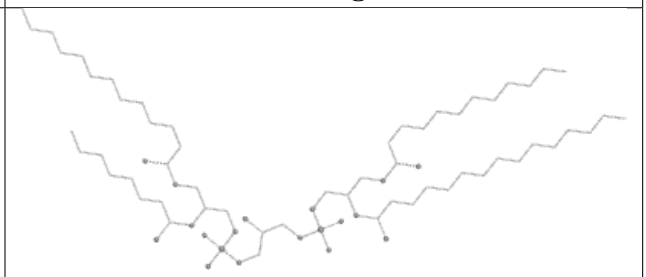
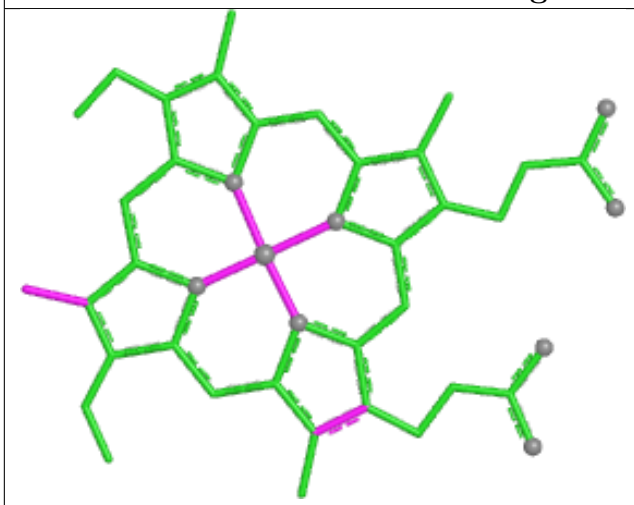


Rings

Ligand HEC I 302



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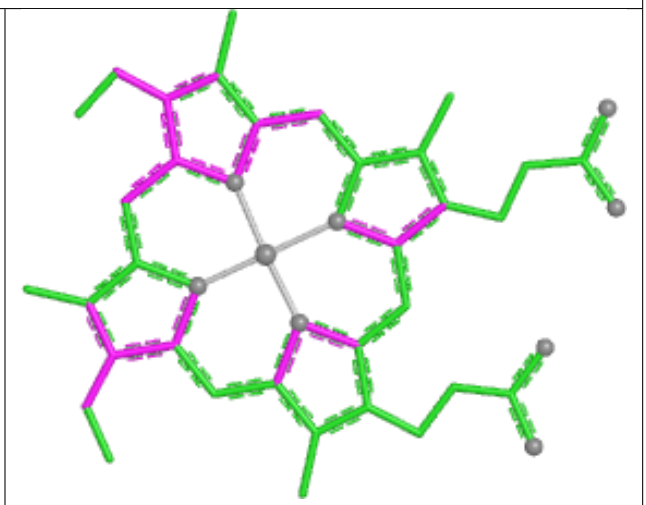
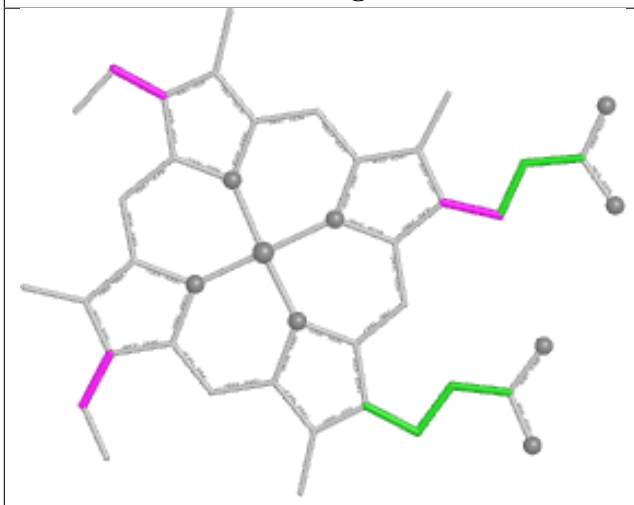
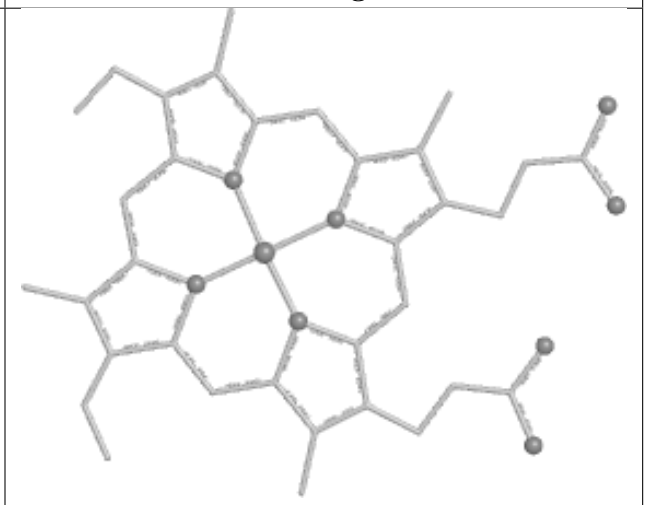


