Full wwPDB EM Validation Report ⓘ

Apr 8, 2025 – 07:35 am BST

PDB ID	:	9GY6 / pdb_00009gy6
EMDB ID	:	EMD-51689
Title	:	Mycobacterial cytochrome bc1:aa3 with inhibitor
Authors	:	lamers, M.H.; Verma, A.K.
Deposited on	:	2024-10-01
Resolution	:	3.10 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

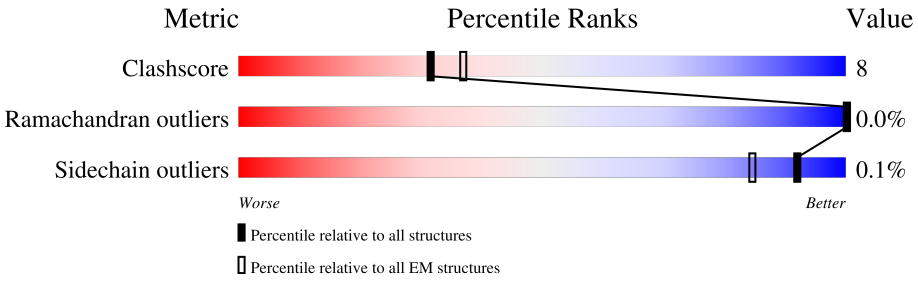
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=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	A	421	79% 10% 10%
1	M	421	75% 14% 10%
2	B	546	81% 16%
2	N	546	81% 16%
3	C	268	68% 15% 17%
3	O	268	70% 13% 17%
4	D	84	67% 21% 12%
4	P	84	5% 69% 19% 12%

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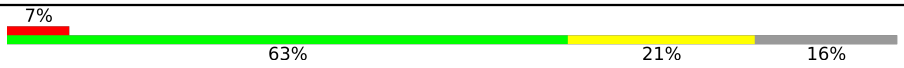
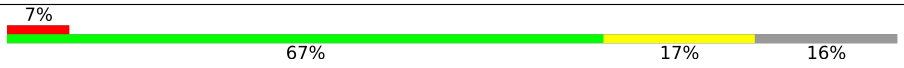
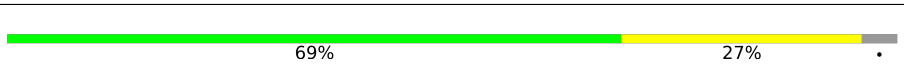
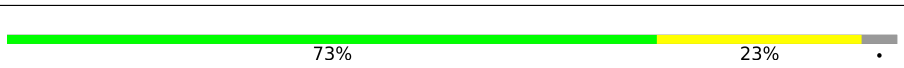
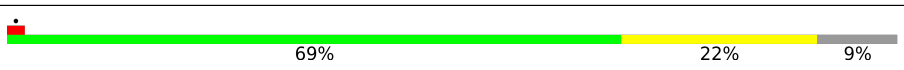
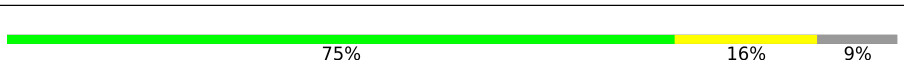
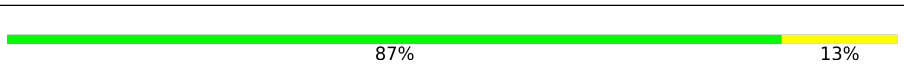
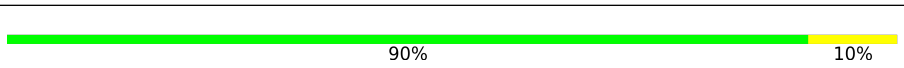
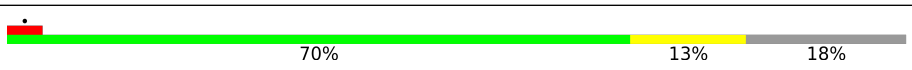
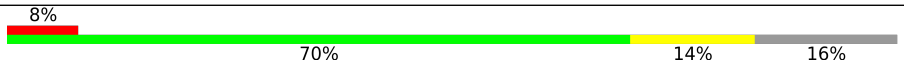
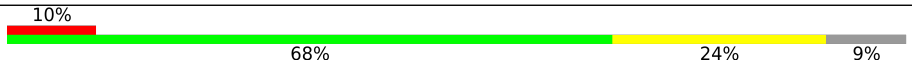
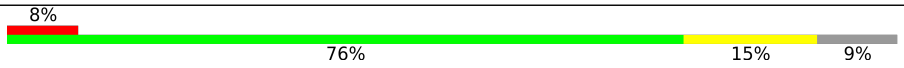
Mol	Chain	Length	Quality of chain
5	E	341	
5	Q	341	
6	F	575	
6	R	575	
7	G	203	
7	S	203	
8	H	139	
8	T	139	
9	I	79	
9	U	79	
10	J	157	
10	V	157	
11	L	236	
11	X	236	

2 Entry composition (i)

There are 25 unique types of molecules in this entry. The entry contains 43307 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cytochrome bc1 complex Rieske iron-sulfur subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	377	Total	C	N	O	S	0	0
			2947	1907	498	531	11		
1	M	377	Total	C	N	O	S	0	0
			2942	1904	496	531	11		

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A0R051
A	2	ASP	-	expression tag	UNP A0R051
A	3	TYR	-	expression tag	UNP A0R051
A	4	ARG	-	expression tag	UNP A0R051
A	5	ASN	-	expression tag	UNP A0R051
A	6	GLY	-	expression tag	UNP A0R051
A	7	GLY	-	expression tag	UNP A0R051
A	8	ARG	-	expression tag	UNP A0R051
A	9	HIS	-	expression tag	UNP A0R051
A	10	ARG	-	expression tag	UNP A0R051
A	11	CYS	-	expression tag	UNP A0R051
A	12	GLY	-	expression tag	UNP A0R051
A	13	HIS	-	expression tag	UNP A0R051
A	14	VAL	-	expression tag	UNP A0R051
M	1	MET	-	initiating methionine	UNP A0R051
M	2	ASP	-	expression tag	UNP A0R051
M	3	TYR	-	expression tag	UNP A0R051
M	4	ARG	-	expression tag	UNP A0R051
M	5	ASN	-	expression tag	UNP A0R051
M	6	GLY	-	expression tag	UNP A0R051
M	7	GLY	-	expression tag	UNP A0R051
M	8	ARG	-	expression tag	UNP A0R051
M	9	HIS	-	expression tag	UNP A0R051
M	10	ARG	-	expression tag	UNP A0R051
M	11	CYS	-	expression tag	UNP A0R051
M	12	GLY	-	expression tag	UNP A0R051

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Chain	Residue	Modelled	Actual	Comment	Reference
M	13	HIS	-	expression tag	UNP A0R051
M	14	VAL	-	expression tag	UNP A0R051

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	531	Total	C	N	O	S	0	0
			4153	2734	705	696	18		
2	N	534	Total	C	N	O	S	0	0
			4176	2747	710	701	18		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	156	TYR	PHE	engineered mutation	UNP A0R052
B	182	MET	ILE	engineered mutation	UNP A0R052
B	189	LEU	MET	engineered mutation	UNP A0R052
B	309	GLU	ASP	engineered mutation	UNP A0R052
B	312	ALA	ILE	engineered mutation	UNP A0R052
N	156	TYR	PHE	engineered mutation	UNP A0R052
N	182	MET	ILE	engineered mutation	UNP A0R052
N	189	LEU	MET	engineered mutation	UNP A0R052
N	309	GLU	ASP	engineered mutation	UNP A0R052
N	312	ALA	ILE	engineered mutation	UNP A0R052

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

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

- Molecule 4 is a protein called Transmembrane protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	74	Total	C	N	O	S	0	0
			590	387	108	91	4		
4	P	74	Total	C	N	O	S	0	0
			590	387	108	91	4		

- Molecule 5 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	285	Total	C	N	O	S	0	0
			2271	1472	375	415	9		
5	Q	285	Total	C	N	O	S	0	0
			2271	1472	375	415	9		

- Molecule 6 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	551	Total	C	N	O	S	0	0
			4364	2933	694	711	26		
6	R	551	Total	C	N	O	S	0	0
			4364	2933	694	711	26		

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	1	MET	-	initiating methionine	UNP A0A2U9PNL2
F	2	VAL	-	expression tag	UNP A0A2U9PNL2
F	3	ALA	-	expression tag	UNP A0A2U9PNL2
F	4	GLU	-	expression tag	UNP A0A2U9PNL2
F	5	ALA	-	expression tag	UNP A0A2U9PNL2
F	6	PRO	-	expression tag	UNP A0A2U9PNL2
F	7	PRO	-	expression tag	UNP A0A2U9PNL2
F	8	ILE	-	expression tag	UNP A0A2U9PNL2
F	9	GLY	-	expression tag	UNP A0A2U9PNL2
F	10	GLU	-	expression tag	UNP A0A2U9PNL2
F	11	LEU	-	expression tag	UNP A0A2U9PNL2
F	12	GLU	-	expression tag	UNP A0A2U9PNL2
F	13	ALA	-	expression tag	UNP A0A2U9PNL2
F	14	ARG	-	expression tag	UNP A0A2U9PNL2
F	15	ARG	-	expression tag	UNP A0A2U9PNL2
F	16	PRO	-	expression tag	UNP A0A2U9PNL2
F	17	PHE	-	expression tag	UNP A0A2U9PNL2
F	18	PRO	-	expression tag	UNP A0A2U9PNL2
F	19	GLU	-	expression tag	UNP A0A2U9PNL2
F	20	ARG	-	expression tag	UNP A0A2U9PNL2
R	1	MET	-	initiating methionine	UNP A0A2U9PNL2
R	2	VAL	-	expression tag	UNP A0A2U9PNL2
R	3	ALA	-	expression tag	UNP A0A2U9PNL2
R	4	GLU	-	expression tag	UNP A0A2U9PNL2
R	5	ALA	-	expression tag	UNP A0A2U9PNL2
R	6	PRO	-	expression tag	UNP A0A2U9PNL2
R	7	PRO	-	expression tag	UNP A0A2U9PNL2

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Chain	Residue	Modelled	Actual	Comment	Reference
R	8	ILE	-	expression tag	UNP A0A2U9PNL2
R	9	GLY	-	expression tag	UNP A0A2U9PNL2
R	10	GLU	-	expression tag	UNP A0A2U9PNL2
R	11	LEU	-	expression tag	UNP A0A2U9PNL2
R	12	GLU	-	expression tag	UNP A0A2U9PNL2
R	13	ALA	-	expression tag	UNP A0A2U9PNL2
R	14	ARG	-	expression tag	UNP A0A2U9PNL2
R	15	ARG	-	expression tag	UNP A0A2U9PNL2
R	16	PRO	-	expression tag	UNP A0A2U9PNL2
R	17	PHE	-	expression tag	UNP A0A2U9PNL2
R	18	PRO	-	expression tag	UNP A0A2U9PNL2
R	19	GLU	-	expression tag	UNP A0A2U9PNL2
R	20	ARG	-	expression tag	UNP A0A2U9PNL2

- Molecule 7 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	185	Total	C	N	O	S	0	0
			1449	973	230	239	7		
7	S	185	Total	C	N	O	S	0	0
			1449	973	230	239	7		

- Molecule 8 is a protein called Cytochrome c oxidase polypeptide 4.

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

- Molecule 9 is a protein called Secreted protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	65	Total	C	N	O	S	0	0
			490	324	83	82	1		
9	U	66	Total	C	N	O	S	0	0
			498	329	84	83	2		

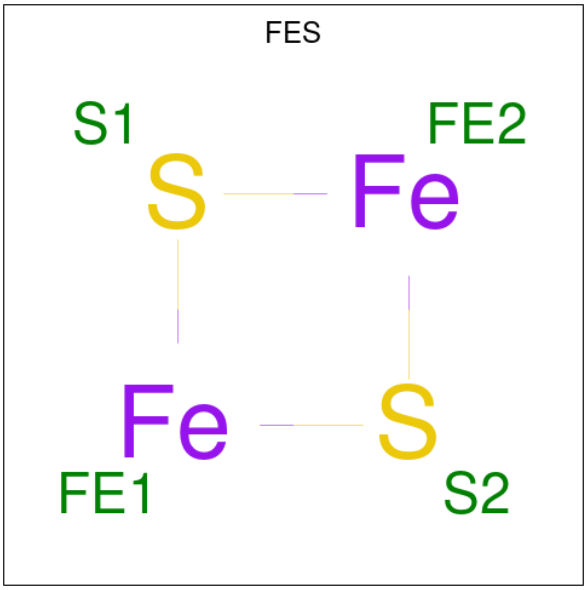
- Molecule 10 is a protein called DUF5130 domain-containing protein.

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

- Molecule 11 is a protein called Superoxide dismutase [Cu-Zn].

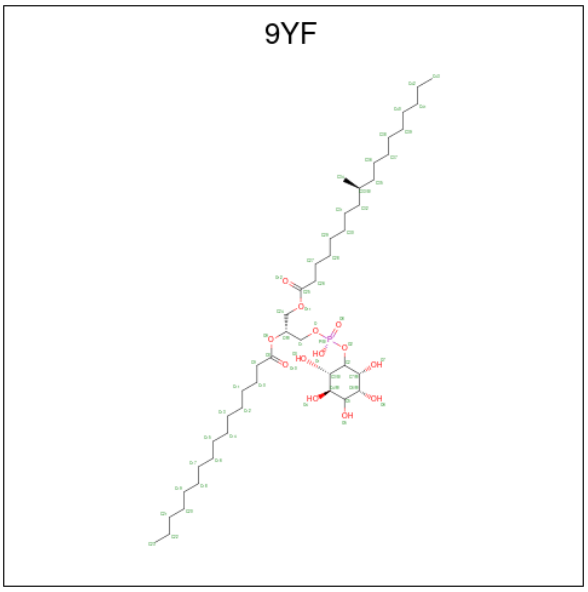
Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	28	Total	C	N	O	S	0	0
			185	113	29	42	1		
11	X	28	Total	C	N	O	S	0	0
			185	113	29	42	1		

- Molecule 12 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



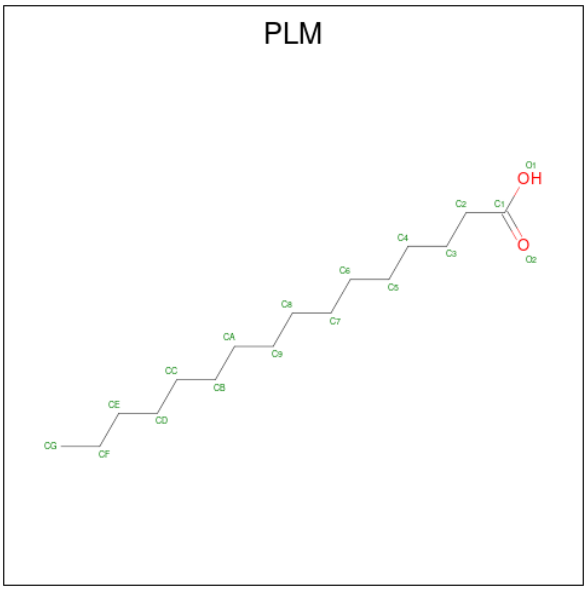
Mol	Chain	Residues	Atoms			AltConf
12	A	1	Total	Fe	S	0
			4	2	2	
12	M	1	Total	Fe	S	0
			4	2	2	

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



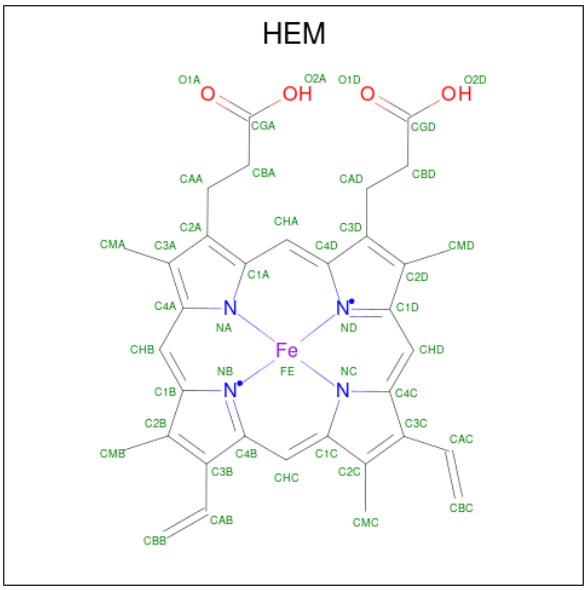
Mol	Chain	Residues	Atoms				AltConf
13	A	1	Total	C	O	P	0
			58	44	13	1	
13	C	1	Total	C	O	P	0
			58	44	13	1	
13	M	1	Total	C	O	P	0
			58	44	13	1	
13	O	1	Total	C	O	P	0
			58	44	13	1	

- Molecule 14 is PALMITIC ACID (CCD ID: PLM) (formula: $C_{16}H_{32}O_2$).



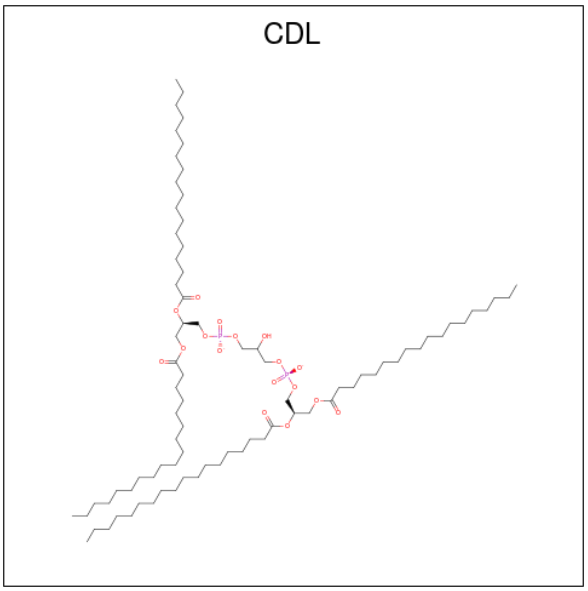
Mol	Chain	Residues	Atoms			AltConf
14	A	1	Total	C	O	0
			17	16	1	
14	G	1	Total	C	O	0
			17	16	1	
14	M	1	Total	C	O	0
			17	16	1	
14	T	1	Total	C	O	0
			17	16	1	

- Molecule 15 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					AltConf
15	B	1	Total	C	Fe	N	O	0
			42	33	1	4	4	
15	B	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
15	N	1	Total	C	Fe	N	O	0
			42	33	1	4	4	
15	N	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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



Mol	Chain	Residues	Atoms				AltConf
16	B	1	Total	C	O	P	0
			74	55	17	2	
16	B	1	Total	C	O	P	0
			77	58	17	2	
16	B	1	Total	C	O	P	0
			79	60	17	2	
16	C	1	Total	C	O	P	0
			79	60	17	2	
16	D	1	Total	C	O	P	0
			88	69	17	2	
16	D	1	Total	C	O	P	0
			95	76	17	2	
16	F	1	Total	C	O	P	0
			76	57	17	2	
16	F	1	Total	C	O	P	0
			81	62	17	2	
16	M	1	Total	C	O	P	0
			74	55	17	2	
16	N	1	Total	C	O	P	0
			74	55	17	2	
16	N	1	Total	C	O	P	0
			77	58	17	2	
16	N	1	Total	C	O	P	0
			79	60	17	2	
16	N	1	Total	C	O	P	0
			79	60	17	2	
16	P	1	Total	C	O	P	0
			88	69	17	2	

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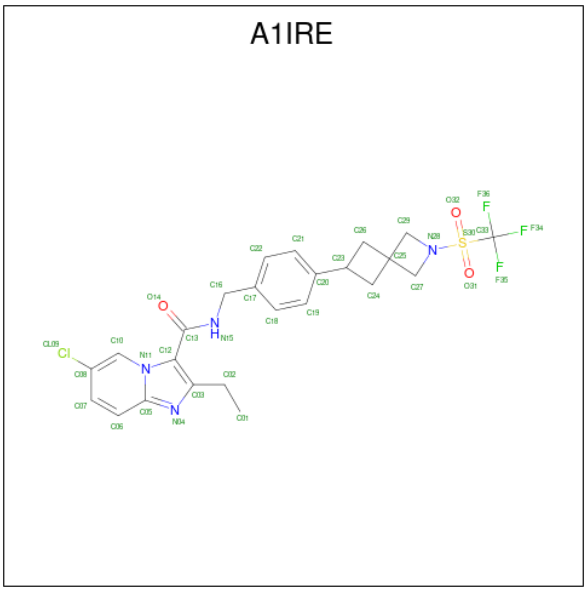
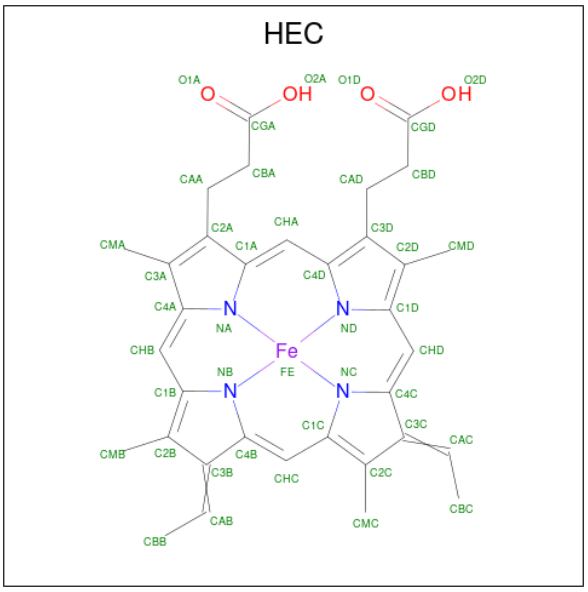
Mol	Chain	Residues	Atoms				AltConf
16	P	1	Total	C	O	P	0
			95	76	17	2	
16	R	1	Total	C	O	P	0
			76	57	17	2	
16	R	1	Total	C	O	P	0
			81	62	17	2	

- Molecule 17 is 6-chloranyl-2-ethyl-N-[[4-[2-(trifluoromethylsulfonyl)-2-azaspiro[3.3]heptan-6-yl]phenyl]methyl]imidazo[1,2-a]pyridine-3-carboxamide (CCD ID: A1IRE) (formula: $C_{24}H_{24}ClF_3N_4O_3S$).



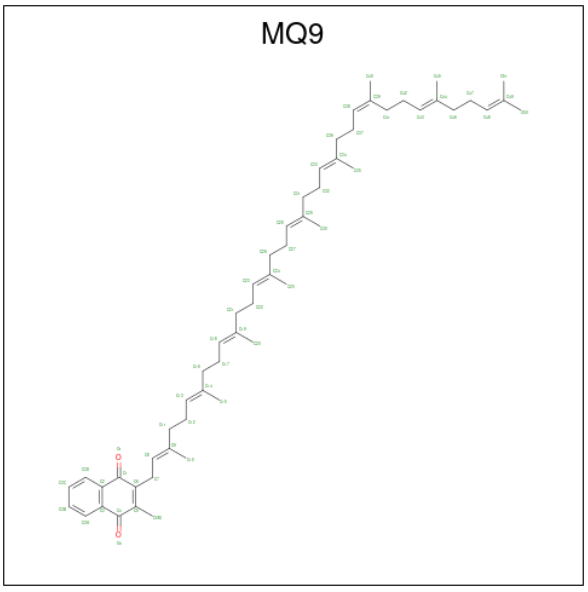
Mol	Chain	Residues	Atoms							AltConf
17	B	1	Total	C	Cl	F	N	O	S	0
			36	24	1	3	4	3	1	
17	N	1	Total	C	Cl	F	N	O	S	0
			36	24	1	3	4	3	1	

- Molecule 18 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



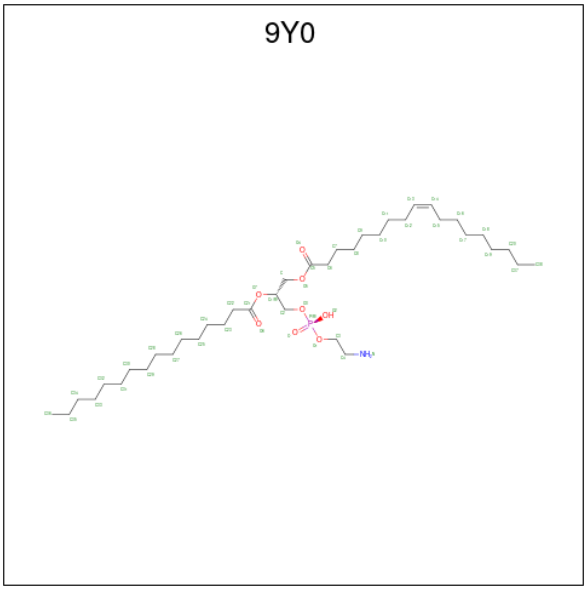
Mol	Chain	Residues	Atoms					AltConf
18	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
18	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
18	O	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
18	O	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 19 is MENAQUINONE-9 (CCD ID: MQ9) (formula: $C_{56}H_{80}O_2$).



Mol	Chain	Residues	Atoms	AltConf
19	C	1	Total C O 58 56 2	0
19	O	1	Total C O 58 56 2	0

- Molecule 20 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
20	D	1	Total C N O P 41 31 1 8 1	0
20	G	1	Total C N O P 43 33 1 8 1	0
20	P	1	Total C N O P 41 31 1 8 1	0
20	S	1	Total C N O P 43 33 1 8 1	0

- Molecule 21 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms	AltConf
21	E	2	Total Cu 2 2	0
21	F	2	Total Cu 2 2	0
21	Q	2	Total Cu 2 2	0

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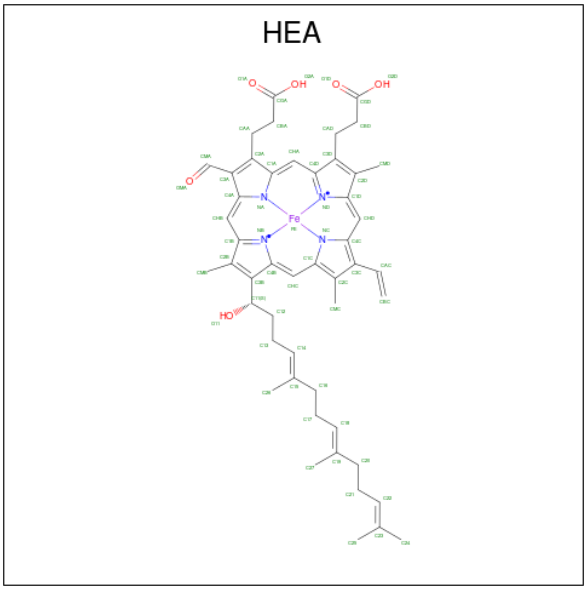
Mol	Chain	Residues	Atoms		AltConf
21	R	2	Total 2	Cu 2	0

- Molecule 22 is HEME-A (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).

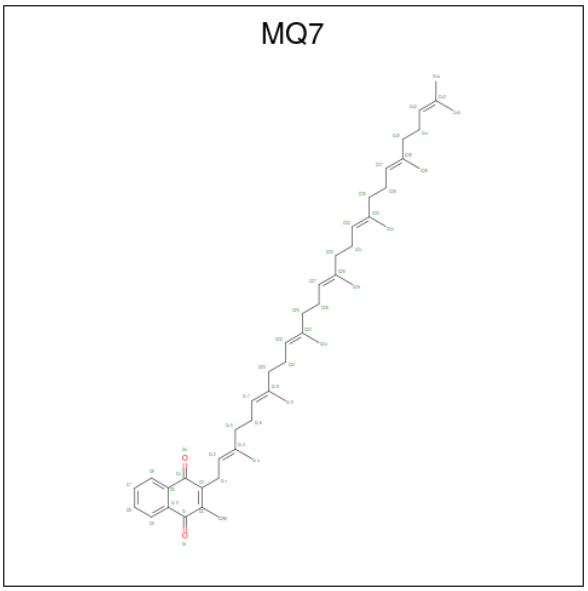


Mol	Chain	Residues	Atoms					AltConf
22	F	1	Total 60	C 49	Fe 1	N 4	O 6	0
22	F	1	Total 60	C 49	Fe 1	N 4	O 6	0
22	R	1	Total 60	C 49	Fe 1	N 4	O 6	0
22	R	1	Total 60	C 49	Fe 1	N 4	O 6	0

- Molecule 23 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
23	F	1	Total 1	Ca 1	0
23	R	1	Total 1	Ca 1	0

- Molecule 24 is MENAQUINONE-7 (CCD ID: MQ7) (formula: $C_{46}H_{64}O_2$).



Mol	Chain	Residues	Atoms	AltConf
24	H	1	Total C O 48 46 2	0
24	O	1	Total C O 48 46 2	0

- Molecule 25 is water.

Mol	Chain	Residues	Atoms	AltConf
25	A	25	Total O 25 25	0
25	B	45	Total O 45 45	0
25	C	10	Total O 10 10	0
25	D	4	Total O 4 4	0
25	E	8	Total O 8 8	0
25	F	25	Total O 25 25	0
25	G	1	Total O 1 1	0
25	H	5	Total O 5 5	0
25	J	1	Total O 1 1	0
25	L	1	Total O 1 1	0

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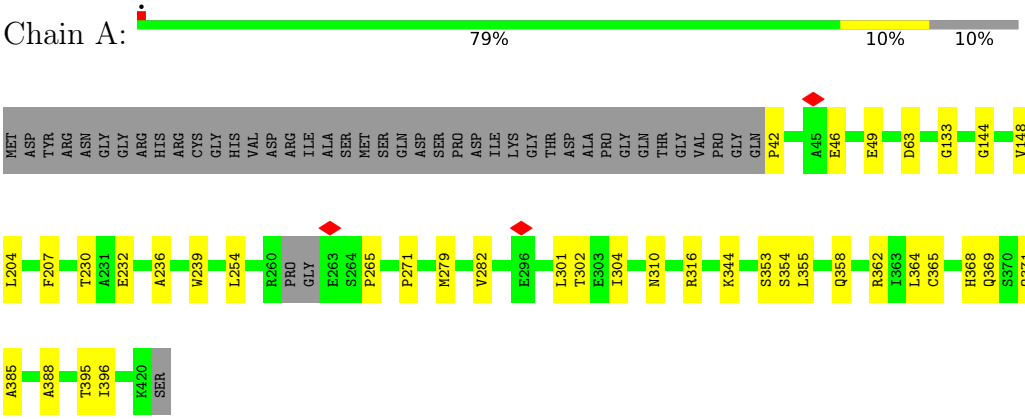
Mol	Chain	Residues	Atoms	AltConf
25	M	21	Total O 21 21	0
25	N	43	Total O 43 43	0
25	O	2	Total O 2 2	0
25	P	3	Total O 3 3	0
25	Q	1	Total O 1 1	0
25	R	11	Total O 11 11	0
25	S	2	Total O 2 2	0
25	T	2	Total O 2 2	0
25	U	1	Total O 1 1	0

3 Residue-property plots (i)

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

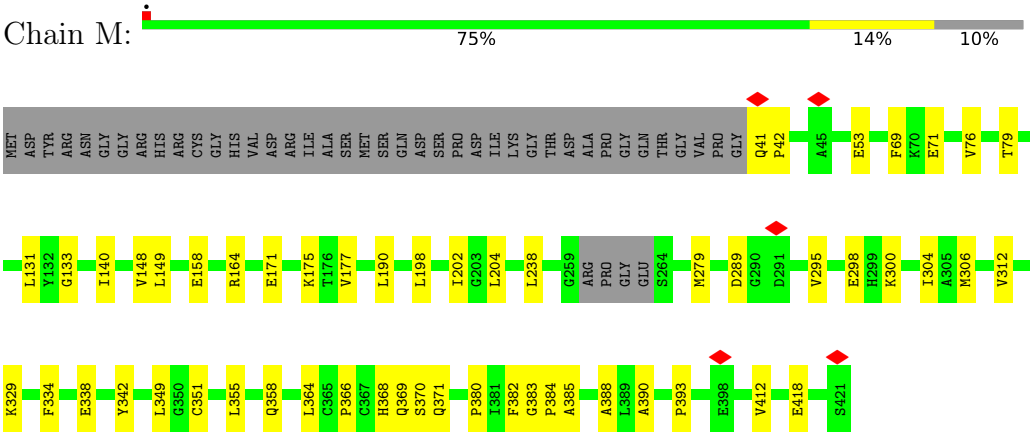
• Molecule 1: Cytochrome bc1 complex Rieske iron-sulfur subunit

Chain A:



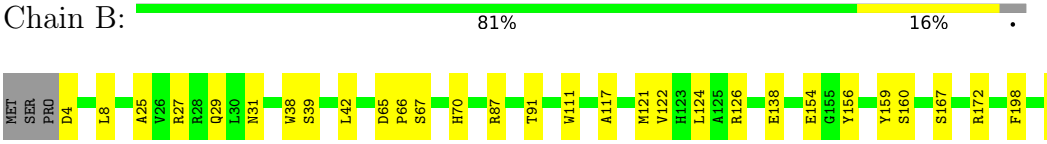
• Molecule 1: Cytochrome bc1 complex Rieske iron-sulfur subunit

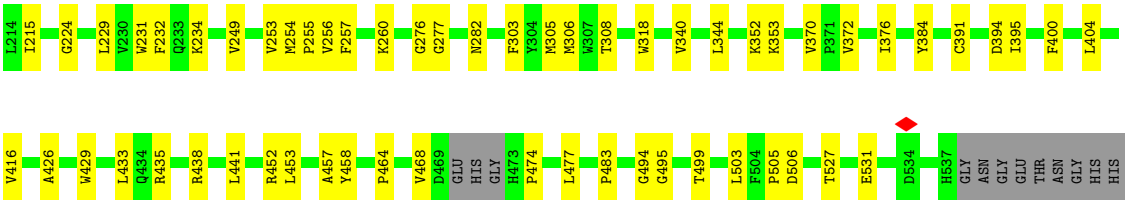
Chain M:



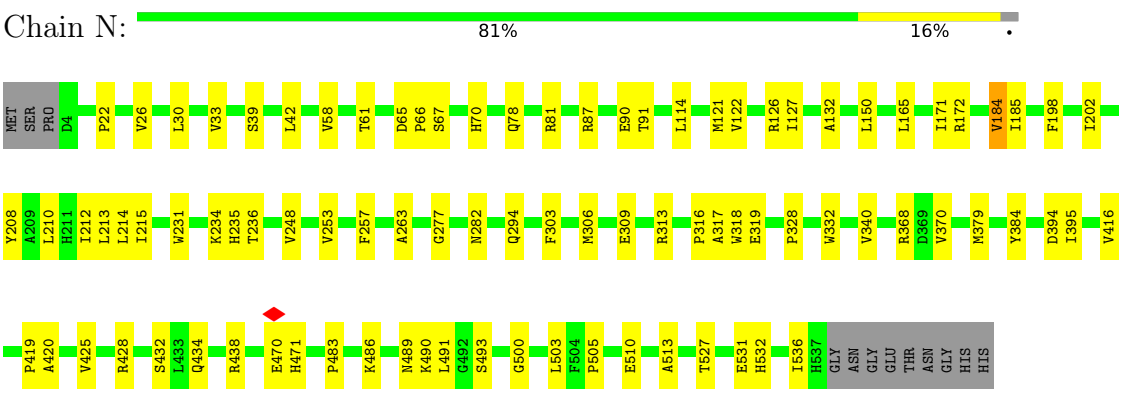
• Molecule 2: Cytochrome bc1 complex cytochrome b subunit

Chain B:

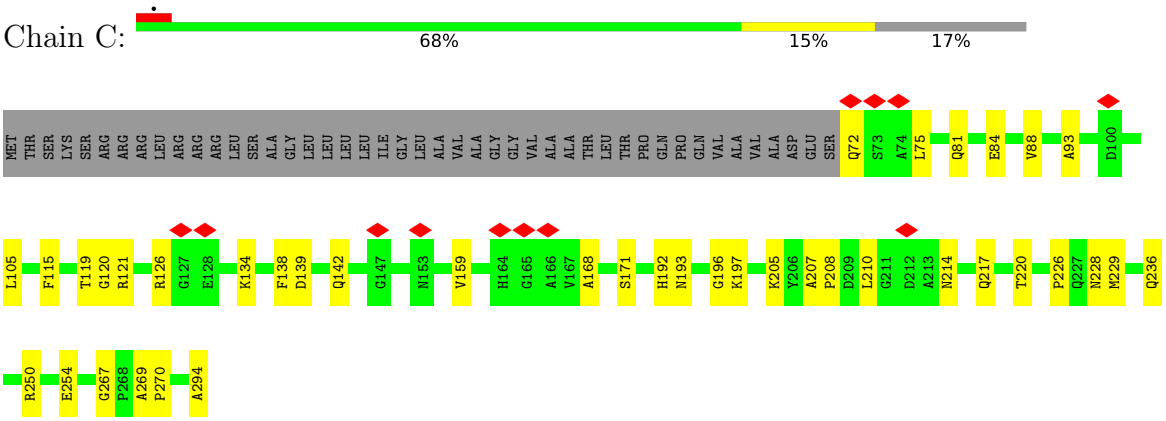




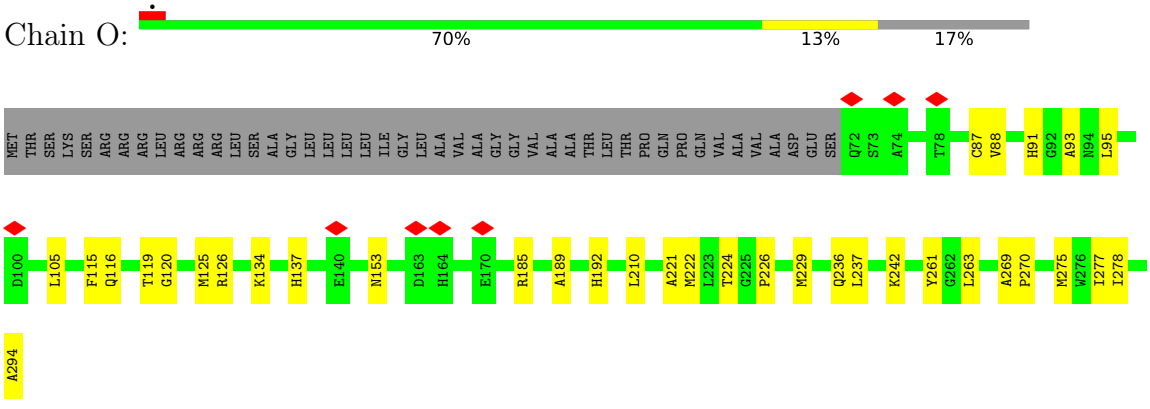
• Molecule 2: Cytochrome bc1 complex cytochrome b subunit



• Molecule 3: Cytochrome bc1 complex cytochrome c subunit

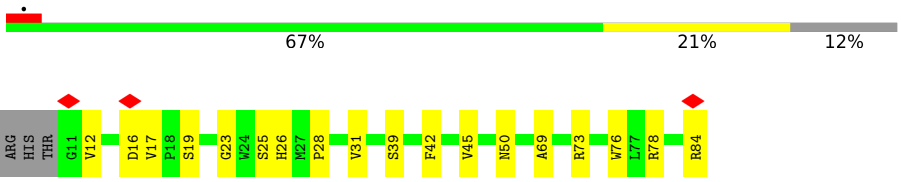


• Molecule 3: Cytochrome bc1 complex cytochrome c subunit



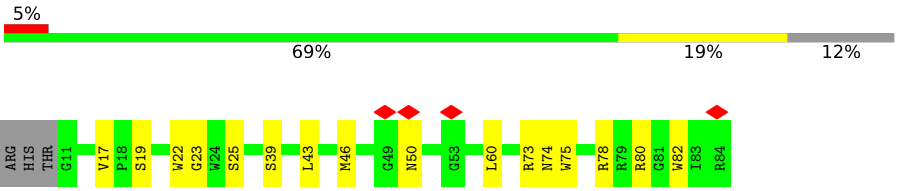
• Molecule 4: Transmembrane protein

Chain D:



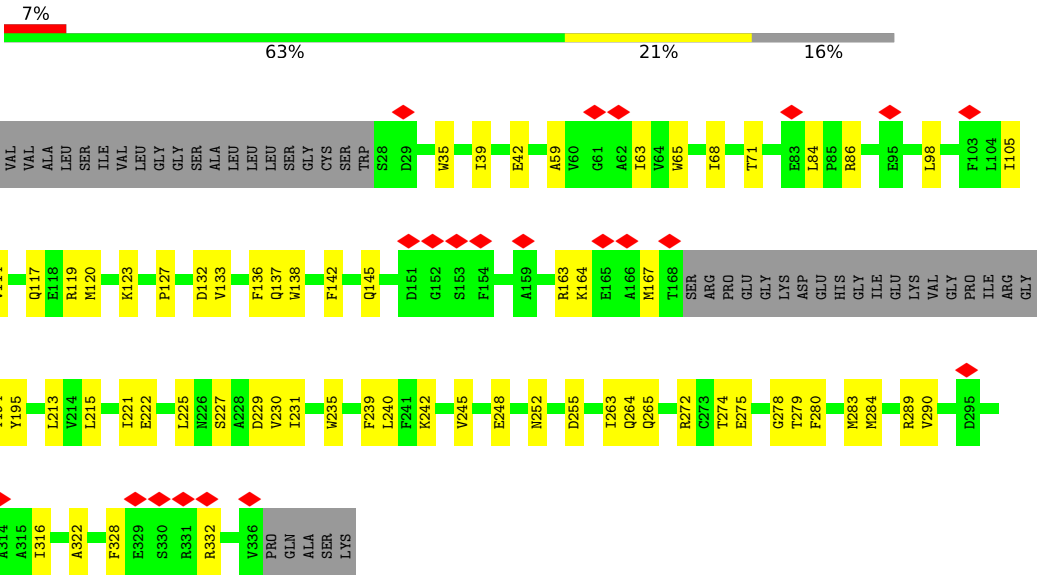
• Molecule 4: Transmembrane protein

Chain P:



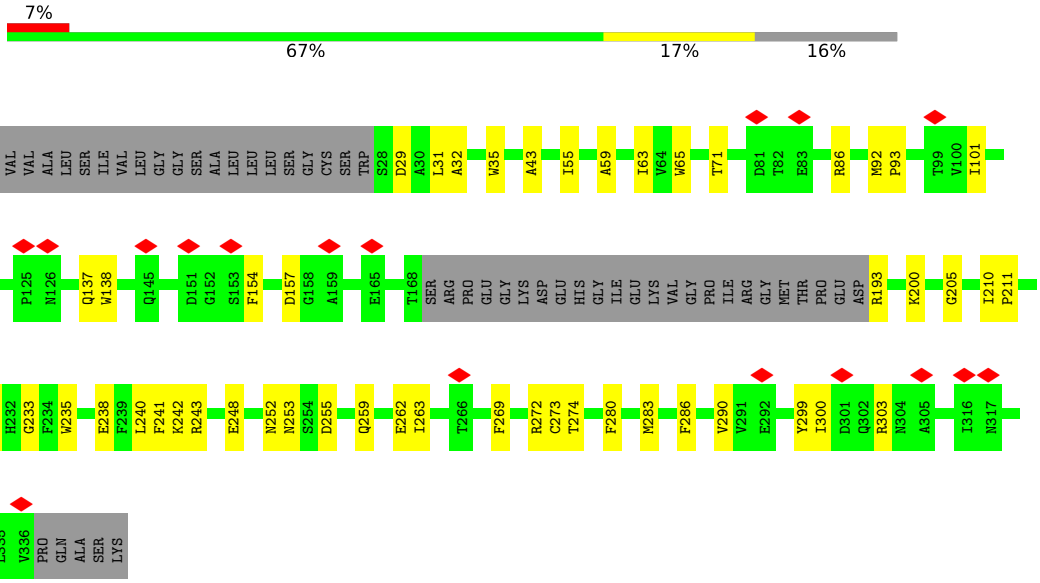
• Molecule 5: Cytochrome c oxidase subunit 2

Chain E:



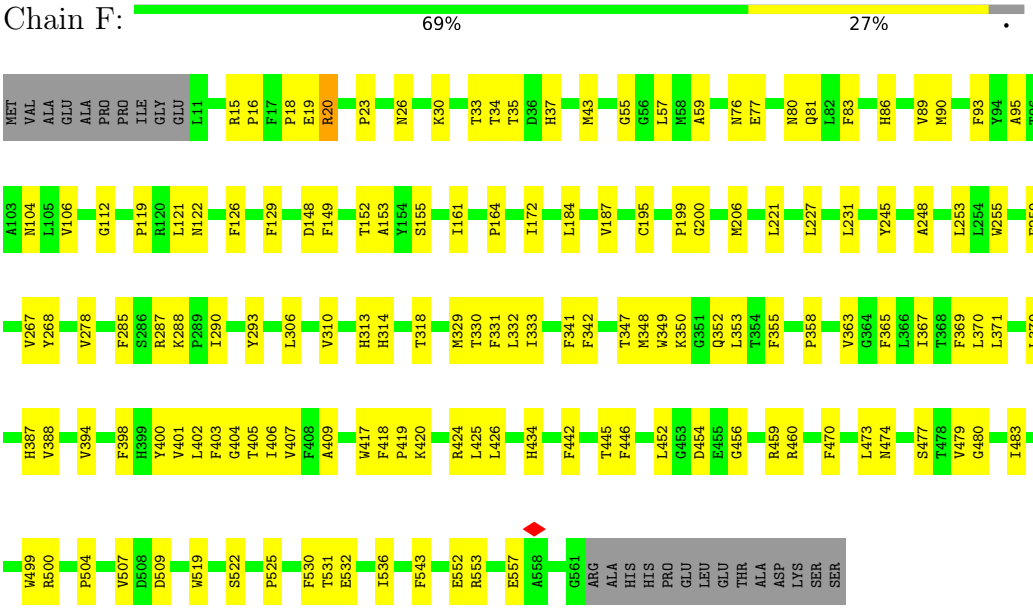
• Molecule 5: Cytochrome c oxidase subunit 2

Chain Q:



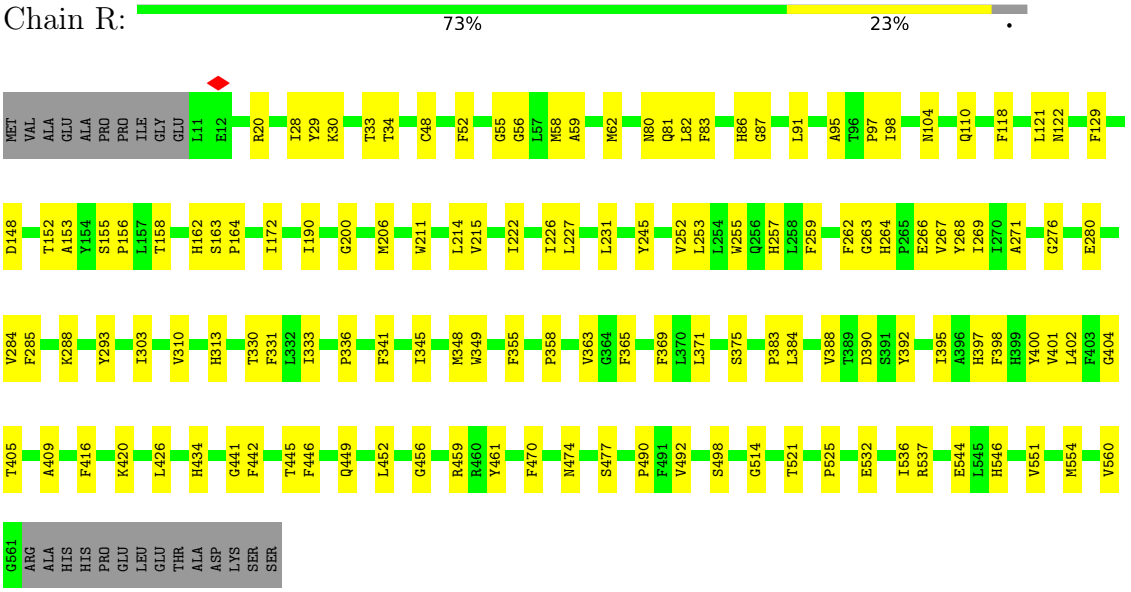
• Molecule 6: Cytochrome c oxidase subunit 1

Chain F:



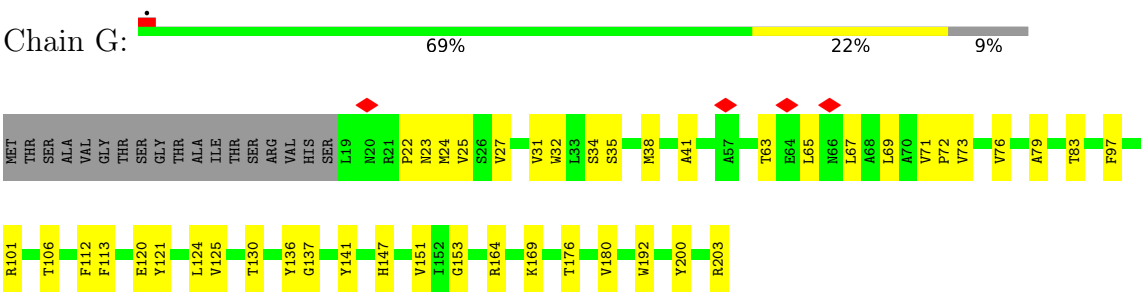
• Molecule 6: Cytochrome c oxidase subunit 1

Chain R:



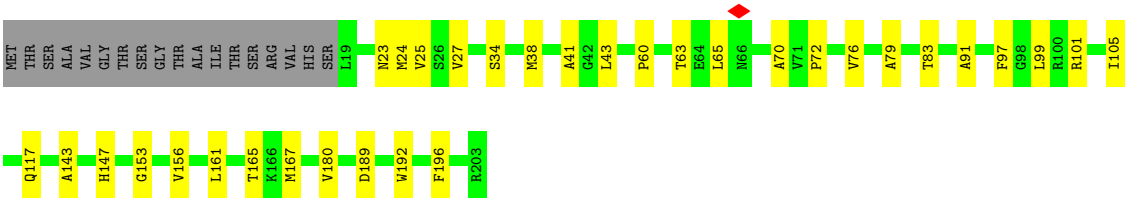
• Molecule 7: Cytochrome c oxidase subunit 3

Chain G:



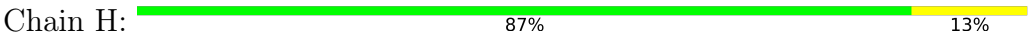
• Molecule 7: Cytochrome c oxidase subunit 3

Chain S:



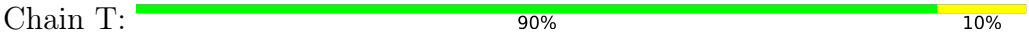
• Molecule 8: Cytochrome c oxidase polypeptide 4

Chain H:



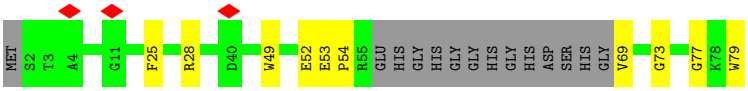
• Molecule 8: Cytochrome c oxidase polypeptide 4

Chain T:



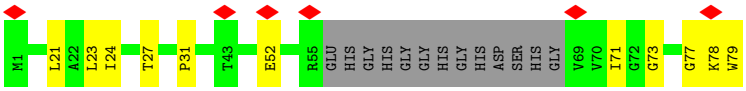
• Molecule 9: Secreted protein

Chain I:



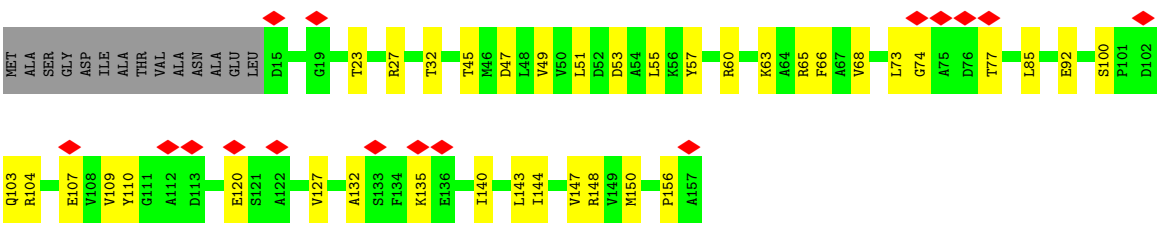
• Molecule 9: Secreted protein

Chain U:



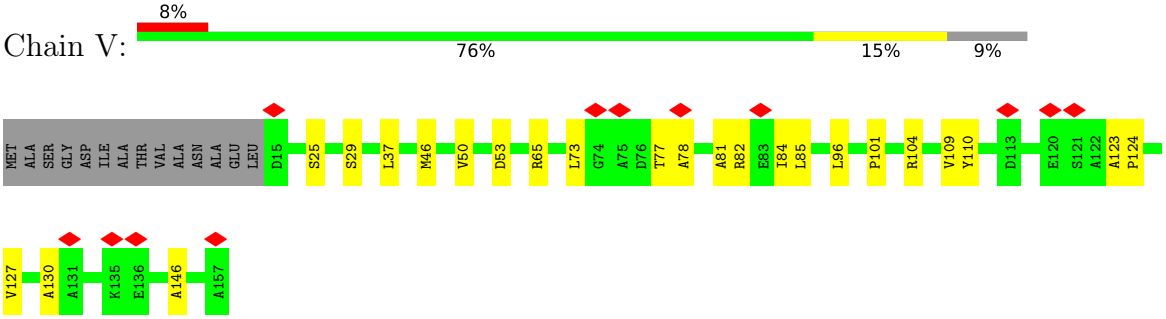
• Molecule 10: DUF5130 domain-containing protein

Chain J:



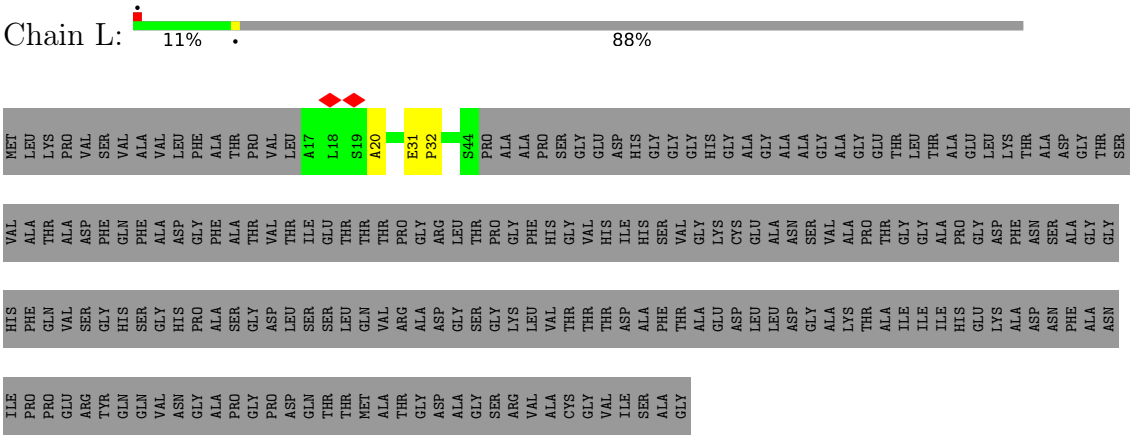
• Molecule 10: DUF5130 domain-containing protein

Chain V:



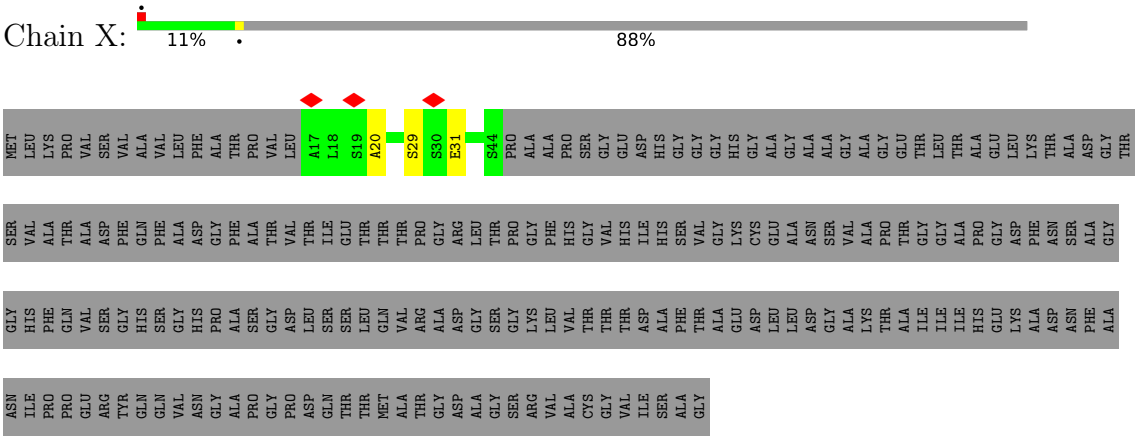
• Molecule 11: Superoxide dismutase [Cu-Zn]

Chain L:



• Molecule 11: Superoxide dismutase [Cu-Zn]

Chain X:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	42000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.063	Depositor
Minimum map value	-0.031	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.009	Depositor
Map size (Å)	351.12003, 351.12003, 351.12003	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8360001, 0.8360001, 0.8360001	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MQ7, A1IRE, CDL, 9Y0, FES, CU, HEA, MQ9, 9YF, HEM, PLM, CA, HEC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.27	0/3024	0.43	0/4096
1	M	0.27	0/3019	0.44	0/4091
2	B	0.28	0/4284	0.42	0/5841
2	N	0.28	0/4309	0.43	0/5876
3	C	0.28	0/1660	0.46	0/2250
3	O	0.27	0/1660	0.46	0/2250
4	D	0.24	0/610	0.39	0/830
4	P	0.23	0/610	0.40	0/830
5	E	0.28	0/2332	0.47	0/3173
5	Q	0.27	0/2332	0.45	0/3173
6	F	0.29	0/4524	0.46	0/6180
6	R	0.30	0/4524	0.46	0/6180
7	G	0.30	0/1496	0.44	0/2043
7	S	0.31	0/1496	0.44	0/2043
8	H	0.30	0/1112	0.47	0/1524
8	T	0.27	0/1112	0.45	0/1524
9	I	0.26	0/506	0.49	0/692
9	U	0.25	0/514	0.50	0/702
10	J	0.27	0/1042	0.46	0/1423
10	V	0.27	0/1042	0.45	0/1423
11	L	0.25	0/191	0.48	0/265
11	X	0.24	0/191	0.48	0/265
All	All	0.28	0/41590	0.45	0/56674