Bond angles

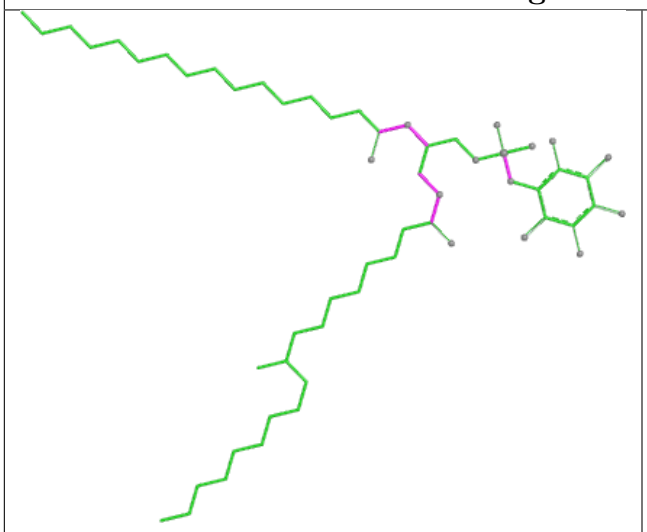


Torsions

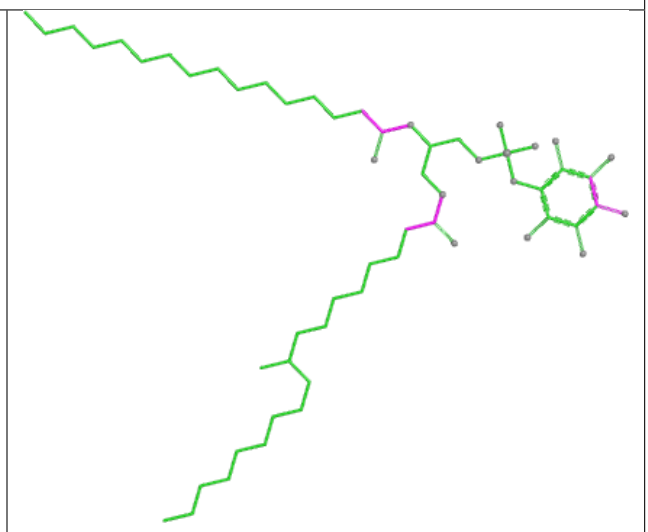


Rings

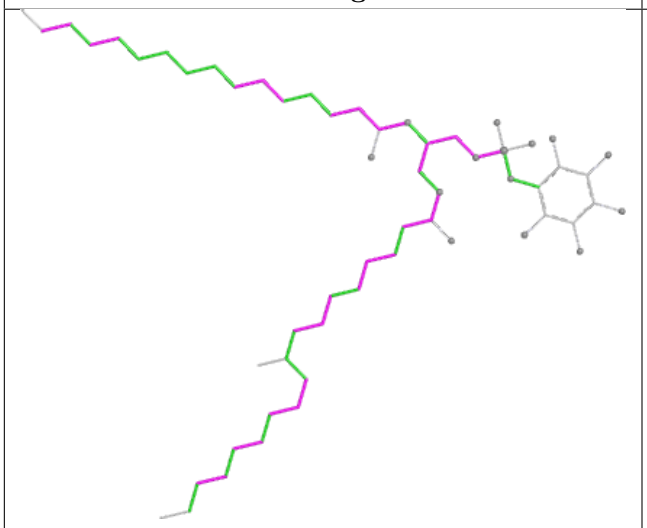
Ligand 9YF O 303



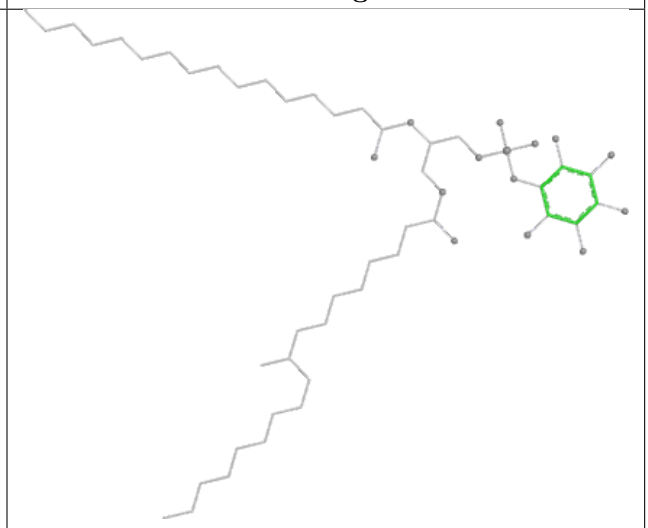
Bond lengths



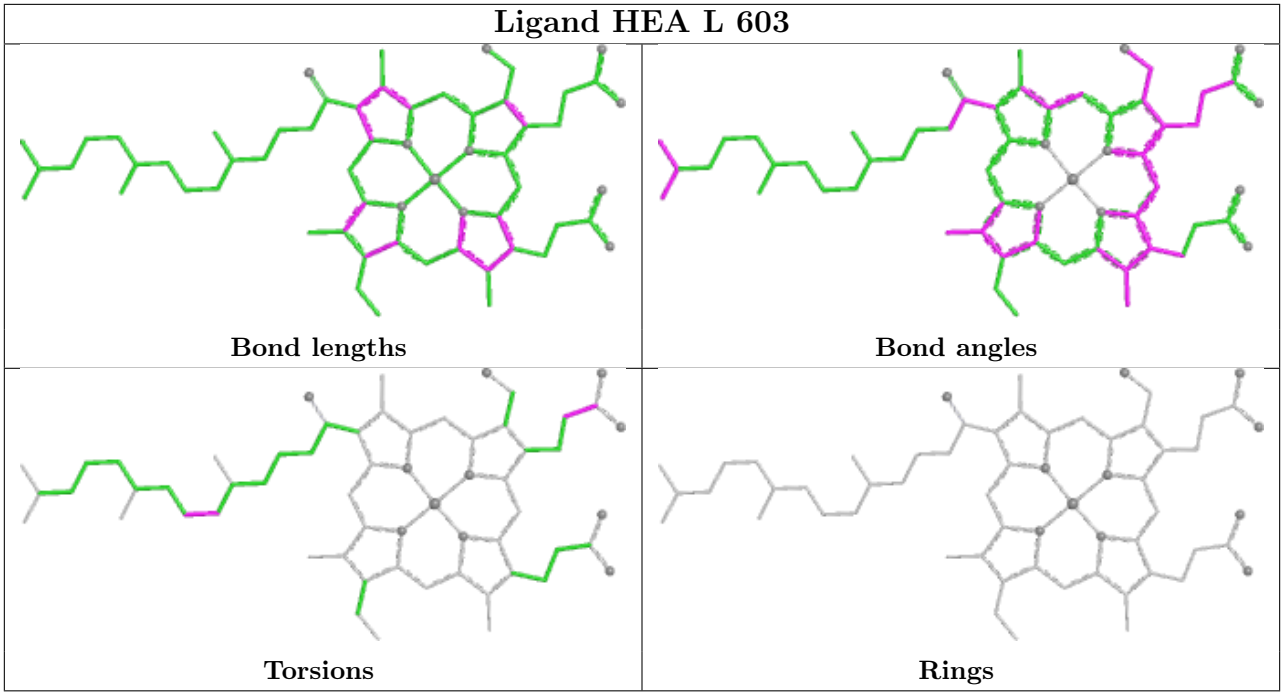
Bond angles