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (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	A	2947	0	2958	29	0
1	M	2942	0	2951	44	0
2	B	4153	0	4176	67	0
2	N	4176	0	4195	69	0
3	C	1623	0	1560	33	0
3	O	1623	0	1560	29	0
4	D	590	0	581	14	0
4	P	590	0	581	14	0
5	E	2271	0	2228	59	0
5	Q	2271	0	2228	43	0
6	F	4364	0	4343	124	0
6	R	4364	0	4343	109	0
7	G	1449	0	1450	38	0
7	S	1449	0	1450	27	0
8	H	1077	0	1058	14	0
8	T	1077	0	1058	13	0
9	I	490	0	498	11	0
9	U	498	0	510	11	0
10	J	1024	0	1035	30	0
10	V	1024	0	1035	20	0
11	L	185	0	170	3	0
11	X	185	0	170	3	0
12	A	4	0	0	1	0
12	M	4	0	0	1	0
13	A	58	0	0	0	0
13	C	58	0	0	1	0
13	M	58	0	0	0	0
13	O	58	0	0	0	0
14	A	17	0	31	0	0
14	G	17	0	31	1	0
14	M	17	0	31	1	0
14	T	17	0	31	4	0
15	B	85	0	57	5	0
15	N	85	0	57	5	0
16	B	230	0	294	13	0
16	C	79	0	105	3	0
16	D	183	0	269	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	F	157	0	205	15	0
16	M	74	0	92	6	0
16	N	309	0	400	12	0
16	P	183	0	269	11	0
16	R	157	0	208	6	0
17	B	36	0	0	0	0
17	N	36	0	0	1	0
18	C	86	0	60	2	0
18	O	86	0	60	2	0
19	C	58	0	80	7	0
19	O	58	0	80	7	0
20	D	41	0	0	0	0
20	G	43	0	0	0	0
20	P	41	0	0	1	0
20	S	43	0	0	0	0
21	E	2	0	0	0	0
21	F	2	0	0	0	0
21	Q	2	0	0	0	0
21	R	2	0	0	0	0
22	F	120	0	108	19	0
22	R	120	0	108	12	0
23	F	1	0	0	0	0
23	R	1	0	0	0	0
24	H	48	0	64	2	0
24	O	48	0	64	2	0
25	A	25	0	0	0	0
25	B	45	0	0	0	0
25	C	10	0	0	0	0
25	D	4	0	0	0	0
25	E	8	0	0	0	0
25	F	25	0	0	2	0
25	G	1	0	0	0	0
25	H	5	0	0	0	0
25	J	1	0	0	0	0
25	L	1	0	0	0	0
25	M	21	0	0	0	0
25	N	43	0	0	1	0
25	O	2	0	0	0	0
25	P	3	0	0	0	0
25	Q	1	0	0	0	0
25	R	11	0	0	0	0
25	S	2	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	T	2	0	0	0	0
25	U	1	0	0	0	0
All	All	43307	0	42842	730	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (730) 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)
6:F:406:ILE:HD11	22:F:602:HEA:HBC2	1.31	1.07
6:F:406:ILE:HD11	22:F:602:HEA:CBC	1.91	0.99
6:F:402:LEU:HD13	22:F:602:HEA:HAC	1.45	0.98
6:F:406:ILE:CD1	22:F:602:HEA:HBC2	2.02	0.89
1:A:133:GLY:HA3	2:B:277:GLY:HA3	1.63	0.80
7:G:25:VAL:HG12	7:G:180:VAL:HG11	1.66	0.76
1:A:358:GLN:NE2	3:C:229:MET:O	2.19	0.75
2:N:184:VAL:HG23	2:N:185:ILE:HG23	1.69	0.74
6:R:211:TRP:HZ3	8:T:7:LEU:HD21	1.53	0.73
6:R:20:ARG:NH2	10:V:53:ASP:OD1	2.22	0.73
6:F:80:ASN:HA	6:F:83:PHE:CE2	2.25	0.72
6:R:267:VAL:HB	22:R:601:HEA:HAC	1.71	0.72
6:F:19:GLU:O	6:F:424:ARG:NH2	2.22	0.72
10:J:132:ALA:HA	10:J:135:LYS:HD2	1.71	0.72
2:N:67:SER:HB3	2:N:87:ARG:HB3	1.72	0.71
16:D:101:CDL:H711	16:F:606:CDL:H721	1.72	0.71
6:R:271:ALA:HA	6:R:405:THR:HG21	1.72	0.71
24:O:301:MQ7:H142	24:O:301:MQ7:H2M1	1.73	0.70
1:A:271:PRO:O	1:A:316:ARG:NH1	2.23	0.70
6:F:310:VAL:O	6:F:313:HIS:ND1	2.24	0.70
6:R:470:PHE:O	6:R:474:ASN:ND2	2.24	0.69
1:M:321:ASP:OD1	1:M:324:ARG:NH1	2.26	0.69
1:M:279:MET:O	3:O:236:GLN:NE2	2.26	0.68
3:O:126:ARG:HH22	6:R:163:SER:HA	1.58	0.68
6:F:509:ASP:HB2	6:F:519:TRP:HB3	1.76	0.67
7:S:167:MET:HG2	14:T:201:PLM:H41	1.76	0.67
10:J:140:ILE:O	10:J:144:ILE:HG12	1.95	0.67
6:F:267:VAL:HB	22:F:601:HEA:HAC	1.74	0.67
6:F:33:THR:HG22	8:H:90:TRP:HB3	1.77	0.66
2:N:438:ARG:HH12	4:P:19:SER:HB3	1.60	0.66
6:F:341:PHE:HZ	6:F:369:PHE:HD1	1.43	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:101:CDL:H182	16:P:101:CDL:H331	1.77	0.66
1:A:362:ARG:HD3	1:A:381:ILE:HD11	1.76	0.66
6:R:288:LYS:NZ	6:R:349:TRP:O	2.23	0.66
6:F:470:PHE:O	6:F:474:ASN:ND2	2.29	0.66
3:C:121:ARG:HH12	3:C:208:PRO:HG3	1.61	0.65
7:G:65:LEU:HB2	7:G:203:ARG:HH11	1.61	0.65
5:Q:220:ARG:NH1	5:Q:259:GLN:OE1	2.29	0.65
6:F:35:THR:HB	6:F:119:PRO:HB2	1.78	0.65
1:M:79:THR:HG22	2:N:510:GLU:HG2	1.78	0.65
6:F:18:PRO:O	6:F:20:ARG:NH1	2.29	0.65
6:R:206:MET:O	6:R:293:TYR:OH	2.09	0.65
7:S:25:VAL:HG12	7:S:180:VAL:HG11	1.77	0.65
6:R:402:LEU:HD13	22:R:602:HEA:HAC	1.78	0.65
6:F:97:PRO:HG3	6:F:129:PHE:CE1	2.33	0.64
5:Q:71:THR:HG21	6:R:348:MET:HB3	1.78	0.64
2:N:500:GLY:HA3	2:N:505:PRO:HA	1.79	0.64
3:O:137:HIS:O	5:Q:193:ARG:NH2	2.30	0.64
4:D:69:ALA:HA	16:D:103:CDL:H582	1.79	0.64
1:M:133:GLY:HA3	2:N:277:GLY:HA3	1.79	0.63
5:Q:32:ALA:HB1	5:Q:35:TRP:HB2	1.80	0.63
5:Q:243:ARG:NH1	5:Q:255:ASP:O	2.31	0.63
1:A:355:LEU:HD22	1:A:364:LEU:HD23	1.80	0.63
2:B:213:LEU:HD21	15:N:602:HEM:HBC1	1.79	0.63
6:R:532:GLU:HB3	10:V:25:SER:HB3	1.80	0.63
5:Q:272:ARG:NH1	6:R:456:GLY:O	2.31	0.63
9:I:52:GLU:HA	10:J:65:ARG:HH11	1.64	0.62
5:E:252:ASN:HB3	6:F:253:LEU:HD23	1.81	0.62
7:G:24:MET:HA	7:G:27:VAL:HG22	1.82	0.62
5:E:106:ILE:HB	6:F:331:PHE:HB3	1.80	0.62
6:R:104:ASN:OD1	6:R:122:ASN:ND2	2.29	0.62
10:J:85:LEU:HD12	10:J:109:VAL:HG23	1.82	0.62
2:B:305:MET:O	2:B:308:THR:OG1	2.16	0.61
7:G:34:SER:HB2	8:H:48:LEU:HG	1.81	0.61
6:R:110:GLN:NE2	6:R:280:GLU:OE2	2.32	0.61
7:S:34:SER:HB3	8:T:48:LEU:HG	1.81	0.61
5:E:117:GLN:HB3	6:F:383:PRO:HD3	1.81	0.61
6:F:221:LEU:HD22	7:G:35:SER:HB3	1.81	0.61
5:Q:252:ASN:HB3	6:R:253:LEU:HD23	1.82	0.61
2:N:87:ARG:NH1	2:N:90:GLU:OE2	2.33	0.61
2:N:486:LYS:NZ	16:N:605:CDL:OB3	2.34	0.61
6:R:264:HIS:CD2	6:R:268:TYR:HE2	2.18	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:74:GLY:O	10:J:103:GLN:NE2	2.33	0.61
7:S:147:HIS:CE1	7:S:192:TRP:HB2	2.36	0.60
3:C:214:ASN:OD1	3:C:217:GLN:NE2	2.32	0.60
6:F:398:PHE:HA	6:F:401:VAL:HG22	1.81	0.60
16:C:305:CDL:H522	14:G:302:PLM:H81	1.84	0.60
5:E:123:LYS:NZ	5:E:255:ASP:OD1	2.26	0.60
7:G:27:VAL:HG12	8:H:55:PHE:HE2	1.66	0.60
6:F:153:ALA:O	6:F:255:TRP:NE1	2.34	0.60
7:G:120:GLU:OE2	7:G:200:TYR:OH	2.19	0.60
2:B:384:TYR:HB2	19:C:304:MQ9:H362	1.84	0.60
7:S:24:MET:HA	7:S:27:VAL:HG22	1.83	0.59
9:U:52:GLU:HA	10:V:65:ARG:HE	1.66	0.59
6:F:268:TYR:OH	22:F:601:HEA:O11	2.20	0.59
6:F:507:VAL:HG21	10:J:32:THR:HG23	1.84	0.59
6:R:303:ILE:HG13	6:R:336:PRO:HB2	1.85	0.59
10:V:130:ALA:HB2	10:V:146:ALA:HB2	1.85	0.59
2:B:212:ILE:HD11	2:N:212:ILE:HD11	1.84	0.59
15:B:602:HEM:HBB2	15:B:602:HEM:HMB2	1.83	0.59
10:J:63:LYS:HG3	10:J:156:PRO:HB3	1.85	0.59
1:A:164:ARG:O	2:B:234:LYS:NZ	2.36	0.59
6:F:403:PHE:HE1	22:F:602:HEA:HMC2	1.68	0.59
6:R:544:GLU:HB2	6:R:551:VAL:HG22	1.83	0.59
2:B:527:THR:O	2:B:531:GLU:HG2	2.03	0.58
10:J:23:THR:OG1	10:J:27:ARG:O	2.20	0.58
1:M:390:ALA:HB3	1:M:412:VAL:HG12	1.84	0.58
8:H:118:VAL:O	8:H:122:ILE:HG12	2.04	0.58
6:R:33:THR:HG22	8:T:90:TRP:HB3	1.83	0.58
2:B:65:ASP:HB3	2:B:91:THR:HG21	1.83	0.58
5:Q:280:PHE:HB3	5:Q:283:MET:HB2	1.86	0.58
10:J:144:ILE:O	10:J:148:ARG:HG3	2.03	0.58
16:P:103:CDL:H272	6:R:492:VAL:HG21	1.85	0.58
2:N:394:ASP:OD1	2:N:395:ILE:N	2.36	0.57
16:P:103:CDL:H761	16:P:103:CDL:H342	1.85	0.57
9:I:54:PRO:O	10:J:65:ARG:NH2	2.33	0.57
5:Q:138:TRP:CD1	5:Q:280:PHE:HB2	2.40	0.57
7:G:125:VAL:HG13	7:G:130:THR:HG22	1.86	0.57
10:J:55:LEU:HD23	10:J:147:VAL:HG11	1.85	0.57
3:C:88:VAL:HG12	3:C:93:ALA:HA	1.85	0.57
2:N:379:MET:HG2	2:N:419:PRO:HB3	1.86	0.57
3:C:121:ARG:NH2	18:C:302:HEC:O2A	2.35	0.57
2:N:65:ASP:HB3	2:N:91:THR:HG21	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:17:VAL:HG11	4:P:25:SER:HB2	1.86	0.57
7:S:43:LEU:HD13	7:S:143:ALA:HA	1.86	0.57
2:B:468:VAL:HA	2:B:474:PRO:HA	1.87	0.57
4:P:75:TRP:O	20:P:102:9Y0:N	2.37	0.57
2:B:253:VAL:HA	2:B:257:PHE:HB3	1.87	0.57
6:R:97:PRO:HG3	6:R:129:PHE:CE1	2.40	0.57
24:H:201:MQ7:H242	24:H:201:MQ7:H393	1.87	0.57
2:B:435:ARG:NH1	4:D:16:ASP:O	2.37	0.56
6:F:499:TRP:HE1	16:F:606:CDL:HB4	1.70	0.56
1:M:295:VAL:O	1:M:298:GLU:HG3	2.05	0.56
2:N:42:LEU:HD13	2:N:122:VAL:HG12	1.87	0.56
3:O:95:LEU:HD13	3:O:153:ASN:ND2	2.19	0.56
2:B:224:GLY:HA2	16:B:603:CDL:H791	1.87	0.56
6:R:398:PHE:HA	6:R:401:VAL:HG22	1.88	0.56
10:V:73:LEU:HD13	10:V:77:THR:HB	1.87	0.56
2:B:303:PHE:HB2	19:C:304:MQ9:H3A	1.86	0.56
6:F:349:TRP:CD1	6:F:350:LYS:HG2	2.39	0.56
6:R:341:PHE:HZ	6:R:369:PHE:HD1	1.53	0.56
2:B:494:GLY:O	7:G:169:LYS:HG2	2.05	0.56
10:J:100:SER:O	10:J:104:ARG:N	2.39	0.56
1:M:95:LEU:HD22	16:M:503:CDL:H771	1.88	0.56
6:F:16:PRO:HD3	9:I:49:TRP:HB3	1.88	0.56
9:I:69:VAL:N	10:J:92:GLU:OE2	2.38	0.56
1:M:385:ALA:O	4:P:50:ASN:ND2	2.38	0.56
2:N:234:LYS:NZ	25:N:701:HOH:O	2.36	0.56
7:G:147:HIS:CE1	7:G:192:TRP:HB2	2.40	0.56
6:F:355:PHE:HE1	6:F:363:VAL:HG21	1.72	0.55
2:B:318:TRP:HD1	11:L:20:ALA:HB2	1.71	0.55
6:R:80:ASN:HA	6:R:83:PHE:CE2	2.42	0.55
6:R:276:GLY:O	6:R:280:GLU:HG2	2.06	0.55
7:S:167:MET:HA	14:T:201:PLM:H22	1.87	0.55
2:B:438:ARG:HH12	4:D:19:SER:HB2	1.71	0.55
16:F:605:CDL:H571	8:H:125:VAL:HG11	1.89	0.55
5:E:136:PHE:O	5:E:138:TRP:N	2.40	0.55
6:R:536:ILE:O	6:R:537:ARG:NH1	2.37	0.55
6:R:87:GLY:HA3	22:R:602:HEA:HBD1	1.88	0.55
6:F:420:LYS:NZ	6:F:522:SER:O	2.37	0.55
7:G:23:ASN:HD21	7:G:176:THR:HG23	1.72	0.55
9:I:73:GLY:HA3	10:J:110:TYR:CZ	2.41	0.55
2:N:370:VAL:HG22	4:P:23:GLY:HA3	1.89	0.55
16:P:103:CDL:H331	16:P:103:CDL:H582	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:372:VAL:O	2:B:376:ILE:HG12	2.06	0.55
6:F:26:ASN:O	6:F:30:LYS:HE3	2.07	0.55
6:F:434:HIS:CD2	6:F:491:PHE:HB2	2.42	0.54
6:R:95:ALA:O	6:R:98:ILE:HG22	2.06	0.54
1:M:76:VAL:HG21	2:N:513:ALA:HB1	1.88	0.54
2:N:78:GLN:HA	2:N:81:ARG:HG3	1.88	0.54
25:F:702:HOH:O	7:G:164:ARG:NH2	2.39	0.54
9:I:52:GLU:HA	10:J:65:ARG:NH1	2.23	0.54
5:Q:235:TRP:CD1	5:Q:242:LYS:HB3	2.42	0.54
3:O:115:PHE:O	3:O:119:THR:OG1	2.17	0.54
6:R:118:PHE:HB3	16:R:605:CDL:HA31	1.89	0.54
10:J:110:TYR:OH	10:J:120:GLU:OE1	2.15	0.54
3:C:226:PRO:HD2	3:C:229:MET:SD	2.48	0.54
6:F:532:GLU:HG3	10:J:23:THR:HB	1.90	0.54
6:R:284:VAL:HG22	6:R:514:GLY:HA2	1.88	0.54
5:E:263:ILE:HG21	5:E:290:VAL:HG21	1.90	0.54
6:F:206:MET:O	6:F:293:TYR:OH	2.12	0.54
2:N:236:THR:OG1	15:N:601:HEM:O1D	2.25	0.54
6:F:59:ALA:HB2	6:F:86:HIS:CE1	2.42	0.53
16:N:604:CDL:H522	16:N:604:CDL:H722	1.90	0.53
9:U:21:LEU:HA	9:U:24:ILE:HG22	1.89	0.53
6:F:200:GLY:HA3	6:F:536:ILE:HB	1.91	0.53
6:R:190:ILE:HG12	6:R:214:LEU:HD12	1.91	0.53
2:N:33:VAL:HG12	2:N:248:VAL:HG12	1.90	0.53
2:B:42:LEU:HD13	2:B:122:VAL:HG12	1.89	0.53
5:E:272:ARG:NH1	6:F:456:GLY:O	2.41	0.53
2:B:138:GLU:OE2	2:B:352:LYS:NZ	2.38	0.53
2:N:282:ASN:ND2	15:N:602:HEM:O2A	2.40	0.53
4:P:80:ARG:NH2	16:P:103:CDL:OB4	2.41	0.53
15:B:601:HEM:HMB1	15:B:601:HEM:HBB2	1.90	0.53
16:B:603:CDL:HA4	16:N:603:CDL:H521	1.90	0.53
3:C:193:ASN:ND2	3:C:197:LYS:HB2	2.24	0.53
5:E:133:VAL:HB	5:E:225:LEU:HD23	1.90	0.53
2:N:416:VAL:HG13	4:P:39:SER:HB2	1.91	0.53
1:M:355:LEU:HB2	1:M:364:LEU:O	2.09	0.53
6:R:59:ALA:HB2	6:R:86:HIS:CE1	2.44	0.53
5:E:42:GLU:HG2	5:E:120:MET:HA	1.91	0.52
2:B:340:VAL:HG13	19:C:304:MQ9:H412	1.91	0.52
4:D:73:ARG:NH1	16:D:103:CDL:OA7	2.42	0.52
3:O:95:LEU:HD13	3:O:153:ASN:HD22	1.74	0.52
5:Q:238:GLU:HG3	5:Q:269:PHE:HD1	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:153:ALA:HB1	6:R:158:THR:HG21	1.92	0.52
15:N:601:HEM:HMB1	15:N:601:HEM:HBB2	1.91	0.52
6:F:187:VAL:HG22	7:G:31:VAL:HG23	1.92	0.52
10:J:47:ASP:HB3	10:J:140:ILE:HG21	1.90	0.52
6:R:369:PHE:HZ	22:R:601:HEA:HMC3	1.74	0.52
2:B:483:PRO:HG2	3:C:294:ALA:HA	1.91	0.52
6:R:81:GLN:HG3	6:R:148:ASP:HB3	1.91	0.52
6:R:441:GLY:O	6:R:445:THR:HG22	2.10	0.52
1:A:355:LEU:HB2	1:A:364:LEU:HB3	1.91	0.52
4:D:12:VAL:HG13	4:D:26:HIS:HB2	1.90	0.52
1:M:355:LEU:HD13	1:M:366:PRO:HD3	1.91	0.52
5:Q:137:GLN:HB3	5:Q:138:TRP:CE3	2.45	0.52
2:B:27:ARG:HB2	1:M:177:VAL:HG22	1.91	0.52
5:E:114:VAL:HA	5:E:117:GLN:HG2	1.92	0.52
5:E:138:TRP:HA	5:E:284:MET:SD	2.50	0.52
5:E:332:ARG:NH2	6:F:77:GLU:OE1	2.41	0.52
2:N:39:SER:HB2	2:N:126:ARG:HG3	1.92	0.52
6:R:384:LEU:O	6:R:388:VAL:HG22	2.10	0.52
4:D:78:ARG:NH2	16:D:101:CDL:OA4	2.42	0.52
2:B:66:PRO:HG3	2:B:208:TYR:CD2	2.46	0.51
2:B:370:VAL:HG22	4:D:23:GLY:HA3	1.92	0.51
6:F:445:THR:HG23	6:F:446:PHE:CD2	2.45	0.51
8:T:54:THR:HG22	8:T:58:PHE:CE2	2.45	0.51
5:E:137:GLN:HG2	5:E:229:ASP:OD2	2.10	0.51
2:N:309:GLU:HG3	17:N:606:A1IRE:N04	2.25	0.51
7:S:147:HIS:NE2	7:S:192:TRP:HB2	2.25	0.51
2:B:318:TRP:CD1	11:L:20:ALA:HB2	2.46	0.51
16:D:103:CDL:HA31	6:F:496:PHE:HE2	1.76	0.51
5:E:264:GLN:HB2	5:E:265:GLN:OE1	2.09	0.51
1:M:148:VAL:HG23	2:N:263:ALA:HB1	1.93	0.51
10:V:46:MET:O	10:V:50:VAL:HG23	2.11	0.51
2:B:282:ASN:ND2	15:B:602:HEM:O2A	2.42	0.51
3:C:269:ALA:HB3	3:C:270:PRO:HD3	1.93	0.51
1:M:418:GLU:OE1	1:M:418:GLU:N	2.44	0.51
6:F:405:THR:O	6:F:409:ALA:HB3	2.11	0.51
3:O:269:ALA:HB3	3:O:270:PRO:HD3	1.92	0.51
6:R:48:CYS:SG	6:R:97:PRO:HB2	2.51	0.51
6:R:426:LEU:HD23	6:R:498:SER:HB2	1.93	0.51
6:F:480:GLY:HA2	6:F:483:ILE:HD12	1.92	0.51
16:F:605:CDL:H402	7:G:32:TRP:CZ2	2.46	0.51
2:N:253:VAL:HA	2:N:257:PHE:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Q:59:ALA:O	5:Q:63:ILE:HG12	2.11	0.51
6:R:537:ARG:CZ	8:T:72:ASP:HA	2.40	0.51
1:A:161:VAL:HG22	2:B:249:VAL:HG22	1.93	0.51
6:F:264:HIS:NE2	6:F:268:TYR:HE2	2.09	0.51
5:E:164:LYS:NZ	5:E:194:THR:O	2.39	0.50
6:R:400:TYR:HA	6:R:442:PHE:HZ	1.76	0.50
2:B:452:ARG:NH2	2:B:458:TYR:OH	2.45	0.50
22:F:602:HEA:HBC1	22:F:602:HEA:HMC1	1.93	0.50
6:R:392:TYR:CE1	6:R:459:ARG:HA	2.46	0.50
9:U:78:LYS:HG3	10:V:104:ARG:O	2.12	0.50
6:R:341:PHE:HZ	6:R:369:PHE:CD1	2.28	0.50
6:R:402:LEU:CD1	22:R:602:HEA:HAC	2.42	0.50
6:R:420:LYS:NZ	6:R:521:THR:O	2.45	0.50
3:C:192:HIS:CE1	3:C:207:ALA:HB1	2.46	0.50
1:M:149:LEU:HD21	16:M:503:CDL:HA22	1.94	0.50
16:D:103:CDL:H201	16:F:606:CDL:H772	1.94	0.50
5:E:71:THR:HG21	6:F:348:MET:HB3	1.93	0.50
5:E:84:LEU:HD13	6:F:543:PHE:HZ	1.77	0.50
5:E:215:LEU:HD13	5:E:221:ILE:HD13	1.94	0.50
6:F:172:ILE:HG23	6:F:231:LEU:HD22	1.93	0.50
2:N:527:THR:O	2:N:531:GLU:HG2	2.11	0.50
1:M:53:GLU:OE2	1:M:53:GLU:N	2.43	0.49
5:Q:248:GLU:O	5:Q:252:ASN:ND2	2.35	0.49
6:R:445:THR:HG23	6:R:446:PHE:CD2	2.48	0.49
2:B:499:THR:HG23	2:B:506:ASP:HB2	1.94	0.49
3:C:197:LYS:HE3	13:C:303:9YF:O7	2.11	0.49
10:J:51:LEU:HD13	10:J:144:ILE:HD13	1.93	0.49
2:N:202:ILE:HG13	2:N:202:ILE:O	2.11	0.49
6:R:264:HIS:O	6:R:267:VAL:HG22	2.12	0.49
6:R:284:VAL:HG21	6:R:416:PHE:HZ	1.77	0.49
6:R:546:HIS:NE2	10:V:29:SER:OG	2.39	0.49
7:S:70:ALA:HB1	7:S:196:PHE:HE1	1.77	0.49
3:O:125:MET:HG3	6:R:162:HIS:HA	1.93	0.49
9:U:73:GLY:HA3	10:V:110:TYR:CZ	2.48	0.49
3:C:168:ALA:HB1	3:C:171:SER:HB3	1.95	0.49
5:E:235:TRP:CD1	5:E:242:LYS:HB3	2.47	0.49
6:F:106:VAL:HG11	6:F:417:TRP:CE2	2.47	0.49
7:S:60:PRO:O	7:S:63:THR:HG22	2.12	0.49
10:V:78:ALA:O	10:V:82:ARG:HD3	2.12	0.49
1:A:279:MET:O	3:C:236:GLN:NE2	2.45	0.49
2:N:340:VAL:HA	19:O:305:MQ9:H401	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:199:PRO:HG3	8:H:78:GLY:HA3	1.95	0.49
2:B:426:ALA:HA	16:B:604:CDL:H332	1.95	0.49
3:C:121:ARG:NH1	3:C:208:PRO:HG3	2.27	0.49
5:E:138:TRP:CD1	5:E:280:PHE:HB2	2.47	0.49
6:F:95:ALA:O	6:F:98:ILE:HG22	2.13	0.49
6:F:310:VAL:HG12	6:F:329:MET:HB3	1.95	0.49
7:G:22:PRO:HD3	8:H:66:ARG:HD3	1.94	0.49
5:Q:235:TRP:CH2	6:R:456:GLY:HA2	2.47	0.49
7:S:117:GLN:NE2	25:S:401:HOH:O	2.35	0.49
2:B:435:ARG:NH1	6:F:23:PRO:HB2	2.27	0.49
6:F:152:THR:HA	6:F:259:PHE:CZ	2.47	0.49
7:S:156:VAL:HG22	14:T:201:PLM:HG1	1.93	0.49
5:E:65:TRP:CD1	6:F:370:LEU:HD23	2.48	0.49
2:N:503:LEU:HD22	7:S:101:ARG:HG2	1.94	0.49
6:R:200:GLY:HA3	6:R:536:ILE:HB	1.93	0.49
10:J:77:THR:OG1	10:J:107:GLU:OE2	2.30	0.48
6:R:59:ALA:HA	6:R:62:MET:HE2	1.95	0.48
3:O:185:ARG:HA	3:O:189:ALA:HB3	1.94	0.48
5:Q:218:GLY:HA2	5:Q:262:GLU:HB2	1.95	0.48
6:F:155:SER:HB2	6:F:255:TRP:HB3	1.95	0.48
2:N:150:LEU:HD22	2:N:215:ILE:HG23	1.96	0.48
2:N:489:ASN:OD1	2:N:490:LYS:N	2.46	0.48
6:R:155:SER:HB2	6:R:255:TRP:HB3	1.96	0.48
2:B:154:GLU:HB2	2:B:215:ILE:HG21	1.95	0.48
2:B:400:PHE:HA	8:H:108:LEU:HD13	1.95	0.48
16:D:101:CDL:H152	16:D:101:CDL:H311	1.95	0.48
9:U:79:TRP:CH2	10:V:104:ARG:HA	2.48	0.48
5:E:316:ILE:HG22	5:E:316:ILE:O	2.14	0.48
6:F:30:LYS:O	6:F:34:THR:HB	2.13	0.48
6:F:330:THR:O	6:F:333:ILE:HG22	2.14	0.48
2:N:532:HIS:O	2:N:536:ILE:HG12	2.13	0.48
3:O:116:GLN:HG3	18:O:302:HEC:HMA2	1.95	0.48
2:B:67:SER:HB3	2:B:87:ARG:HB3	1.95	0.48
5:E:98:LEU:HB3	6:F:342:PHE:CD2	2.48	0.48
24:O:301:MQ7:H241	24:O:301:MQ7:H261	1.72	0.48
2:N:318:TRP:CD1	11:X:20:ALA:HB2	2.49	0.48
3:O:87:CYS:O	3:O:91:HIS:HB2	2.13	0.48
3:O:134:LYS:HD3	6:R:164:PRO:HG3	1.96	0.48
7:S:38:MET:HE1	8:T:45:THR:HA	1.94	0.48
10:V:85:LEU:HD13	10:V:109:VAL:HG12	1.94	0.48
6:F:460:ARG:H	22:F:602:HEA:CGA	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:210:LEU:HA	2:N:214:LEU:HB2	1.96	0.48
3:C:250:ARG:NH2	3:C:254:GLU:OE2	2.47	0.48
6:F:264:HIS:HE2	6:F:268:TYR:HE2	1.61	0.48
7:G:23:ASN:HD21	7:G:176:THR:CG2	2.26	0.48
2:N:66:PRO:HG3	2:N:208:TYR:CD2	2.49	0.48
5:Q:222:GLU:HG3	5:Q:259:GLN:HG2	1.96	0.48
3:C:81:GLN:HB2	5:E:163:ARG:HH11	1.78	0.47
7:S:91:ALA:HB2	7:S:99:LEU:HD13	1.95	0.47
6:F:459:ARG:HG3	6:F:460:ARG:HG3	1.96	0.47
7:G:69:LEU:HD23	7:G:120:GLU:HB2	1.95	0.47
10:J:53:ASP:O	10:J:57:TYR:HD2	1.97	0.47
1:M:306:MET:SD	2:N:70:HIS:NE2	2.85	0.47
2:N:491:LEU:O	2:N:493:SER:N	2.42	0.47
4:P:74:ASN:O	4:P:78:ARG:HG3	2.14	0.47
6:R:434:HIS:HB2	6:R:490:PRO:HB2	1.95	0.47
3:C:138:PHE:HB3	3:C:142:GLN:HB2	1.96	0.47
10:V:81:ALA:HA	10:V:84:ILE:HG12	1.96	0.47
1:A:265:PRO:HG2	1:A:301:LEU:HD23	1.95	0.47
3:O:277:ILE:HG23	3:O:278:ILE:HG13	1.96	0.47
5:Q:157:ASP:O	5:Q:200:LYS:NZ	2.47	0.47
6:R:371:LEU:HD23	6:R:400:TYR:CE2	2.49	0.47
7:S:161:LEU:O	7:S:165:THR:HG23	2.14	0.47
2:B:495:GLY:HA3	7:G:169:LYS:HE3	1.97	0.47
3:C:72:GLN:HG3	3:C:75:LEU:H	1.79	0.47
5:E:229:ASP:OD1	5:E:230:VAL:N	2.46	0.47
6:F:102:PHE:O	6:F:106:VAL:HG22	2.13	0.47
8:H:47:GLY:O	8:H:51:ILE:HG12	2.14	0.47
3:O:120:GLY:O	3:O:134:LYS:HE3	2.14	0.47
6:F:264:HIS:O	6:F:267:VAL:HG22	2.15	0.47
2:N:22:PRO:HB2	2:N:26:VAL:HG23	1.96	0.47
1:A:207:PHE:CE1	1:M:140:ILE:HB	2.49	0.47
2:B:453:LEU:HB2	2:B:457:ALA:HB3	1.96	0.47
3:C:139:ASP:OD2	3:C:142:GLN:NE2	2.47	0.47
6:F:112:GLY:HA2	6:F:530:PHE:CE2	2.50	0.47
6:F:499:TRP:NE1	16:F:606:CDL:HB4	2.30	0.47
16:F:605:CDL:H392	16:F:605:CDL:H151	1.96	0.47
1:M:358:GLN:NE2	3:O:229:MET:O	2.39	0.47
6:F:288:LYS:HB3	6:F:288:LYS:HE2	1.65	0.47
6:F:452:LEU:HD13	6:F:473:LEU:HB2	1.96	0.47
7:G:121:TYR:O	7:G:125:VAL:HG23	2.14	0.47
3:O:237:LEU:O	3:O:242:LYS:NZ	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Q:233:GLY:HA3	5:Q:274:THR:H	1.80	0.47
16:C:305:CDL:HB22	8:H:137:GLU:HG3	1.97	0.47
6:F:37:HIS:ND1	6:F:104:ASN:O	2.37	0.47
16:M:503:CDL:H542	16:M:503:CDL:HA61	1.97	0.47
5:Q:231:ILE:HD11	6:R:252:VAL:HG13	1.97	0.47
15:B:602:HEM:HBC1	2:N:213:LEU:HD21	1.96	0.47
4:D:76:TRP:CD1	16:D:103:CDL:H511	2.50	0.47
5:E:113:THR:CG2	6:F:382:PRO:HD2	2.45	0.47
6:F:55:GLY:O	6:F:86:HIS:ND1	2.44	0.47
1:M:370:SER:HA	1:M:383:GLY:HA3	1.96	0.47
2:N:428:ARG:HH22	16:P:101:CDL:H1	1.80	0.47
2:B:441:LEU:HD22	2:B:477:LEU:HB2	1.97	0.46
6:F:227:LEU:HD22	6:F:262:PHE:CZ	2.50	0.46
9:U:23:LEU:O	9:U:27:THR:OG1	2.19	0.46
19:C:304:MQ9:H43	19:C:304:MQ9:H471	1.65	0.46
5:E:240:LEU:HA	6:F:387:HIS:ND1	2.30	0.46
8:H:91:TRP:O	8:H:95:ILE:HG13	2.16	0.46
3:O:88:VAL:HG23	3:O:93:ALA:HB2	1.97	0.46
5:Q:235:TRP:CE3	5:Q:274:THR:HG21	2.50	0.46
6:R:30:LYS:O	6:R:34:THR:HB	2.16	0.46
4:D:78:ARG:NH1	4:D:84:ARG:O	2.46	0.46
22:F:602:HEA:H261	22:F:602:HEA:H172	1.57	0.46
16:M:503:CDL:HA62	16:N:607:CDL:H571	1.97	0.46
6:F:531:THR:OG1	6:F:532:GLU:OE1	2.28	0.46
16:B:605:CDL:HA61	8:H:90:TRP:HZ2	1.79	0.46
6:F:81:GLN:HG3	6:F:148:ASP:HB3	1.97	0.46
6:F:371:LEU:HD23	6:F:400:TYR:CE1	2.50	0.46
6:F:379:LEU:HD21	6:F:394:VAL:HG22	1.97	0.46
7:G:79:ALA:O	7:G:83:THR:HG23	2.16	0.46
2:N:231:TRP:CG	16:N:603:CDL:H731	2.51	0.46
16:D:101:CDL:H341	16:D:101:CDL:H312	1.43	0.46
19:O:305:MQ9:H253	19:O:305:MQ9:H271	1.65	0.46
6:R:211:TRP:CZ3	8:T:7:LEU:HD21	2.43	0.46
6:R:226:ILE:HG13	7:S:38:MET:HG3	1.97	0.46
1:M:106:VAL:HG11	1:M:131:LEU:HB3	1.98	0.46
9:U:79:TRP:HH2	10:V:101:PRO:HA	1.81	0.46
1:M:69:PHE:CE1	1:M:71:GLU:HG2	2.51	0.46
2:N:384:TYR:HB2	19:O:305:MQ9:H362	1.97	0.46
19:O:305:MQ9:H353	19:O:305:MQ9:H412	1.97	0.46
16:R:606:CDL:H612	16:R:606:CDL:H581	1.55	0.46
19:C:304:MQ9:H253	19:C:304:MQ9:H271	1.65	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:479:VAL:O	6:F:483:ILE:HG13	2.16	0.46
15:N:602:HEM:HMB1	15:N:602:HEM:HBB2	1.97	0.46
5:Q:263:ILE:HG21	5:Q:290:VAL:HG21	1.98	0.46
1:A:304:ILE:O	1:A:310:ASN:ND2	2.44	0.46
1:A:369:GLN:HG3	2:B:404:LEU:HD11	1.98	0.46
19:C:304:MQ9:H372	19:C:304:MQ9:H411	1.71	0.46
16:C:305:CDL:H542	16:C:305:CDL:H572	1.62	0.46
5:E:195:TYR:CD2	5:E:248:GLU:HG2	2.50	0.46
7:G:83:THR:OG1	7:G:106:THR:OG1	2.27	0.46
1:A:344:LYS:HE2	1:A:354:SER:HB3	1.99	0.45
4:D:42:PHE:HA	4:D:45:VAL:HG12	1.98	0.45
6:F:104:ASN:CG	6:F:122:ASN:HD21	2.20	0.45
1:M:349:LEU:HD12	1:M:368:HIS:CE1	2.50	0.45
2:N:58:VAL:O	2:N:61:THR:OG1	2.31	0.45
3:O:115:PHE:CE1	3:O:221:ALA:HB2	2.51	0.45
6:R:369:PHE:CZ	22:R:601:HEA:HMC3	2.51	0.45
16:B:605:CDL:HA61	16:B:605:CDL:H312	1.82	0.45
6:F:420:LYS:O	6:F:525:PRO:HD3	2.16	0.45
2:N:420:ALA:HB2	16:P:101:CDL:H191	1.97	0.45
16:N:607:CDL:H592	14:T:201:PLM:H71	1.98	0.45
1:M:371:GLN:HB2	1:M:382:PHE:HB3	1.99	0.45
5:E:231:ILE:HG22	5:E:275:GLU:HG2	1.99	0.45
2:N:505:PRO:HB3	7:S:97:PHE:CE2	2.51	0.45
3:O:192:HIS:CE1	3:O:210:LEU:HD21	2.52	0.45
5:Q:86:ARG:HH21	6:R:560:VAL:HA	1.81	0.45
2:B:39:SER:HB2	2:B:126:ARG:HG3	1.98	0.45
2:B:503:LEU:HD22	7:G:101:ARG:HG2	1.97	0.45
6:R:156:PRO:O	6:R:162:HIS:ND1	2.48	0.45
2:B:117:ALA:O	2:B:121:MET:HG3	2.17	0.45
2:B:160:SER:HA	2:B:167:SER:HB2	1.98	0.45
16:D:101:CDL:H732	16:F:606:CDL:H721	1.98	0.45
5:E:35:TRP:HD1	6:F:454:ASP:HB3	1.81	0.45
6:F:403:PHE:HZ	22:F:602:HEA:O11	1.99	0.45
6:R:310:VAL:O	6:R:313:HIS:ND1	2.50	0.45
3:C:134:LYS:HD2	6:F:161:ILE:HA	1.98	0.45
5:E:227:SER:HB2	5:E:245:VAL:HG12	1.97	0.45
16:N:607:CDL:H831	16:N:607:CDL:H801	1.61	0.45
6:R:172:ILE:HG23	6:R:231:LEU:HD22	1.98	0.45
16:R:605:CDL:H761	7:S:153:GLY:HA3	1.98	0.45
16:D:101:CDL:H151	16:D:101:CDL:H181	1.67	0.45
5:E:119:ARG:HE	5:E:119:ARG:HA	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:235:TRP:CE3	5:E:274:THR:HG21	2.51	0.45
3:O:229:MET:HG3	18:O:303:HEC:NC	2.32	0.45
6:R:152:THR:HA	6:R:259:PHE:CZ	2.51	0.45
16:D:103:CDL:OA3	6:F:500:ARG:NH1	2.45	0.45
5:E:299:TYR:OH	5:E:309:ASN:OD1	2.17	0.45
5:Q:154:PHE:HZ	5:Q:300:ILE:HG21	1.80	0.45
7:S:72:PRO:O	7:S:76:VAL:HG23	2.16	0.45
7:S:79:ALA:O	7:S:83:THR:HG23	2.15	0.45
5:E:59:ALA:O	5:E:63:ILE:HG12	2.17	0.45
7:G:147:HIS:NE2	7:G:192:TRP:HB2	2.32	0.45
5:Q:238:GLU:HG3	5:Q:269:PHE:CD1	2.51	0.45
6:R:449:GLN:HA	6:R:452:LEU:HB2	1.97	0.45
4:D:17:VAL:HG11	4:D:25:SER:HB2	1.99	0.44
16:D:103:CDL:H151	16:D:103:CDL:H182	1.81	0.44
6:F:285:PHE:CZ	6:F:358:PRO:HG2	2.52	0.44
6:F:445:THR:HA	6:F:477:SER:HA	1.98	0.44
3:O:115:PHE:CE2	3:O:226:PRO:HB3	2.52	0.44
2:B:254:MET:HA	2:B:255:PRO:HA	1.65	0.44
7:G:83:THR:HG1	7:G:106:THR:HG1	1.58	0.44
2:N:121:MET:HB3	19:O:305:MQ9:H262	1.98	0.44
1:A:368:HIS:HB2	12:A:501:FES:S2	2.57	0.44
1:A:385:ALA:O	4:D:50:ASN:ND2	2.49	0.44
10:J:73:LEU:HG	10:J:100:SER:HB2	1.99	0.44
1:M:380:PRO:HD3	1:M:388:ALA:HA	1.99	0.44
3:O:222:MET:HA	3:O:229:MET:HE2	1.99	0.44
2:B:124:LEU:HD11	2:B:344:LEU:HD11	1.99	0.44
6:F:148:ASP:OD2	25:F:701:HOH:O	2.20	0.44
6:F:306:LEU:HD21	6:F:332:LEU:HG	1.99	0.44
5:Q:106:ILE:HB	6:R:331:PHE:HB3	1.99	0.44
5:E:113:THR:HG23	6:F:383:PRO:HD2	2.00	0.44
5:E:137:GLN:HB3	5:E:138:TRP:CE3	2.52	0.44
6:F:57:LEU:HD13	22:F:602:HEA:H202	1.99	0.44
6:F:90:MET:HE3	22:F:602:HEA:HHC	1.99	0.44
5:Q:101:ILE:O	5:Q:104:LEU:HG	2.18	0.44
5:Q:299:TYR:OH	5:Q:303:ARG:NH2	2.48	0.44
3:C:193:ASN:OD1	3:C:196:GLY:N	2.51	0.44
5:E:132:ASP:OD2	5:E:145:GLN:HB2	2.17	0.44
6:F:253:LEU:HD11	6:F:318:THR:HG21	1.98	0.44
24:H:201:MQ7:H212	24:H:201:MQ7:H191	1.83	0.44
5:Q:43:ALA:HB1	5:Q:240:LEU:HD12	1.99	0.44
5:Q:113:THR:HG23	6:R:383:PRO:HD2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:ALA:HB3	1:A:239:TRP:CD1	2.51	0.44
1:A:380:PRO:HD3	1:A:388:ALA:HA	2.00	0.44
16:F:605:CDL:H112	16:F:605:CDL:H372	1.99	0.44
2:N:470:GLU:HG2	2:N:471:HIS:H	1.83	0.44
16:P:101:CDL:H831	16:P:101:CDL:H862	1.51	0.44
16:B:604:CDL:H381	16:B:605:CDL:H591	2.00	0.44
6:F:18:PRO:HG2	6:F:504:PRO:HB3	2.00	0.44
2:N:368:ARG:O	2:N:434:GLN:NE2	2.33	0.44
16:N:605:CDL:H791	16:R:606:CDL:H661	2.00	0.44
8:T:54:THR:HG22	8:T:58:PHE:HE2	1.82	0.44
3:C:267:GLY:O	3:C:270:PRO:HD2	2.18	0.44
16:D:103:CDL:H841	16:D:103:CDL:H872	1.82	0.44
8:H:3:ILE:O	8:H:7:LEU:HD23	2.18	0.44
1:M:289:ASP:HA	1:M:300:LYS:HE3	2.00	0.44
16:M:503:CDL:HB4	16:M:503:CDL:H512	1.77	0.44
2:N:316:PRO:HG2	2:N:318:TRP:CZ2	2.53	0.44
3:O:91:HIS:CE1	3:O:105:LEU:HG	2.52	0.44
5:Q:233:GLY:O	5:Q:273:CYS:HA	2.18	0.44
6:R:121:LEU:HB2	16:R:605:CDL:HA32	1.99	0.44
2:B:232:PHE:HZ	16:B:603:CDL:HB61	1.83	0.43
7:G:67:LEU:HD13	7:G:200:TYR:HB3	1.99	0.43
9:I:25:PHE:HA	9:I:28:ARG:HD2	2.00	0.43
9:I:77:GLY:HA3	10:J:127:VAL:HG11	2.00	0.43
6:R:211:TRP:O	6:R:215:VAL:HG23	2.18	0.43
2:N:483:PRO:HG2	3:O:294:ALA:HA	2.01	0.43
2:B:38:TRP:CH2	16:B:604:CDL:H711	2.54	0.43
6:F:552:GLU:HB2	6:F:553:ARG:NH2	2.33	0.43
7:G:76:VAL:HG21	7:G:112:PHE:CE2	2.53	0.43
5:Q:65:TRP:HH2	6:R:371:LEU:HD13	1.84	0.43
2:N:26:VAL:O	2:N:30:LEU:HG	2.17	0.43
16:N:605:CDL:H132	16:N:607:CDL:HA4	2.00	0.43
6:R:58:MET:HG2	6:R:82:LEU:HD22	2.00	0.43
6:R:395:ILE:HA	6:R:398:PHE:CE2	2.54	0.43
7:G:71:VAL:HB	7:G:72:PRO:HD3	2.00	0.43
7:G:147:HIS:O	7:G:151:VAL:HG23	2.19	0.43
1:M:88:LEU:HD13	16:M:503:CDL:H712	2.01	0.43
1:M:384:PRO:HA	2:N:317:ALA:HB2	1.99	0.43
6:R:365:PHE:HD1	6:R:404:GLY:O	2.01	0.43
6:R:405:THR:O	6:R:409:ALA:HB3	2.18	0.43
6:R:420:LYS:O	6:R:525:PRO:HD3	2.19	0.43
16:D:103:CDL:H221	16:D:103:CDL:H192	1.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:190:LEU:HD22	14:M:504:PLM:HC1	2.00	0.43
6:R:257:HIS:NE2	8:T:35:GLU:OE2	2.51	0.43
5:E:119:ARG:HA	5:E:119:ARG:NE	2.34	0.43
6:F:400:TYR:HA	6:F:442:PHE:HZ	1.82	0.43
7:G:63:THR:HG21	7:G:136:TYR:CE1	2.54	0.43
7:G:137:GLY:O	7:G:141:TYR:HD2	2.01	0.43
10:J:143:LEU:O	10:J:147:VAL:HG23	2.19	0.43
2:N:303:PHE:HA	2:N:306:MET:HG3	2.00	0.43
2:N:432:SER:OG	6:R:29:TYR:HB2	2.18	0.43
6:R:267:VAL:HB	22:R:601:HEA:CAC	2.45	0.43
6:R:390:ASP:HA	6:R:459:ARG:HD3	1.99	0.43
6:R:402:LEU:HB3	22:R:602:HEA:HAC	1.99	0.43
9:U:77:GLY:HA3	10:V:127:VAL:HG11	2.01	0.43
1:A:144:GLY:O	1:A:148:VAL:HG23	2.19	0.43
16:D:103:CDL:H412	16:D:103:CDL:H821	2.01	0.43
6:F:418:PHE:CD2	6:F:426:LEU:HG	2.54	0.43
1:M:131:LEU:HD23	1:M:131:LEU:HA	1.87	0.43
2:N:184:VAL:HG23	2:N:185:ILE:N	2.34	0.43
2:N:425:VAL:HG13	6:R:28:ILE:HD11	1.99	0.43
6:R:226:ILE:HD11	7:S:38:MET:SD	2.59	0.43
6:R:551:VAL:HA	6:R:554:MET:HE2	2.01	0.43
5:E:235:TRP:HZ2	6:F:387:HIS:CE1	2.37	0.43
16:N:605:CDL:H571	16:N:605:CDL:H601	1.69	0.43
5:Q:29:ASP:OD1	5:Q:29:ASP:N	2.49	0.43
6:R:355:PHE:HE1	6:R:363:VAL:HG21	1.83	0.43
10:V:123:ALA:HB3	10:V:124:PRO:HD3	2.01	0.43
2:B:4:ASP:O	2:B:8:LEU:HG	2.19	0.43
5:E:279:THR:O	6:F:76:ASN:HB3	2.19	0.43
1:M:334:PHE:CE2	1:M:393:PRO:HG3	2.54	0.43
5:Q:241:PHE:HZ	5:Q:243:ARG:HH21	1.64	0.43
5:Q:272:ARG:HB3	6:R:461:TYR:OH	2.19	0.43
6:R:52:PHE:HE1	22:R:602:HEA:HMC3	1.84	0.43
22:R:602:HEA:H261	22:R:602:HEA:H172	1.75	0.43
2:B:156:TYR:HA	2:B:159:TYR:CE2	2.54	0.42
1:A:230:THR:HG22	1:A:232:GLU:H	1.84	0.42
16:D:103:CDL:H181	16:F:606:CDL:H752	2.01	0.42
11:L:31:GLU:OE2	11:L:32:PRO:HD2	2.19	0.42
1:M:164:ARG:NH1	2:N:235:HIS:O	2.49	0.42
6:R:155:SER:OG	6:R:245:TYR:HB3	2.19	0.42
3:C:120:GLY:HA3	3:C:134:LYS:O	2.19	0.42
3:C:208:PRO:HG2	18:C:302:HEC:HBA1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:15:ARG:HD2	9:I:52:GLU:OE2	2.20	0.42
16:F:605:CDL:H771	7:G:153:GLY:HA3	2.01	0.42
9:I:53:GLU:HG2	10:J:60:ARG:HB2	2.00	0.42
3:O:126:ARG:NH2	6:R:163:SER:HA	2.31	0.42
5:Q:331:ARG:NE	5:Q:333:GLY:O	2.52	0.42
6:R:375:SER:OG	6:R:397:HIS:ND1	2.50	0.42
3:C:159:VAL:HG12	3:C:220:THR:HG21	2.02	0.42
5:E:167:MET:SD	5:E:193:ARG:HB2	2.60	0.42
2:N:172:ARG:HB2	2:N:198:PHE:CZ	2.54	0.42
6:R:227:LEU:HD22	6:R:262:PHE:CZ	2.54	0.42
6:R:345:ILE:HD13	6:R:345:ILE:HA	1.88	0.42
16:D:101:CDL:H782	16:D:103:CDL:H222	2.01	0.42
5:E:138:TRP:HZ2	5:E:278:GLY:HA3	1.85	0.42
2:N:114:LEU:HB3	3:O:275:MET:HG2	2.00	0.42
2:N:171:ILE:HG22	2:N:198:PHE:HE1	1.84	0.42
6:R:222:ILE:O	7:S:38:MET:HG2	2.20	0.42
8:T:13:ALA:O	8:T:17:LEU:HD23	2.20	0.42
2:B:111:TRP:HD1	2:B:276:GLY:HA2	1.84	0.42
3:C:119:THR:HG21	3:C:121:ARG:NH2	2.35	0.42
3:C:134:LYS:HD3	6:F:164:PRO:HG3	2.01	0.42
6:F:121:LEU:HD11	6:F:184:LEU:HD13	2.01	0.42
16:F:606:CDL:H871	16:F:606:CDL:H841	1.82	0.42
2:N:319:GLU:OE1	2:N:328:PRO:HA	2.20	0.42
5:Q:205:GLY:HA3	5:Q:211:PRO:HD3	2.01	0.42
6:R:392:TYR:CD1	6:R:395:ILE:HG13	2.55	0.42
10:V:85:LEU:HD12	10:V:96:LEU:HB3	2.00	0.42
5:Q:92:MET:HB2	5:Q:93:PRO:HD3	2.01	0.42
6:R:330:THR:HG22	22:R:601:HEA:HMB2	2.01	0.42
7:S:38:MET:O	7:S:41:ALA:HB3	2.20	0.42
7:S:167:MET:HE2	8:T:130:PHE:CD1	2.55	0.42
3:C:205:LYS:HD2	3:C:228:ASN:ND2	2.34	0.42
5:E:65:TRP:HD1	5:E:68:ILE:HD12	1.85	0.42
1:M:69:PHE:O	1:M:158:GLU:HA	2.20	0.42
1:M:366:PRO:O	1:M:369:GLN:NE2	2.52	0.42
2:N:416:VAL:CG1	4:P:39:SER:HB2	2.49	0.42
2:B:429:TRP:HH2	16:B:605:CDL:H742	1.85	0.42
5:E:86:ARG:HG3	6:F:557:GLU:OE1	2.19	0.42
16:N:603:CDL:H771	16:N:603:CDL:H741	1.70	0.42
4:P:80:ARG:HB2	4:P:82:TRP:CD1	2.55	0.42
6:R:55:GLY:O	6:R:86:HIS:ND1	2.49	0.42
6:R:285:PHE:CZ	6:R:358:PRO:HG2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:341:PHE:CZ	6:R:369:PHE:HD1	2.35	0.42
1:A:204:LEU:HD23	1:A:204:LEU:HA	1.87	0.42
2:B:505:PRO:HB3	7:G:97:PHE:CE2	2.54	0.42
3:C:192:HIS:CE1	3:C:210:LEU:HD21	2.55	0.42
3:O:261:TYR:CE2	3:O:263:LEU:HD23	2.54	0.42
3:C:84:GLU:HA	3:C:88:VAL:HG13	2.02	0.41
5:E:265:GLN:OE1	5:E:265:GLN:N	2.53	0.41
6:F:149:PHE:HE1	6:F:153:ALA:HB2	1.84	0.41
2:N:470:GLU:HG2	2:N:471:HIS:N	2.35	0.41
5:Q:299:TYR:O	5:Q:303:ARG:HG2	2.20	0.41
1:A:353:SER:HA	1:A:365:CYS:HA	2.01	0.41
5:E:39:ILE:HD11	5:E:239:PHE:CE1	2.55	0.41
5:E:227:SER:OG	5:E:230:VAL:O	2.21	0.41
5:E:289:ARG:HH12	5:E:322:ALA:HA	1.83	0.41
6:F:419:PRO:HG3	6:F:425:LEU:HD23	2.02	0.41
1:M:171:GLU:O	1:M:175:LYS:HG2	2.20	0.41
3:O:224:THR:O	3:O:224:THR:OG1	2.35	0.41
1:A:371:GLN:HB2	1:A:382:PHE:HB3	2.03	0.41
4:D:28:PRO:HG2	4:D:31:VAL:HG23	2.02	0.41
6:F:495:VAL:HG11	16:F:606:CDL:H812	2.02	0.41
10:J:45:THR:O	10:J:49:VAL:HG23	2.20	0.41
10:J:73:LEU:HD13	10:J:77:THR:HB	2.01	0.41
19:O:305:MQ9:H153	19:O:305:MQ9:H172	1.65	0.41
6:R:537:ARG:HA	6:R:537:ARG:HD3	1.86	0.41
7:S:65:LEU:HD23	7:S:65:LEU:HA	1.89	0.41
1:A:46:GLU:HA	1:A:49:GLU:HG2	2.01	0.41
1:A:254:LEU:HD23	1:A:282:VAL:HG21	2.02	0.41
5:E:284:MET:O	5:E:284:MET:HG2	2.21	0.41
6:F:195:CYS:SG	7:G:24:MET:HB3	2.60	0.41
1:M:329:LYS:HA	11:X:29:SER:HB3	2.03	0.41
2:N:165:LEU:HD11	2:N:294:GLN:O	2.21	0.41
2:N:318:TRP:O	2:N:332:TRP:NE1	2.47	0.41
4:P:19:SER:HB2	4:P:22:TRP:CD1	2.56	0.41
2:B:306:MET:HG2	2:B:391:CYS:SG	2.60	0.41
5:E:113:THR:HG21	6:F:382:PRO:HD2	2.03	0.41
6:F:89:VAL:HG22	6:F:93:PHE:HD2	1.85	0.41
6:F:267:VAL:HB	22:F:601:HEA:CAC	2.46	0.41
9:I:79:TRP:CD2	10:J:104:ARG:HG3	2.55	0.41
1:M:289:ASP:OD2	1:M:304:ILE:HD11	2.20	0.41
1:M:312:VAL:HG13	1:M:342:TYR:O	2.21	0.41
4:P:43:LEU:O	4:P:60:LEU:HD22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:ASP:OD2	2:B:31:ASN:ND2	2.44	0.41
1:A:302:THR:HG21	2:B:70:HIS:CD2	2.56	0.41
3:C:115:PHE:CE2	3:C:226:PRO:HG3	2.55	0.41
6:F:43:MET:HB3	6:F:126:PHE:CZ	2.56	0.41
16:F:606:CDL:H591	16:F:606:CDL:H562	1.79	0.41
6:R:330:THR:O	6:R:333:ILE:HG22	2.20	0.41
9:U:79:TRP:CH2	10:V:101:PRO:HA	2.56	0.41
1:A:395:THR:OG1	1:A:396:ILE:N	2.53	0.41
2:B:256:VAL:HG12	2:B:260:LYS:HE2	2.03	0.41
3:C:115:PHE:HE2	3:C:226:PRO:HG3	1.85	0.41
5:E:248:GLU:OE1	6:F:248:ALA:HA	2.20	0.41
6:F:403:PHE:HZ	22:F:602:HEA:HO1	1.68	0.41
6:F:532:GLU:OE1	6:F:532:GLU:N	2.54	0.41
6:R:263:GLY:O	6:R:267:VAL:HG13	2.20	0.41
2:B:416:VAL:HG13	4:D:39:SER:HB2	2.02	0.41
6:F:287:ARG:HD3	6:F:352:GLN:O	2.20	0.41
6:F:290:ILE:HD12	6:F:347:THR:OG1	2.20	0.41
6:F:365:PHE:HD1	6:F:404:GLY:O	2.03	0.41
6:F:398:PHE:CD2	22:F:601:HEA:HAD1	2.55	0.41
8:T:9:GLU:OE2	8:T:57:ARG:NH1	2.43	0.41
2:B:231:TRP:CE2	16:B:603:CDL:H712	2.56	0.41
2:B:394:ASP:OD1	2:B:395:ILE:N	2.53	0.41
2:B:433:LEU:HD11	16:B:605:CDL:OB7	2.20	0.41
2:B:464:PRO:HB3	2:B:474:PRO:HB3	2.02	0.41
5:E:65:TRP:HE1	6:F:367:ILE:HA	1.86	0.41
6:F:245:TYR:CZ	6:F:255:TRP:HE3	2.39	0.41
6:F:406:ILE:CD1	22:F:602:HEA:CBC	2.74	0.41
16:F:605:CDL:H402	7:G:32:TRP:HZ2	1.85	0.41
10:J:68:VAL:HG11	10:J:143:LEU:HD13	2.02	0.41
1:M:204:LEU:HD23	1:M:204:LEU:HA	1.92	0.41
1:M:238:LEU:HD23	1:M:238:LEU:HA	1.89	0.41
16:N:604:CDL:H341	16:N:605:CDL:H552	2.03	0.41
16:P:101:CDL:H811	16:P:101:CDL:H842	1.74	0.41
7:S:101:ARG:O	7:S:105:ILE:HG12	2.20	0.41
9:U:31:PRO:HB2	10:V:37:LEU:CD2	2.51	0.41
10:V:123:ALA:O	10:V:127:VAL:HG23	2.21	0.41
1:A:42:PRO:HA	1:A:46:GLU:OE2	2.21	0.41
2:B:38:TRP:HZ2	16:B:604:CDL:HB4	1.86	0.41
3:C:105:LEU:HD23	3:C:105:LEU:HA	1.94	0.41
22:F:602:HEA:CBC	22:F:602:HEA:HMC1	2.51	0.41
8:H:5:ALA:O	8:H:9:GLU:OE1	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:66:PHE:HE2	10:J:150:MET:HB3	1.86	0.41
2:N:127:ILE:HG23	2:N:132:ALA:HB3	2.03	0.41
2:N:309:GLU:CD	2:N:313:ARG:HH22	2.23	0.41
16:P:101:CDL:H152	16:P:101:CDL:H311	2.03	0.41
2:B:124:LEU:HD12	15:B:601:HEM:HMC2	2.02	0.40
5:E:65:TRP:CE2	6:F:367:ILE:HG23	2.57	0.40
5:E:127:PRO:HG3	5:E:222:GLU:OE1	2.20	0.40
6:F:278:VAL:HG21	6:F:365:PHE:CE2	2.55	0.40
7:G:73:VAL:HB	7:G:113:PHE:CD1	2.56	0.40
2:N:316:PRO:HG3	4:P:46:MET:HG2	2.03	0.40
6:R:445:THR:HA	6:R:477:SER:HA	2.03	0.40
2:B:503:LEU:O	7:G:101:ARG:NH1	2.51	0.40
5:E:105:ILE:O	5:E:108:VAL:HG12	2.20	0.40
5:E:142:PHE:CE2	5:E:213:LEU:HB2	2.56	0.40
5:E:283:MET:HG2	5:E:328:PHE:CG	2.57	0.40
6:F:384:LEU:O	6:F:388:VAL:HG22	2.21	0.40
6:F:403:PHE:HA	6:F:407:VAL:HB	2.03	0.40
3:O:126:ARG:HH12	6:R:163:SER:HA	1.86	0.40
19:O:305:MQ9:H412	19:O:305:MQ9:H372	1.84	0.40
5:Q:253:ASN:HB3	8:T:31:THR:HB	2.03	0.40
11:X:31:GLU:N	11:X:31:GLU:OE1	2.53	0.40
2:B:25:ALA:O	2:B:29:GLN:HG2	2.21	0.40
5:E:71:THR:HG22	6:F:353:LEU:HD11	2.04	0.40
6:F:314:HIS:ND1	22:F:601:HEA:HAA2	2.36	0.40
7:G:124:LEU:HD23	7:G:124:LEU:HA	1.92	0.40
1:M:41:GLN:HA	1:M:42:PRO:HD3	1.90	0.40
6:R:56:GLY:HA3	22:R:602:HEA:H161	2.03	0.40
6:R:91:LEU:HA	6:R:91:LEU:HD23	1.81	0.40
6:R:392:TYR:HB3	6:R:449:GLN:HB3	2.03	0.40
2:B:229:LEU:HD23	16:B:603:CDL:H121	2.03	0.40
7:G:38:MET:O	7:G:41:ALA:HB3	2.20	0.40
1:M:198:LEU:O	1:M:202:ILE:HG12	2.21	0.40
1:M:351:CYS:HB2	12:M:501:FES:S1	2.62	0.40
5:Q:31:LEU:HD13	5:Q:55:ILE:HD11	2.04	0.40
5:Q:331:ARG:NH2	5:Q:334:GLU:HA	2.36	0.40
9:U:71:ILE:HD11	9:U:73:GLY:O	2.20	0.40
2:B:121:MET:HB3	19:C:304:MQ9:H262	2.03	0.40
2:B:172:ARG:HB2	2:B:198:PHE:CZ	2.57	0.40
1:M:322:MET:CE	1:M:338:GLU:HA	2.51	0.40
2:N:425:VAL:HG22	16:R:606:CDL:H122	2.03	0.40
4:P:73:ARG:HH12	16:P:103:CDL:HA32	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Q:210:ILE:HG23	5:Q:286:PHE:HA	2.03	0.40
6:R:266:GLU:HA	6:R:269:ILE:HD12	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	373/421 (89%)	362 (97%)	11 (3%)	0	100	100
1	M	373/421 (89%)	362 (97%)	11 (3%)	0	100	100
2	B	527/546 (96%)	508 (96%)	19 (4%)	0	100	100
2	N	532/546 (97%)	513 (96%)	18 (3%)	1 (0%)	44	74
3	C	221/268 (82%)	210 (95%)	11 (5%)	0	100	100
3	O	221/268 (82%)	210 (95%)	11 (5%)	0	100	100
4	D	72/84 (86%)	71 (99%)	1 (1%)	0	100	100
4	P	72/84 (86%)	70 (97%)	2 (3%)	0	100	100
5	E	281/341 (82%)	267 (95%)	14 (5%)	0	100	100
5	Q	281/341 (82%)	269 (96%)	12 (4%)	0	100	100
6	F	549/575 (96%)	536 (98%)	13 (2%)	0	100	100
6	R	549/575 (96%)	528 (96%)	21 (4%)	0	100	100
7	G	183/203 (90%)	182 (100%)	1 (0%)	0	100	100
7	S	183/203 (90%)	180 (98%)	3 (2%)	0	100	100
8	H	137/139 (99%)	133 (97%)	4 (3%)	0	100	100
8	T	137/139 (99%)	133 (97%)	4 (3%)	0	100	100
9	I	61/79 (77%)	58 (95%)	3 (5%)	0	100	100
9	U	62/79 (78%)	57 (92%)	5 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	J	141/157 (90%)	138 (98%)	3 (2%)	0	100	100
10	V	141/157 (90%)	138 (98%)	3 (2%)	0	100	100
11	L	26/236 (11%)	25 (96%)	1 (4%)	0	100	100
11	X	26/236 (11%)	24 (92%)	2 (8%)	0	100	100
All	All	5148/6098 (84%)	4974 (97%)	173 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	N	184	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	A	309/343 (90%)	309 (100%)	0	100	100
1	M	309/343 (90%)	309 (100%)	0	100	100
2	B	426/437 (98%)	425 (100%)	1 (0%)	92	96
2	N	428/437 (98%)	428 (100%)	0	100	100
3	C	163/197 (83%)	162 (99%)	1 (1%)	84	91
3	O	163/197 (83%)	163 (100%)	0	100	100
4	D	58/67 (87%)	58 (100%)	0	100	100
4	P	58/67 (87%)	58 (100%)	0	100	100
5	E	243/288 (84%)	243 (100%)	0	100	100
5	Q	243/288 (84%)	243 (100%)	0	100	100
6	F	452/471 (96%)	451 (100%)	1 (0%)	92	96
6	R	452/471 (96%)	452 (100%)	0	100	100
7	G	147/161 (91%)	147 (100%)	0	100	100
7	S	147/161 (91%)	145 (99%)	2 (1%)	62	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	H	106/106 (100%)	106 (100%)	0	100	100
8	T	106/106 (100%)	106 (100%)	0	100	100
9	I	50/59 (85%)	50 (100%)	0	100	100
9	U	51/59 (86%)	51 (100%)	0	100	100
10	J	105/114 (92%)	105 (100%)	0	100	100
10	V	105/114 (92%)	105 (100%)	0	100	100
11	L	21/167 (13%)	21 (100%)	0	100	100
11	X	21/167 (13%)	21 (100%)	0	100	100
All	All	4163/4820 (86%)	4158 (100%)	5 (0%)	92	97

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	353	LYS
3	C	126	ARG
6	F	20	ARG
7	S	23	ASN
7	S	189	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	519	HIS
6	F	434	HIS
7	G	23	ASN
3	O	153	ASN
6	R	387	HIS

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 59 ligands modelled in this entry, 10 are monoatomic - leaving 49 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	$\#\|Z\| > 2$
16	CDL	P	101	-	87,87,99	1.30	10 (11%)	93,99,111	1.10	5 (5%)
16	CDL	N	605	-	78,78,99	1.34	9 (11%)	84,90,111	1.11	4 (4%)
17	A1IRE	B	606	-	37,40,40	2.40	12 (32%)	47,63,63	4.17	16 (34%)
22	HEA	R	601	6	57,67,67	2.05	17 (29%)	61,103,103	2.49	28 (45%)
15	HEM	B	601	2	41,49,50	1.27	3 (7%)	46,81,82	1.33	6 (13%)
20	9Y0	S	301	-	42,42,48	0.94	4 (9%)	44,47,53	1.11	2 (4%)
16	CDL	B	605	-	78,78,99	1.33	10 (12%)	84,90,111	1.14	4 (4%)
13	9YF	M	502	-	58,58,58	0.88	4 (6%)	69,71,71	1.17	5 (7%)
18	HEC	C	301	3	32,50,50	2.17	3 (9%)	24,82,82	1.56	3 (12%)
16	CDL	C	305	-	78,78,99	1.35	11 (14%)	84,90,111	1.13	4 (4%)
24	MQ7	O	301	-	49,49,49	1.69	5 (10%)	60,63,63	1.63	15 (25%)
18	HEC	C	302	3	32,50,50	2.18	3 (9%)	24,82,82	1.49	3 (12%)
16	CDL	N	607	-	78,78,99	1.34	11 (14%)	84,90,111	1.14	4 (4%)
19	MQ9	C	304	-	59,59,59	1.55	5 (8%)	72,75,75	1.63	20 (27%)
18	HEC	O	302	3	32,50,50	2.15	3 (9%)	24,82,82	1.66	6 (25%)
16	CDL	M	503	-	73,73,99	1.41	12 (16%)	79,85,111	1.17	5 (6%)
14	PLM	A	503	-	16,16,17	0.52	0	15,15,17	0.42	0
16	CDL	F	605	-	75,75,99	1.38	10 (13%)	81,87,111	1.15	4 (4%)
19	MQ9	O	305	-	59,59,59	1.56	5 (8%)	72,75,75	1.63	20 (27%)
20	9Y0	G	301	-	42,42,48	0.95	4 (9%)	44,47,53	1.07	2 (4%)
24	MQ7	H	201	-	49,49,49	1.72	5 (10%)	60,63,63	1.62	14 (23%)
14	PLM	M	504	-	16,16,17	0.52	0	15,15,17	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	9Y0	D	102	-	40,40,48	0.95	4 (10%)	43,45,53	1.10	2 (4%)
16	CDL	B	603	-	73,73,99	1.38	10 (13%)	79,85,111	1.17	4 (5%)
16	CDL	R	605	-	75,75,99	1.38	11 (14%)	81,87,111	1.13	4 (4%)
12	FES	A	501	1	0,4,4	-	-	-		
16	CDL	P	103	-	94,94,99	1.29	11 (11%)	100,106,111	1.09	4 (4%)
16	CDL	R	606	-	80,80,99	1.34	9 (11%)	86,92,111	1.06	4 (4%)
13	9YF	C	303	-	58,58,58	0.87	4 (6%)	69,71,71	1.02	2 (2%)
22	HEA	F	602	6	57,67,67	2.17	19 (33%)	61,103,103	2.40	27 (44%)
22	HEA	F	601	-	57,67,67	2.06	16 (28%)	61,103,103	2.43	25 (40%)
13	9YF	A	502	-	58,58,58	0.87	4 (6%)	69,71,71	1.12	6 (8%)
14	PLM	T	201	-	16,16,17	0.54	0	15,15,17	0.43	0
12	FES	M	501	1	0,4,4	-	-	-		
16	CDL	D	101	-	87,87,99	1.30	10 (11%)	93,99,111	1.11	4 (4%)
16	CDL	D	103	-	94,94,99	1.29	9 (9%)	100,106,111	1.09	4 (4%)
16	CDL	N	603	-	73,73,99	1.38	10 (13%)	79,85,111	1.12	4 (5%)
16	CDL	N	604	-	76,76,99	1.35	10 (13%)	82,88,111	1.17	4 (4%)
15	HEM	N	602	2	41,50,50	1.45	4 (9%)	45,82,82	1.35	8 (17%)
18	HEC	O	303	3	32,50,50	2.19	3 (9%)	24,82,82	1.45	3 (12%)
20	9Y0	P	102	-	40,40,48	0.96	2 (5%)	43,45,53	1.03	2 (4%)
15	HEM	N	601	2	41,49,50	1.27	3 (7%)	46,81,82	1.35	7 (15%)
22	HEA	R	602	6	57,67,67	2.11	18 (31%)	61,103,103	2.39	26 (42%)
13	9YF	O	304	-	58,58,58	0.87	4 (6%)	69,71,71	1.07	3 (4%)
14	PLM	G	302	-	16,16,17	0.53	0	15,15,17	0.42	0
17	A1IRE	N	606	-	37,40,40	2.42	12 (32%)	47,63,63	4.30	14 (29%)
16	CDL	F	606	-	80,80,99	1.34	10 (12%)	86,92,111	1.08	4 (4%)
15	HEM	B	602	2	41,50,50	1.45	3 (7%)	45,82,82	1.30	6 (13%)
16	CDL	B	604	-	76,76,99	1.36	10 (13%)	82,88,111	1.16	4 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CDL	P	101	-	-	59/98/98/110	-
16	CDL	N	605	-	-	53/89/89/110	-
17	A1IRE	B	606	-	-	15/24/50/50	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	HEA	R	601	6	-	5/32/76/76	-
15	HEM	B	601	2	-	2/12/52/54	-
20	9Y0	S	301	-	-	19/46/46/52	-
16	CDL	B	605	-	-	51/89/89/110	-
13	9YF	M	502	-	-	23/54/78/78	0/1/1/1
18	HEC	C	301	3	-	2/10/54/54	-
16	CDL	C	305	-	-	47/89/89/110	-
24	MQ7	O	301	-	-	11/41/61/61	0/2/2/2
18	HEC	C	302	3	-	5/10/54/54	-
16	CDL	N	607	-	-	59/89/89/110	-
19	MQ9	C	304	-	-	17/53/73/73	0/2/2/2
18	HEC	O	302	3	-	1/10/54/54	-
16	CDL	M	503	-	-	41/84/84/110	-
14	PLM	A	503	-	-	1/13/14/15	-
16	CDL	F	605	-	-	46/86/86/110	-
19	MQ9	O	305	-	-	22/53/73/73	0/2/2/2
20	9Y0	G	301	-	-	22/46/46/52	-
24	MQ7	H	201	-	-	12/41/61/61	0/2/2/2
14	PLM	M	504	-	-	5/13/14/15	-
20	9Y0	D	102	-	-	21/44/44/52	-
16	CDL	B	603	-	-	42/84/84/110	-
16	CDL	R	605	-	-	42/86/86/110	-
16	CDL	P	103	-	-	63/105/105/110	-
16	CDL	R	606	-	-	56/91/91/110	-
22	HEA	F	602	6	-	9/32/76/76	-
13	9YF	C	303	-	-	34/54/78/78	0/1/1/1
12	FES	A	501	1	-	-	0/1/1/1
22	HEA	F	601	-	-	5/32/76/76	-
13	9YF	A	502	-	-	26/54/78/78	0/1/1/1
12	FES	M	501	1	-	-	0/1/1/1
14	PLM	T	201	-	-	6/13/14/15	-
20	9Y0	P	102	-	-	22/44/44/52	-
16	CDL	D	101	-	-	54/98/98/110	-
16	CDL	D	103	-	-	62/105/105/110	-
16	CDL	N	603	-	-	38/84/84/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CDL	N	604	-	-	44/87/87/110	-
15	HEM	N	602	2	-	1/12/54/54	-
18	HEC	O	303	3	-	1/10/54/54	-
22	HEA	R	602	6	-	6/32/76/76	-
15	HEM	N	601	2	-	4/12/52/54	-
13	9YF	O	304	-	-	36/54/78/78	0/1/1/1
14	PLM	G	302	-	-	4/13/14/15	-
17	A1IRE	N	606	-	-	13/24/50/50	0/5/5/5
16	CDL	F	606	-	-	44/91/91/110	-
15	HEM	B	602	2	-	2/12/54/54	-
16	CDL	B	604	-	-	43/87/87/110	-

All (342) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	H	201	MQ7	C3-C2	7.74	1.49	1.35
19	O	305	MQ9	C6-C5	7.42	1.48	1.35
24	O	301	MQ7	C3-C2	7.41	1.48	1.35
19	C	304	MQ9	C6-C5	7.40	1.48	1.35
17	N	606	A1IRE	S30-N28	6.76	1.71	1.59
17	B	606	A1IRE	S30-N28	6.64	1.70	1.59
18	O	303	HEC	C3C-C2C	-6.63	1.33	1.40
18	C	302	HEC	C3C-C2C	-6.52	1.33	1.40
18	C	301	HEC	C2B-C3B	-6.37	1.34	1.40
17	N	606	A1IRE	C27-C25	-6.23	1.48	1.54
18	C	302	HEC	C2B-C3B	-6.18	1.34	1.40
18	O	302	HEC	C3C-C2C	-6.15	1.34	1.40
18	O	302	HEC	C2B-C3B	-6.13	1.34	1.40
18	O	303	HEC	C2B-C3B	-6.13	1.34	1.40
18	C	301	HEC	C3C-C2C	-6.05	1.34	1.40
17	B	606	A1IRE	C27-C25	-6.02	1.49	1.54
17	B	606	A1IRE	C29-C25	-5.90	1.49	1.54
17	N	606	A1IRE	C29-C25	-5.86	1.49	1.54
22	F	602	HEA	C3B-C2B	5.71	1.47	1.34
22	F	602	HEA	C3A-C2A	5.66	1.48	1.40
22	R	602	HEA	C3B-C2B	5.58	1.47	1.34
18	C	301	HEC	C3D-C2D	5.55	1.54	1.37
22	R	602	HEA	C3A-C2A	5.43	1.47	1.40
18	O	303	HEC	C3D-C2D	5.43	1.53	1.37
18	O	302	HEC	C3D-C2D	5.42	1.53	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	F	601	HEA	C3B-C2B	5.42	1.46	1.34
22	R	601	HEA	C3B-C2B	5.41	1.46	1.34
18	C	302	HEC	C3D-C2D	5.36	1.53	1.37
17	B	606	A1IRE	C13-N15	5.32	1.45	1.33
17	N	606	A1IRE	C13-N15	5.28	1.45	1.33
22	R	601	HEA	C3A-C2A	5.23	1.47	1.40
22	F	602	HEA	CHD-C1D	5.17	1.48	1.35
22	F	601	HEA	C3A-C2A	5.17	1.47	1.40
22	F	602	HEA	C3D-C2D	5.16	1.47	1.36
22	R	602	HEA	CHD-C1D	5.12	1.48	1.35
22	R	602	HEA	C3D-C2D	5.11	1.47	1.36
22	F	601	HEA	C3D-C2D	5.08	1.47	1.36
22	F	602	HEA	CHC-C4B	5.02	1.47	1.35
22	R	601	HEA	C3D-C2D	4.97	1.47	1.36
19	C	304	MQ9	C3-C4	4.87	1.57	1.48
19	O	305	MQ9	C3-C4	4.84	1.57	1.48
22	R	602	HEA	CHC-C4B	4.80	1.47	1.35
24	O	301	MQ7	C5-C4	4.78	1.57	1.48
22	F	601	HEA	CHD-C1D	4.78	1.47	1.35
24	H	201	MQ7	C5-C4	4.77	1.57	1.48
22	F	601	HEA	CHC-C4B	4.77	1.47	1.35
19	O	305	MQ9	C2-C1	4.74	1.57	1.48
22	R	601	HEA	CHD-C1D	4.72	1.47	1.35
24	O	301	MQ7	C10-C1	4.72	1.57	1.48
24	H	201	MQ7	C10-C1	4.69	1.57	1.48
22	R	601	HEA	CHC-C4B	4.65	1.46	1.35
22	F	602	HEA	C3C-C2C	4.63	1.46	1.40
19	C	304	MQ9	C2-C1	4.57	1.56	1.48
22	F	601	HEA	C3C-C2C	4.44	1.46	1.40
22	R	602	HEA	C3C-C2C	4.37	1.46	1.40
22	R	601	HEA	C3C-C2C	4.33	1.46	1.40
15	B	602	HEM	C3C-C2C	-4.30	1.34	1.40
15	N	602	HEM	C3C-C2C	-4.16	1.34	1.40
16	R	606	CDL	OA8-CA7	3.88	1.44	1.33
16	B	603	CDL	OA8-CA7	3.81	1.44	1.33
16	D	103	CDL	OA8-CA7	3.80	1.44	1.33
16	N	603	CDL	OA8-CA7	3.79	1.44	1.33
16	F	606	CDL	OA8-CA7	3.79	1.44	1.33
16	D	101	CDL	OA8-CA7	3.79	1.44	1.33
16	P	103	CDL	OA8-CA7	3.77	1.44	1.33
16	B	605	CDL	OA8-CA7	3.75	1.44	1.33
16	R	605	CDL	OA8-CA7	3.74	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	M	503	CDL	OA8-CA7	3.72	1.44	1.33
16	C	305	CDL	OA8-CA7	3.72	1.44	1.33
16	P	101	CDL	OA8-CA7	3.71	1.44	1.33
16	N	607	CDL	OA8-CA7	3.70	1.44	1.33
16	F	605	CDL	OA8-CA7	3.69	1.44	1.33
16	N	605	CDL	OA8-CA7	3.69	1.44	1.33
16	M	503	CDL	OB8-CB7	3.67	1.44	1.33
16	B	604	CDL	OA8-CA7	3.66	1.44	1.33
16	P	101	CDL	OB8-CB7	3.61	1.43	1.33
16	D	103	CDL	OB8-CB7	3.60	1.43	1.33
16	F	606	CDL	OB8-CB7	3.59	1.43	1.33
16	B	604	CDL	OB8-CB7	3.59	1.43	1.33
16	C	305	CDL	OB8-CB7	3.59	1.43	1.33
16	D	101	CDL	OB8-CB7	3.58	1.43	1.33
16	F	606	CDL	OA6-CA5	3.57	1.44	1.34
16	N	604	CDL	OA8-CA7	3.57	1.43	1.33
16	D	103	CDL	OA6-CA5	3.55	1.44	1.34
16	N	607	CDL	OB8-CB7	3.55	1.43	1.33
16	F	605	CDL	OB8-CB7	3.54	1.43	1.33
16	R	606	CDL	OA6-CA5	3.54	1.44	1.34
16	P	103	CDL	OB8-CB7	3.54	1.43	1.33
16	N	604	CDL	OB8-CB7	3.53	1.43	1.33
16	R	605	CDL	OB8-CB7	3.51	1.43	1.33
16	R	606	CDL	OB8-CB7	3.50	1.43	1.33
16	B	605	CDL	OB8-CB7	3.49	1.43	1.33
16	B	603	CDL	OB8-CB7	3.48	1.43	1.33
15	B	602	HEM	C3C-CAC	3.46	1.54	1.47
16	N	603	CDL	OB8-CB7	3.44	1.43	1.33
16	P	103	CDL	OA6-CA5	3.40	1.43	1.34
16	N	605	CDL	OA6-CA5	3.39	1.43	1.34
16	B	605	CDL	OA6-CA5	3.37	1.43	1.34
15	N	602	HEM	C3C-CAC	3.35	1.54	1.47
16	N	605	CDL	OB8-CB7	3.34	1.43	1.33
16	F	605	CDL	OA6-CA5	3.33	1.43	1.34
16	P	101	CDL	OA6-CA5	3.31	1.43	1.34
16	R	605	CDL	OA6-CA5	3.29	1.43	1.34
16	D	101	CDL	OA6-CA5	3.29	1.43	1.34
16	M	503	CDL	OA6-CA5	3.25	1.43	1.34
17	B	606	A1IRE	C05-N04	3.25	1.36	1.33
16	B	604	CDL	OA6-CA5	3.25	1.43	1.34
16	C	305	CDL	OA6-CA5	3.19	1.43	1.34
16	N	603	CDL	OA6-CA5	3.19	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	603	CDL	OA6-CA5	3.17	1.43	1.34
16	N	607	CDL	OA6-CA5	3.16	1.43	1.34
16	N	604	CDL	OA6-CA5	3.14	1.43	1.34
22	F	602	HEA	C4B-NB	-3.13	1.34	1.40
22	R	602	HEA	C4B-NB	-3.11	1.34	1.40
22	R	601	HEA	FE-ND	3.06	2.12	1.96
22	R	601	HEA	FE-NB	3.05	2.12	1.96
22	F	601	HEA	FE-NB	3.04	2.11	1.96
17	N	606	A1IRE	O31-S30	3.02	1.46	1.42
22	F	601	HEA	FE-ND	3.00	2.11	1.96
17	B	606	A1IRE	O31-S30	2.98	1.46	1.42
17	N	606	A1IRE	C05-N04	2.98	1.36	1.33
16	F	605	CDL	OB6-CB5	2.97	1.42	1.34
22	F	602	HEA	C2A-C1A	2.95	1.49	1.42
15	B	601	HEM	CAB-C3B	2.94	1.55	1.47
15	N	601	HEM	CAB-C3B	2.93	1.55	1.47
22	R	602	HEA	C1D-ND	-2.92	1.35	1.40
22	R	602	HEA	FE-ND	2.91	2.11	1.96
17	N	606	A1IRE	O32-S30	2.90	1.46	1.42
16	D	103	CDL	OB6-CB5	2.89	1.42	1.34
16	F	606	CDL	OB6-CB5	2.88	1.42	1.34
22	R	602	HEA	FE-NB	2.88	2.11	1.96
16	N	605	CDL	OB6-CB5	2.88	1.42	1.34
15	B	602	HEM	CAB-C3B	2.87	1.55	1.47
16	M	503	CDL	OB6-CB5	2.87	1.42	1.34
15	N	602	HEM	CAB-C3B	2.87	1.55	1.47
22	R	602	HEA	C2A-C1A	2.87	1.49	1.42
22	F	602	HEA	C1D-ND	-2.86	1.35	1.40
17	B	606	A1IRE	C26-C23	-2.86	1.52	1.55
22	F	602	HEA	FE-ND	2.86	2.11	1.96
16	R	606	CDL	OB6-CB5	2.85	1.42	1.34
16	F	606	CDL	OB6-CB4	-2.85	1.39	1.46
16	B	604	CDL	OB6-CB4	-2.84	1.39	1.46
22	F	601	HEA	C2A-C1A	2.84	1.49	1.42
22	R	601	HEA	C1D-ND	-2.84	1.35	1.40
16	N	603	CDL	OB6-CB4	-2.83	1.39	1.46
17	N	606	A1IRE	C26-C23	-2.83	1.52	1.55
13	A	502	9YF	O9-C	-2.83	1.39	1.46
16	P	103	CDL	OB6-CB4	-2.82	1.39	1.46
16	P	101	CDL	OB6-CB4	-2.81	1.39	1.46
16	N	604	CDL	OB6-CB4	-2.81	1.39	1.46
16	D	101	CDL	OB6-CB5	2.79	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	D	103	CDL	OB6-CB4	-2.79	1.39	1.46
16	B	604	CDL	OB6-CB5	2.79	1.42	1.34
16	B	603	CDL	OB6-CB5	2.79	1.42	1.34
22	R	601	HEA	C2A-C1A	2.78	1.48	1.42
16	R	606	CDL	OB6-CB4	-2.78	1.39	1.46
16	B	605	CDL	OB6-CB4	-2.77	1.39	1.46
16	N	607	CDL	OB6-CB5	2.77	1.42	1.34
16	N	607	CDL	OB6-CB4	-2.77	1.39	1.46
16	C	305	CDL	OB6-CB5	2.77	1.42	1.34
16	N	604	CDL	OB6-CB5	2.77	1.42	1.34
22	F	601	HEA	C1D-ND	-2.77	1.35	1.40
22	F	602	HEA	FE-NB	2.76	2.10	1.96
16	R	605	CDL	OB6-CB5	2.75	1.42	1.34
16	D	101	CDL	OB6-CB4	-2.75	1.39	1.46
16	B	605	CDL	OB6-CB5	2.75	1.42	1.34
16	R	605	CDL	OB6-CB4	-2.75	1.39	1.46
16	M	503	CDL	OB6-CB4	-2.74	1.39	1.46
16	B	603	CDL	OB6-CB4	-2.74	1.39	1.46
16	C	305	CDL	OB6-CB4	-2.73	1.39	1.46
16	N	603	CDL	OB6-CB5	2.73	1.42	1.34
16	P	101	CDL	OB6-CB5	2.72	1.42	1.34
16	P	103	CDL	OB6-CB5	2.71	1.42	1.34
22	F	601	HEA	C4B-NB	-2.71	1.35	1.40
22	R	601	HEA	C4B-NB	-2.70	1.35	1.40
13	M	502	9YF	O9-C	-2.67	1.39	1.46
17	B	606	A1IRE	O32-S30	2.66	1.46	1.42
16	N	605	CDL	OB6-CB4	-2.66	1.39	1.46
20	G	301	9Y0	O7-C1	-2.65	1.40	1.46
13	C	303	9YF	O9-C	-2.63	1.40	1.46
17	N	606	A1IRE	C24-C23	-2.62	1.53	1.55
22	F	601	HEA	C4B-C3B	2.60	1.49	1.44
20	P	102	9Y0	O5-C5	2.58	1.40	1.33
22	R	601	HEA	C4B-C3B	2.58	1.48	1.44
20	S	301	9Y0	O7-C1	-2.56	1.40	1.46
16	F	605	CDL	OB6-CB4	-2.55	1.40	1.46
22	F	602	HEA	C1C-CHC	2.52	1.48	1.41
13	O	304	9YF	O9-C	-2.52	1.40	1.46
22	R	602	HEA	C4B-C3B	2.51	1.48	1.44
20	P	102	9Y0	O7-C21	2.49	1.41	1.34
22	F	602	HEA	C4C-CHD	2.47	1.47	1.41
13	O	304	9YF	O11-C25	2.45	1.40	1.33
22	R	602	HEA	C4C-CHD	2.45	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	D	102	9Y0	O7-C1	-2.44	1.40	1.46
20	S	301	9Y0	O5-C5	2.44	1.40	1.33
22	F	602	HEA	C4B-C3B	2.44	1.48	1.44
13	C	303	9YF	O11-C25	2.43	1.40	1.33
13	M	502	9YF	O11-C25	2.42	1.40	1.33
16	F	606	CDL	C11-CA5	2.42	1.57	1.50
20	D	102	9Y0	O5-C5	2.42	1.40	1.33
17	B	606	A1IRE	C24-C23	-2.40	1.53	1.55
15	N	601	HEM	FE-ND	2.40	2.08	1.96
16	N	603	CDL	OA6-CA4	-2.39	1.40	1.46
16	F	605	CDL	C11-CA5	2.39	1.57	1.50
20	G	301	9Y0	O5-C5	2.39	1.40	1.33
16	N	604	CDL	OA6-CA4	-2.38	1.40	1.46
16	R	606	CDL	C11-CA5	2.38	1.57	1.50
16	R	605	CDL	C11-CA5	2.37	1.57	1.50
16	M	503	CDL	PB2-OB5	2.36	1.68	1.59
16	P	103	CDL	C11-CA5	2.36	1.57	1.50
16	N	607	CDL	OA6-CA4	-2.36	1.40	1.46
16	D	101	CDL	C11-CA5	2.35	1.57	1.50
16	N	604	CDL	C11-CA5	2.35	1.57	1.50
16	P	101	CDL	C11-CA5	2.34	1.57	1.50
16	D	103	CDL	C11-CA5	2.34	1.57	1.50
15	N	601	HEM	C2C-C3C	-2.34	1.33	1.41
22	F	602	HEA	C1D-C2D	2.33	1.49	1.44
16	M	503	CDL	OA6-CA4	-2.32	1.40	1.46
16	M	503	CDL	C11-CA5	2.32	1.57	1.50
16	D	101	CDL	PB2-OB5	2.32	1.68	1.59
16	B	603	CDL	C11-CA5	2.32	1.57	1.50
13	A	502	9YF	O11-C25	2.32	1.40	1.33
22	F	602	HEA	C4D-C3D	2.31	1.49	1.45
16	C	305	CDL	PB2-OB5	2.29	1.68	1.59
16	N	605	CDL	PB2-OB5	2.29	1.68	1.59
16	F	605	CDL	PB2-OB5	2.28	1.68	1.59
16	B	605	CDL	C11-CA5	2.28	1.57	1.50
16	N	603	CDL	C11-CA5	2.28	1.57	1.50
24	O	301	MQ7	O1-C1	-2.28	1.18	1.23
16	B	603	CDL	OA6-CA4	-2.28	1.40	1.46
16	M	503	CDL	PB2-OB2	2.27	1.68	1.59
16	B	604	CDL	OA6-CA4	-2.27	1.40	1.46
16	R	605	CDL	PB2-OB5	2.27	1.68	1.59
15	B	601	HEM	C2C-C3C	-2.27	1.34	1.41
22	F	601	HEA	C4C-CHD	2.27	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	D	103	CDL	PB2-OB2	2.27	1.68	1.59
16	R	605	CDL	OA6-CA4	-2.27	1.40	1.46
16	R	605	CDL	PA1-OA5	2.27	1.68	1.59
16	P	101	CDL	PB2-OB2	2.26	1.68	1.59
16	P	101	CDL	OA6-CA4	-2.26	1.40	1.46
16	P	103	CDL	PA1-OA5	2.26	1.68	1.59
16	N	607	CDL	PB2-OB5	2.26	1.68	1.59
16	B	603	CDL	PB2-OB5	2.26	1.68	1.59
16	C	305	CDL	OA6-CA4	-2.26	1.41	1.46
16	P	101	CDL	PA1-OA5	2.25	1.68	1.59
22	R	602	HEA	C1C-CHC	2.25	1.47	1.41
16	D	103	CDL	PB2-OB5	2.25	1.68	1.59
22	F	602	HEA	CHB-C1B	2.25	1.47	1.41
16	B	605	CDL	PB2-OB5	2.24	1.68	1.59
16	M	503	CDL	PA1-OA5	2.24	1.68	1.59
22	F	601	HEA	C1D-C2D	2.24	1.48	1.44
16	N	605	CDL	C11-CA5	2.24	1.57	1.50
13	A	502	9YF	O11-C24	-2.24	1.40	1.45
16	F	605	CDL	PA1-OA5	2.24	1.68	1.59
16	B	604	CDL	C11-CA5	2.23	1.57	1.50
19	C	304	MQ9	O1-C1	-2.23	1.18	1.23
16	D	101	CDL	PA1-OA5	2.23	1.68	1.59
16	P	103	CDL	PB2-OB5	2.23	1.68	1.59
16	C	305	CDL	C11-CA5	2.23	1.57	1.50
16	D	101	CDL	OA6-CA4	-2.23	1.41	1.46
16	D	103	CDL	PA1-OA5	2.23	1.68	1.59
16	N	603	CDL	PA1-OA5	2.23	1.68	1.59
13	C	303	9YF	O9-C8	2.23	1.40	1.34
16	N	607	CDL	C11-CA5	2.23	1.57	1.50
16	P	103	CDL	PB2-OB2	2.22	1.68	1.59
19	O	305	MQ9	O4-C4	-2.22	1.18	1.23
16	C	305	CDL	PB2-OB2	2.22	1.68	1.59
16	R	605	CDL	PB2-OB2	2.22	1.68	1.59
16	P	101	CDL	PB2-OB5	2.22	1.68	1.59
16	N	603	CDL	PB2-OB2	2.22	1.68	1.59
16	N	605	CDL	PA1-OA5	2.21	1.68	1.59
16	B	604	CDL	PB2-OB5	2.21	1.68	1.59
16	F	605	CDL	OA6-CA4	-2.21	1.41	1.46
16	F	606	CDL	PB2-OB2	2.21	1.68	1.59
19	O	305	MQ9	O1-C1	-2.20	1.18	1.23
20	G	301	9Y0	O5-C	-2.20	1.40	1.45
16	N	607	CDL	PB2-OB2	2.20	1.68	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	N	603	CDL	PB2-OB5	2.20	1.68	1.59
22	R	602	HEA	C1D-C2D	2.20	1.48	1.44
13	O	304	9YF	O9-C8	2.20	1.40	1.34
16	B	603	CDL	PA1-OA5	2.20	1.68	1.59
16	N	604	CDL	PB2-OB5	2.19	1.68	1.59
16	C	305	CDL	PA1-OA5	2.19	1.68	1.59
16	R	606	CDL	PA1-OA5	2.19	1.68	1.59
16	N	607	CDL	PA1-OA5	2.19	1.68	1.59
16	F	605	CDL	PB2-OB2	2.18	1.68	1.59
16	R	606	CDL	PB2-OB5	2.18	1.68	1.59
16	D	101	CDL	PB2-OB2	2.17	1.68	1.59
16	B	604	CDL	PB2-OB2	2.17	1.68	1.59
24	H	201	MQ7	O1-C1	-2.17	1.18	1.23
17	N	606	A1IRE	C24-C25	-2.17	1.52	1.54
16	P	103	CDL	OA6-CA4	-2.16	1.41	1.46
16	N	605	CDL	PB2-OB2	2.16	1.68	1.59
15	B	601	HEM	FE-ND	2.16	2.07	1.96
22	R	601	HEA	C1B-C2B	2.15	1.48	1.44
16	B	603	CDL	PB2-OB2	2.15	1.68	1.59
16	F	606	CDL	PA1-OA5	2.15	1.68	1.59
13	M	502	9YF	O9-C8	2.15	1.40	1.34
24	O	301	MQ7	O4-C4	-2.15	1.18	1.23
22	R	601	HEA	C1D-C2D	2.15	1.48	1.44
22	F	602	HEA	CHA-C4D	2.14	1.47	1.41
13	C	303	9YF	O11-C24	-2.14	1.40	1.45
20	D	102	9Y0	O7-C21	2.13	1.40	1.34
16	B	605	CDL	PA1-OA5	2.13	1.67	1.59
20	D	102	9Y0	O5-C	-2.13	1.40	1.45
20	S	301	9Y0	O5-C	-2.13	1.40	1.45
16	B	604	CDL	PA1-OA5	2.13	1.67	1.59
20	S	301	9Y0	O7-C21	2.13	1.40	1.34
24	H	201	MQ7	O4-C4	-2.12	1.18	1.23
22	F	601	HEA	C1C-CHC	2.12	1.46	1.41
17	N	606	A1IRE	O14-C13	-2.12	1.19	1.23
16	N	604	CDL	PB2-OB2	2.12	1.67	1.59
17	B	606	A1IRE	O14-C13	-2.12	1.19	1.23
13	M	502	9YF	O11-C24	-2.12	1.40	1.45
16	R	606	CDL	PB2-OB2	2.12	1.67	1.59
19	C	304	MQ9	O4-C4	-2.11	1.18	1.23
22	R	601	HEA	C1C-CHC	2.11	1.46	1.41
22	F	602	HEA	C1B-C2B	2.10	1.48	1.44
22	R	601	HEA	C4C-CHD	2.10	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	605	CDL	PB2-OB2	2.10	1.67	1.59
20	G	301	9Y0	O7-C21	2.10	1.40	1.34
17	B	606	A1IRE	C26-C25	-2.10	1.52	1.54
16	F	606	CDL	PB2-OB5	2.10	1.67	1.59
22	R	601	HEA	C4D-C3D	2.09	1.48	1.45
13	O	304	9YF	O11-C24	-2.08	1.40	1.45
16	N	604	CDL	PA1-OA5	2.08	1.67	1.59
13	A	502	9YF	O9-C8	2.08	1.40	1.34
16	M	503	CDL	PA1-OA2	2.07	1.67	1.59
22	R	602	HEA	C4D-C3D	2.06	1.48	1.45
16	B	605	CDL	OA6-CA4	-2.05	1.41	1.46
22	R	602	HEA	CHA-C4D	2.05	1.47	1.41
16	C	305	CDL	C31-CA7	2.05	1.56	1.50
17	B	606	A1IRE	C08-CL09	2.04	1.79	1.74
16	R	605	CDL	C31-CA7	2.04	1.56	1.50
22	R	602	HEA	CHB-C1B	2.04	1.46	1.41
16	P	103	CDL	C31-CA7	2.04	1.56	1.50
16	F	606	CDL	C31-CA7	2.04	1.56	1.50
22	F	601	HEA	C1B-C2B	2.03	1.48	1.44
15	N	602	HEM	CMB-C2B	2.03	1.55	1.50
16	N	607	CDL	C31-CA7	2.02	1.56	1.50
16	M	503	CDL	C31-CA7	2.00	1.56	1.50
17	N	606	A1IRE	C08-CL09	2.00	1.78	1.74