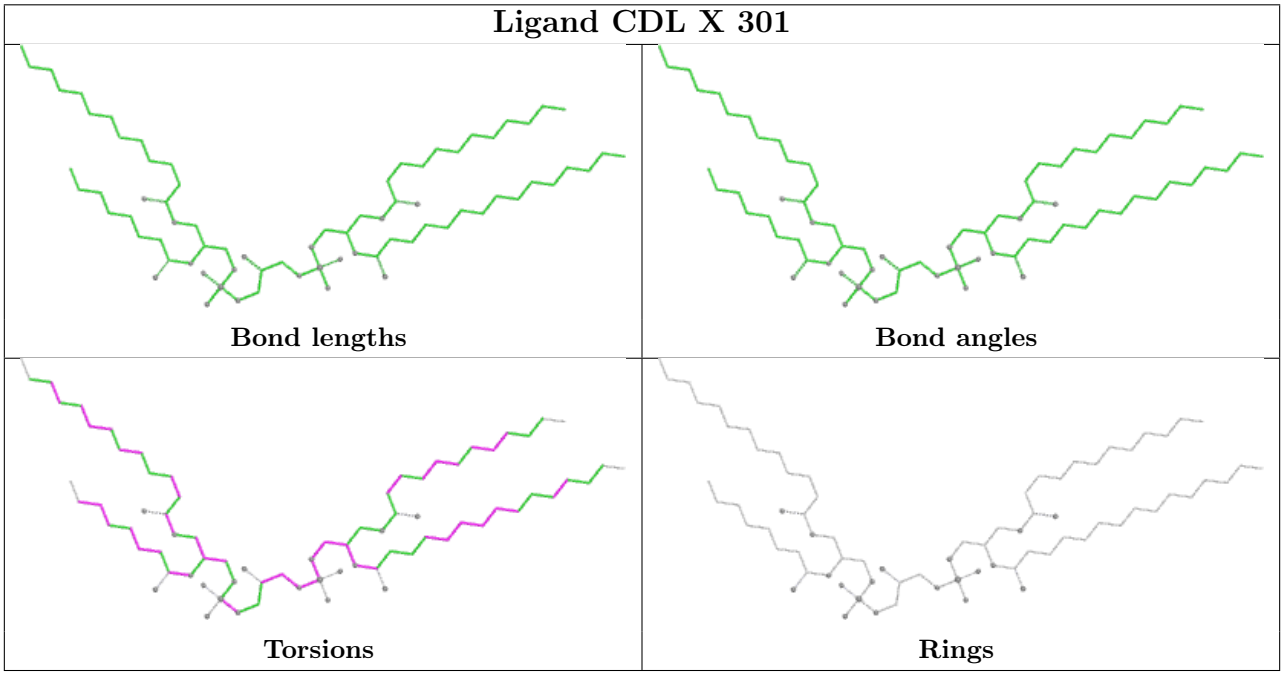


Torsions



Rings





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

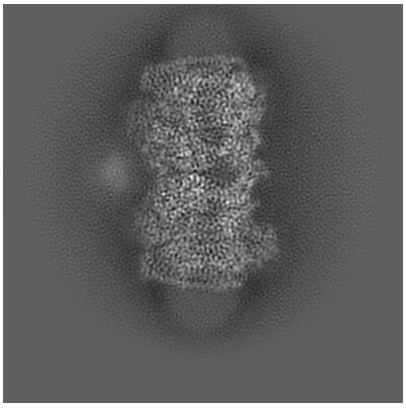
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-24455. These allow visual inspection of the internal detail of the map and identification of artifacts.

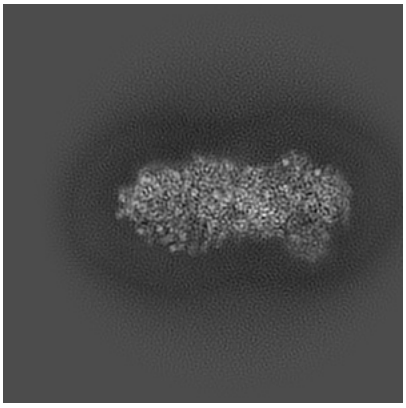
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

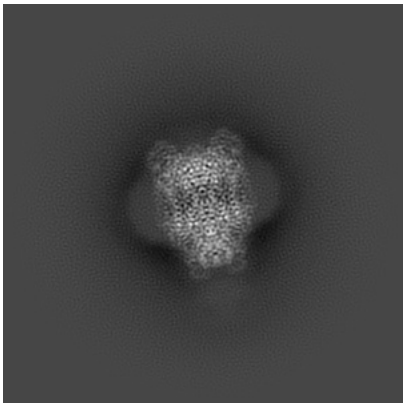
6.1.1 Primary map



X



Y

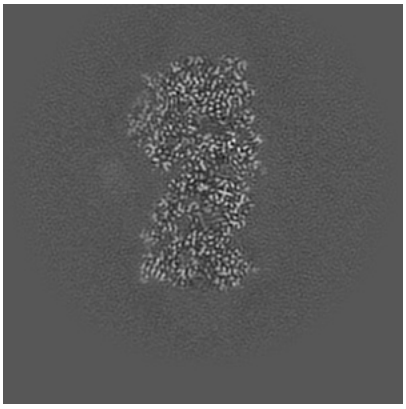


Z

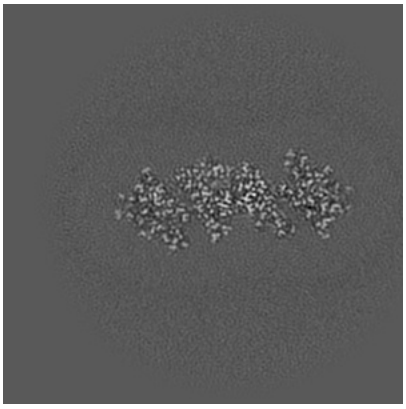
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

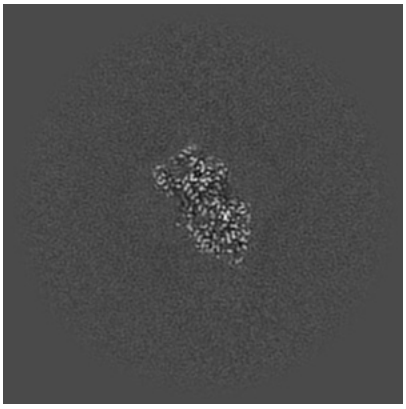
6.2.1 Primary map



X Index: 165



Y Index: 165

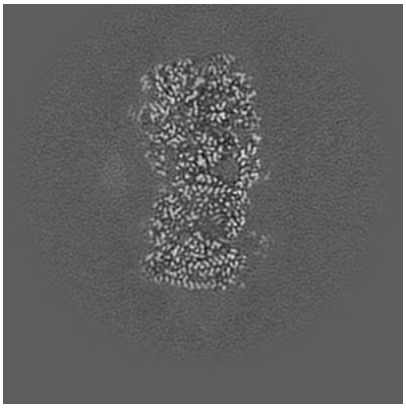


Z Index: 165

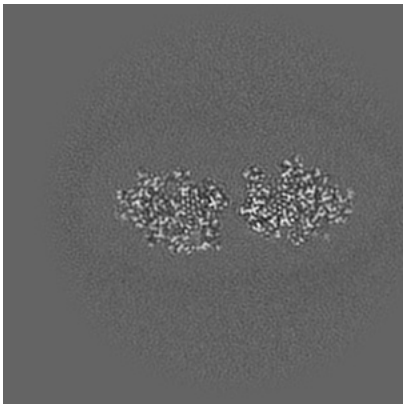
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

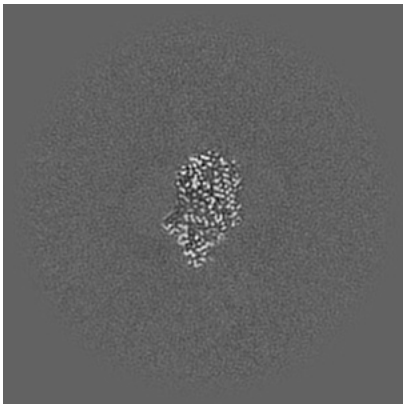
6.3.1 Primary map



X Index: 170



Y Index: 182

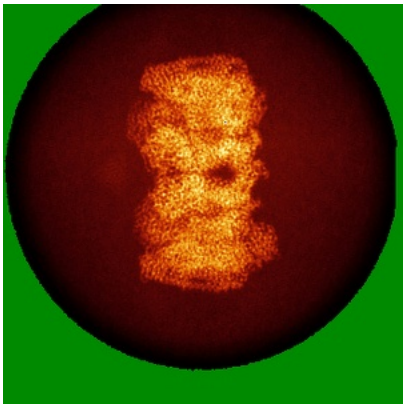


Z Index: 208

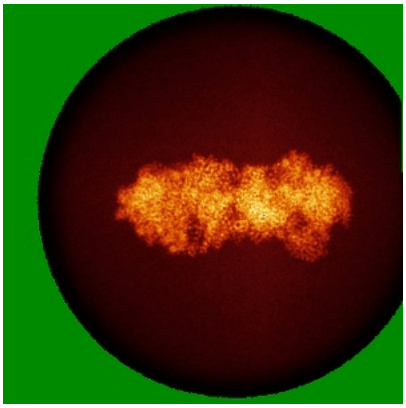
The images above show the largest variance slices of the map in three orthogonal directions.