All (341) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	N	606	A1IRE	C26-C25-C29	16.41	169.33	120.79
17	B	606	A1IRE	C26-C25-C29	16.28	168.93	120.79
17	N	606	A1IRE	O32-S30-O31	-10.50	100.97	120.87
17	B	606	A1IRE	O32-S30-O31	-10.13	101.67	120.87
17	N	606	A1IRE	C24-C23-C20	-8.79	105.47	119.33
17	N	606	A1IRE	C24-C25-C29	-8.07	96.92	120.79
17	B	606	A1IRE	C24-C25-C29	-8.00	97.14	120.79
17	B	606	A1IRE	C26-C25-C27	-7.75	97.85	120.79
17	N	606	A1IRE	C24-C25-C27	-7.65	98.16	120.79
17	B	606	A1IRE	C24-C23-C20	-7.63	107.30	119.33
17	N	606	A1IRE	C26-C25-C27	-7.43	98.80	120.79
17	N	606	A1IRE	C26-C23-C20	7.37	130.94	119.33
17	B	606	A1IRE	C24-C25-C27	-7.20	99.49	120.79
22	R	601	HEA	C3D-C4D-ND	6.71	116.85	110.36
22	F	601	HEA	C3D-C4D-ND	6.66	116.81	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B	606	A1IRE	C26-C23-C20	6.25	129.18	119.33
22	R	602	HEA	C3D-C4D-ND	5.89	116.06	110.36
17	B	606	A1IRE	C29-N28-S30	5.68	135.25	122.96
22	R	601	HEA	C2D-C1D-ND	5.66	116.54	109.84
22	F	602	HEA	CHA-C4D-ND	-5.60	118.35	124.43
22	R	601	HEA	C2B-C1B-NB	5.56	116.55	109.88
22	R	601	HEA	C3B-C4B-NB	5.56	116.43	109.84
22	F	601	HEA	C2B-C1B-NB	5.54	116.52	109.88
22	F	602	HEA	C3D-C4D-ND	5.43	115.62	110.36
17	B	606	A1IRE	C27-N28-S30	5.36	134.54	122.96
22	F	601	HEA	C2D-C1D-ND	5.33	116.15	109.84
22	F	601	HEA	C3B-C4B-NB	5.29	116.11	109.84
17	N	606	A1IRE	C29-N28-S30	5.29	134.40	122.96
17	N	606	A1IRE	C27-N28-S30	5.14	134.07	122.96
22	R	602	HEA	C3B-C4B-NB	5.13	115.92	109.84
22	R	602	HEA	C2B-C1B-NB	5.07	115.96	109.88
16	M	503	CDL	OB6-CB5-C51	4.70	121.62	111.50
22	R	602	HEA	CHA-C4D-ND	-4.66	119.37	124.43
17	B	606	A1IRE	C33-S30-N28	4.64	110.40	104.65
17	B	606	A1IRE	O31-S30-C33	4.63	111.52	104.35
17	N	606	A1IRE	C17-C16-N15	-4.63	103.13	113.05
17	N	606	A1IRE	C33-S30-N28	4.58	110.32	104.65
16	D	103	CDL	OB6-CB5-C51	4.57	121.35	111.50
22	F	602	HEA	C2B-C1B-NB	4.53	115.31	109.88
17	N	606	A1IRE	O31-S30-C33	4.51	111.34	104.35
16	B	603	CDL	OB6-CB5-C51	4.49	121.17	111.50
22	R	602	HEA	C2D-C1D-ND	4.48	115.15	109.84
16	N	605	CDL	OB6-CB5-C51	4.46	121.12	111.50
16	F	605	CDL	OB6-CB5-C51	4.43	121.06	111.50
22	F	602	HEA	C3B-C4B-NB	4.42	115.08	109.84
22	R	601	HEA	C1D-C2D-C3D	-4.37	102.36	106.96
22	R	602	HEA	CBA-CAA-C2A	-4.35	105.27	112.60
24	O	301	MQ7	C11-C12-C13	-4.31	119.61	126.79
22	F	601	HEA	C1D-C2D-C3D	-4.26	102.47	106.96
17	N	606	A1IRE	O32-S30-C33	4.24	110.91	104.35
16	N	604	CDL	OB6-CB5-C51	4.21	120.58	111.50
22	F	602	HEA	C2D-C1D-ND	4.21	114.83	109.84
16	C	305	CDL	OB6-CB5-C51	4.20	120.56	111.50
16	B	605	CDL	OB6-CB5-C51	4.20	120.55	111.50
16	B	604	CDL	OA6-CA5-C11	4.19	120.54	111.50
16	M	503	CDL	OA6-CA5-C11	4.18	120.52	111.50
16	P	103	CDL	OA6-CA5-C11	4.16	120.46	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	F	602	HEA	C13-C12-C11	-4.16	108.10	114.35
17	B	606	A1IRE	O32-S30-C33	4.15	110.77	104.35
16	N	607	CDL	OA6-CA5-C11	4.07	120.26	111.50
16	C	305	CDL	OA6-CA5-C11	4.04	120.21	111.50
24	H	201	MQ7	C11-C12-C13	-4.03	120.08	126.79
16	R	605	CDL	OB6-CB5-C51	4.03	120.19	111.50
19	O	305	MQ9	C7-C8-C9	-4.02	120.09	126.79
13	M	502	9YF	O9-C8-C9	4.02	120.16	111.50
16	P	101	CDL	OA6-CA5-C11	4.02	120.16	111.50
16	P	103	CDL	OB6-CB5-C51	4.01	120.15	111.50
16	N	607	CDL	OB6-CB5-C51	4.01	120.14	111.50
22	R	601	HEA	C3C-C4C-NC	3.99	114.37	109.21
22	F	601	HEA	C3C-C4C-NC	3.98	114.36	109.21
16	N	603	CDL	OB6-CB5-C51	3.98	120.08	111.50
20	D	102	9Y0	O7-C21-C22	3.97	120.07	111.50
16	F	605	CDL	OA6-CA5-C11	3.97	120.06	111.50
16	B	604	CDL	OB6-CB5-C51	3.95	120.02	111.50
16	R	605	CDL	OA6-CA5-C11	3.95	120.01	111.50
16	D	101	CDL	OA6-CA5-C11	3.92	119.94	111.50
16	R	606	CDL	OB6-CB5-C51	3.89	119.88	111.50
16	D	103	CDL	OA6-CA5-C11	3.89	119.87	111.50
16	N	604	CDL	OA6-CA5-C11	3.87	119.83	111.50
16	D	101	CDL	OB6-CB5-C51	3.85	119.80	111.50
22	F	602	HEA	C4D-CHA-C1A	-3.85	117.48	122.56
16	P	101	CDL	OB6-CB5-C51	3.83	119.76	111.50
16	B	603	CDL	OA6-CA5-C11	3.83	119.76	111.50
19	C	304	MQ9	C7-C8-C9	-3.82	120.44	126.79
16	B	605	CDL	OA6-CA5-C11	3.79	119.68	111.50
16	N	603	CDL	OA6-CA5-C11	3.79	119.67	111.50
13	O	304	9YF	O9-C8-C9	3.77	119.63	111.50
20	S	301	9Y0	O7-C21-C22	3.75	119.58	111.50
18	C	301	HEC	CMC-C2C-C1C	-3.74	122.71	128.46
22	F	601	HEA	C1B-C2B-C3B	-3.66	102.42	106.80
13	A	502	9YF	O9-C8-C9	3.63	119.33	111.50
22	R	601	HEA	C1B-C2B-C3B	-3.61	102.48	106.80
22	R	602	HEA	C1D-C2D-C3D	-3.61	103.16	106.96
22	F	602	HEA	C1D-C2D-C3D	-3.60	103.17	106.96
16	N	605	CDL	OA6-CA5-C11	3.58	119.23	111.50
22	F	602	HEA	CBA-CAA-C2A	-3.57	106.59	112.60
22	F	602	HEA	C13-C14-C15	-3.56	119.08	127.66
22	F	602	HEA	C1B-C2B-C3B	-3.56	102.54	106.80
16	F	606	CDL	OB6-CB5-C51	3.54	119.12	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	R	602	HEA	C1B-C2B-C3B	-3.52	102.59	106.80
13	C	303	9YF	O9-C8-C9	3.48	119.00	111.50
19	O	305	MQ9	C17-C18-C19	-3.43	119.41	127.66
22	R	601	HEA	C13-C12-C11	-3.41	109.22	114.35
22	R	602	HEA	C13-C12-C11	-3.41	109.23	114.35
24	H	201	MQ7	C24-C23-C25	3.39	120.97	115.27
20	G	301	9Y0	O7-C21-C22	3.35	118.72	111.50
16	F	606	CDL	OA6-CA5-C11	3.34	118.69	111.50
22	R	602	HEA	C4D-C3D-C2D	-3.33	102.04	106.90
24	O	301	MQ7	C36-C37-C38	-3.33	119.65	127.66
22	R	601	HEA	C4D-C3D-C2D	-3.27	102.13	106.90
22	R	602	HEA	C17-C18-C19	-3.27	119.78	127.66
18	C	302	HEC	CBA-CAA-C2A	-3.27	107.09	112.60
24	O	301	MQ7	C24-C23-C25	3.26	120.75	115.27
22	F	601	HEA	C4D-C3D-C2D	-3.26	102.15	106.90
24	H	201	MQ7	C36-C37-C38	-3.26	119.82	127.66
22	F	601	HEA	C13-C14-C15	-3.24	119.86	127.66
24	O	301	MQ7	C31-C32-C33	-3.22	119.92	127.66
19	C	304	MQ9	C32-C33-C34	-3.21	119.94	127.66
16	R	606	CDL	OA6-CA5-C11	3.21	118.41	111.50
22	F	602	HEA	C4D-C3D-C2D	-3.20	102.23	106.90
22	R	601	HEA	CHA-C4D-ND	-3.19	120.97	124.43
18	O	302	HEC	CMC-C2C-C1C	-3.17	123.59	128.46
22	F	601	HEA	C27-C19-C20	3.16	120.59	115.27
22	R	602	HEA	C13-C14-C15	-3.16	120.04	127.66
19	C	304	MQ9	C25-C24-C26	3.16	120.59	115.27
19	C	304	MQ9	C45-C44-C46	3.16	120.58	115.27
22	F	602	HEA	CAD-C3D-C4D	3.16	130.17	124.66
19	O	305	MQ9	C15-C14-C16	3.15	120.57	115.27
20	P	102	9Y0	O7-C21-C22	3.14	118.26	111.50
22	R	601	HEA	C13-C14-C15	-3.12	120.14	127.66
22	R	602	HEA	C3C-C4C-NC	3.12	113.24	109.21
24	H	201	MQ7	C21-C22-C23	-3.11	120.18	127.66
22	R	601	HEA	CHB-C1B-NB	-3.10	121.06	124.43
22	F	602	HEA	CHB-C1B-NB	-3.10	121.07	124.43
24	H	201	MQ7	C26-C27-C28	-3.07	120.26	127.66
22	F	602	HEA	C17-C18-C19	-3.06	120.29	127.66
22	R	601	HEA	CBA-CAA-C2A	-3.02	107.51	112.60
18	O	302	HEC	CMB-C2B-C1B	-3.02	123.83	128.46
22	R	602	HEA	C4D-CHA-C1A	-3.01	118.58	122.56
24	O	301	MQ7	C26-C27-C28	-3.01	120.41	127.66
19	C	304	MQ9	C37-C38-C39	-3.00	120.43	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	F	602	HEA	CAD-CBD-CGD	-2.98	107.18	113.60
19	O	305	MQ9	C32-C33-C34	-2.98	120.49	127.66
22	R	602	HEA	C4B-C3B-C2B	-2.97	102.33	107.41
22	R	601	HEA	C4B-C3B-C2B	-2.97	102.33	107.41
24	H	201	MQ7	C14-C13-C15	2.97	120.27	115.27
19	O	305	MQ9	C25-C24-C26	2.96	120.25	115.27
22	R	601	HEA	CMB-C2B-C1B	2.91	129.48	125.04
15	N	601	HEM	C4D-ND-C1D	2.90	108.07	105.07
24	H	201	MQ7	C31-C32-C33	-2.89	120.69	127.66
13	M	502	9YF	C7-C6-C5	2.88	115.84	110.82
22	F	602	HEA	C3C-C4C-NC	2.88	112.93	109.21
24	O	301	MQ7	C29-C28-C30	2.87	120.10	115.27
19	C	304	MQ9	C15-C14-C16	2.87	120.10	115.27
22	R	601	HEA	C1D-ND-C4D	-2.86	102.12	105.07
17	B	606	A1IRE	C17-C16-N15	-2.86	106.92	113.05
22	R	601	HEA	CMC-C2C-C3C	2.85	130.01	124.68
22	F	601	HEA	C4B-C3B-C2B	-2.85	102.54	107.41
22	F	601	HEA	CBA-CAA-C2A	-2.85	107.80	112.60
19	C	304	MQ9	C22-C23-C24	-2.84	120.81	127.66
19	O	305	MQ9	C12-C13-C14	-2.84	120.82	127.66
19	C	304	MQ9	C12-C13-C14	-2.84	120.83	127.66
24	H	201	MQ7	C34-C33-C35	2.83	120.03	115.27
22	R	602	HEA	CHB-C1B-NB	-2.82	121.37	124.43
19	C	304	MQ9	C5M-C5-C6	-2.80	119.83	124.40
15	B	602	HEM	C1B-NB-C4B	2.79	107.96	105.07
22	R	602	HEA	CMC-C2C-C3C	2.79	129.89	124.68
15	B	601	HEM	C4D-ND-C1D	2.78	107.94	105.07
22	R	601	HEA	C25-C23-C24	2.77	120.73	114.60
22	R	601	HEA	C4B-NB-C1B	-2.77	102.22	105.07
19	O	305	MQ9	C42-C43-C44	-2.76	121.00	127.66
24	H	201	MQ7	C29-C28-C30	2.75	119.90	115.27
15	B	601	HEM	C1B-NB-C4B	2.75	107.91	105.07
24	H	201	MQ7	C19-C18-C20	2.74	119.89	115.27
19	O	305	MQ9	C22-C23-C24	-2.74	121.06	127.66
16	M	503	CDL	OA8-CA7-C31	2.74	120.49	111.91
18	C	302	HEC	CMB-C2B-C1B	-2.73	124.27	128.46
17	B	606	A1IRE	C26-C23-C24	2.73	90.24	88.08
13	M	502	9YF	O11-C25-C26	2.72	120.44	111.91
16	B	603	CDL	OA8-CA7-C31	2.70	120.39	111.91
16	M	503	CDL	OB8-CB7-C71	2.70	120.39	111.91
22	R	601	HEA	C27-C19-C20	2.70	119.81	115.27
22	F	601	HEA	CAD-CBD-CGD	-2.70	107.80	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	B	604	CDL	OB8-CB7-C71	2.70	120.37	111.91
24	O	301	MQ7	C21-C22-C23	-2.70	121.17	127.66
22	F	601	HEA	C25-C23-C24	2.70	120.56	114.60
15	N	602	HEM	C4D-ND-C1D	2.69	107.86	105.07
15	N	601	HEM	C1B-NB-C4B	2.69	107.86	105.07
22	F	601	HEA	CMB-C2B-C1B	2.69	129.14	125.04
16	F	605	CDL	OA8-CA7-C31	2.68	120.32	111.91
22	F	601	HEA	CHB-C1B-NB	-2.68	121.52	124.43
22	F	601	HEA	CMC-C2C-C3C	2.67	129.68	124.68
24	O	301	MQ7	C34-C33-C35	2.67	119.76	115.27
22	F	602	HEA	C4B-C3B-C2B	-2.67	102.86	107.41
15	B	602	HEM	C4B-CHC-C1C	2.65	126.06	122.56
16	R	605	CDL	OA8-CA7-C31	2.65	120.23	111.91
16	N	607	CDL	OA8-CA7-C31	2.65	120.22	111.91
22	R	602	HEA	C27-C19-C20	2.65	119.73	115.27
13	O	304	9YF	O11-C25-C26	2.65	120.22	111.91
16	B	603	CDL	OB8-CB7-C71	2.65	120.22	111.91
18	C	301	HEC	CMB-C2B-C1B	-2.64	124.40	128.46
19	O	305	MQ9	C45-C44-C46	2.64	119.72	115.27
16	N	603	CDL	OB8-CB7-C71	2.63	120.17	111.91
16	C	305	CDL	OA8-CA7-C31	2.63	120.17	111.91
16	D	101	CDL	OA8-CA7-C31	2.63	120.17	111.91
16	C	305	CDL	OB8-CB7-C71	2.63	120.16	111.91
16	D	103	CDL	OA8-CA7-C31	2.63	120.15	111.91
16	N	604	CDL	OB8-CB7-C71	2.63	120.15	111.91
20	G	301	9Y0	O5-C5-C6	2.62	120.14	111.91
22	F	601	HEA	C26-C15-C16	2.62	119.68	115.27
19	O	305	MQ9	C35-C34-C36	2.62	119.67	115.27
19	O	305	MQ9	C37-C38-C39	-2.61	121.37	127.66
22	R	602	HEA	CAD-C3D-C4D	2.61	129.22	124.66
16	P	103	CDL	OB8-CB7-C71	2.60	120.08	111.91
16	R	605	CDL	OB8-CB7-C71	2.60	120.07	111.91
19	C	304	MQ9	C35-C34-C36	2.60	119.64	115.27
22	F	602	HEA	C27-C19-C20	2.60	119.64	115.27
24	H	201	MQ7	C16-C17-C18	-2.60	121.40	127.66
16	N	607	CDL	OB8-CB7-C71	2.60	120.05	111.91
16	P	103	CDL	OA8-CA7-C31	2.59	120.04	111.91
13	A	502	9YF	O11-C25-C26	2.59	120.04	111.91
22	F	601	HEA	C13-C12-C11	-2.59	110.46	114.35
16	B	604	CDL	OA8-CA7-C31	2.59	120.03	111.91
16	N	603	CDL	OA8-CA7-C31	2.59	120.03	111.91
16	N	604	CDL	OA8-CA7-C31	2.59	120.02	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	C	304	MQ9	C40-C39-C41	2.58	119.61	115.27
16	R	606	CDL	OB8-CB7-C71	2.58	120.01	111.91
22	F	601	HEA	C4B-NB-C1B	-2.58	102.41	105.07
16	D	103	CDL	OB8-CB7-C71	2.58	120.01	111.91
24	H	201	MQ7	C39-C38-C40	2.58	119.60	115.27
22	F	601	HEA	C1D-ND-C4D	-2.57	102.42	105.07
24	O	301	MQ7	C19-C18-C20	2.57	119.60	115.27
20	S	301	9Y0	O5-C5-C6	2.56	119.96	111.91
16	F	606	CDL	OA8-CA7-C31	2.56	119.94	111.91
22	F	602	HEA	C26-C15-C16	2.56	119.58	115.27
19	C	304	MQ9	C17-C18-C19	-2.56	121.50	127.66
16	F	605	CDL	OB8-CB7-C71	2.55	119.92	111.91
13	O	304	9YF	C7-C2-C3	2.54	114.51	110.85
18	O	303	HEC	CMB-C2B-C1B	-2.53	124.57	128.46
15	N	602	HEM	C4B-CHC-C1C	2.53	125.90	122.56
17	N	606	A1IRE	C03-C12-C13	-2.53	126.39	131.24
19	O	305	MQ9	C10-C9-C11	2.53	119.52	115.27
16	B	605	CDL	OB8-CB7-C71	2.52	119.83	111.91
19	C	304	MQ9	C5M-C5-C4	2.52	120.45	116.27
19	O	305	MQ9	C5M-C5-C6	-2.52	120.29	124.40
16	P	101	CDL	OA8-CA7-C31	2.52	119.81	111.91
13	C	303	9YF	O11-C25-C26	2.51	119.79	111.91
20	P	102	9Y0	O5-C5-C6	2.50	119.74	111.91
13	M	502	9YF	C6-C5-C4	2.49	115.17	110.82
16	D	101	CDL	OB8-CB7-C71	2.48	119.70	111.91
24	O	301	MQ7	C45-C43-C44	2.48	120.09	114.60
20	D	102	9Y0	O5-C5-C6	2.47	119.67	111.91
19	O	305	MQ9	C30-C29-C31	2.47	119.43	115.27
18	O	303	HEC	CBD-CAD-C3D	-2.47	108.40	112.62
19	O	305	MQ9	C27-C28-C29	-2.46	121.73	127.66
16	P	101	CDL	OB8-CB7-C71	2.46	119.64	111.91
19	C	304	MQ9	C42-C43-C44	-2.46	121.73	127.66
16	R	606	CDL	OA8-CA7-C31	2.46	119.62	111.91
22	F	602	HEA	CMB-C2B-C1B	2.45	128.77	125.04
24	O	301	MQ7	C2M-C2-C3	-2.44	120.42	124.40
18	C	301	HEC	C1D-C2D-C3D	-2.43	105.31	107.00
15	N	602	HEM	CMC-C2C-C3C	2.43	129.22	124.68
15	N	602	HEM	C4C-CHD-C1D	2.43	125.76	122.56
15	B	602	HEM	C4D-ND-C1D	2.42	107.57	105.07
22	F	602	HEA	C25-C23-C24	2.42	119.94	114.60
24	O	301	MQ7	C16-C17-C18	-2.42	121.84	127.66
24	H	201	MQ7	C45-C43-C44	2.41	119.92	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	R	602	HEA	C25-C23-C24	2.40	119.90	114.60
16	F	606	CDL	OB8-CB7-C71	2.40	119.43	111.91
24	O	301	MQ7	C41-C42-C43	-2.39	119.57	127.75
19	O	305	MQ9	C40-C39-C41	2.39	119.30	115.27
16	N	605	CDL	OA8-CA7-C31	2.39	119.42	111.91
22	F	601	HEA	CHA-C4D-ND	-2.39	121.83	124.43
15	N	601	HEM	C4B-CHC-C1C	2.39	125.71	122.56
19	O	305	MQ9	C51-C49-C50	2.39	119.88	114.60
22	R	601	HEA	C17-C18-C19	-2.38	121.92	127.66
15	N	602	HEM	C1B-NB-C4B	2.38	107.53	105.07
19	C	304	MQ9	C10-C9-C11	2.38	119.27	115.27
22	R	602	HEA	CAD-CBD-CGD	-2.37	108.50	113.60
15	B	601	HEM	C4B-CHC-C1C	2.37	125.69	122.56
17	B	606	A1IRE	C03-C12-C13	-2.37	126.69	131.24
22	F	601	HEA	CHA-C4D-C3D	-2.37	121.36	124.84
19	C	304	MQ9	C20-C19-C21	2.36	119.24	115.27
15	N	602	HEM	CBA-CAA-C2A	-2.35	108.61	112.62
22	R	602	HEA	C26-C15-C16	2.34	119.22	115.27
22	R	601	HEA	CHD-C1D-C2D	-2.34	120.26	126.72
16	B	605	CDL	OA8-CA7-C31	2.34	119.24	111.91
22	R	601	HEA	C26-C15-C16	2.33	119.19	115.27
22	F	602	HEA	CMD-C2D-C1D	2.33	128.58	125.04
22	F	602	HEA	CHC-C4B-NB	-2.32	121.52	124.38
19	O	305	MQ9	C47-C48-C49	-2.32	119.83	127.75
18	C	302	HEC	CMC-C2C-C1C	-2.31	124.91	128.46
22	F	602	HEA	CMC-C2C-C3C	2.29	128.97	124.68
16	N	605	CDL	OB8-CB7-C71	2.28	119.08	111.91
19	O	305	MQ9	C20-C19-C21	2.28	119.11	115.27
19	O	305	MQ9	C5M-C5-C4	2.28	120.04	116.27
24	O	301	MQ7	C39-C38-C40	2.28	119.10	115.27
19	C	304	MQ9	C27-C28-C29	-2.28	122.18	127.66
18	O	303	HEC	C1D-C2D-C3D	-2.27	105.42	107.00
22	R	601	HEA	C21-C22-C23	-2.25	120.06	127.75
13	A	502	9YF	C7-C6-C5	2.25	114.75	110.82
22	R	602	HEA	CHC-C4B-NB	-2.24	121.61	124.38
15	N	601	HEM	CMA-C3A-C4A	-2.23	125.03	128.46
24	O	301	MQ7	C14-C13-C15	2.23	119.03	115.27
13	A	502	9YF	C31-C32-C33	-2.20	108.81	115.92
18	O	302	HEC	CBD-CAD-C3D	-2.19	108.88	112.62
22	F	601	HEA	CHD-C1D-C2D	-2.18	120.68	126.72
22	R	602	HEA	CMB-C2B-C1B	2.18	128.35	125.04
15	N	602	HEM	CMA-C3A-C4A	-2.17	125.12	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	H	201	MQ7	C41-C42-C43	-2.17	120.34	127.75
15	B	601	HEM	C3C-C2C-C1C	2.14	108.33	106.85
22	R	601	HEA	CAD-C3D-C4D	2.14	128.40	124.66
19	C	304	MQ9	C51-C49-C50	2.14	119.32	114.60
15	N	601	HEM	C3D-C4D-ND	-2.14	107.79	110.17
18	O	302	HEC	C1D-C2D-C3D	-2.13	105.51	107.00
19	C	304	MQ9	C47-C48-C49	-2.12	120.50	127.75
22	R	601	HEA	CAD-CBD-CGD	-2.12	109.05	113.60
17	B	606	A1IRE	C29-C25-C27	2.12	88.98	85.68
16	P	101	CDL	CB4-OB6-CB5	-2.11	112.59	117.79
15	B	601	HEM	C3D-C4D-ND	-2.10	107.83	110.17
13	A	502	9YF	C6-C5-C4	2.10	114.49	110.82
13	M	502	9YF	C31-C32-C33	-2.10	109.14	115.92
18	O	302	HEC	CAA-CBA-CGA	-2.09	107.90	113.76
22	F	601	HEA	C17-C18-C19	-2.08	122.64	127.66
15	N	601	HEM	C3C-C2C-C1C	2.07	108.28	106.85
22	R	602	HEA	C21-C22-C23	-2.07	120.69	127.75
13	A	502	9YF	C36-C35-C33	-2.06	109.27	115.92
15	B	602	HEM	CMC-C2C-C3C	2.05	128.52	124.68
15	B	602	HEM	C4A-C3A-C2A	2.05	108.42	107.00
22	F	602	HEA	C21-C22-C23	-2.05	120.76	127.75
22	R	602	HEA	OMA-CMA-C3A	-2.04	120.47	124.91
22	R	601	HEA	CMD-C2D-C1D	2.04	128.14	125.04
22	F	602	HEA	OMA-CMA-C3A	-2.04	120.48	124.91
16	M	503	CDL	OB6-CB5-OB7	-2.02	118.81	123.70
15	N	601	HEM	CBD-CAD-C3D	-2.02	107.01	112.63
15	N	602	HEM	C4A-C3A-C2A	2.02	108.40	107.00
22	R	601	HEA	CHC-C4B-C3B	-2.02	120.60	125.80
18	O	302	HEC	CMB-C2B-C3B	2.01	128.19	125.82
15	B	601	HEM	C3B-C2B-C1B	2.00	107.97	106.49
19	C	304	MQ9	C30-C29-C31	2.00	118.64	115.27
15	B	602	HEM	CAD-CBD-CGD	-2.00	109.30	113.60

There are no chirality outliers.

All (1196) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	502	9YF	C1-O-P-O1
13	A	502	9YF	C1-O-P-O8
13	A	502	9YF	O9-C-C1-O
13	C	303	9YF	C2-O2-P-O
13	C	303	9YF	C1-O-P-O1

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Mol	Chain	Res	Type	Atoms
13	C	303	9YF	C1-O-P-O8
13	M	502	9YF	C1-O-P-O1
13	M	502	9YF	C1-O-P-O2
13	M	502	9YF	C1-O-P-O8
13	M	502	9YF	O9-C-C1-O
13	O	304	9YF	C1-O-P-O1
13	O	304	9YF	C1-O-P-O8
16	B	603	CDL	CA2-OA2-PA1-OA3
16	B	603	CDL	CA2-OA2-PA1-OA4
16	B	603	CDL	CA3-OA5-PA1-OA4
16	B	603	CDL	C11-CA5-OA6-CA4
16	B	604	CDL	CA2-OA2-PA1-OA4
16	B	604	CDL	CB2-OB2-PB2-OB3
16	B	604	CDL	CB2-OB2-PB2-OB4
16	B	604	CDL	CB3-OB5-PB2-OB4
16	B	604	CDL	C51-CB5-OB6-CB4
16	B	605	CDL	CA2-OA2-PA1-OA3
16	B	605	CDL	CA2-OA2-PA1-OA4
16	B	605	CDL	CA2-OA2-PA1-OA5
16	B	605	CDL	CA3-OA5-PA1-OA4
16	B	605	CDL	CB3-OB5-PB2-OB3
16	B	605	CDL	CB3-OB5-PB2-OB4
16	B	605	CDL	OB7-CB5-OB6-CB4
16	C	305	CDL	CA2-OA2-PA1-OA3
16	C	305	CDL	CA3-OA5-PA1-OA3
16	C	305	CDL	CB3-OB5-PB2-OB4
16	D	101	CDL	CB2-C1-CA2-OA2
16	D	101	CDL	CA2-OA2-PA1-OA3
16	D	101	CDL	CA2-OA2-PA1-OA4
16	D	101	CDL	CA3-OA5-PA1-OA3
16	D	101	CDL	CA3-OA5-PA1-OA4
16	D	101	CDL	C51-CB5-OB6-CB4
16	D	103	CDL	CB3-OB5-PB2-OB3
16	D	103	CDL	OB7-CB5-OB6-CB4
16	D	103	CDL	C51-CB5-OB6-CB4
16	F	605	CDL	CA2-OA2-PA1-OA3
16	F	605	CDL	CA2-OA2-PA1-OA4
16	F	605	CDL	CB2-OB2-PB2-OB3
16	F	605	CDL	CB2-OB2-PB2-OB4
16	F	605	CDL	CB3-OB5-PB2-OB3
16	F	605	CDL	CB3-OB5-PB2-OB4
16	F	605	CDL	C51-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
16	F	606	CDL	O1-C1-CB2-OB2
16	F	606	CDL	CB2-OB2-PB2-OB3
16	F	606	CDL	CB3-OB5-PB2-OB3
16	M	503	CDL	CA2-OA2-PA1-OA3
16	M	503	CDL	CA2-OA2-PA1-OA4
16	M	503	CDL	CA3-OA5-PA1-OA3
16	M	503	CDL	CA3-OA5-PA1-OA4
16	M	503	CDL	C11-CA5-OA6-CA4
16	M	503	CDL	CB2-OB2-PB2-OB3
16	M	503	CDL	CB2-OB2-PB2-OB4
16	M	503	CDL	OB6-CB4-CB6-OB8
16	M	503	CDL	OB7-CB5-OB6-CB4
16	M	503	CDL	C51-CB5-OB6-CB4
16	M	503	CDL	OB9-CB7-OB8-CB6
16	M	503	CDL	C71-CB7-OB8-CB6
16	N	603	CDL	CB3-OB5-PB2-OB3
16	N	603	CDL	CB3-OB5-PB2-OB4
16	N	604	CDL	O1-C1-CA2-OA2
16	N	604	CDL	CA2-OA2-PA1-OA3
16	N	604	CDL	CA3-OA5-PA1-OA3
16	N	604	CDL	CB3-OB5-PB2-OB2
16	N	604	CDL	CB3-OB5-PB2-OB3
16	N	604	CDL	OB7-CB5-OB6-CB4
16	N	604	CDL	C51-CB5-OB6-CB4
16	N	605	CDL	O1-C1-CB2-OB2
16	N	605	CDL	CB3-OB5-PB2-OB4
16	N	605	CDL	OB7-CB5-OB6-CB4
16	N	605	CDL	C51-CB5-OB6-CB4
16	N	607	CDL	CA3-OA5-PA1-OA2
16	N	607	CDL	CB2-OB2-PB2-OB4
16	N	607	CDL	CB2-OB2-PB2-OB5
16	N	607	CDL	OB9-CB7-OB8-CB6
16	P	101	CDL	O1-C1-CB2-OB2
16	P	101	CDL	CA2-C1-CB2-OB2
16	P	101	CDL	CA3-OA5-PA1-OA3
16	P	101	CDL	OA5-CA3-CA4-OA6
16	P	101	CDL	CB2-OB2-PB2-OB3
16	P	101	CDL	CB2-OB2-PB2-OB4
16	P	101	CDL	CB2-OB2-PB2-OB5
16	P	101	CDL	C51-CB5-OB6-CB4
16	P	103	CDL	O1-C1-CA2-OA2
16	P	103	CDL	C11-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
16	P	103	CDL	CB2-OB2-PB2-OB3
16	P	103	CDL	CB2-OB2-PB2-OB5
16	R	605	CDL	CA2-C1-CB2-OB2
16	R	605	CDL	CA3-OA5-PA1-OA3
16	R	605	CDL	CB3-OB5-PB2-OB3
16	R	606	CDL	CA2-C1-CB2-OB2
16	R	606	CDL	CA2-OA2-PA1-OA3
16	R	606	CDL	CA2-OA2-PA1-OA4
16	R	606	CDL	CB2-OB2-PB2-OB3
16	R	606	CDL	CB2-OB2-PB2-OB4
16	R	606	CDL	CB2-OB2-PB2-OB5
16	R	606	CDL	CB3-OB5-PB2-OB2
16	R	606	CDL	CB3-OB5-PB2-OB3
16	R	606	CDL	CB3-OB5-PB2-OB4
16	R	606	CDL	OB5-CB3-CB4-OB6
17	B	606	A1IRE	C01-C02-C03-C12
17	N	606	A1IRE	C01-C02-C03-C12
17	N	606	A1IRE	C27-N28-S30-O32
17	N	606	A1IRE	C29-N28-S30-O32
19	C	304	MQ9	C9-C11-C12-C13
19	C	304	MQ9	C14-C16-C17-C18
19	O	305	MQ9	C9-C11-C12-C13
19	O	305	MQ9	C13-C14-C16-C17
19	O	305	MQ9	C15-C14-C16-C17
19	O	305	MQ9	C14-C16-C17-C18
19	O	305	MQ9	C19-C21-C22-C23
19	O	305	MQ9	C38-C39-C41-C42
19	O	305	MQ9	C40-C39-C41-C42
20	D	102	9Y0	C22-C21-O7-C1
20	D	102	9Y0	O1-C3-C4-N
20	D	102	9Y0	C3-O1-P-O
20	G	301	9Y0	O5-C-C1-O7
20	G	301	9Y0	C13-C14-C15-C16
20	G	301	9Y0	C3-O1-P-O
20	G	301	9Y0	C3-O1-P-O2
20	P	102	9Y0	O1-C3-C4-N
20	P	102	9Y0	C3-O1-P-O
20	P	102	9Y0	C3-O1-P-O3
20	P	102	9Y0	C2-O3-P-O
20	P	102	9Y0	C2-O3-P-O2
20	S	301	9Y0	C13-C14-C15-C16
20	S	301	9Y0	O1-C3-C4-N

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Mol	Chain	Res	Type	Atoms
22	F	602	HEA	C19-C20-C21-C22
22	R	601	HEA	C2A-CAA-CBA-CGA
22	R	602	HEA	C19-C20-C21-C22
24	H	201	MQ7	C12-C13-C15-C16
24	H	201	MQ7	C14-C13-C15-C16
24	H	201	MQ7	C13-C15-C16-C17
24	H	201	MQ7	C17-C18-C20-C21
24	H	201	MQ7	C19-C18-C20-C21
24	H	201	MQ7	C22-C23-C25-C26
24	H	201	MQ7	C24-C23-C25-C26
24	O	301	MQ7	C24-C23-C25-C26
13	C	303	9YF	O12-C25-O11-C24
16	B	605	CDL	OA9-CA7-OA8-CA6
16	D	101	CDL	OB9-CB7-OB8-CB6
13	C	303	9YF	C26-C25-O11-C24
16	B	603	CDL	C31-CA7-OA8-CA6
16	B	605	CDL	C31-CA7-OA8-CA6
16	D	101	CDL	C71-CB7-OB8-CB6
16	B	603	CDL	OA9-CA7-OA8-CA6
16	D	103	CDL	OA9-CA7-OA8-CA6
16	B	603	CDL	OA7-CA5-OA6-CA4
16	B	604	CDL	OB7-CB5-OB6-CB4
16	D	101	CDL	OB7-CB5-OB6-CB4
16	F	605	CDL	OB7-CB5-OB6-CB4
16	M	503	CDL	OA7-CA5-OA6-CA4
16	P	103	CDL	OA7-CA5-OA6-CA4
20	D	102	9Y0	O6-C21-O7-C1
13	O	304	9YF	C26-C25-O11-C24
16	C	305	CDL	C71-CB7-OB8-CB6
16	N	607	CDL	C71-CB7-OB8-CB6
16	P	103	CDL	C31-CA7-OA8-CA6
16	B	605	CDL	C51-CB5-OB6-CB4
19	O	305	MQ9	C35-C34-C36-C37
22	F	602	HEA	C26-C15-C16-C17
24	O	301	MQ7	C19-C18-C20-C21
22	F	602	HEA	C14-C15-C16-C17
16	D	103	CDL	C15-C16-C17-C18
16	D	103	CDL	C31-CA7-OA8-CA6
16	R	606	CDL	C71-CB7-OB8-CB6
20	P	102	9Y0	C6-C5-O5-C
16	P	101	CDL	OB7-CB5-OB6-CB4
13	O	304	9YF	O12-C25-O11-C24

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Mol	Chain	Res	Type	Atoms
16	C	305	CDL	OB9-CB7-OB8-CB6
16	P	103	CDL	OA9-CA7-OA8-CA6
16	R	606	CDL	OB9-CB7-OB8-CB6
13	O	304	9YF	C14-C15-C16-C17
16	B	603	CDL	O1-C1-CA2-OA2
16	B	604	CDL	O1-C1-CA2-OA2
16	B	604	CDL	O1-C1-CB2-OB2
16	D	101	CDL	O1-C1-CA2-OA2
16	D	101	CDL	O1-C1-CB2-OB2
16	D	103	CDL	O1-C1-CA2-OA2
16	N	603	CDL	O1-C1-CB2-OB2
16	R	606	CDL	O1-C1-CB2-OB2
13	O	304	9YF	C9-C8-O9-C
16	D	101	CDL	C11-CA5-OA6-CA4
16	F	606	CDL	C51-CB5-OB6-CB4
16	R	606	CDL	C51-CB5-OB6-CB4
16	N	603	CDL	C74-C75-C76-C77
13	M	502	9YF	C17-C18-C19-C20
16	D	103	CDL	C31-C32-C33-C34
16	M	503	CDL	C18-C19-C20-C21
16	M	503	CDL	C51-C52-C53-C54
16	P	103	CDL	C19-C20-C21-C22
20	P	102	9Y0	O4-C5-O5-C
13	C	303	9YF	C14-C15-C16-C17
19	C	304	MQ9	C25-C24-C26-C27
19	O	305	MQ9	C25-C24-C26-C27
19	C	304	MQ9	C23-C24-C26-C27
19	O	305	MQ9	C23-C24-C26-C27
19	O	305	MQ9	C33-C34-C36-C37
24	O	301	MQ7	C22-C23-C25-C26
16	D	101	CDL	C15-C16-C17-C18
19	C	304	MQ9	C39-C41-C42-C43
19	O	305	MQ9	C39-C41-C42-C43
22	F	602	HEA	C15-C16-C17-C18
24	H	201	MQ7	C38-C40-C41-C42
16	P	101	CDL	C31-CA7-OA8-CA6
16	R	605	CDL	C71-CB7-OB8-CB6
16	N	603	CDL	C76-C77-C78-C79
16	R	605	CDL	OB9-CB7-OB8-CB6
16	D	103	CDL	CA2-C1-CB2-OB2
16	F	605	CDL	CB2-C1-CA2-OA2
16	F	606	CDL	CA2-C1-CB2-OB2

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Mol	Chain	Res	Type	Atoms
16	N	603	CDL	CA2-C1-CB2-OB2
16	N	604	CDL	CB2-C1-CA2-OA2
16	N	605	CDL	CB2-C1-CA2-OA2
16	N	605	CDL	CA2-C1-CB2-OB2
16	N	607	CDL	CB2-C1-CA2-OA2
16	P	101	CDL	CB2-C1-CA2-OA2
16	P	103	CDL	CA2-C1-CB2-OB2
16	R	606	CDL	CB2-C1-CA2-OA2
13	O	304	9YF	O10-C8-O9-C
16	D	101	CDL	OA7-CA5-OA6-CA4
16	R	606	CDL	OB7-CB5-OB6-CB4
13	M	502	9YF	C26-C25-O11-C24
20	S	301	9Y0	C6-C5-O5-C
17	N	606	A1IRE	F34-C33-S30-O31
16	B	605	CDL	OB5-CB3-CB4-OB6
16	D	101	CDL	OA5-CA3-CA4-OA6
16	B	605	CDL	O1-C1-CA2-OA2
16	D	103	CDL	O1-C1-CB2-OB2
16	N	603	CDL	O1-C1-CA2-OA2
16	N	604	CDL	O1-C1-CB2-OB2
16	N	605	CDL	O1-C1-CA2-OA2
16	P	101	CDL	O1-C1-CA2-OA2
16	P	103	CDL	O1-C1-CB2-OB2
16	R	606	CDL	O1-C1-CA2-OA2
13	A	502	9YF	C11-C10-C9-C8
16	N	605	CDL	CB7-C71-C72-C73
16	P	103	CDL	OB6-CB4-CB6-OB8
16	P	103	CDL	C76-C77-C78-C79
24	O	301	MQ7	C17-C18-C20-C21
13	O	304	9YF	C34-C33-C35-C36
13	C	303	9YF	C9-C10-C11-C12
16	D	103	CDL	C19-C20-C21-C22
16	B	605	CDL	C11-CA5-OA6-CA4
16	N	607	CDL	C11-CA5-OA6-CA4
14	G	302	PLM	C7-C8-C9-CA
16	N	607	CDL	CA5-C11-C12-C13
16	R	606	CDL	CA5-C11-C12-C13
20	S	301	9Y0	O4-C5-O5-C
16	D	101	CDL	C31-C32-C33-C34
16	M	503	CDL	CA7-C31-C32-C33
20	S	301	9Y0	C21-C22-C23-C24
13	A	502	9YF	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
16	B	605	CDL	CB7-C71-C72-C73
16	D	101	CDL	CB5-C51-C52-C53
16	D	103	CDL	CA5-C11-C12-C13
16	F	605	CDL	CA7-C31-C32-C33
16	F	605	CDL	CB7-C71-C72-C73
16	F	606	CDL	CB5-C51-C52-C53
16	M	503	CDL	CA5-C11-C12-C13
16	M	503	CDL	CB7-C71-C72-C73
16	N	607	CDL	CB7-C71-C72-C73
16	R	605	CDL	CB7-C71-C72-C73
16	R	606	CDL	CB5-C51-C52-C53
20	S	301	9Y0	C5-C6-C7-C8
16	N	605	CDL	C57-C58-C59-C60
17	B	606	A1IRE	F35-C33-S30-O32
16	F	606	CDL	OB7-CB5-OB6-CB4
16	N	605	CDL	C77-C78-C79-C80
16	R	606	CDL	C58-C59-C60-C61
17	B	606	A1IRE	F34-C33-S30-O32
17	N	606	A1IRE	F35-C33-S30-O31
17	N	606	A1IRE	F36-C33-S30-O31
13	A	502	9YF	C33-C35-C36-C37
16	D	101	CDL	C74-C75-C76-C77
16	N	607	CDL	C80-C81-C82-C83
16	R	606	CDL	C51-C52-C53-C54
17	B	606	A1IRE	F36-C33-S30-O32
13	M	502	9YF	O12-C25-O11-C24
19	C	304	MQ9	C24-C26-C27-C28
19	C	304	MQ9	C34-C36-C37-C38
19	C	304	MQ9	C44-C46-C47-C48
19	O	305	MQ9	C24-C26-C27-C28
19	O	305	MQ9	C34-C36-C37-C38
19	O	305	MQ9	C44-C46-C47-C48
22	R	602	HEA	C15-C16-C17-C18
24	O	301	MQ7	C13-C15-C16-C17
24	O	301	MQ7	C28-C30-C31-C32
24	O	301	MQ7	C38-C40-C41-C42
16	B	603	CDL	O1-C1-CB2-OB2
16	F	606	CDL	O1-C1-CA2-OA2
16	R	605	CDL	O1-C1-CB2-OB2
16	B	605	CDL	OA7-CA5-OA6-CA4
17	B	606	A1IRE	F36-C33-S30-N28
17	N	606	A1IRE	F36-C33-S30-N28

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Mol	Chain	Res	Type	Atoms
16	F	605	CDL	C71-CB7-OB8-CB6
16	P	101	CDL	OA9-CA7-OA8-CA6
16	F	606	CDL	CA5-C11-C12-C13
16	C	305	CDL	C74-C75-C76-C77
16	R	606	CDL	C73-C74-C75-C76
16	C	305	CDL	C11-CA5-OA6-CA4
13	A	502	9YF	C1-O-P-O2
13	C	303	9YF	C1-O-P-O2
16	B	603	CDL	CA2-OA2-PA1-OA5
16	B	603	CDL	CA3-OA5-PA1-OA2
16	B	604	CDL	CA2-OA2-PA1-OA5
16	B	604	CDL	CB2-OB2-PB2-OB5
16	B	604	CDL	CB3-OB5-PB2-OB2
16	B	605	CDL	CA3-OA5-PA1-OA2
16	B	605	CDL	CB3-OB5-PB2-OB2
16	C	305	CDL	CA3-OA5-PA1-OA2
16	C	305	CDL	CB3-OB5-PB2-OB2
16	D	101	CDL	CA2-OA2-PA1-OA5
16	D	101	CDL	CA3-OA5-PA1-OA2
16	D	103	CDL	CA3-OA5-PA1-OA2
16	D	103	CDL	CB2-OB2-PB2-OB5
16	F	605	CDL	CA2-OA2-PA1-OA5
16	F	605	CDL	CB2-OB2-PB2-OB5
16	F	605	CDL	CB3-OB5-PB2-OB2
16	M	503	CDL	CA2-OA2-PA1-OA5
16	M	503	CDL	CA3-OA5-PA1-OA2
16	M	503	CDL	CB2-OB2-PB2-OB5
16	N	603	CDL	CB3-OB5-PB2-OB2
16	N	604	CDL	CA3-OA5-PA1-OA2
16	N	605	CDL	CB3-OB5-PB2-OB2
16	N	607	CDL	CB3-OB5-PB2-OB2
16	P	101	CDL	CA3-OA5-PA1-OA2
16	P	103	CDL	CA2-OA2-PA1-OA5
16	R	606	CDL	CA2-OA2-PA1-OA5
20	D	102	9Y0	C3-O1-P-O3
20	G	301	9Y0	C3-O1-P-O3
20	P	102	9Y0	C2-O3-P-O1
17	B	606	A1IRE	F34-C33-S30-O31
17	B	606	A1IRE	F35-C33-S30-O31
17	N	606	A1IRE	F34-C33-S30-O32
17	N	606	A1IRE	F35-C33-S30-O32
16	B	603	CDL	C57-C58-C59-C60

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Mol	Chain	Res	Type	Atoms
16	P	101	CDL	C22-C23-C24-C25
16	N	603	CDL	CB5-C51-C52-C53
20	G	301	9Y0	C5-C6-C7-C8
16	B	603	CDL	CA2-C1-CB2-OB2
16	B	604	CDL	CB2-C1-CA2-OA2
16	B	605	CDL	CB2-C1-CA2-OA2
16	C	305	CDL	OA7-CA5-OA6-CA4
16	D	103	CDL	OA7-CA5-OA6-CA4
16	N	607	CDL	OA7-CA5-OA6-CA4
16	D	103	CDL	C13-C14-C15-C16
17	B	606	A1IRE	F36-C33-S30-O31
17	N	606	A1IRE	F36-C33-S30-O32
16	N	604	CDL	CA7-C31-C32-C33
13	C	303	9YF	C26-C27-C28-C29
13	M	502	9YF	C13-C14-C15-C16
16	F	605	CDL	C13-C14-C15-C16
16	N	603	CDL	C55-C56-C57-C58
16	D	103	CDL	C11-CA5-OA6-CA4
16	N	605	CDL	C11-CA5-OA6-CA4
16	P	101	CDL	C11-CA5-OA6-CA4
13	C	303	9YF	C10-C11-C12-C13
14	G	302	PLM	C8-C9-CA-CB
16	B	603	CDL	C16-C17-C18-C19
16	B	605	CDL	C14-C15-C16-C17
16	C	305	CDL	C51-C52-C53-C54
16	C	305	CDL	C71-C72-C73-C74
16	C	305	CDL	C83-C84-C85-C86
16	F	605	CDL	C52-C53-C54-C55
16	N	605	CDL	C20-C21-C22-C23
16	N	607	CDL	C74-C75-C76-C77
16	P	101	CDL	C76-C77-C78-C79
16	P	103	CDL	C11-C12-C13-C14
16	P	103	CDL	C13-C14-C15-C16
16	P	103	CDL	C32-C33-C34-C35
16	P	103	CDL	C35-C36-C37-C38
16	P	103	CDL	C51-C52-C53-C54
16	P	103	CDL	C55-C56-C57-C58
13	A	502	9YF	C12-C13-C14-C15
13	M	502	9YF	C15-C16-C17-C18
16	D	101	CDL	C20-C21-C22-C23
16	D	103	CDL	C21-C22-C23-C24
16	D	103	CDL	C61-C62-C63-C64

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Mol	Chain	Res	Type	Atoms
16	F	605	CDL	C60-C61-C62-C63
16	N	603	CDL	C14-C15-C16-C17
16	N	603	CDL	C51-C52-C53-C54
16	N	604	CDL	C13-C14-C15-C16
16	P	101	CDL	C53-C54-C55-C56
20	P	102	9Y0	C7-C8-C9-C10
16	N	605	CDL	OA7-CA5-OA6-CA4
16	P	101	CDL	OA7-CA5-OA6-CA4
16	D	101	CDL	C13-C14-C15-C16
16	D	101	CDL	C55-C56-C57-C58
16	F	605	CDL	C51-C52-C53-C54
16	F	605	CDL	C55-C56-C57-C58
16	N	604	CDL	C36-C37-C38-C39
16	R	606	CDL	C60-C61-C62-C63
20	G	301	9Y0	C7-C8-C9-C10
13	C	303	9YF	C27-C28-C29-C30
16	B	604	CDL	C55-C56-C57-C58
16	B	605	CDL	C11-C12-C13-C14
16	B	605	CDL	C18-C19-C20-C21
16	D	103	CDL	C56-C57-C58-C59
16	D	103	CDL	C79-C80-C81-C82
16	M	503	CDL	C75-C76-C77-C78
16	N	603	CDL	C78-C79-C80-C81
20	P	102	9Y0	C25-C26-C27-C28
20	S	301	9Y0	C27-C28-C29-C30
16	F	605	CDL	O1-C1-CA2-OA2
16	N	607	CDL	O1-C1-CA2-OA2
15	N	602	HEM	C3D-CAD-CBD-CGD
16	B	603	CDL	C76-C77-C78-C79
16	B	604	CDL	C51-C52-C53-C54
16	D	101	CDL	C79-C80-C81-C82
16	N	607	CDL	C76-C77-C78-C79
16	P	101	CDL	C11-C12-C13-C14
16	P	101	CDL	C83-C84-C85-C86
17	B	606	A1IRE	F34-C33-S30-N28
17	B	606	A1IRE	F35-C33-S30-N28
17	N	606	A1IRE	F34-C33-S30-N28
13	O	304	9YF	C13-C14-C15-C16
16	B	605	CDL	C21-C22-C23-C24
16	D	103	CDL	C34-C35-C36-C37
16	F	606	CDL	C12-C13-C14-C15
16	F	606	CDL	C76-C77-C78-C79

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Mol	Chain	Res	Type	Atoms
16	N	603	CDL	C58-C59-C60-C61
16	P	103	CDL	C16-C17-C18-C19
16	P	103	CDL	C78-C79-C80-C81
16	R	606	CDL	C76-C77-C78-C79
20	D	102	9Y0	C24-C25-C26-C27
20	D	102	9Y0	C7-C8-C9-C10
14	T	201	PLM	C8-C9-CA-CB
16	B	604	CDL	C17-C18-C19-C20
16	C	305	CDL	C31-C32-C33-C34
16	D	101	CDL	C52-C53-C54-C55
16	N	603	CDL	C79-C80-C81-C82
16	P	103	CDL	C79-C80-C81-C82
16	R	605	CDL	C59-C60-C61-C62
20	P	102	9Y0	C22-C23-C24-C25
13	C	303	9YF	C11-C10-C9-C8
16	D	103	CDL	CB5-C51-C52-C53
13	A	502	9YF	C38-C39-C40-C41
16	B	604	CDL	C13-C14-C15-C16
16	B	604	CDL	C74-C75-C76-C77
16	F	605	CDL	C36-C37-C38-C39
16	N	607	CDL	C77-C78-C79-C80
16	P	103	CDL	C81-C82-C83-C84
13	A	502	9YF	C30-C31-C32-C33
16	B	603	CDL	C79-C80-C81-C82
16	D	103	CDL	C18-C19-C20-C21
16	D	103	CDL	C62-C63-C64-C65
16	F	605	CDL	C31-C32-C33-C34
16	N	604	CDL	C72-C73-C74-C75
16	N	605	CDL	C15-C16-C17-C18
16	R	605	CDL	C51-CB5-OB6-CB4
16	B	605	CDL	C51-C52-C53-C54
16	D	103	CDL	C60-C61-C62-C63
16	B	604	CDL	CA5-C11-C12-C13
16	D	101	CDL	CB7-C71-C72-C73
16	N	607	CDL	CB5-C51-C52-C53
13	A	502	9YF	C13-C14-C15-C16
13	A	502	9YF	C27-C28-C29-C30
13	C	303	9YF	C17-C18-C19-C20
14	T	201	PLM	C2-C3-C4-C5
14	T	201	PLM	C7-C8-C9-CA
16	B	603	CDL	C74-C75-C76-C77
16	C	305	CDL	C52-C53-C54-C55