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

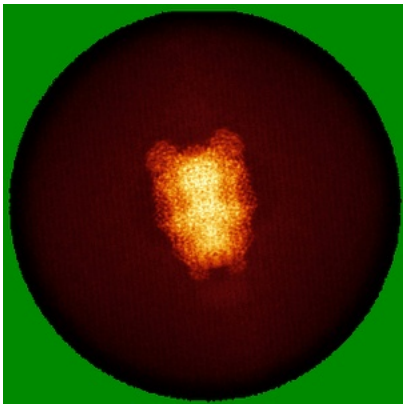
6.4.1 Primary map



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 1.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

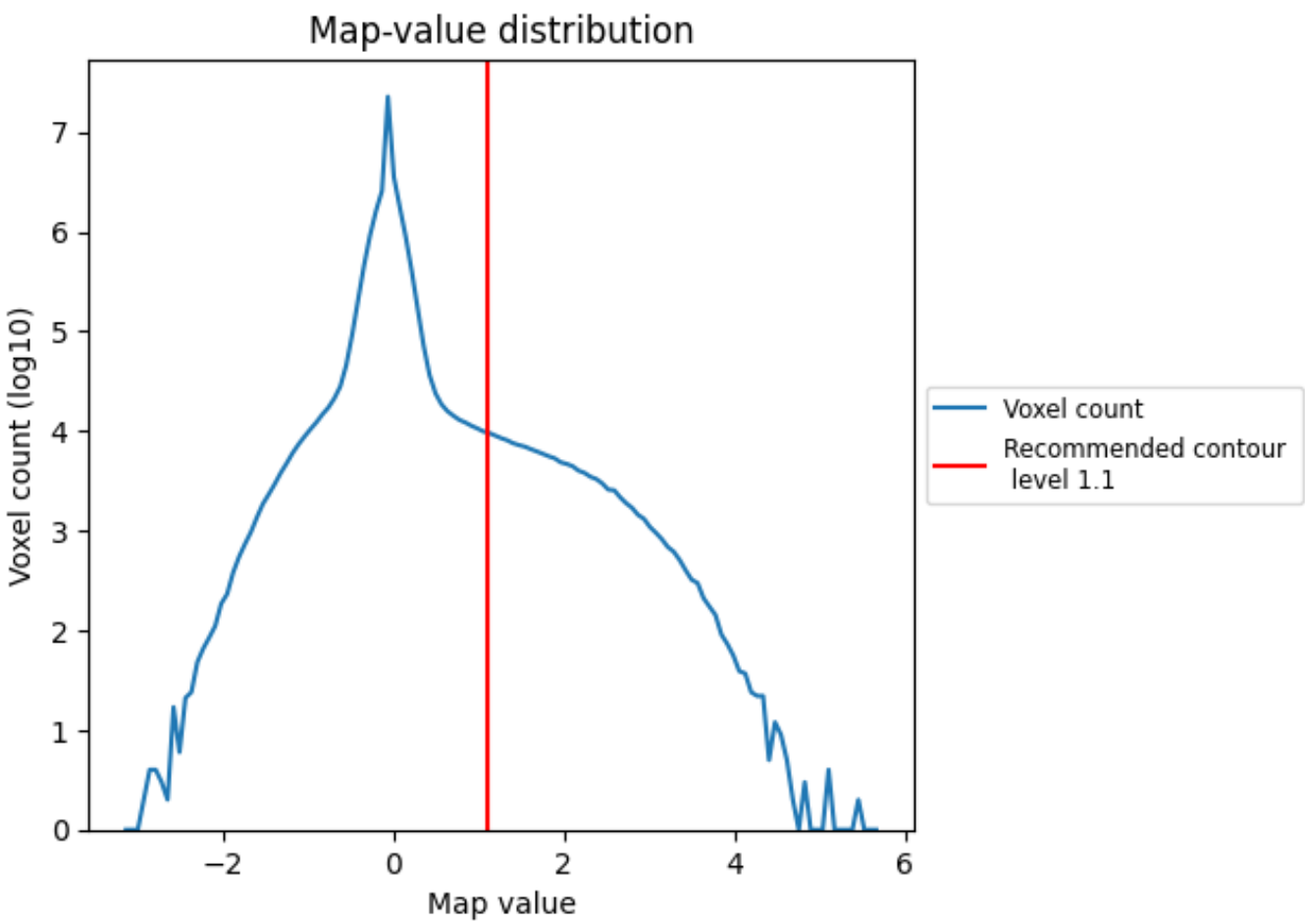
6.6 Mask visualisation (i)

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

7 Map analysis (i)

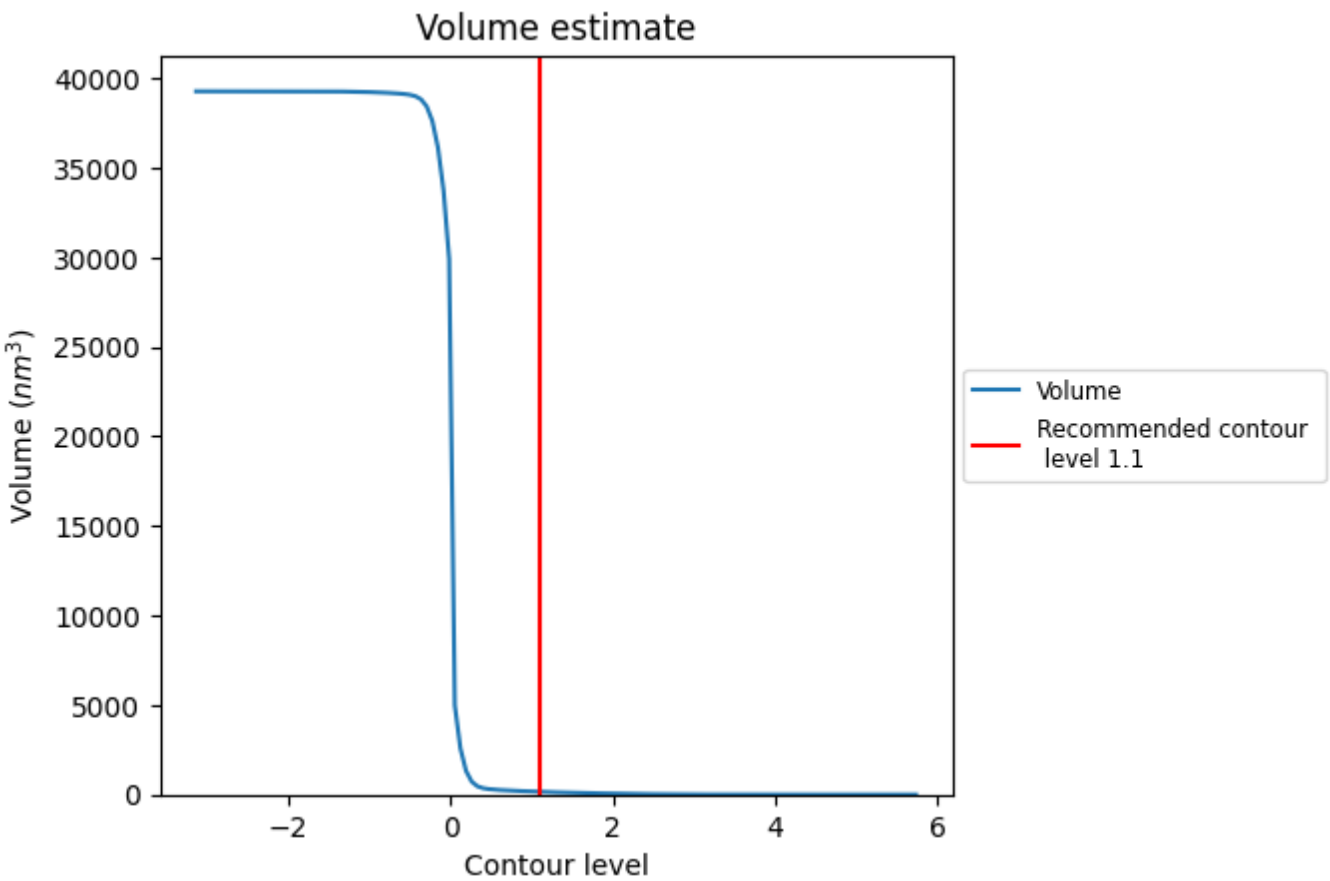
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

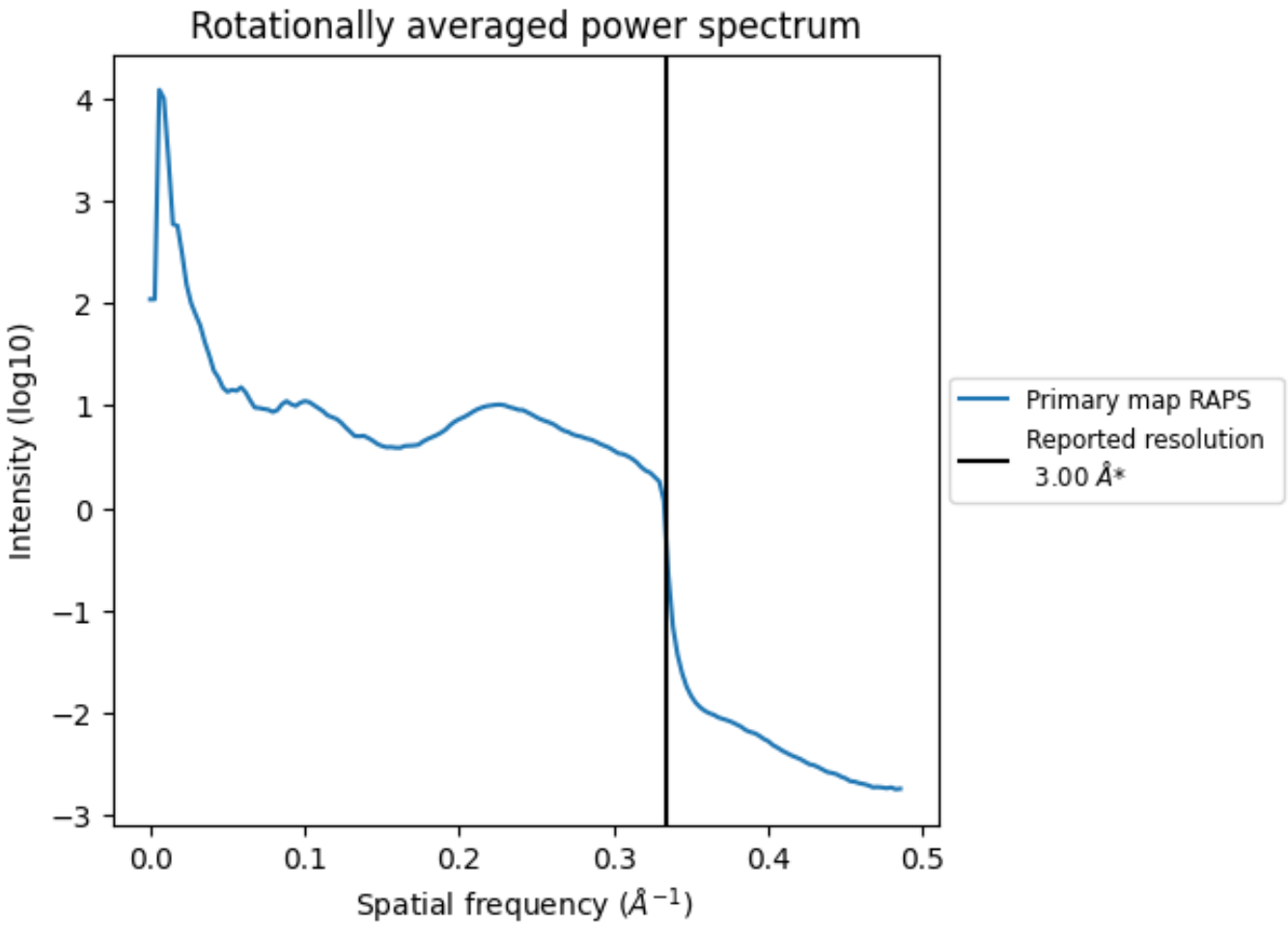
7.2 Volume estimate (i)