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Mol	Chain	Res	Type	Atoms
16	D	101	CDL	C17-C18-C19-C20
16	D	101	CDL	C80-C81-C82-C83
16	D	103	CDL	C16-C17-C18-C19
16	F	605	CDL	C35-C36-C37-C38
16	F	605	CDL	C57-C58-C59-C60
16	N	604	CDL	C14-C15-C16-C17
16	N	605	CDL	C74-C75-C76-C77
16	N	607	CDL	C14-C15-C16-C17
16	N	607	CDL	C34-C35-C36-C37
16	P	103	CDL	C18-C19-C20-C21
16	P	103	CDL	C58-C59-C60-C61
16	P	103	CDL	C74-C75-C76-C77
16	R	606	CDL	C59-C60-C61-C62
16	N	607	CDL	OA5-CA3-CA4-CA6
13	O	304	9YF	C38-C39-C40-C41
14	M	504	PLM	CA-CB-CC-CD
16	B	604	CDL	C59-C60-C61-C62
16	P	101	CDL	C51-C52-C53-C54
16	R	606	CDL	C33-C34-C35-C36
16	B	603	CDL	C72-C73-C74-C75
16	C	305	CDL	C81-C82-C83-C84
16	D	101	CDL	C37-C38-C39-C40
16	F	606	CDL	C31-C32-C33-C34
16	F	606	CDL	C78-C79-C80-C81
16	N	604	CDL	C57-C58-C59-C60
16	N	607	CDL	C81-C82-C83-C84
16	P	101	CDL	C23-C24-C25-C26
16	P	103	CDL	C57-C58-C59-C60
16	F	605	CDL	C76-C77-C78-C79
16	P	103	CDL	C21-C22-C23-C24
20	P	102	9Y0	C24-C25-C26-C27
16	R	605	CDL	C31-CA7-OA8-CA6
16	B	603	CDL	C18-C19-C20-C21
16	B	605	CDL	C19-C20-C21-C22
16	M	503	CDL	C73-C74-C75-C76
16	N	604	CDL	C12-C13-C14-C15
16	R	606	CDL	C62-C63-C64-C65
16	B	603	CDL	C15-C16-C17-C18
16	N	607	CDL	C57-C58-C59-C60
13	C	303	9YF	C15-C16-C17-C18
13	O	304	9YF	C11-C12-C13-C14
16	B	604	CDL	C52-C53-C54-C55

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Mol	Chain	Res	Type	Atoms
16	B	605	CDL	C57-C58-C59-C60
16	F	605	CDL	C34-C35-C36-C37
16	M	503	CDL	C11-C12-C13-C14
16	R	606	CDL	C53-C54-C55-C56
16	N	605	CDL	CB3-CB4-CB6-OB8
16	R	605	CDL	OB7-CB5-OB6-CB4
16	D	103	CDL	C22-C23-C24-C25
16	N	607	CDL	C16-C17-C18-C19
16	P	101	CDL	C38-C39-C40-C41
16	P	103	CDL	C59-C60-C61-C62
20	G	301	9Y0	C32-C33-C34-C35
16	N	607	CDL	C72-C73-C74-C75
16	R	606	CDL	C83-C84-C85-C86
16	F	605	CDL	OB9-CB7-OB8-CB6
16	B	604	CDL	C71-CB7-OB8-CB6
16	N	607	CDL	C55-C56-C57-C58
16	B	604	CDL	C57-C58-C59-C60
16	B	605	CDL	C75-C76-C77-C78
16	N	604	CDL	C74-C75-C76-C77
16	P	103	CDL	C60-C61-C62-C63
20	D	102	9Y0	C9-C10-C11-C12
16	C	305	CDL	C80-C81-C82-C83
16	D	101	CDL	C18-C19-C20-C21
16	N	604	CDL	C52-C53-C54-C55
16	N	605	CDL	C11-C12-C13-C14
20	P	102	9Y0	C27-C28-C29-C30
16	N	607	CDL	CA7-C31-C32-C33
13	O	304	9YF	C10-C11-C12-C13
16	B	604	CDL	C36-C37-C38-C39
16	C	305	CDL	C35-C36-C37-C38
16	N	607	CDL	C78-C79-C80-C81
16	R	605	CDL	C71-C72-C73-C74
16	R	606	CDL	C55-C56-C57-C58
14	G	302	PLM	C6-C7-C8-C9
16	B	605	CDL	C15-C16-C17-C18
16	B	605	CDL	C22-C23-C24-C25
16	D	103	CDL	C58-C59-C60-C61
16	M	503	CDL	C76-C77-C78-C79
16	B	603	CDL	C59-C60-C61-C62
16	M	503	CDL	C16-C17-C18-C19
16	N	605	CDL	C75-C76-C77-C78
15	B	602	HEM	C3D-CAD-CBD-CGD

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Mol	Chain	Res	Type	Atoms
16	B	605	CDL	C76-C77-C78-C79
16	D	101	CDL	C22-C23-C24-C25
16	F	606	CDL	C81-C82-C83-C84
16	N	605	CDL	C18-C19-C20-C21
16	R	606	CDL	C12-C13-C14-C15
16	N	607	CDL	C33-C34-C35-C36
16	R	605	CDL	C74-C75-C76-C77
16	D	103	CDL	C53-C54-C55-C56
16	P	101	CDL	C57-C58-C59-C60
16	B	604	CDL	OB9-CB7-OB8-CB6
16	R	605	CDL	OA9-CA7-OA8-CA6
16	C	305	CDL	C16-C17-C18-C19
16	M	503	CDL	C74-C75-C76-C77
16	N	603	CDL	C18-C19-C20-C21
16	P	101	CDL	C78-C79-C80-C81
16	C	305	CDL	OB7-CB5-OB6-CB4
16	R	606	CDL	OA7-CA5-OA6-CA4
16	R	605	CDL	CA7-C31-C32-C33
16	P	101	CDL	C71-CB7-OB8-CB6
16	N	605	CDL	C55-C56-C57-C58
16	N	607	CDL	C71-C72-C73-C74
16	F	606	CDL	C83-C84-C85-C86
16	N	607	CDL	C52-C53-C54-C55
20	G	301	9Y0	C25-C26-C27-C28
13	M	502	9YF	C36-C37-C38-C39
16	B	605	CDL	C73-C74-C75-C76
16	C	305	CDL	C76-C77-C78-C79
16	P	103	CDL	C71-C72-C73-C74
24	O	301	MQ7	C33-C35-C36-C37
13	M	502	9YF	C35-C36-C37-C38
16	C	305	CDL	C53-C54-C55-C56
16	D	103	CDL	C83-C84-C85-C86
16	N	604	CDL	C53-C54-C55-C56
16	N	605	CDL	C51-C52-C53-C54
16	N	607	CDL	C83-C84-C85-C86
16	R	605	CDL	C56-C57-C58-C59
16	R	606	CDL	C71-C72-C73-C74
13	M	502	9YF	C25-C26-C27-C28
16	B	603	CDL	C51-CB5-OB6-CB4
16	C	305	CDL	C51-CB5-OB6-CB4
16	N	603	CDL	C51-CB5-OB6-CB4
16	N	607	CDL	C51-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
16	R	606	CDL	C11-CA5-OA6-CA4
20	D	102	9Y0	O7-C1-C2-O3
16	D	101	CDL	C82-C83-C84-C85
16	N	604	CDL	C55-C56-C57-C58
20	D	102	9Y0	C22-C23-C24-C25
16	F	605	CDL	C74-C75-C76-C77
16	B	603	CDL	OB7-CB5-OB6-CB4
17	N	606	A1IRE	F35-C33-S30-N28
16	B	603	CDL	CB5-C51-C52-C53
16	N	605	CDL	C16-C17-C18-C19
16	N	607	CDL	C15-C16-C17-C18
16	R	605	CDL	OA6-CA4-CA6-OA8
13	A	502	9YF	C15-C16-C17-C18
13	C	303	9YF	C16-C17-C18-C19
16	D	103	CDL	C17-C18-C19-C20
16	P	101	CDL	C81-C82-C83-C84
16	R	606	CDL	C79-C80-C81-C82
16	D	103	CDL	C11-C12-C13-C14
16	D	103	CDL	C76-C77-C78-C79
16	P	101	CDL	C18-C19-C20-C21
16	C	305	CDL	CA7-C31-C32-C33
19	C	304	MQ9	C33-C34-C36-C37
16	C	305	CDL	C72-C73-C74-C75
16	D	103	CDL	C37-C38-C39-C40
13	A	502	9YF	C19-C20-C21-C22
16	D	103	CDL	C35-C36-C37-C38
16	N	605	CDL	C22-C23-C24-C25
16	N	607	CDL	C53-C54-C55-C56
13	O	304	9YF	C35-C36-C37-C38
16	R	605	CDL	C77-C78-C79-C80
16	R	606	CDL	C32-C33-C34-C35
20	S	301	9Y0	C6-C7-C8-C9
16	N	607	CDL	OB7-CB5-OB6-CB4
14	G	302	PLM	CB-CC-CD-CE
13	O	304	9YF	C1-O-P-O2
16	D	103	CDL	CB3-OB5-PB2-OB2
16	F	606	CDL	CB2-OB2-PB2-OB5
16	F	606	CDL	CB3-OB5-PB2-OB2
20	D	102	9Y0	C2-O3-P-O1
13	O	304	9YF	C9-C10-C11-C12
16	D	101	CDL	C35-C36-C37-C38
16	N	607	CDL	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
16	B	605	CDL	CA4-CA3-OA5-PA1
16	B	605	CDL	C52-C53-C54-C55
13	A	502	9YF	C24-C-C1-O
13	M	502	9YF	C24-C-C1-O
13	O	304	9YF	C24-C-C1-O
16	B	603	CDL	OB5-CB3-CB4-CB6
16	B	605	CDL	OB5-CB3-CB4-CB6
16	C	305	CDL	OA5-CA3-CA4-CA6
16	D	101	CDL	OA5-CA3-CA4-CA6
16	N	603	CDL	OB5-CB3-CB4-CB6
16	P	101	CDL	OA5-CA3-CA4-CA6
16	R	605	CDL	OA5-CA3-CA4-CA6
16	B	604	CDL	C11-C12-C13-C14
16	F	606	CDL	C73-C74-C75-C76
16	P	101	CDL	C37-C38-C39-C40
16	N	605	CDL	CB5-C51-C52-C53
16	N	604	CDL	C34-C35-C36-C37
16	N	605	CDL	C23-C24-C25-C26
16	N	605	CDL	C78-C79-C80-C81
13	C	303	9YF	C39-C40-C41-C42
13	O	304	9YF	C17-C18-C19-C20
16	F	606	CDL	C62-C63-C64-C65
16	M	503	CDL	C53-C54-C55-C56
16	D	103	CDL	CB2-C1-CA2-OA2
16	P	103	CDL	CB2-C1-CA2-OA2
19	C	304	MQ9	C35-C34-C36-C37
16	R	605	CDL	C60-C61-C62-C63
16	B	605	CDL	C16-C17-C18-C19
16	P	101	CDL	C79-C80-C81-C82
16	R	606	CDL	C78-C79-C80-C81
16	R	606	CDL	C81-C82-C83-C84
16	P	101	CDL	OB9-CB7-OB8-CB6
16	D	101	CDL	C71-C72-C73-C74
16	R	605	CDL	C38-C39-C40-C41
13	C	303	9YF	C20-C21-C22-C23
16	B	603	CDL	CB3-CB4-CB6-OB8
16	B	605	CDL	CB3-CB4-CB6-OB8
16	N	603	CDL	CA3-CA4-CA6-OA8
16	N	605	CDL	C33-C34-C35-C36
16	P	103	CDL	CB3-CB4-CB6-OB8
16	R	605	CDL	CB3-CB4-CB6-OB8
17	B	606	A1IRE	C27-N28-S30-O32

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Mol	Chain	Res	Type	Atoms
20	G	301	9Y0	O5-C-C1-C2
16	C	305	CDL	C79-C80-C81-C82
16	M	503	CDL	C14-C15-C16-C17
22	F	602	HEA	C4D-C3D-CAD-CBD
13	C	303	9YF	C29-C30-C31-C32
13	O	304	9YF	C20-C21-C22-C23
16	D	103	CDL	C64-C65-C66-C67
16	F	605	CDL	C56-C57-C58-C59
16	N	603	CDL	C59-C60-C61-C62
16	R	605	CDL	C76-C77-C78-C79
16	R	605	CDL	CA5-C11-C12-C13
13	A	502	9YF	C29-C30-C31-C32
16	M	503	CDL	C57-C58-C59-C60
16	N	607	CDL	C12-C13-C14-C15
19	O	305	MQ9	C29-C31-C32-C33
24	H	201	MQ7	C23-C25-C26-C27
24	H	201	MQ7	C33-C35-C36-C37
16	B	604	CDL	C18-C19-C20-C21
20	G	301	9Y0	C10-C11-C12-C13
20	S	301	9Y0	C10-C11-C12-C13
16	P	101	CDL	C20-C21-C22-C23
16	D	103	CDL	C57-C58-C59-C60
19	O	305	MQ9	C45-C44-C46-C47
16	B	604	CDL	C76-C77-C78-C79
16	F	605	CDL	C59-C60-C61-C62
16	F	606	CDL	C51-C52-C53-C54
16	R	606	CDL	C15-C16-C17-C18
16	D	101	CDL	C31-CA7-OA8-CA6
16	N	603	CDL	C31-CA7-OA8-CA6
16	D	103	CDL	C20-C21-C22-C23
16	R	606	CDL	C34-C35-C36-C37
16	D	103	CDL	CA3-CA4-OA6-CA5
16	N	605	CDL	CA6-CA4-OA6-CA5
16	P	103	CDL	CA6-CA4-OA6-CA5
16	P	103	CDL	C12-C13-C14-C15
16	B	604	CDL	C58-C59-C60-C61
20	D	102	9Y0	C27-C28-C29-C30
16	N	604	CDL	C16-C17-C18-C19
16	B	603	CDL	OA5-CA3-CA4-OA6
16	B	604	CDL	OB5-CB3-CB4-OB6
13	C	303	9YF	C19-C20-C21-C22
16	D	103	CDL	C74-C75-C76-C77

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Mol	Chain	Res	Type	Atoms
20	P	102	9Y0	C11-C10-C9-C8
22	F	601	HEA	C4D-C3D-CAD-CBD
16	F	606	CDL	C15-C16-C17-C18
16	N	604	CDL	C76-C77-C78-C79
16	B	605	CDL	C79-C80-C81-C82
16	M	503	CDL	C79-C80-C81-C82
16	N	603	CDL	OB7-CB5-OB6-CB4
16	F	605	CDL	C54-C55-C56-C57
13	O	304	9YF	C31-C32-C33-C35
19	O	305	MQ9	C43-C44-C46-C47
16	D	101	CDL	C23-C24-C25-C26
16	D	101	CDL	C51-C52-C53-C54
16	F	606	CDL	C58-C59-C60-C61
13	A	502	9YF	C34-C33-C35-C36
16	D	101	CDL	C11-C12-C13-C14
16	P	101	CDL	C15-C16-C17-C18
16	B	605	CDL	C34-C35-C36-C37
16	C	305	CDL	C15-C16-C17-C18
16	C	305	CDL	C54-C55-C56-C57
16	N	605	CDL	C79-C80-C81-C82
16	P	101	CDL	C16-C17-C18-C19
16	B	604	CDL	OB5-CB3-CB4-CB6
16	R	606	CDL	OB5-CB3-CB4-CB6
20	D	102	9Y0	C-C1-C2-O3
20	S	301	9Y0	C-C1-C2-O3
24	H	201	MQ7	C28-C30-C31-C32
16	C	305	CDL	C14-C15-C16-C17
16	R	606	CDL	CB7-C71-C72-C73
16	N	607	CDL	C11-C12-C13-C14
16	C	305	CDL	CB5-C51-C52-C53
13	A	502	9YF	C9-C10-C11-C12
13	C	303	9YF	C35-C36-C37-C38
16	D	101	CDL	OA9-CA7-OA8-CA6
14	T	201	PLM	C9-CA-CB-CC
16	F	605	CDL	C12-C13-C14-C15
16	P	103	CDL	C36-C37-C38-C39
16	P	103	CDL	C72-C73-C74-C75
16	F	606	CDL	C31-CA7-OA8-CA6
16	R	605	CDL	C52-C51-CB5-OB6
16	D	103	CDL	C71-C72-C73-C74
16	F	606	CDL	C52-C53-C54-C55
16	N	605	CDL	CA4-CA3-OA5-PA1

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Mol	Chain	Res	Type	Atoms
16	N	603	CDL	OA9-CA7-OA8-CA6
20	S	301	9Y0	C7-C8-C9-C10
16	D	101	CDL	C57-C58-C59-C60
16	N	603	CDL	C73-C74-C75-C76
16	P	101	CDL	C39-C40-C41-C42
16	B	604	CDL	C37-C38-C39-C40
16	B	604	CDL	CB3-CB4-CB6-OB8
16	C	305	CDL	CA3-CA4-CA6-OA8
16	D	101	CDL	CA3-CA4-CA6-OA8
16	N	604	CDL	CB3-CB4-CB6-OB8
16	N	607	CDL	CA3-CA4-CA6-OA8
16	N	607	CDL	CB3-CB4-CB6-OB8
16	P	101	CDL	CA3-CA4-CA6-OA8
16	R	605	CDL	CA3-CA4-CA6-OA8
17	B	606	A1IRE	C21-C20-C23-C26
16	R	606	CDL	C13-C14-C15-C16
13	O	304	9YF	C11-C10-C9-C8
14	A	503	PLM	C8-C9-CA-CB
16	P	103	CDL	C33-C34-C35-C36
20	G	301	9Y0	C11-C10-C9-C8
20	S	301	9Y0	C25-C26-C27-C28
16	B	605	CDL	C78-C79-C80-C81
16	B	603	CDL	CB3-OB5-PB2-OB2
16	C	305	CDL	CA2-OA2-PA1-OA5
16	N	607	CDL	CA2-OA2-PA1-OA5
16	B	605	CDL	C71-C72-C73-C74
16	P	103	CDL	C77-C78-C79-C80
13	C	303	9YF	O9-C-C1-O
13	O	304	9YF	O9-C-C1-O
16	C	305	CDL	OA5-CA3-CA4-OA6
16	F	605	CDL	OA5-CA3-CA4-OA6
16	N	603	CDL	OA5-CA3-CA4-OA6
16	N	607	CDL	OA5-CA3-CA4-OA6
16	R	605	CDL	OA5-CA3-CA4-OA6
16	R	606	CDL	OA5-CA3-CA4-OA6
13	O	304	9YF	C19-C20-C21-C22
20	G	301	9Y0	C27-C28-C29-C30
20	P	102	9Y0	C10-C11-C12-C13
16	F	606	CDL	C11-C12-C13-C14
16	M	503	CDL	C71-C72-C73-C74
16	R	606	CDL	C61-C62-C63-C64
16	N	603	CDL	OA6-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
16	P	101	CDL	OA6-CA4-CA6-OA8
13	A	502	9YF	C11-C12-C13-C14
13	M	502	9YF	C26-C27-C28-C29
16	F	605	CDL	C78-C79-C80-C81
16	N	604	CDL	C60-C61-C62-C63
22	F	601	HEA	C2D-C3D-CAD-CBD
16	B	603	CDL	CB2-C1-CA2-OA2
16	D	101	CDL	CA2-C1-CB2-OB2
16	N	604	CDL	C33-C34-C35-C36
13	O	304	9YF	C15-C16-C17-C18
16	P	101	CDL	C33-C34-C35-C36
13	O	304	9YF	C39-C40-C41-C42
16	M	503	CDL	C15-C16-C17-C18
16	B	604	CDL	CB4-CB3-OB5-PB2
16	N	605	CDL	C72-C73-C74-C75
20	D	102	9Y0	C26-C27-C28-C29
16	C	305	CDL	C57-C58-C59-C60
16	R	605	CDL	C78-C79-C80-C81
16	F	605	CDL	C32-C31-CA7-OA8
16	N	605	CDL	C14-C15-C16-C17
16	F	606	CDL	C57-C58-C59-C60
22	F	602	HEA	C2D-C3D-CAD-CBD
16	C	305	CDL	C36-C37-C38-C39
16	F	605	CDL	OA5-CA3-CA4-CA6
16	P	103	CDL	OB5-CB3-CB4-CB6
16	R	605	CDL	OB5-CB3-CB4-CB6
13	A	502	9YF	C32-C33-C35-C36
16	D	103	CDL	CA7-C31-C32-C33
16	N	603	CDL	C13-C14-C15-C16
20	G	301	9Y0	C26-C27-C28-C29
16	R	606	CDL	C56-C57-C58-C59
16	N	604	CDL	C35-C36-C37-C38
16	B	605	CDL	CA6-CA4-OA6-CA5
16	N	605	CDL	CB6-CB4-OB6-CB5
16	B	604	CDL	C35-C36-C37-C38
16	M	503	CDL	C72-C73-C74-C75
16	N	603	CDL	C80-C81-C82-C83
16	N	605	CDL	C76-C77-C78-C79
16	F	606	CDL	C79-C80-C81-C82
16	B	605	CDL	C32-C33-C34-C35
16	B	605	CDL	C1-CA2-OA2-PA1
16	M	503	CDL	CB3-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
16	N	603	CDL	CB3-CB4-CB6-OB8
16	P	101	CDL	CA4-CA3-OA5-PA1
16	R	606	CDL	CB3-CB4-CB6-OB8
20	D	102	9Y0	O5-C-C1-C2
20	D	102	9Y0	C1-C2-O3-P
16	R	605	CDL	C57-C58-C59-C60
16	P	103	CDL	OB5-CB3-CB4-OB6
20	S	301	9Y0	O7-C1-C2-O3
16	R	606	CDL	C32-C31-CA7-OA8
16	D	101	CDL	C32-C33-C34-C35
20	D	102	9Y0	C11-C10-C9-C8
16	B	604	CDL	CA2-C1-CB2-OB2
16	F	606	CDL	CB2-C1-CA2-OA2
16	D	101	CDL	C36-C37-C38-C39
13	C	303	9YF	O9-C-C24-O11
16	B	603	CDL	OB6-CB4-CB6-OB8
16	B	604	CDL	OB6-CB4-CB6-OB8
16	B	605	CDL	OB6-CB4-CB6-OB8
16	C	305	CDL	OB6-CB4-CB6-OB8
16	D	101	CDL	OA6-CA4-CA6-OA8
16	N	603	CDL	OB6-CB4-CB6-OB8
16	N	604	CDL	OB6-CB4-CB6-OB8
16	N	605	CDL	OB6-CB4-CB6-OB8
16	N	607	CDL	OB6-CB4-CB6-OB8
16	R	605	CDL	OB6-CB4-CB6-OB8
20	P	102	9Y0	O5-C-C1-O7
16	F	606	CDL	C32-C33-C34-C35
16	F	606	CDL	OA9-CA7-OA8-CA6
16	N	605	CDL	C13-C14-C15-C16
16	N	607	CDL	C56-C57-C58-C59
16	P	103	CDL	C22-C23-C24-C25
16	D	101	CDL	C54-C55-C56-C57
16	N	607	CDL	C51-C52-C53-C54
16	N	605	CDL	C71-C72-C73-C74
16	P	101	CDL	C84-C85-C86-C87
16	B	604	CDL	C32-C33-C34-C35
16	B	604	CDL	C72-C73-C74-C75
20	S	301	9Y0	C32-C33-C34-C35
16	N	604	CDL	CA2-OA2-PA1-OA5
16	N	605	CDL	CB2-OB2-PB2-OB5
13	A	502	9YF	C26-C27-C28-C29
13	O	304	9YF	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
16	N	604	CDL	C71-C72-C73-C74
16	P	101	CDL	C1-CB2-OB2-PB2
16	P	103	CDL	CB4-CB3-OB5-PB2
16	B	603	CDL	CA3-OA5-PA1-OA3
16	B	604	CDL	CA2-OA2-PA1-OA3
16	B	604	CDL	CA3-OA5-PA1-OA4
16	B	604	CDL	CB3-OB5-PB2-OB3
16	C	305	CDL	CB3-OB5-PB2-OB3
16	D	103	CDL	CA3-OA5-PA1-OA3
16	D	103	CDL	CA3-OA5-PA1-OA4
16	D	103	CDL	CB2-OB2-PB2-OB4
16	N	604	CDL	CA2-OA2-PA1-OA4
16	N	604	CDL	CA3-OA5-PA1-OA4
16	N	605	CDL	CB2-OB2-PB2-OB3
16	N	605	CDL	CB3-OB5-PB2-OB3
16	N	607	CDL	CB2-OB2-PB2-OB3
16	N	607	CDL	CB3-OB5-PB2-OB3
16	N	607	CDL	CB3-OB5-PB2-OB4
16	P	101	CDL	CA2-OA2-PA1-OA3
16	P	101	CDL	CA3-OA5-PA1-OA4
16	P	103	CDL	CA2-OA2-PA1-OA3
16	P	103	CDL	CA2-OA2-PA1-OA4
16	P	103	CDL	CB3-OB5-PB2-OB4
20	D	102	9Y0	C2-O3-P-O
20	D	102	9Y0	C2-O3-P-O2
13	A	502	9YF	C17-C18-C19-C20
16	D	103	CDL	C51-C52-C53-C54
16	N	603	CDL	C19-C20-C21-C22
13	C	303	9YF	C30-C31-C32-C33
13	C	303	9YF	C24-C-C1-O
16	D	103	CDL	OA5-CA3-CA4-CA6
16	F	606	CDL	OA5-CA3-CA4-CA6
16	R	606	CDL	OA5-CA3-CA4-CA6
13	A	502	9YF	C10-C11-C12-C13
16	C	305	CDL	CA5-C11-C12-C13
16	F	606	CDL	C34-C35-C36-C37
16	N	605	CDL	C53-C54-C55-C56
16	F	606	CDL	C64-C65-C66-C67
13	O	304	9YF	C29-C30-C31-C32
20	P	102	9Y0	C14-C15-C16-C17
16	D	101	CDL	C14-C15-C16-C17
16	F	606	CDL	C54-C55-C56-C57

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Mol	Chain	Res	Type	Atoms
13	M	502	9YF	C32-C33-C35-C36
13	O	304	9YF	C32-C33-C35-C36
16	B	603	CDL	OB5-CB3-CB4-OB6
16	D	103	CDL	OA5-CA3-CA4-OA6
16	F	606	CDL	OA5-CA3-CA4-OA6
16	F	606	CDL	CA7-C31-C32-C33
16	M	503	CDL	CB5-C51-C52-C53
16	N	603	CDL	OB5-CB3-CB4-OB6
18	C	302	HEC	C3D-CAD-CBD-CGD
18	O	302	HEC	C2A-CAA-CBA-CGA
18	O	303	HEC	C2A-CAA-CBA-CGA
13	M	502	9YF	C18-C19-C20-C21
16	R	606	CDL	C31-C32-C33-C34
16	D	103	CDL	C80-C81-C82-C83
16	N	607	CDL	O1-C1-CB2-OB2
13	C	303	9YF	C1-C-C24-O11
15	B	602	HEM	C1A-C2A-CAA-CBA
16	B	605	CDL	CA3-CA4-CA6-OA8
16	B	605	CDL	C58-C59-C60-C61
16	C	305	CDL	CB3-CB4-CB6-OB8
17	B	606	A1IRE	C29-N28-S30-O32
18	C	301	HEC	C2D-C3D-CAD-CBD
18	C	301	HEC	C4D-C3D-CAD-CBD
18	C	302	HEC	C2D-C3D-CAD-CBD
18	C	302	HEC	C4D-C3D-CAD-CBD
16	B	605	CDL	OA6-CA4-CA6-OA8
16	C	305	CDL	OA6-CA4-CA6-OA8
16	N	607	CDL	OA6-CA4-CA6-OA8
16	R	606	CDL	OB6-CB4-CB6-OB8
20	D	102	9Y0	O5-C-C1-O7
16	N	604	CDL	C32-C33-C34-C35
16	B	603	CDL	CB4-CB3-OB5-PB2
16	C	305	CDL	C13-C14-C15-C16
16	P	103	CDL	C37-C38-C39-C40
16	R	605	CDL	C51-C52-C53-C54
16	F	605	CDL	C52-C51-CB5-OB6
13	M	502	9YF	C34-C33-C35-C36
16	M	503	CDL	C59-C60-C61-C62
16	N	603	CDL	C15-C16-C17-C18
13	A	502	9YF	C16-C17-C18-C19
16	R	606	CDL	C52-C53-C54-C55
16	F	605	CDL	CB5-C51-C52-C53

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Mol	Chain	Res	Type	Atoms
16	P	101	CDL	C74-C75-C76-C77
16	P	103	CDL	CB5-C51-C52-C53
13	M	502	9YF	C29-C30-C31-C32
13	O	304	9YF	C1-C-O9-C8
16	B	605	CDL	CB6-CB4-OB6-CB5
16	D	101	CDL	CA3-CA4-OA6-CA5
16	F	606	CDL	CA6-CA4-OA6-CA5
16	R	606	CDL	CA6-CA4-OA6-CA5
16	B	603	CDL	OA5-CA3-CA4-CA6
16	N	603	CDL	CB2-C1-CA2-OA2
16	P	103	CDL	OB7-CB5-OB6-CB4
20	G	301	9Y0	C30-C31-C32-C33
13	O	304	9YF	C36-C37-C38-C39
13	O	304	9YF	C33-C35-C36-C37
16	B	603	CDL	C1-CA2-OA2-PA1
16	M	503	CDL	OA5-CA3-CA4-OA6
16	R	605	CDL	OB5-CB3-CB4-OB6
16	F	606	CDL	C72-C71-CB7-OB8
19	C	304	MQ9	C40-C39-C41-C42
16	P	103	CDL	C52-C53-C54-C55
16	B	603	CDL	C19-C20-C21-C22
16	B	605	CDL	C72-C73-C74-C75
20	G	301	9Y0	C23-C24-C25-C26
16	P	103	CDL	C51-CB5-OB6-CB4
13	C	303	9YF	C11-C12-C13-C14
13	O	304	9YF	C26-C27-C28-C29
16	N	603	CDL	C53-C54-C55-C56
16	R	605	CDL	C55-C56-C57-C58
16	C	305	CDL	CB2-OB2-PB2-OB5
16	N	605	CDL	CA3-OA5-PA1-OA2
16	P	103	CDL	CB3-OB5-PB2-OB2
16	R	605	CDL	CB2-OB2-PB2-OB5
16	P	101	CDL	CB3-CB4-CB6-OB8
19	O	305	MQ9	C12-C11-C9-C10
16	P	101	CDL	C56-C57-C58-C59
16	C	305	CDL	C78-C79-C80-C81
13	O	304	9YF	C31-C32-C33-C34
14	T	201	PLM	C6-C7-C8-C9
16	D	103	CDL	C1-CA2-OA2-PA1
20	P	102	9Y0	C13-C14-C15-C16
16	F	605	CDL	C39-C40-C41-C42
16	N	604	CDL	CA2-C1-CB2-OB2

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Mol	Chain	Res	Type	Atoms
16	N	607	CDL	CA2-C1-CB2-OB2
16	N	607	CDL	C73-C74-C75-C76
16	R	605	CDL	C13-C14-C15-C16
14	M	504	PLM	C7-C8-C9-CA
16	N	603	CDL	C16-C17-C18-C19
20	G	301	9Y0	O1-C3-C4-N
15	N	601	HEM	CAA-CBA-CGA-O1A
19	C	304	MQ9	C45-C44-C46-C47
22	R	602	HEA	C26-C15-C16-C17
16	N	607	CDL	C82-C83-C84-C85
19	C	304	MQ9	C43-C44-C46-C47
16	P	103	CDL	C14-C15-C16-C17
16	D	103	CDL	OA6-CA4-CA6-OA8
20	G	301	9Y0	C28-C29-C30-C31
16	N	607	CDL	C79-C80-C81-C82
16	P	101	CDL	C73-C74-C75-C76
14	M	504	PLM	C2-C3-C4-C5
16	D	101	CDL	CA7-C31-C32-C33
16	P	101	CDL	CB5-C51-C52-C53
13	A	502	9YF	C40-C41-C42-C43
13	C	303	9YF	C38-C39-C40-C41
16	F	606	CDL	C53-C54-C55-C56
16	F	606	CDL	C77-C78-C79-C80
16	F	605	CDL	CA2-C1-CB2-OB2
17	B	606	A1IRE	C19-C20-C23-C26
16	P	103	CDL	C34-C35-C36-C37
13	C	303	9YF	C18-C19-C20-C21
13	C	303	9YF	C2-O2-P-O8
16	M	503	CDL	C77-C78-C79-C80
18	C	302	HEC	CAA-CBA-CGA-O1A
22	F	601	HEA	CAD-CBD-CGD-O1D
22	F	601	HEA	CAD-CBD-CGD-O2D
13	C	303	9YF	C31-C32-C33-C35
16	P	101	CDL	C36-C37-C38-C39
16	R	605	CDL	C39-C40-C41-C42
16	M	503	CDL	OA5-CA3-CA4-CA6
13	A	502	9YF	C20-C21-C22-C23
16	D	101	CDL	C81-C82-C83-C84
16	F	606	CDL	C59-C60-C61-C62
16	R	606	CDL	C82-C83-C84-C85
19	C	304	MQ9	C12-C11-C9-C10
19	O	305	MQ9	C20-C19-C21-C22

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Mol	Chain	Res	Type	Atoms
24	O	301	MQ7	C29-C28-C30-C31
16	F	605	CDL	C61-C62-C63-C64
15	N	601	HEM	CAA-CBA-CGA-O2A
15	N	601	HEM	CAD-CBD-CGD-O2D
16	P	101	CDL	C14-C15-C16-C17
16	F	605	CDL	OA6-CA4-CA6-OA8
16	N	604	CDL	C71-CB7-OB8-CB6
16	P	103	CDL	C61-C62-C63-C64
22	R	601	HEA	CAD-CBD-CGD-O1D
13	C	303	9YF	C7-C2-O2-P
19	C	304	MQ9	C19-C21-C22-C23
22	R	601	HEA	CAD-CBD-CGD-O2D
16	N	604	CDL	OB9-CB7-OB8-CB6
16	N	605	CDL	C19-C20-C21-C22
16	D	101	CDL	C56-C57-C58-C59
16	F	605	CDL	C53-C54-C55-C56
16	N	605	CDL	OB9-CB7-OB8-CB6
16	R	606	CDL	C63-C64-C65-C66
16	N	604	CDL	C32-C31-CA7-OA8
17	N	606	A1IRE	C27-N28-S30-O31
13	M	502	9YF	C12-C13-C14-C15
16	N	605	CDL	C71-CB7-OB8-CB6
16	D	103	CDL	C38-C39-C40-C41
20	S	301	9Y0	C28-C29-C30-C31
16	B	603	CDL	C31-C32-C33-C34
16	P	101	CDL	C54-C55-C56-C57
19	O	305	MQ9	C12-C11-C9-C8
15	N	601	HEM	CAD-CBD-CGD-O1D
16	B	604	CDL	C38-C39-C40-C41
16	N	604	CDL	C59-C60-C61-C62
16	B	605	CDL	C55-C56-C57-C58
22	R	601	HEA	C2D-C3D-CAD-CBD
16	D	103	CDL	CB7-C71-C72-C73
16	N	605	CDL	C58-C59-C60-C61
20	G	301	9Y0	C-C1-C2-O3
16	R	605	CDL	C52-C51-CB5-OB7
16	B	603	CDL	C12-C13-C14-C15
22	R	602	HEA	CAD-CBD-CGD-O2D
22	R	601	HEA	C4D-C3D-CAD-CBD
16	N	605	CDL	C1-CA2-OA2-PA1
16	D	103	CDL	OB6-CB4-CB6-OB8
16	R	605	CDL	CB3-OB5-PB2-OB2

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Mol	Chain	Res	Type	Atoms
20	G	301	9Y0	C2-O3-P-O1
20	P	102	9Y0	O7-C21-C22-C23
13	C	303	9YF	C31-C32-C33-C34
16	D	103	CDL	C72-C73-C74-C75
15	B	601	HEM	CAA-CBA-CGA-O1A
20	S	301	9Y0	C9-C10-C11-C12
20	P	102	9Y0	C23-C24-C25-C26
13	O	304	9YF	O11-C25-C26-C27
16	N	607	CDL	C52-C51-CB5-OB6
16	D	101	CDL	CA6-CA4-OA6-CA5
14	T	201	PLM	C5-C6-C7-C8
22	R	602	HEA	CAD-CBD-CGD-O1D
19	C	304	MQ9	C12-C11-C9-C8
19	O	305	MQ9	C18-C19-C21-C22
24	O	301	MQ7	C27-C28-C30-C31
16	P	103	CDL	C12-C11-CA5-OA6
20	G	301	9Y0	C6-C7-C8-C9
16	D	103	CDL	CA3-CA4-CA6-OA8
13	M	502	9YF	C38-C39-C40-C41
18	C	302	HEC	CAA-CBA-CGA-O2A
16	P	101	CDL	C72-C73-C74-C75
16	R	605	CDL	C12-C11-CA5-OA6
16	P	101	CDL	C24-C25-C26-C27
16	N	604	CDL	C51-C52-C53-C54
16	N	603	CDL	OA5-CA3-CA4-CA6
16	P	103	CDL	C31-C32-C33-C34
16	B	604	CDL	C32-C31-CA7-OA8
16	F	606	CDL	C63-C64-C65-C66
20	S	301	9Y0	C29-C30-C31-C32
16	D	103	CDL	C84-C85-C86-C87
13	O	304	9YF	O9-C8-C9-C10
16	M	503	CDL	C80-C81-C82-C83
16	F	606	CDL	C32-C31-CA7-OA8
16	B	603	CDL	C55-C56-C57-C58
16	B	603	CDL	C75-C76-C77-C78
16	P	101	CDL	C32-C31-CA7-OA8
15	B	601	HEM	CAA-CBA-CGA-O2A
22	F	602	HEA	CAD-CBD-CGD-O2D
24	O	301	MQ7	C30-C31-C32-C33
14	M	504	PLM	C9-CA-CB-CC
16	P	101	CDL	CB7-C71-C72-C73
16	R	605	CDL	C61-C62-C63-C64

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Mol	Chain	Res	Type	Atoms
17	B	606	A1IRE	C03-C12-C13-O14
20	P	102	9Y0	O6-C21-C22-C23
16	D	103	CDL	C32-C33-C34-C35
16	N	605	CDL	C52-C53-C54-C55
16	P	103	CDL	C54-C55-C56-C57
16	B	603	CDL	C53-C54-C55-C56
16	B	605	CDL	C13-C14-C15-C16
16	N	605	CDL	C32-C31-CA7-OA8
16	F	605	CDL	C32-C31-CA7-OA9
16	R	605	CDL	CA4-CA3-OA5-PA1
16	P	101	CDL	C32-C31-CA7-OA9
19	C	304	MQ9	C38-C39-C41-C42
16	N	604	CDL	C11-C12-C13-C14
16	B	603	CDL	CB3-OB5-PB2-OB4
16	B	605	CDL	CB2-OB2-PB2-OB3
16	D	103	CDL	CA2-OA2-PA1-OA3
16	N	605	CDL	CA3-OA5-PA1-OA3
16	N	605	CDL	CB2-OB2-PB2-OB4
16	P	103	CDL	C12-C11-CA5-OA7
16	N	604	CDL	C72-C71-CB7-OB8
13	M	502	9YF	C40-C41-C42-C43
16	C	305	CDL	C82-C83-C84-C85
20	S	301	9Y0	C11-C10-C9-C8
16	C	305	CDL	C52-C51-CB5-OB6
22	R	602	HEA	C14-C15-C16-C17
20	D	102	9Y0	C4-C3-O1-P
20	P	102	9Y0	C-C1-O7-C21
20	S	301	9Y0	C4-C3-O1-P
13	O	304	9YF	O12-C25-C26-C27
16	N	607	CDL	C52-C51-CB5-OB7
13	C	303	9YF	C34-C33-C35-C36
16	F	605	CDL	C72-C71-CB7-OB8
16	N	607	CDL	C72-C71-CB7-OB8
16	N	603	CDL	C72-C73-C74-C75
16	N	604	CDL	C75-C76-C77-C78
16	C	305	CDL	CA2-C1-CB2-OB2
22	F	601	HEA	CAA-CBA-CGA-O2A
13	C	303	9YF	C37-C38-C39-C40
16	N	604	CDL	C56-C57-C58-C59
13	O	304	9YF	O10-C8-C9-C10
16	N	605	CDL	C32-C31-CA7-OA9
24	H	201	MQ7	C39-C38-C40-C41

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Mol	Chain	Res	Type	Atoms
20	G	301	9Y0	O7-C1-C2-O3
13	M	502	9YF	O11-C25-C26-C27
16	P	103	CDL	C52-C51-CB5-OB6
16	P	103	CDL	C72-C71-CB7-OB8
16	P	103	CDL	C83-C84-C85-C86
16	N	607	CDL	C32-C31-CA7-OA8
16	D	101	CDL	C38-C39-C40-C41
16	N	607	CDL	C72-C71-CB7-OB9
22	F	602	HEA	CAD-CBD-CGD-O1D
16	P	101	CDL	C19-C20-C21-C22
16	F	606	CDL	C12-C11-CA5-OA6
16	P	103	CDL	C52-C51-CB5-OB7
22	F	602	HEA	CAA-CBA-CGA-O1A
14	M	504	PLM	C3-C4-C5-C6
13	M	502	9YF	O12-C25-C26-C27

There are no ring outliers.