The volume at the recommended contour level is 155 nm^3; this corresponds to an approximate mass of 140 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 0.333 Å^{-1}

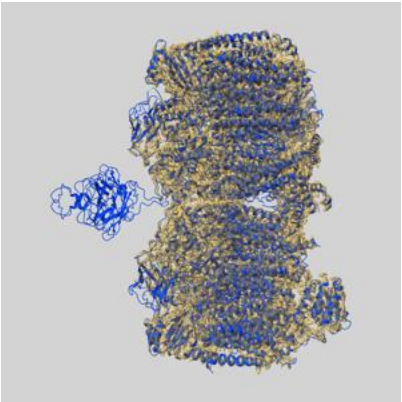
8 Fourier-Shell correlation (i)

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

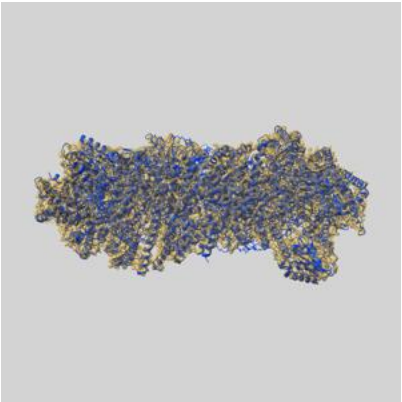
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-24455 and PDB model 7RH5. Per-residue inclusion information can be found in section 3 on page 16.

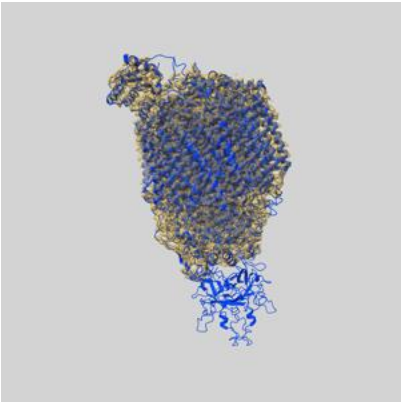
9.1 Map-model overlay (i)



X



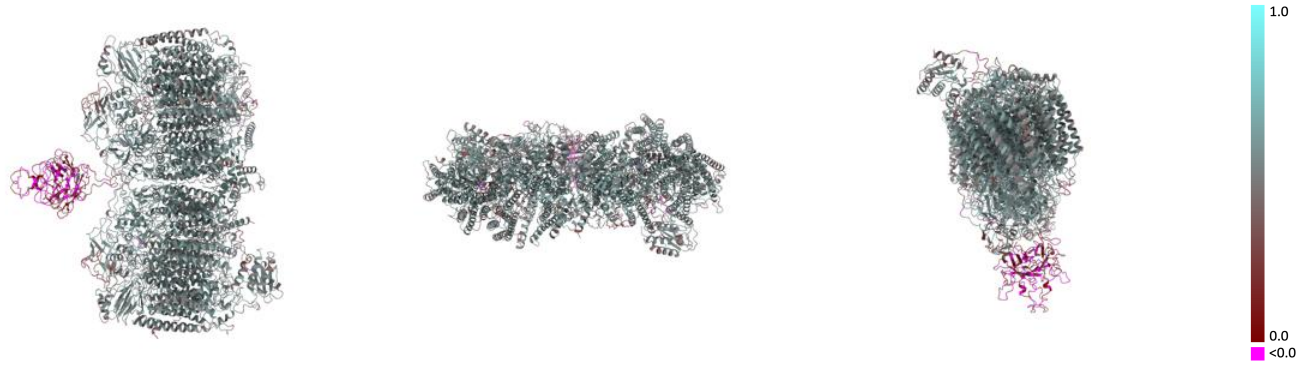
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.1 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.

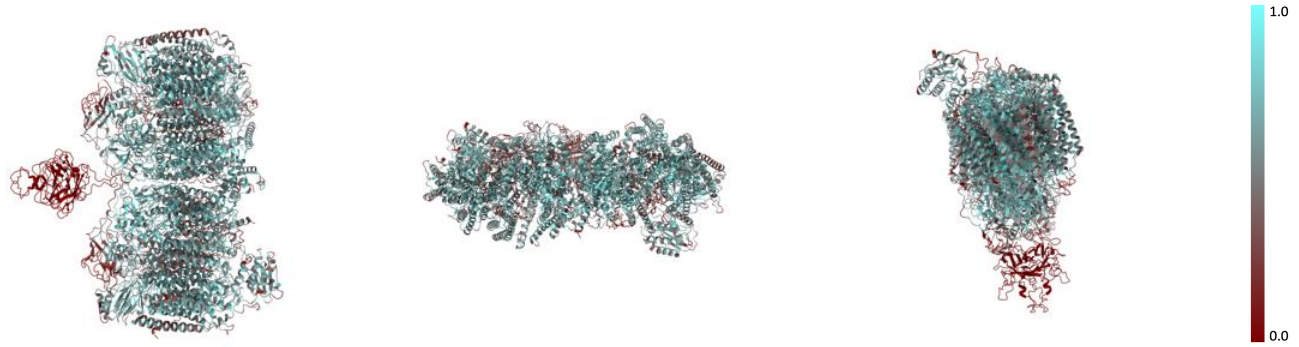
9.2 Q-score mapped to coordinate model (i)



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.

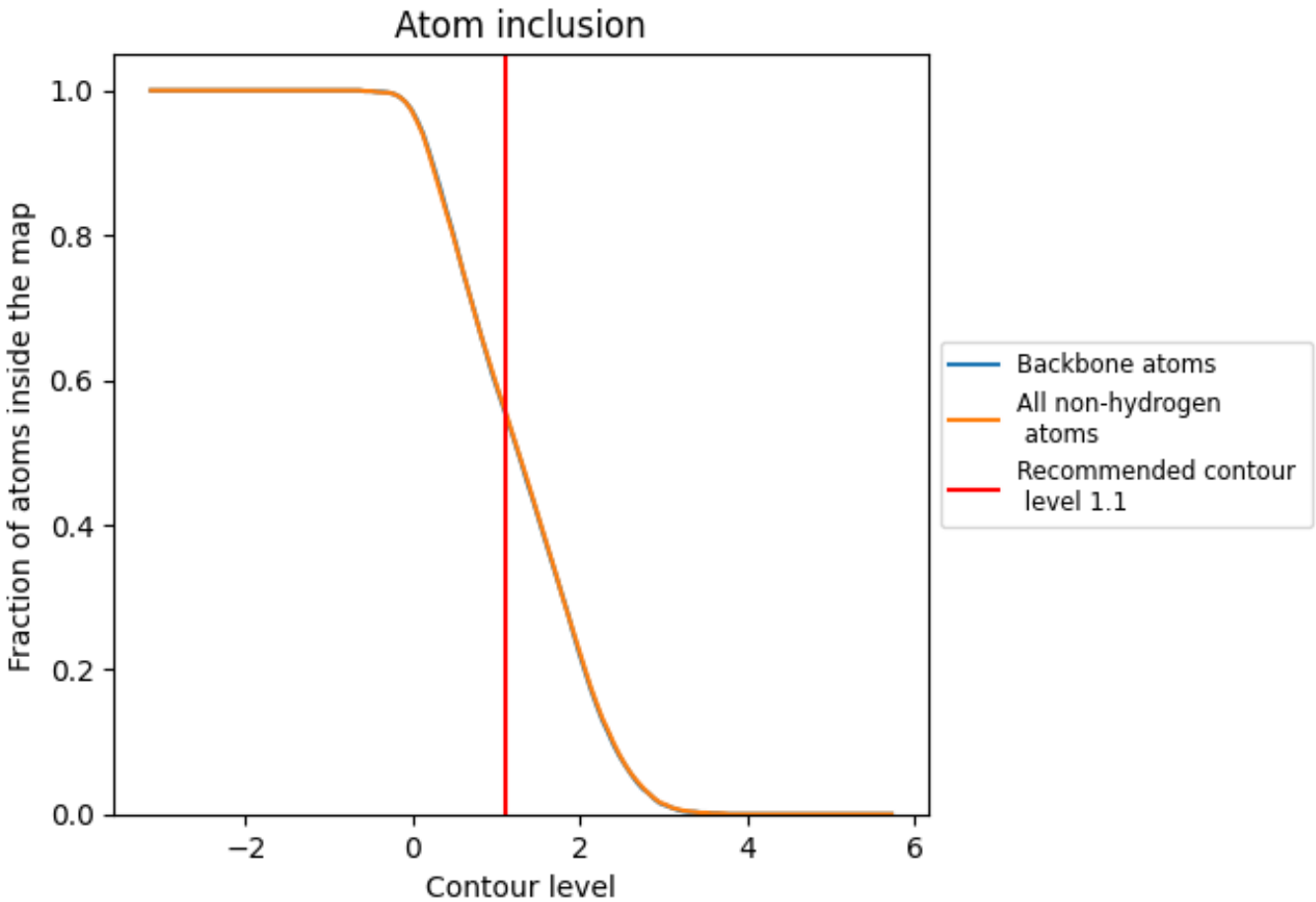
9.3 Atom inclusion mapped to coordinate model (i)



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 (1.1).

9.4 Atom inclusion (i)



At the recommended contour level, 56% of all backbone atoms, 56% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (1.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5600	0.5130
D	0.0790	0.1670
E	0.6810	0.5580
F	0.6870	0.5560
G	0.0850	0.1590
I	0.6130	0.5480
J	0.4740	0.5050
K	0.5030	0.4900
L	0.6620	0.5560
M	0.6750	0.5500
O	0.6400	0.5460
P	0.5140	0.5020
Q	0.5170	0.4950
R	0.6770	0.5550
S	0.5920	0.5140
T	0.5580	0.5220
U	0.4030	0.4330
V	0.5340	0.4920
W	0.2870	0.4550
X	0.5500	0.5160
Y	0.6710	0.5520
Z	0.5480	0.5110
a	0.4060	0.4380
b	0.5250	0.4980
c	0.2540	0.4560