40 monomers are involved in 149 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	P	101	CDL	6	0
16	N	605	CDL	5	0
22	R	601	HEA	5	0
15	B	601	HEM	2	0
16	B	605	CDL	5	0
16	C	305	CDL	3	0
24	O	301	MQ7	2	0
18	C	302	HEC	2	0
16	N	607	CDL	4	0
19	C	304	MQ9	7	0
18	O	302	HEC	1	0
16	M	503	CDL	6	0
16	F	605	CDL	6	0
19	O	305	MQ9	7	0
24	H	201	MQ7	2	0
14	M	504	PLM	1	0
16	B	603	CDL	5	0
16	R	605	CDL	3	0
12	A	501	FES	1	0
16	P	103	CDL	5	0
16	R	606	CDL	3	0
13	C	303	9YF	1	0

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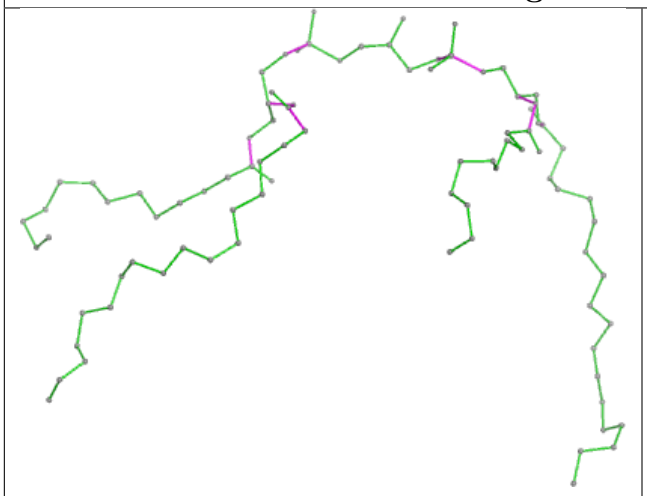
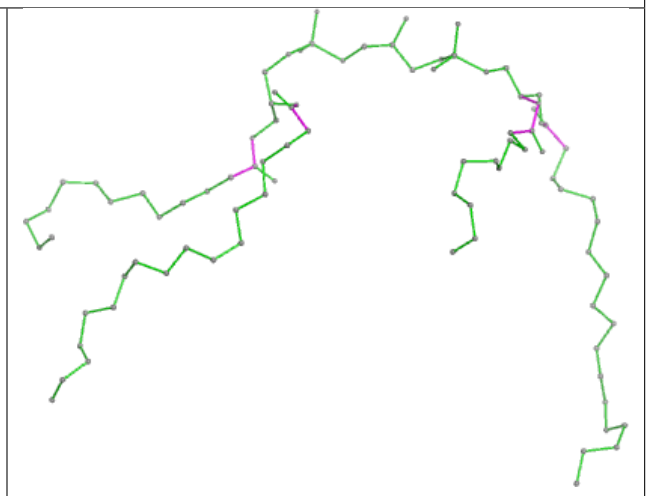
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	F	602	HEA	14	0
22	F	601	HEA	5	0
14	T	201	PLM	4	0
12	M	501	FES	1	0
16	D	101	CDL	7	0
16	D	103	CDL	12	0
16	N	603	CDL	3	0
16	N	604	CDL	2	0
15	N	602	HEM	3	0
18	O	303	HEC	1	0
20	P	102	9Y0	1	0
15	N	601	HEM	2	0
22	R	602	HEA	7	0
14	G	302	PLM	1	0
17	N	606	A1IRE	1	0
16	F	606	CDL	9	0
15	B	602	HEM	3	0
16	B	604	CDL	4	0

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

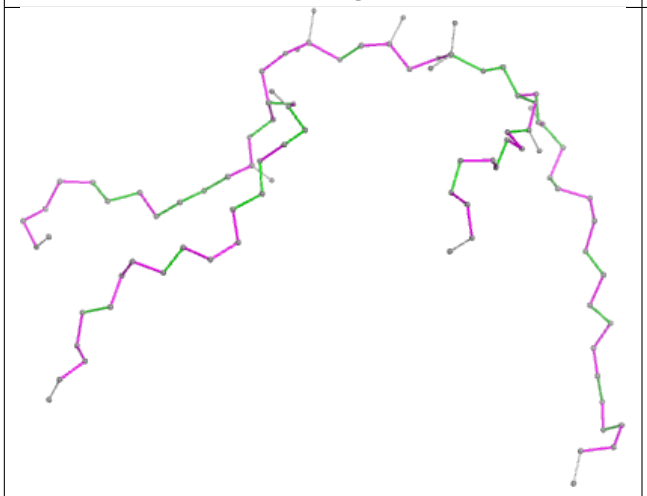
Ligand CDL P 101



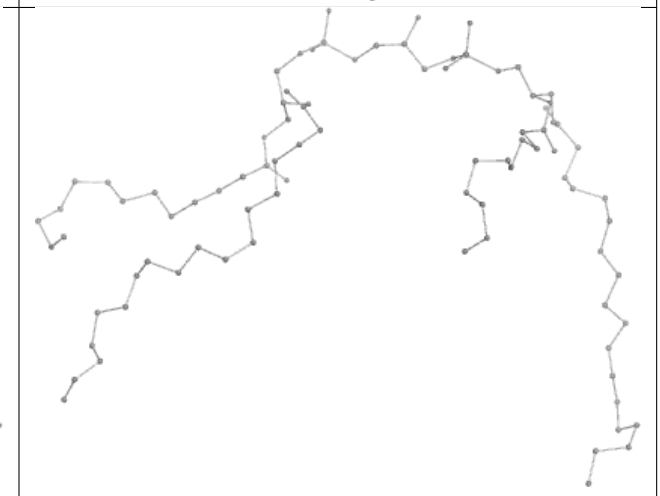
Bond lengths



Bond angles

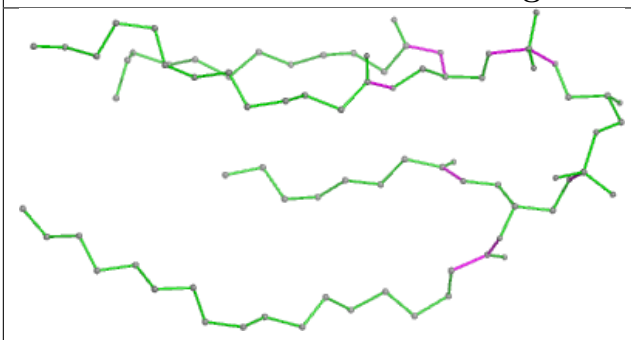


Torsions

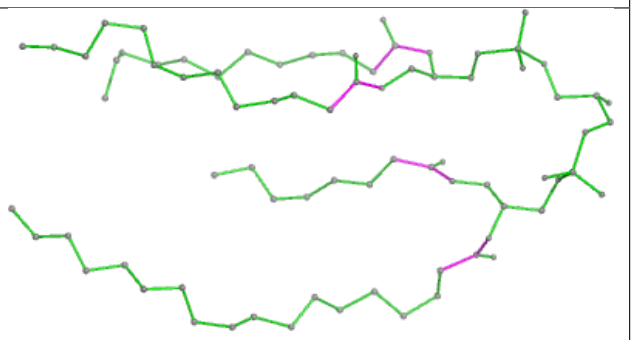


Rings

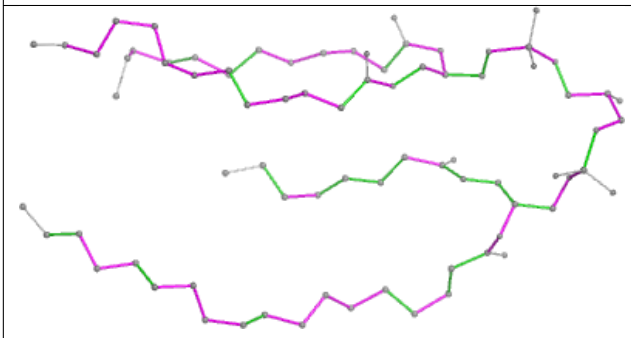
Ligand CDL N 605



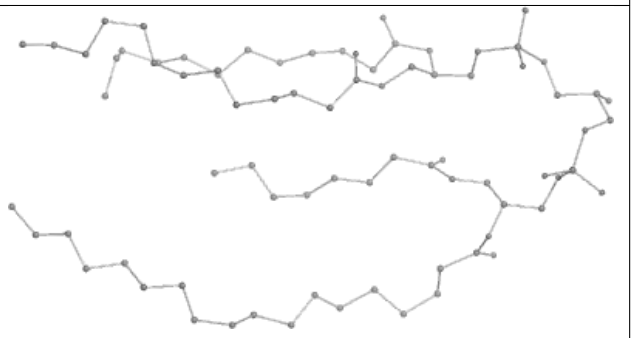
Bond lengths



Bond angles

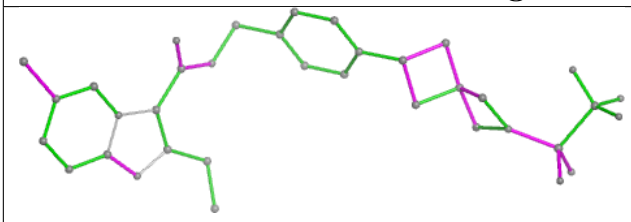


Torsions

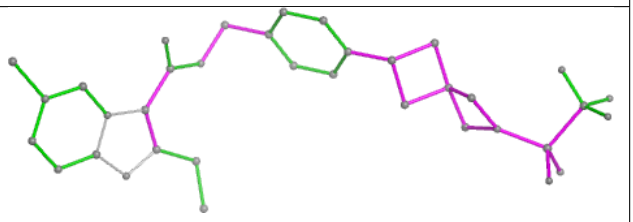


Rings

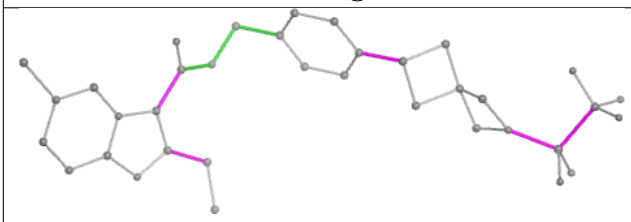
Ligand A1IRE B 606



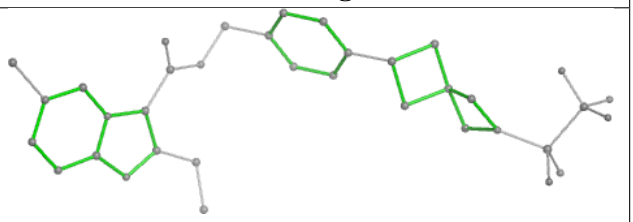
Bond lengths



Bond angles

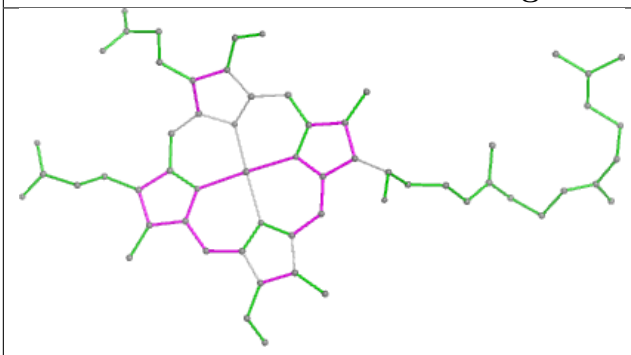


Torsions



Rings

Ligand HEA R 601



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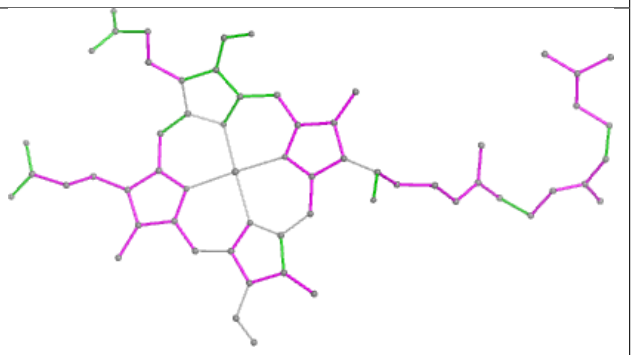
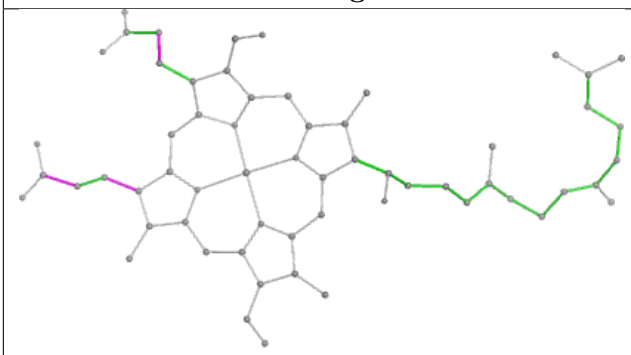
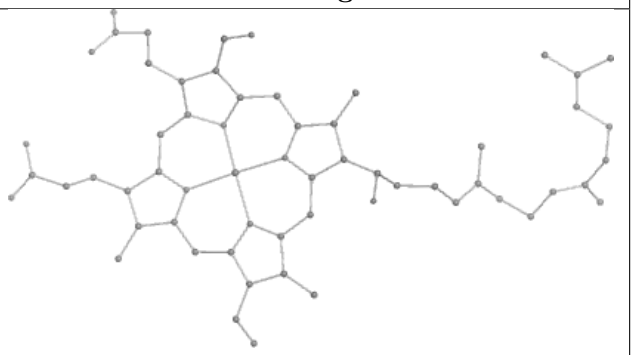


Bond angles

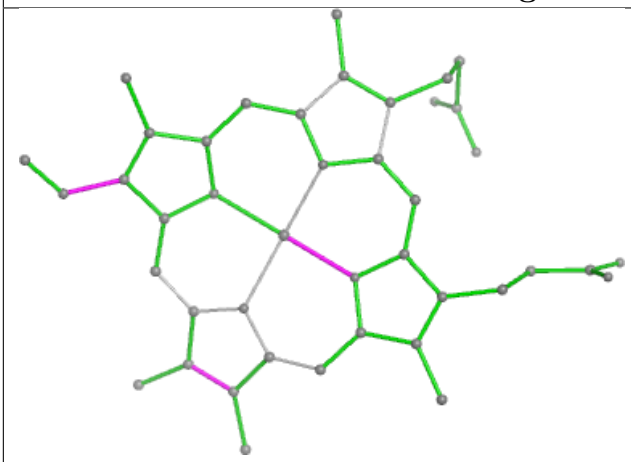


Torsions



Rings

Ligand HEM B 601



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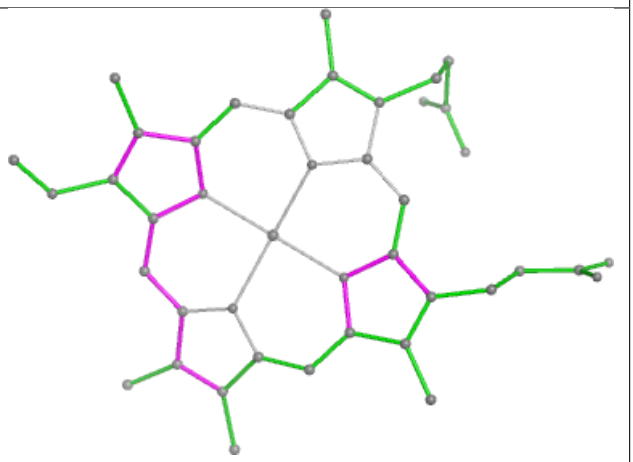
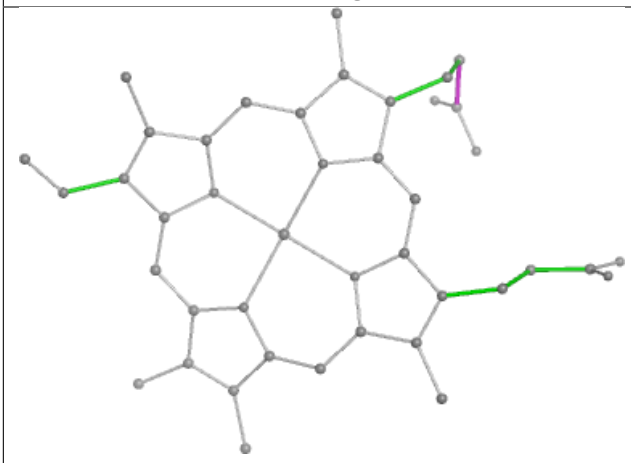
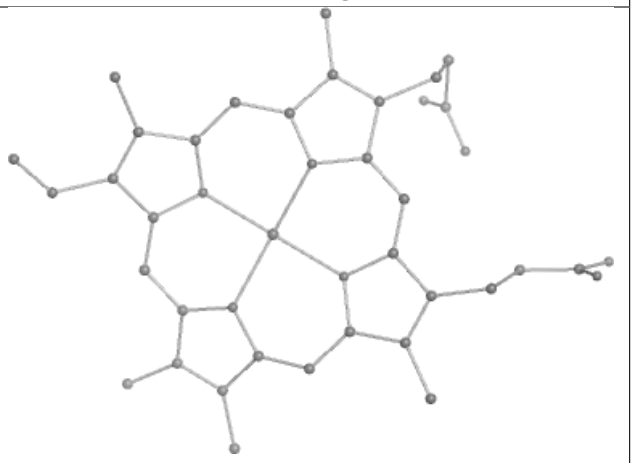


Bond angles

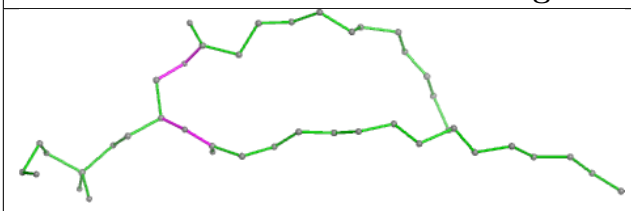


Torsions



Rings

Ligand 9Y0 S 301



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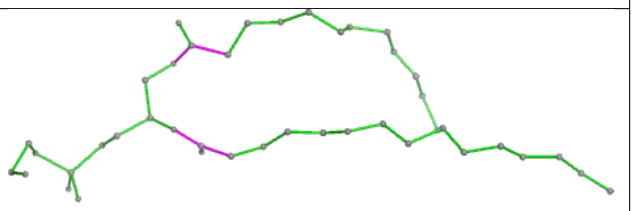
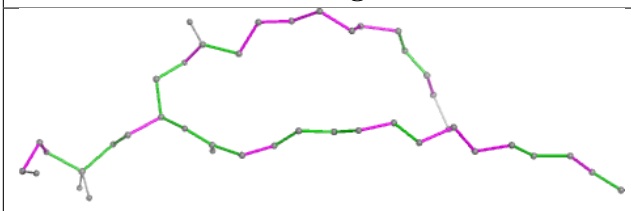
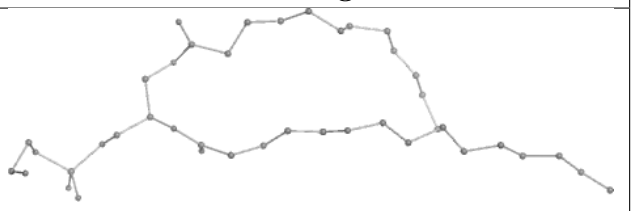


Bond angles

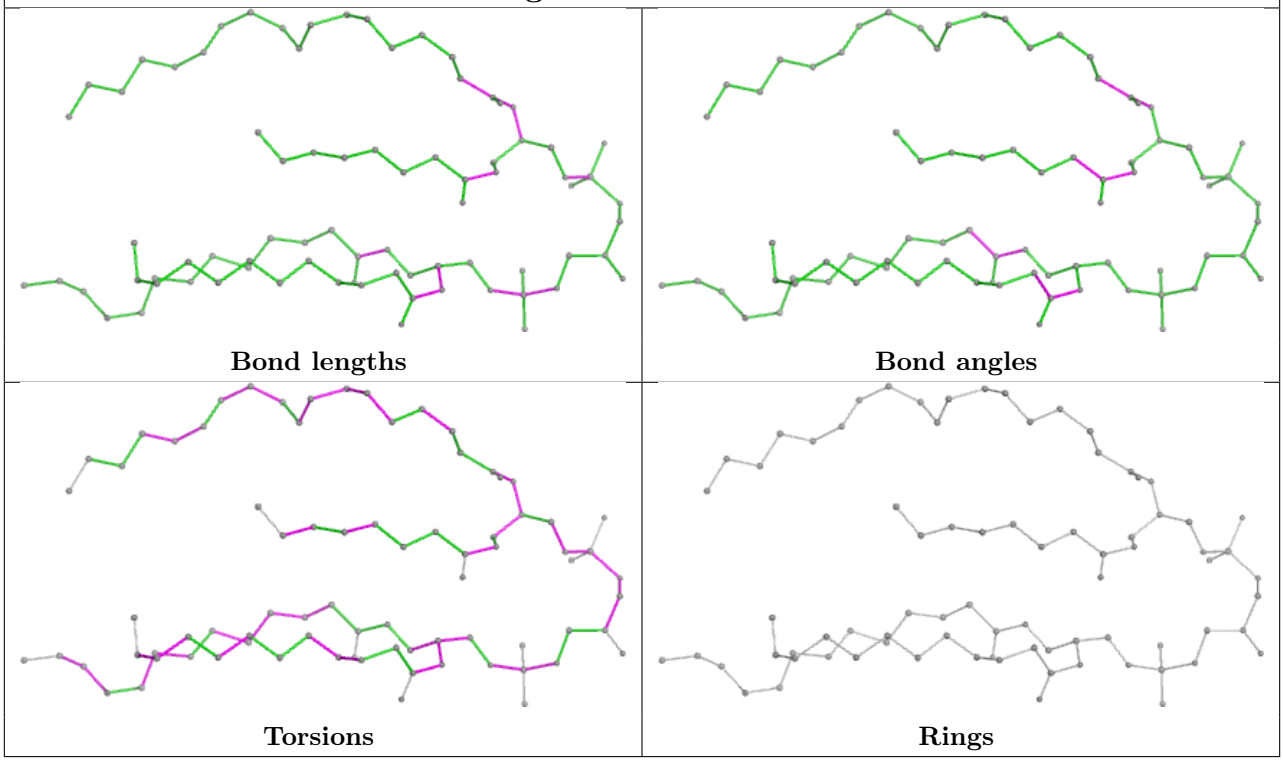


Torsions

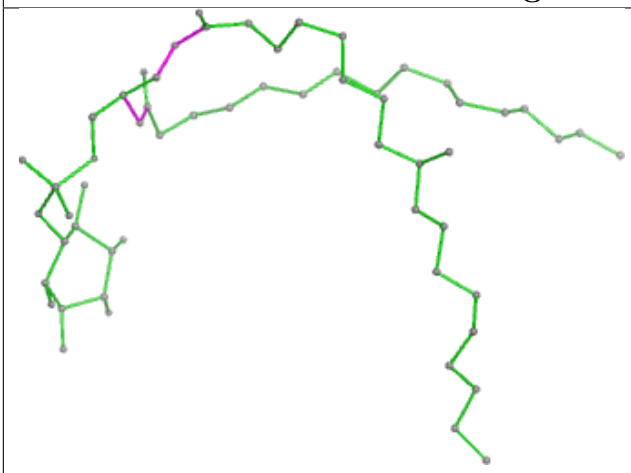


Rings

Ligand CDL B 605



Ligand 9YF M 502



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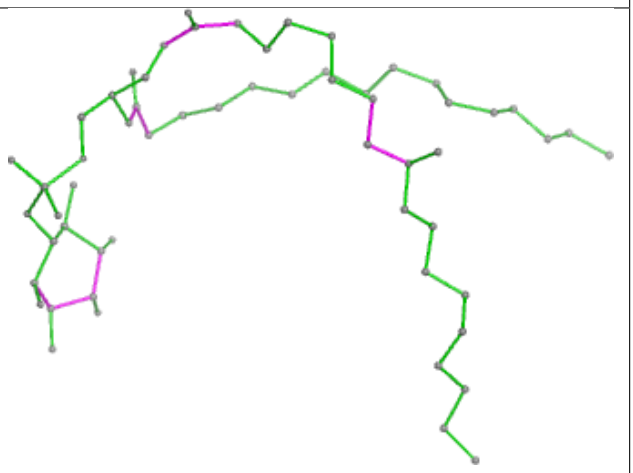
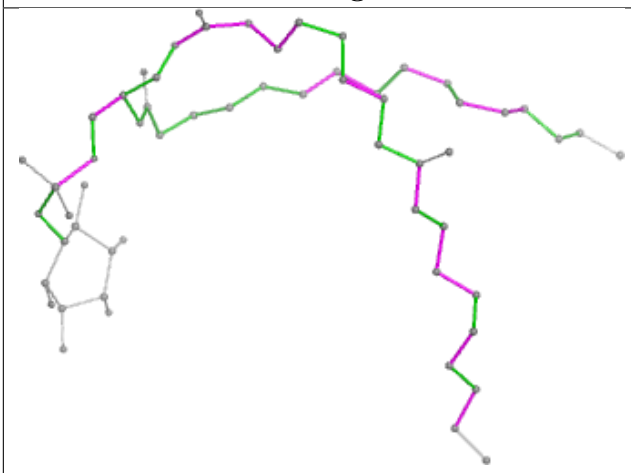


Bond angles



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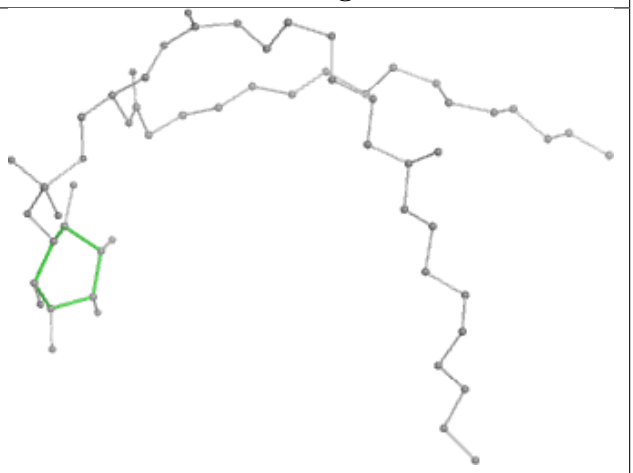
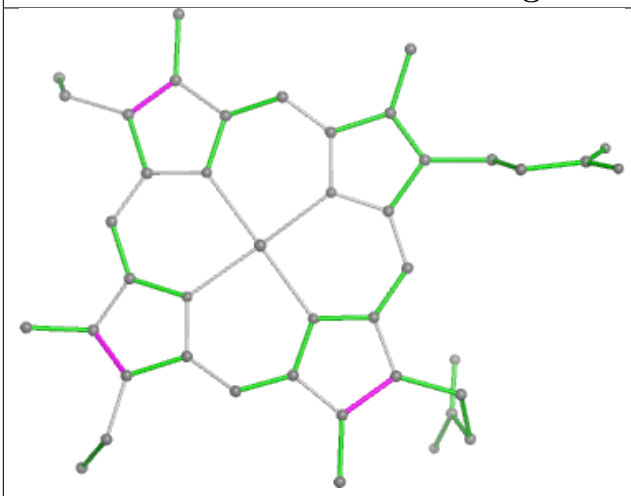


Rings

Ligand HEC C 301



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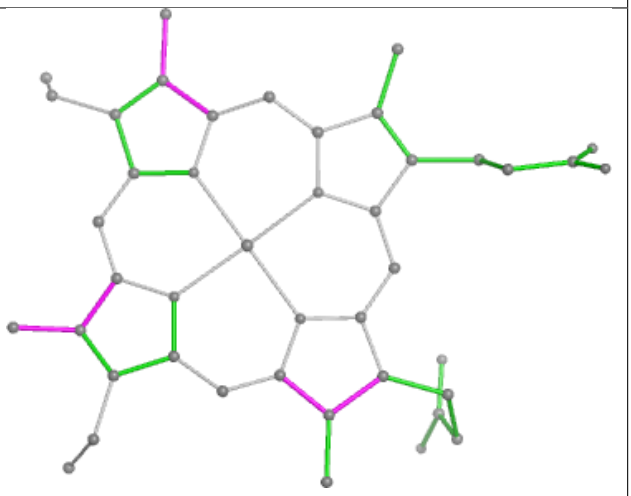
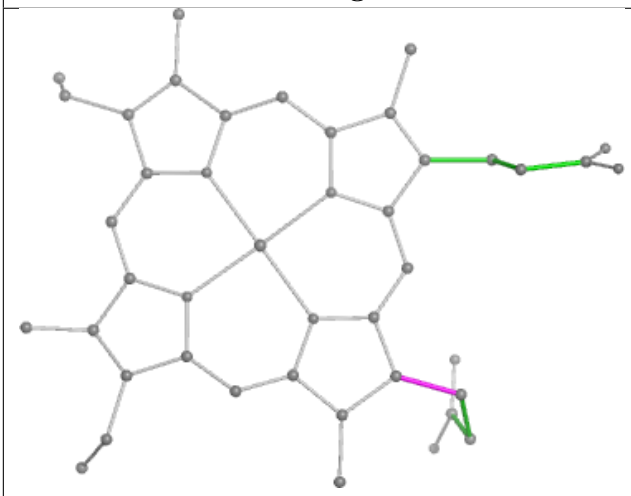


Bond angles



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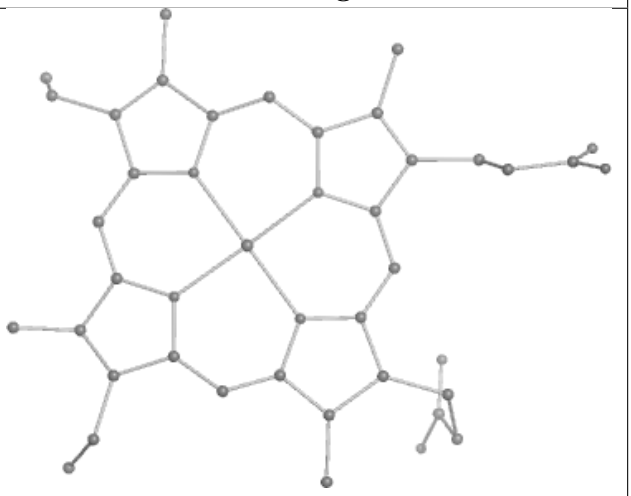
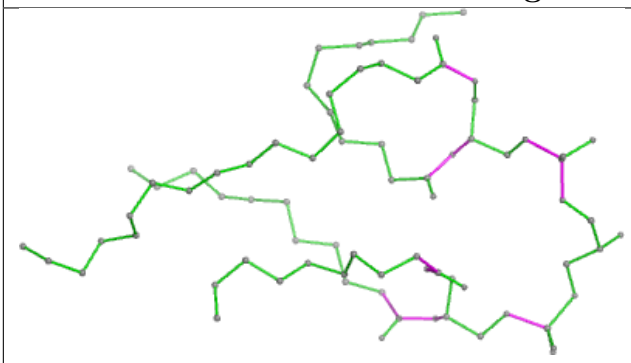


Rings

Ligand CDL C 305



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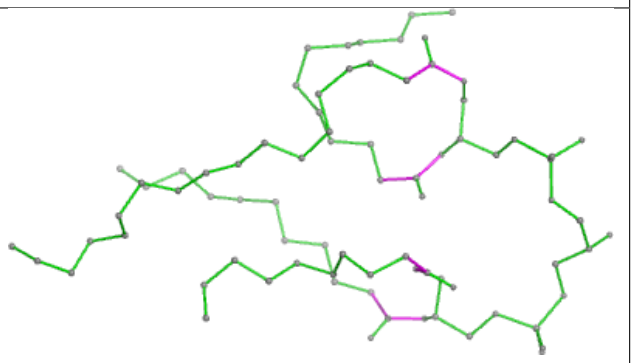
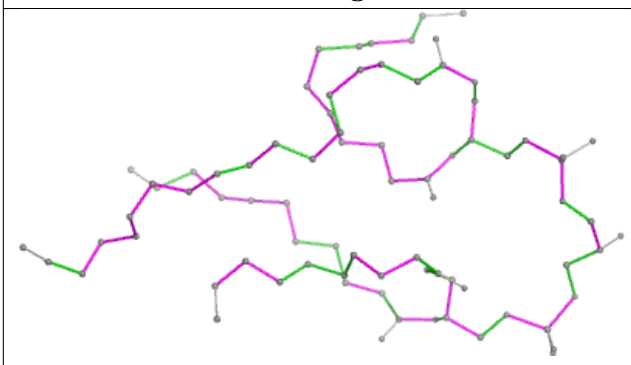


Bond angles



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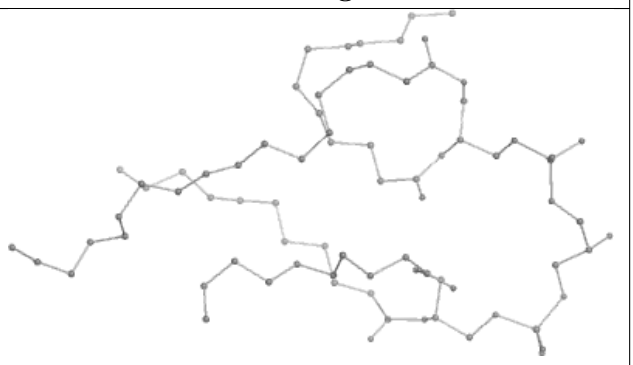
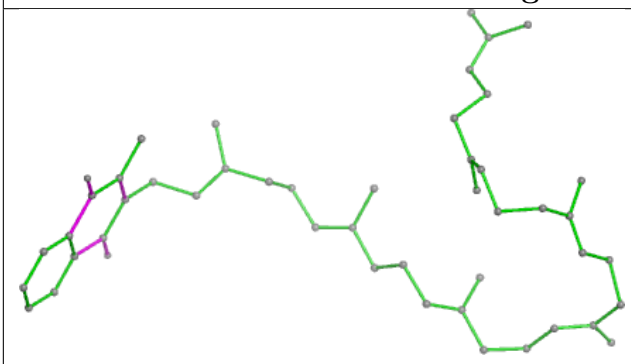


Rings

Ligand MQ7 O 301



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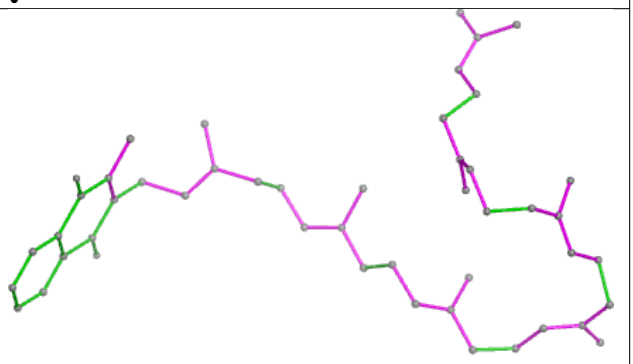
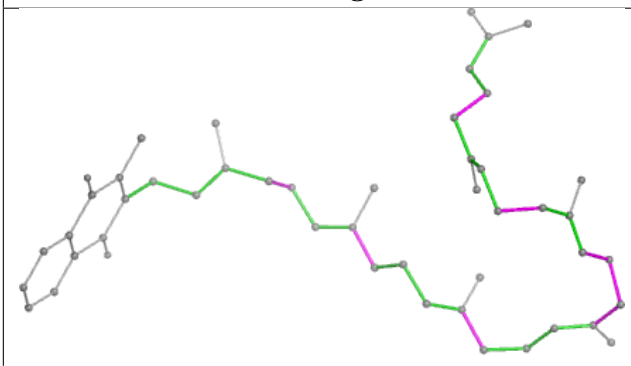
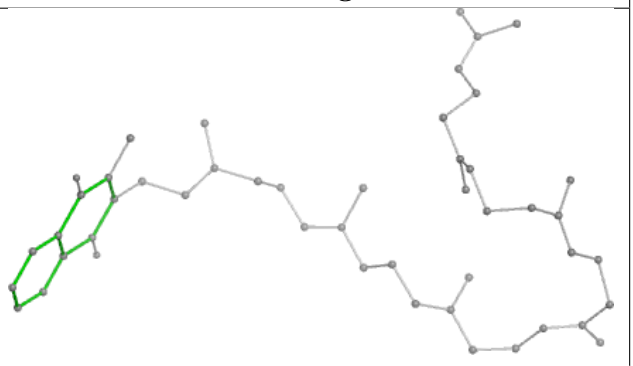


Bond angles

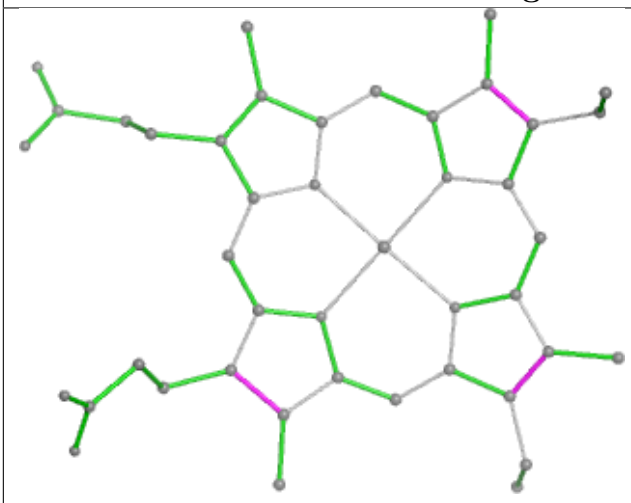


Torsions



Rings

Ligand HEC C 302



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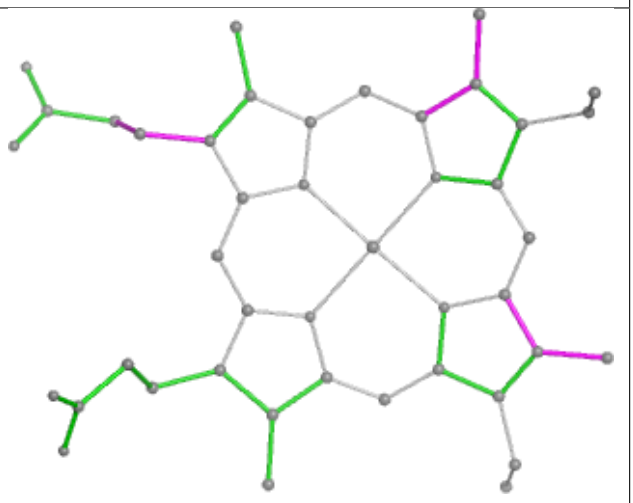
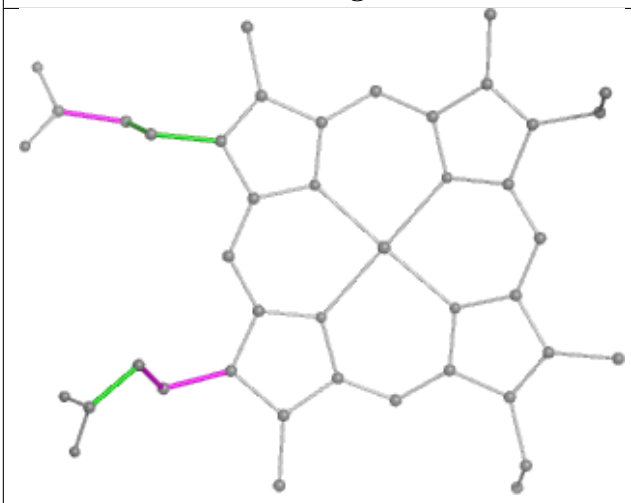


Bond angles



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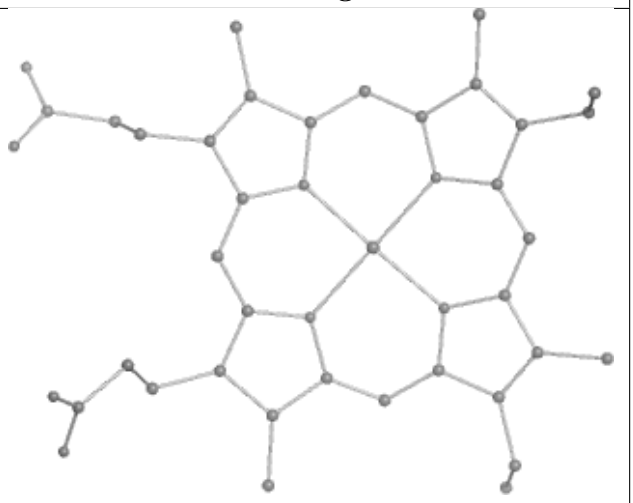
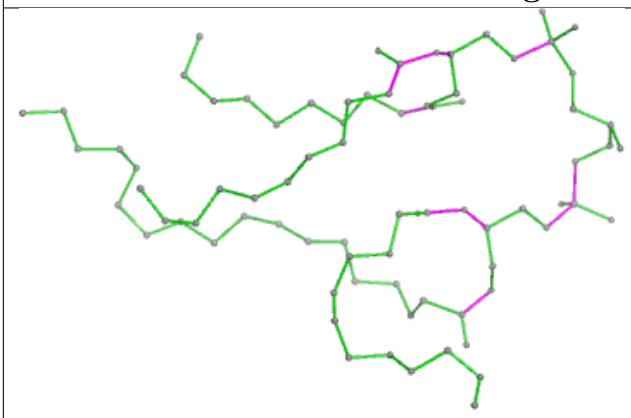


Rings

Ligand CDL N 607



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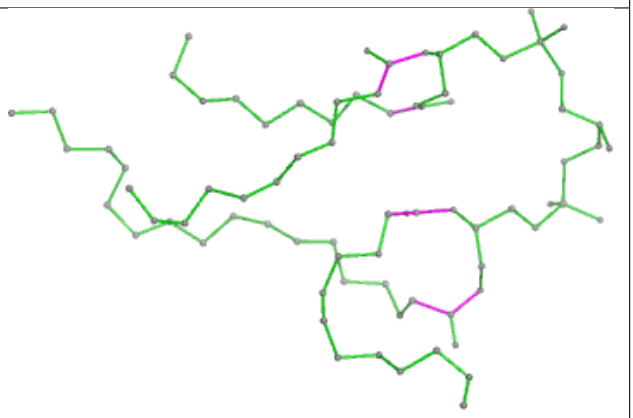
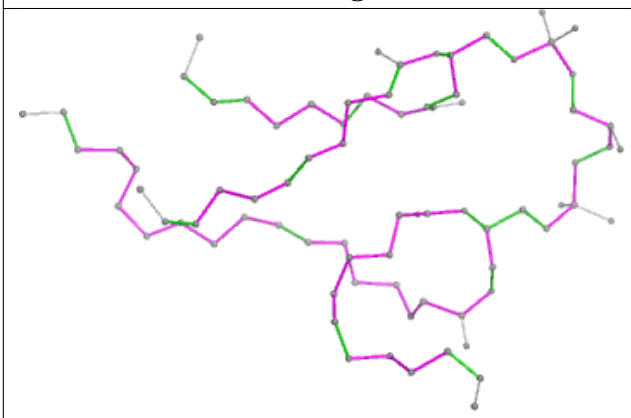


Bond angles



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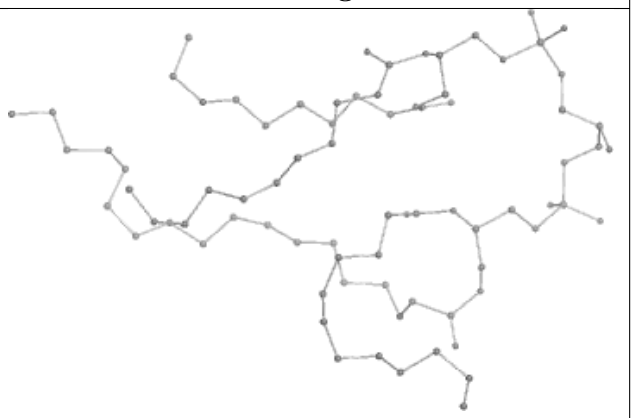
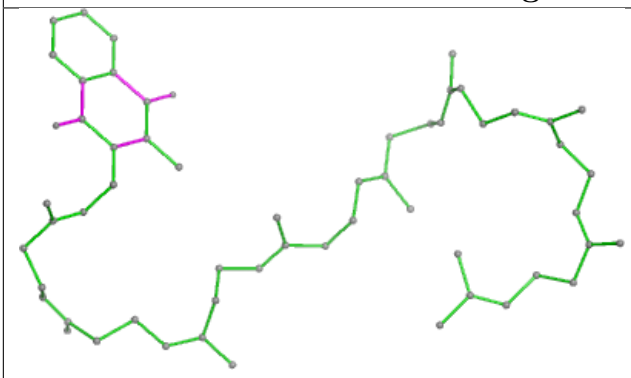


Rings

Ligand MQ9 C 304



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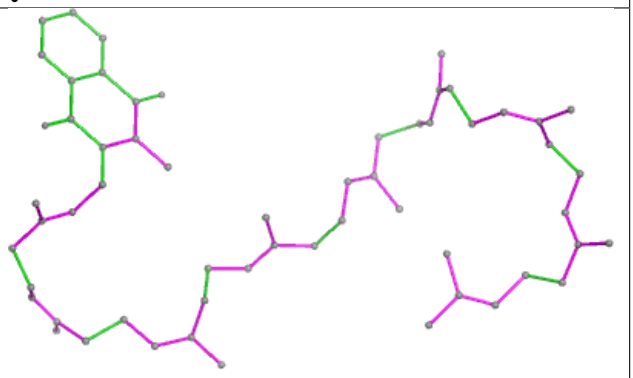
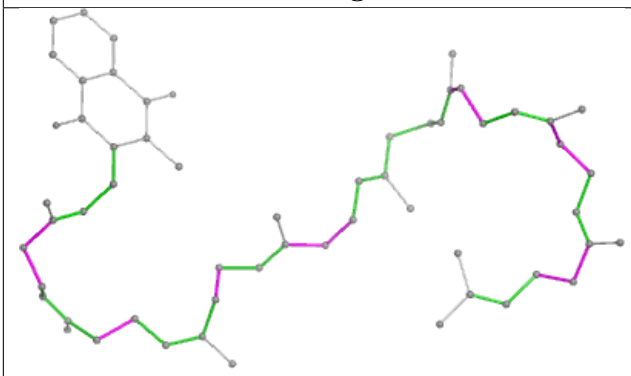


Bond angles



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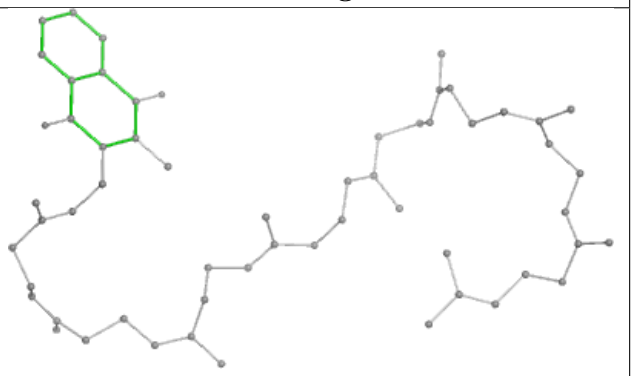
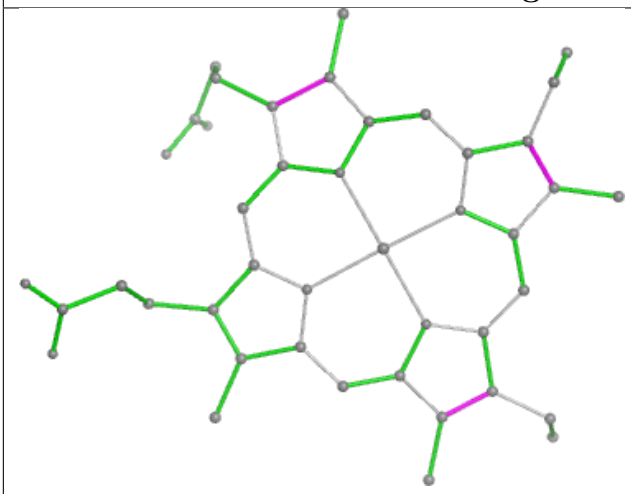


Rings

Ligand HEC O 302



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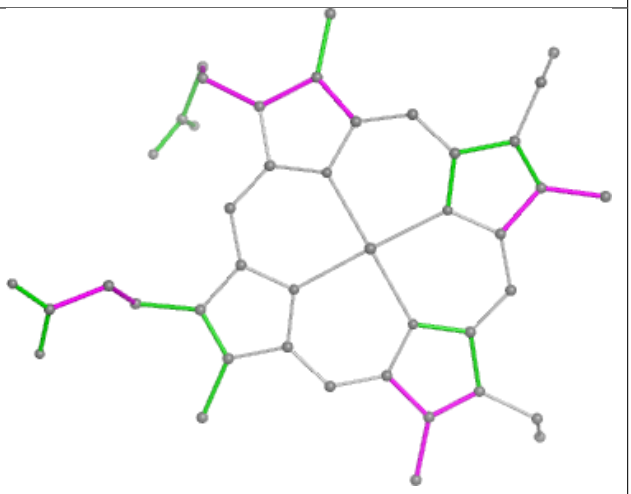
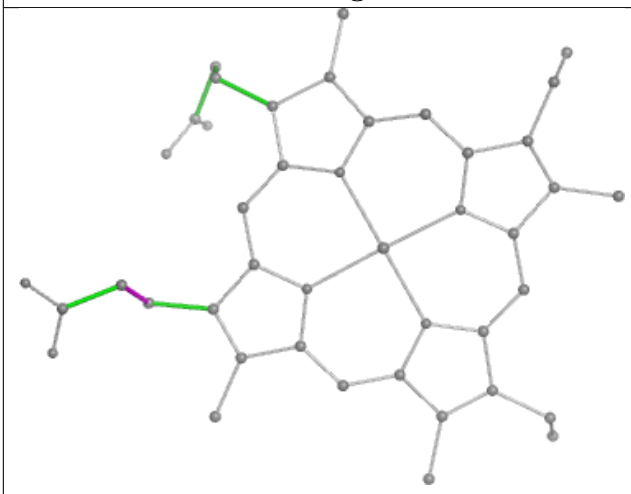
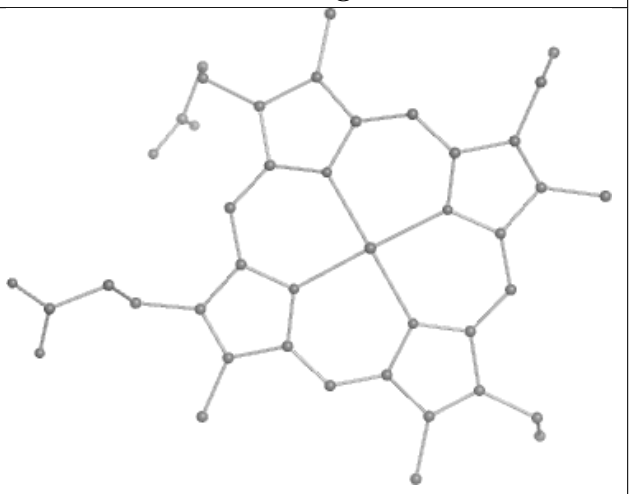


Bond angles

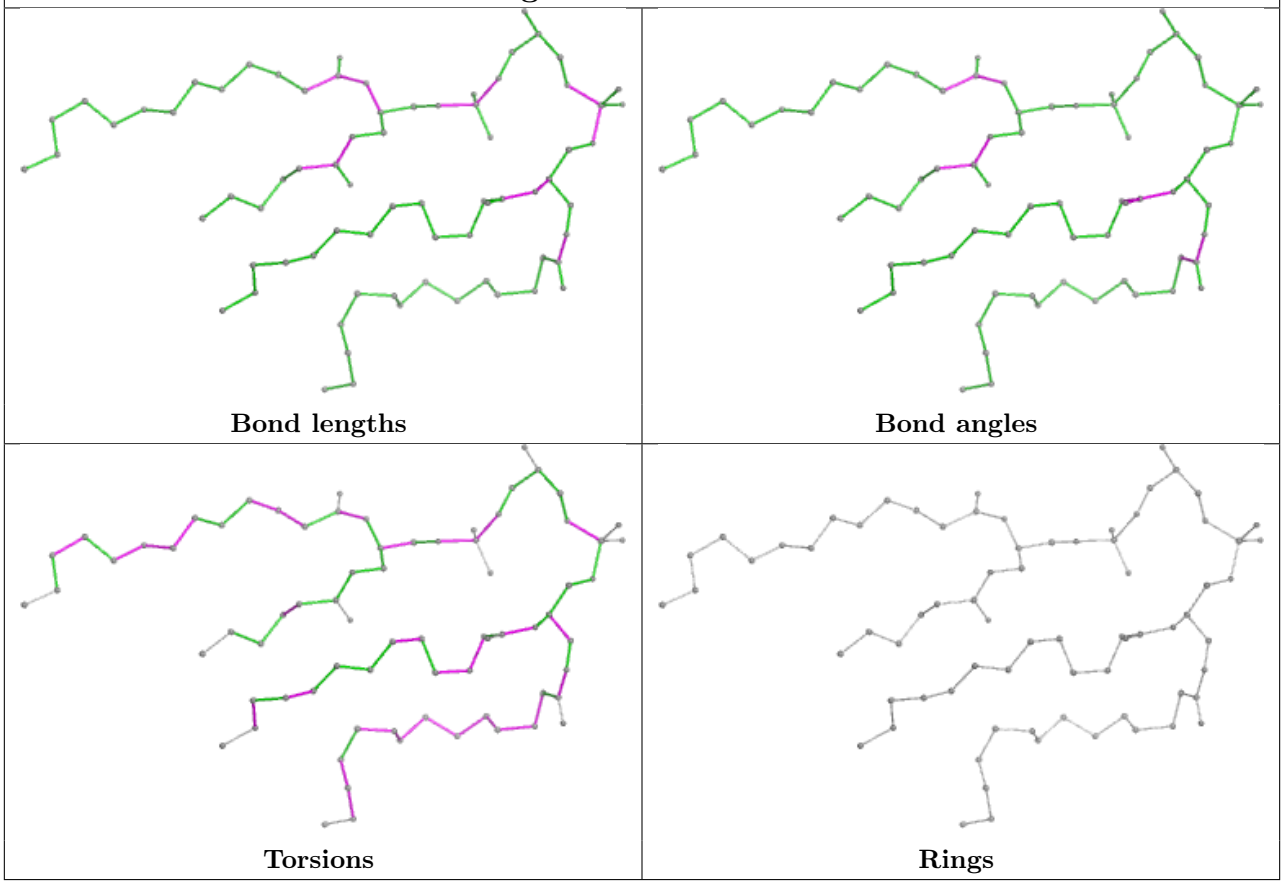


Torsions

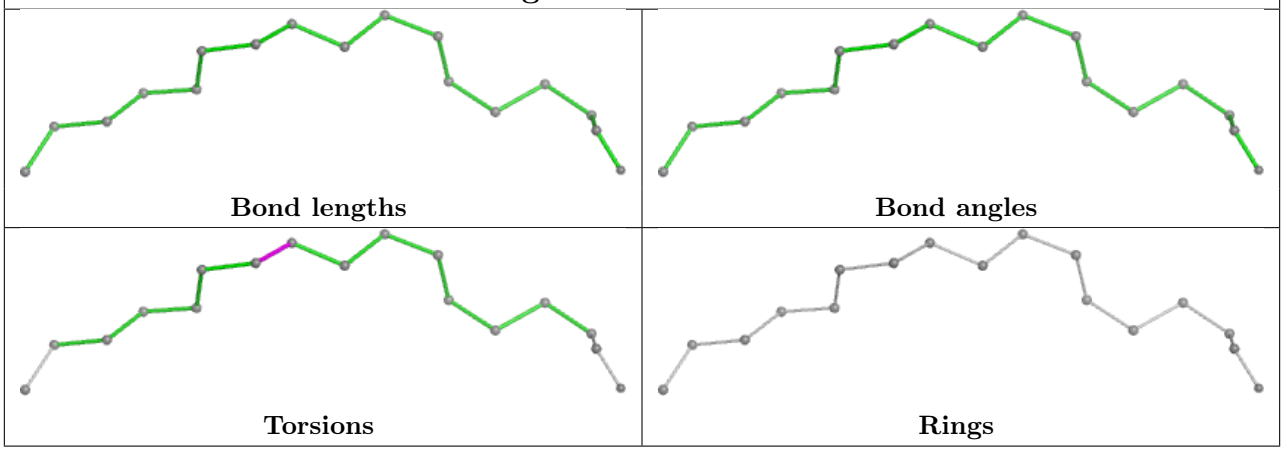


Rings

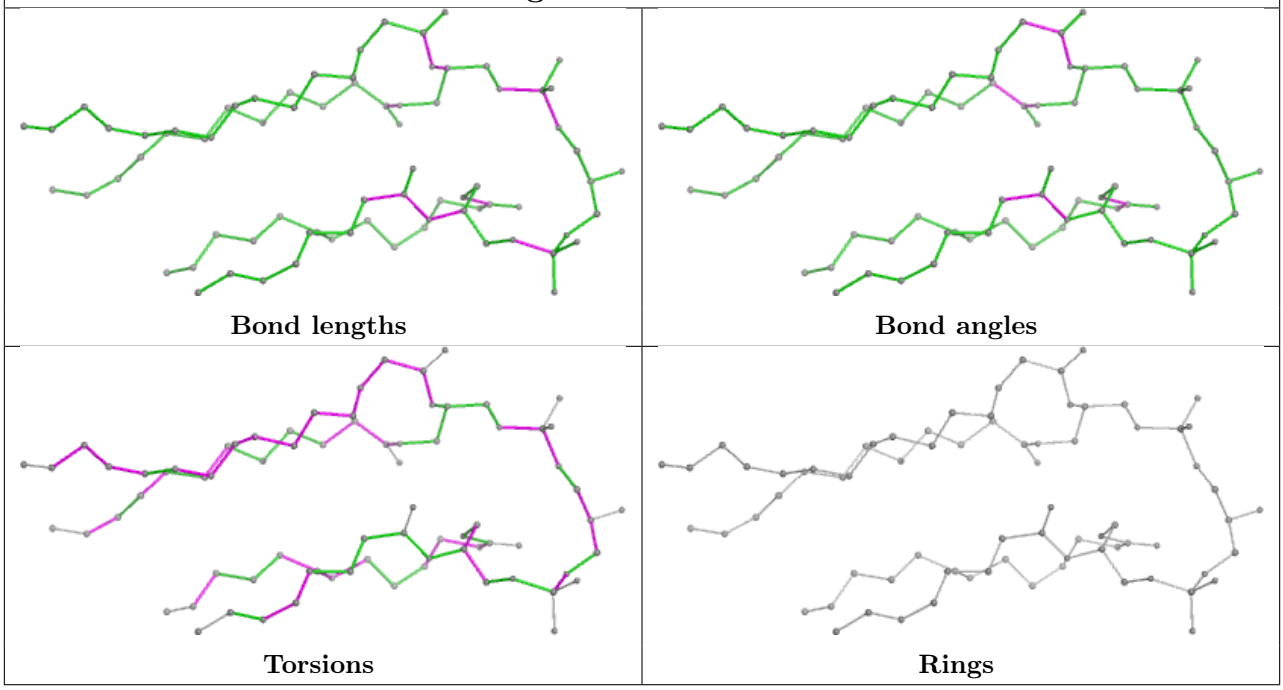
Ligand CDL M 503



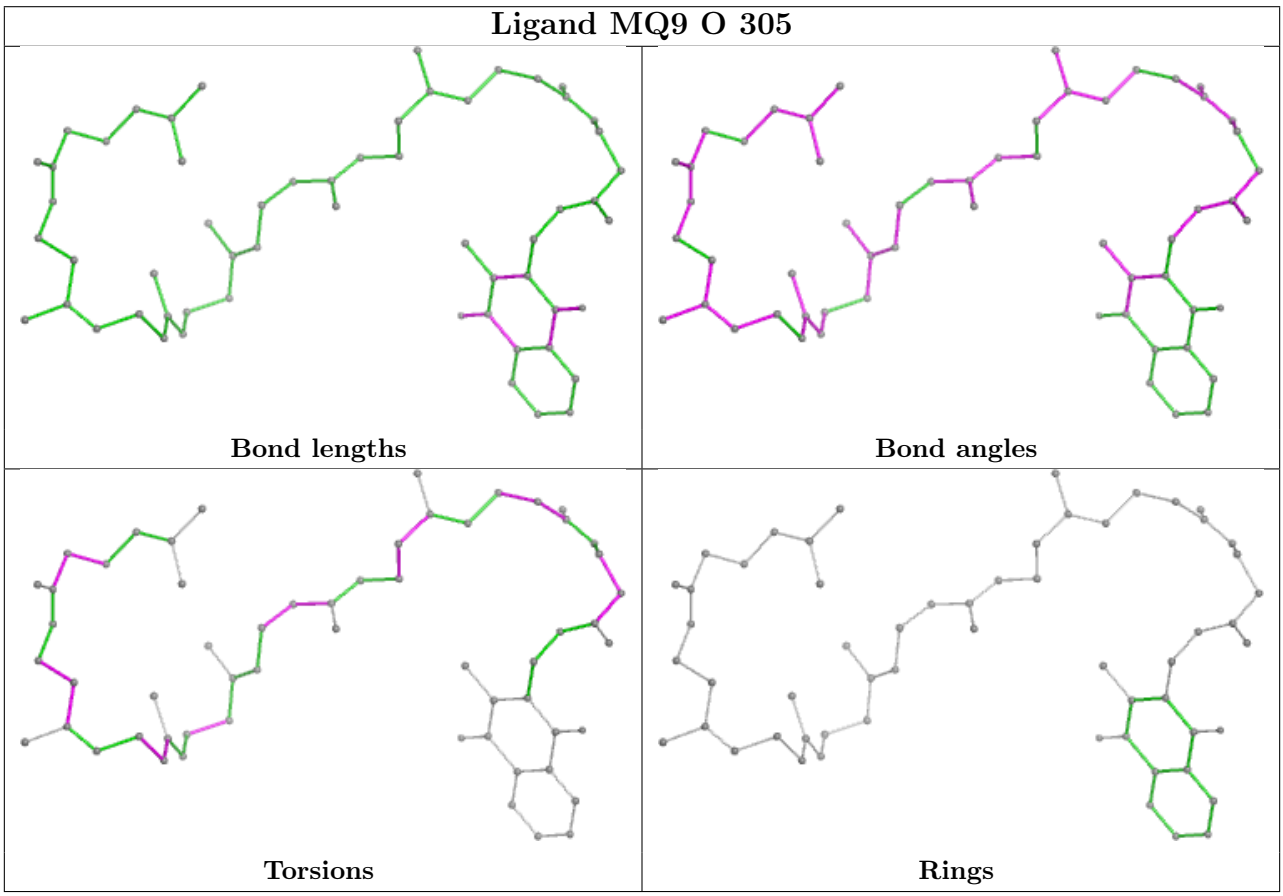
Ligand PLM A 503



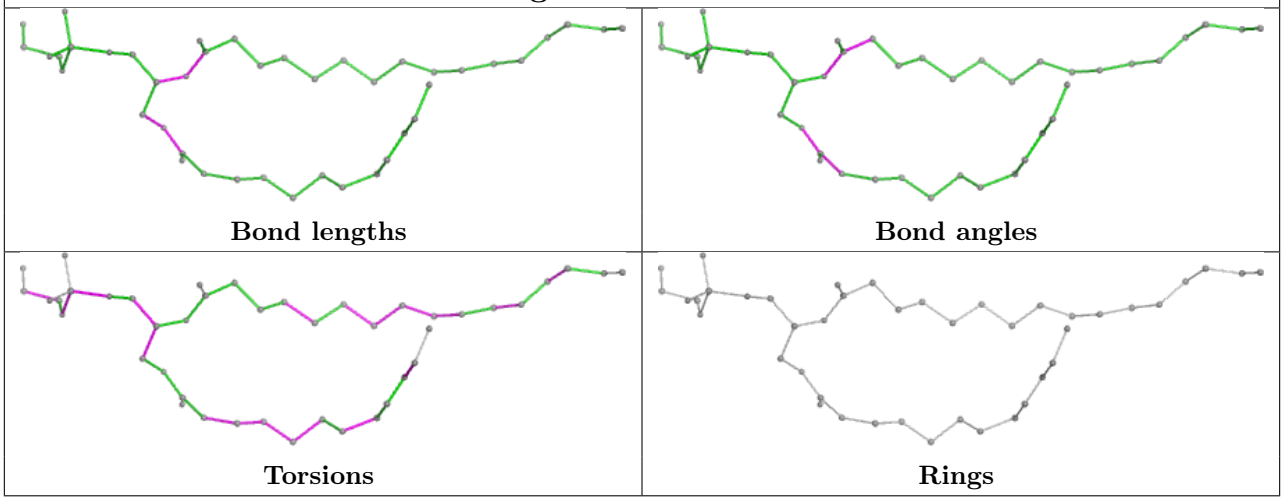
Ligand CDL F 605



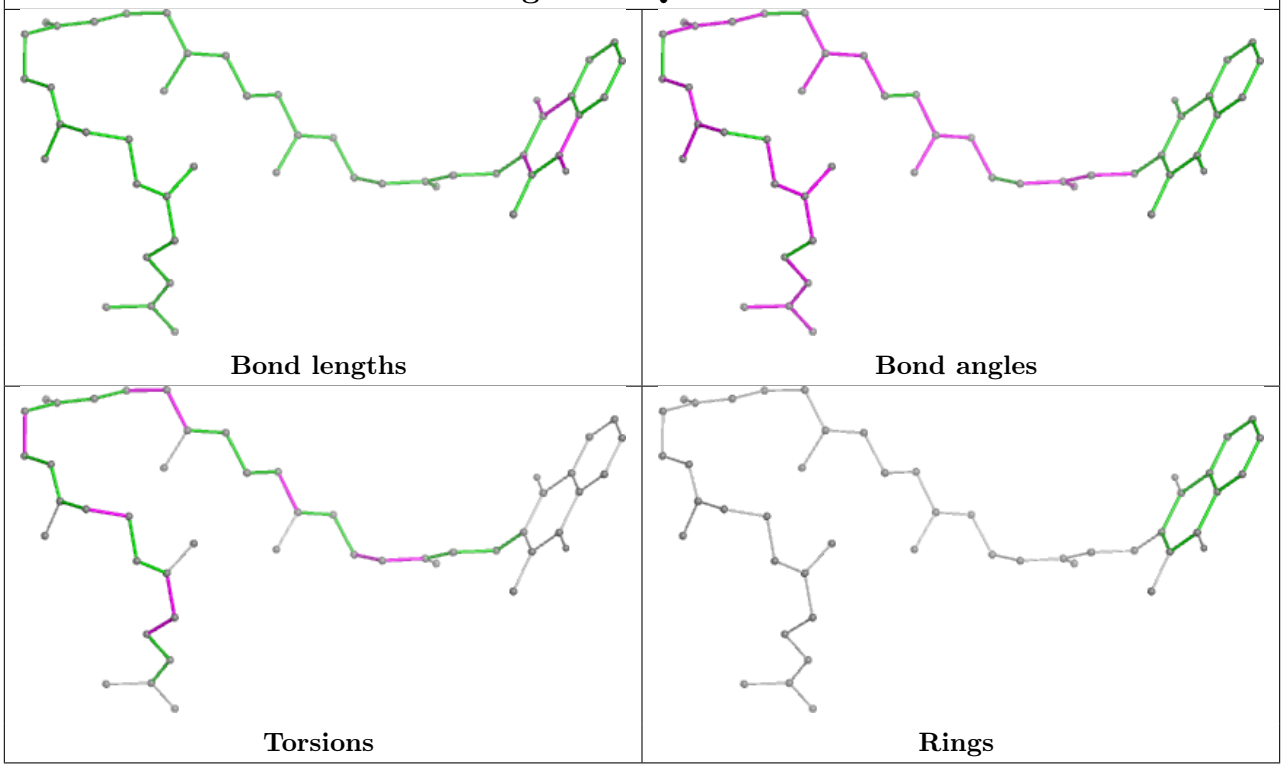
Ligand MQ9 O 305



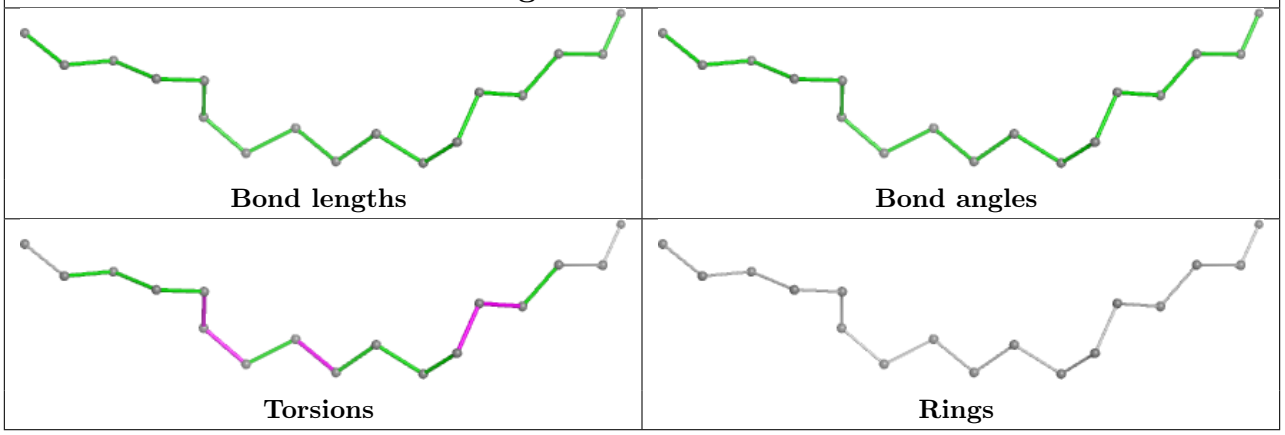
Ligand 9Y0 G 301



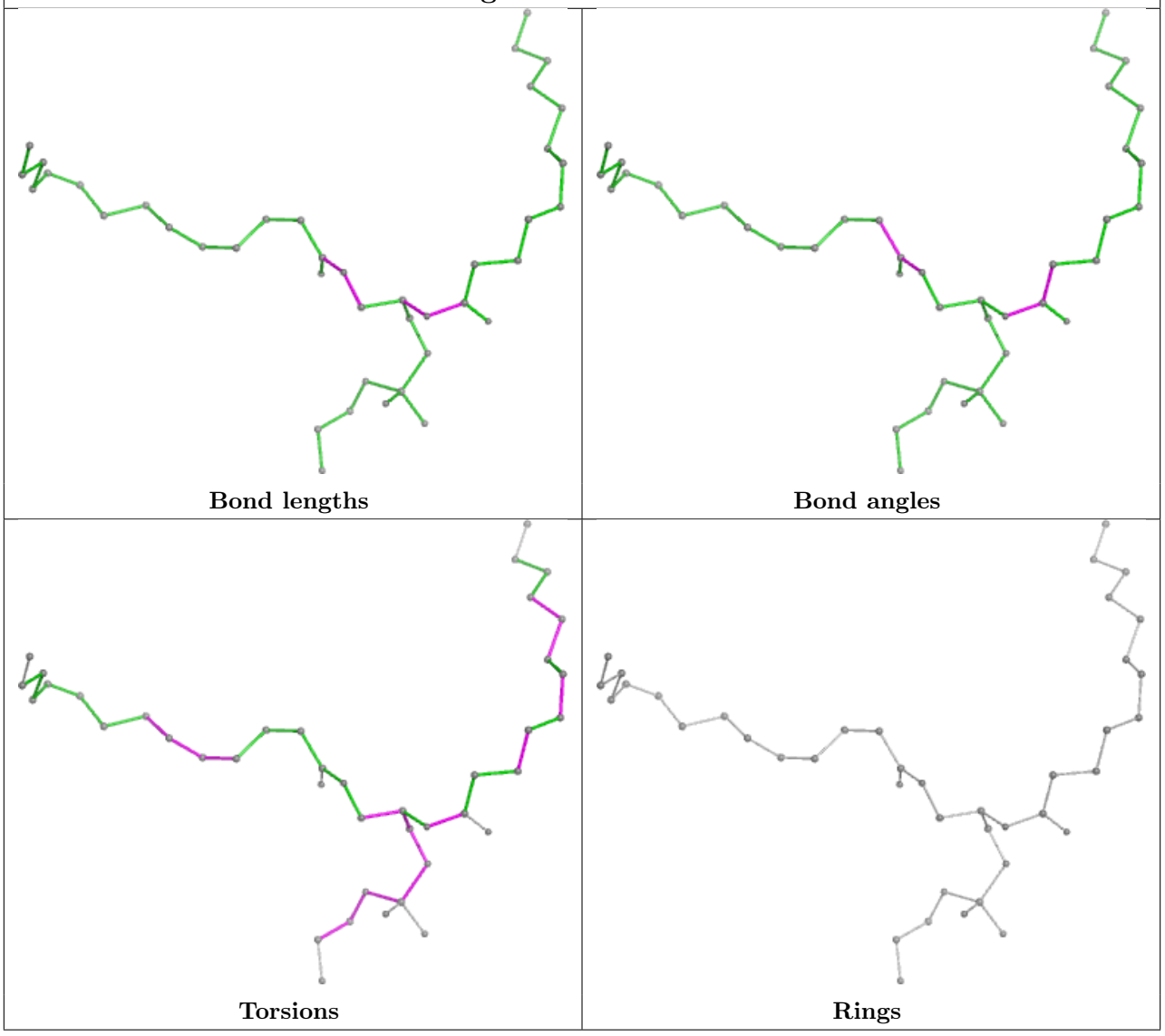
Ligand MQ7 H 201



Ligand PLM M 504

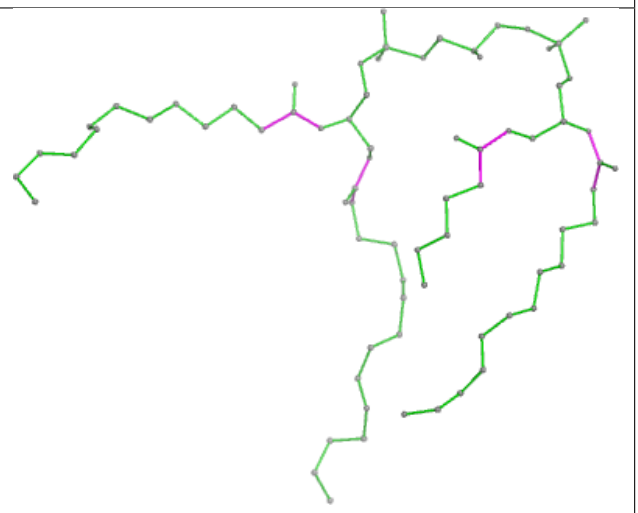


Ligand 9Y0 D 102

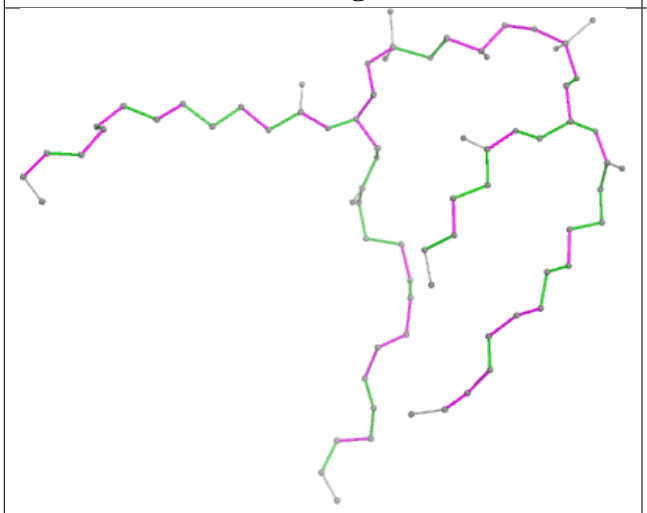


Ligand CDL B 603

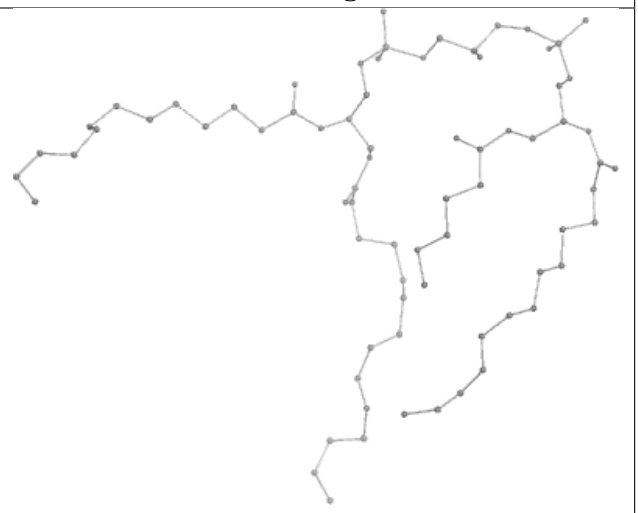
Bond lengths



Bond angles

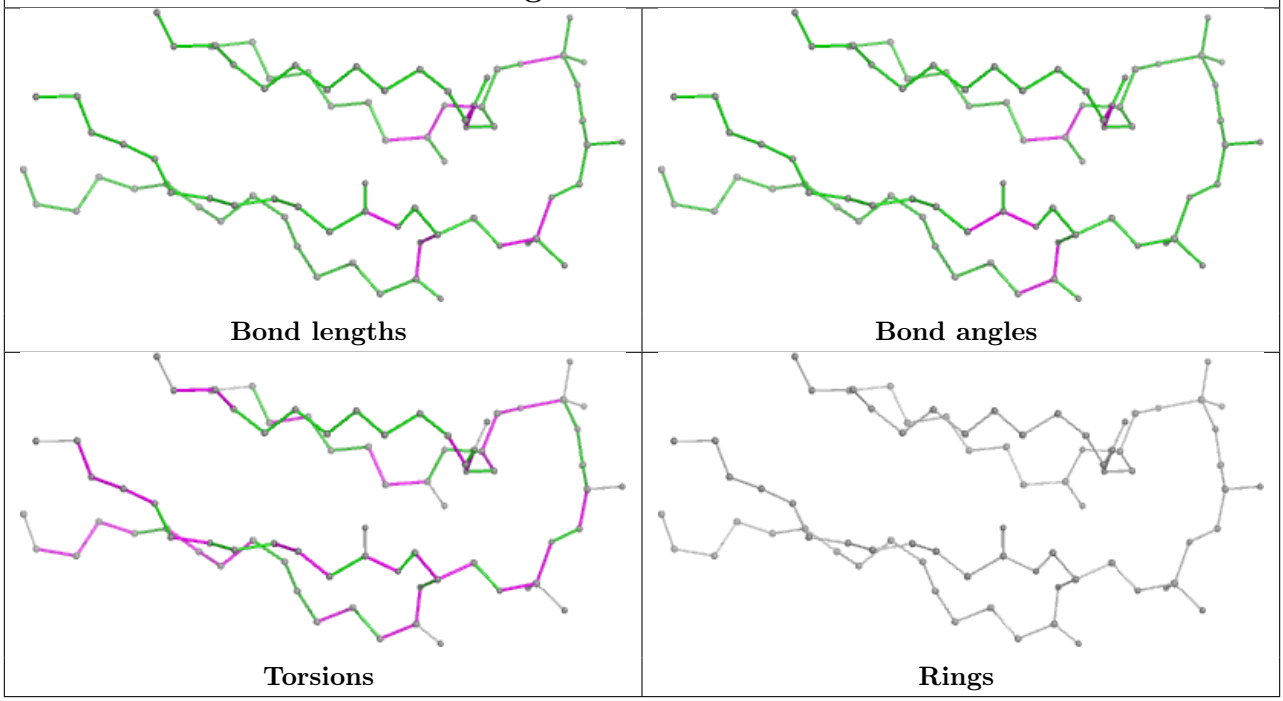


Torsions

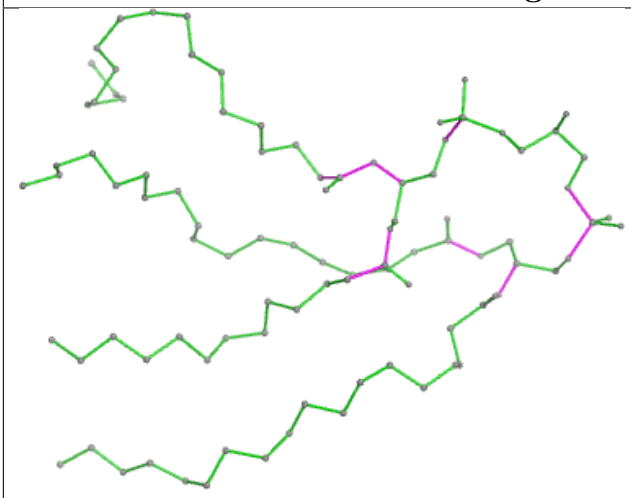


Rings

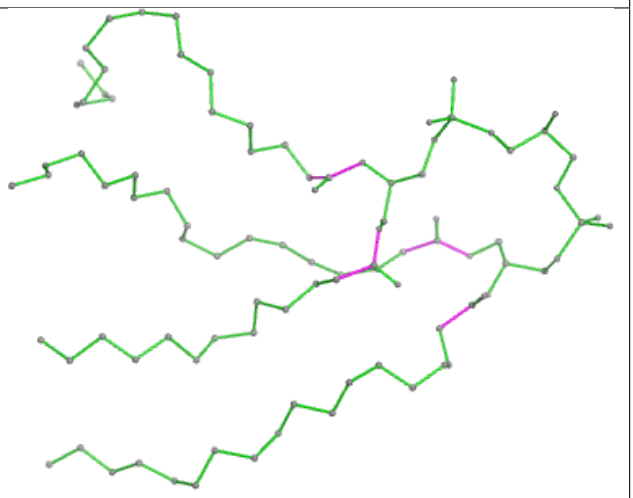
Ligand CDL R 605



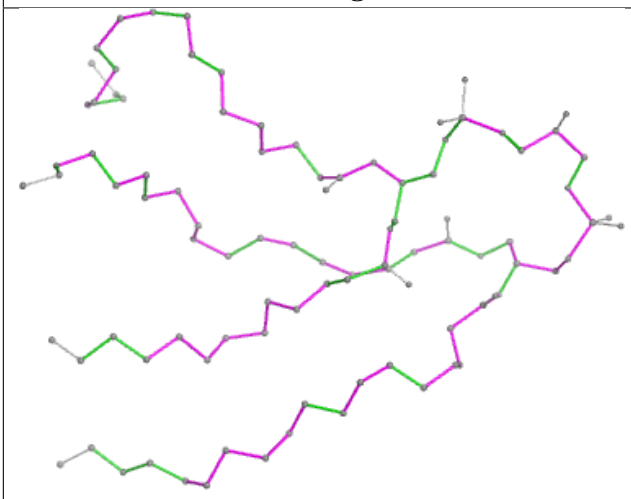
Ligand CDL P 103



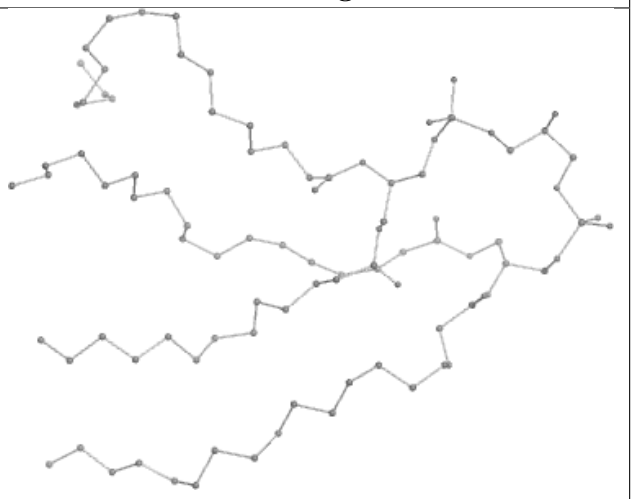
Bond lengths



Bond angles

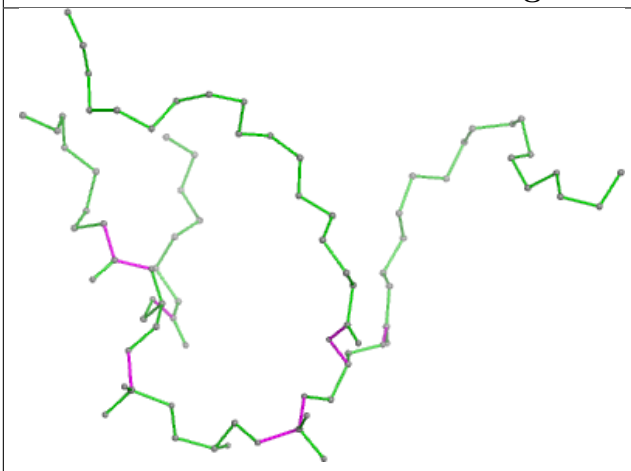


Torsions

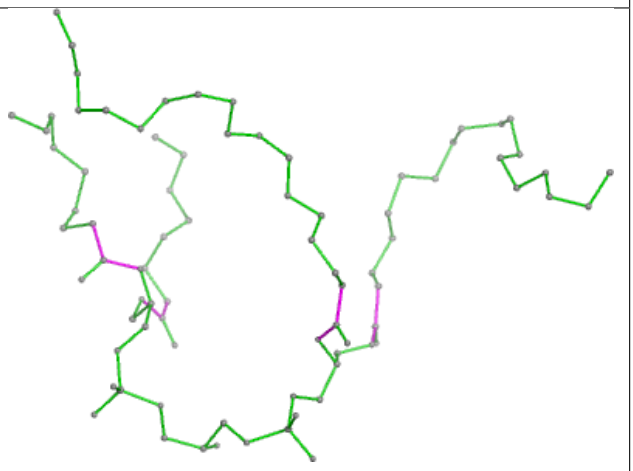


Rings

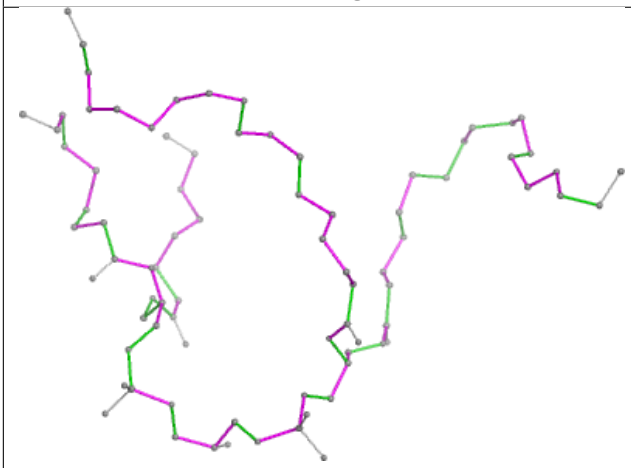
Ligand CDL R 606



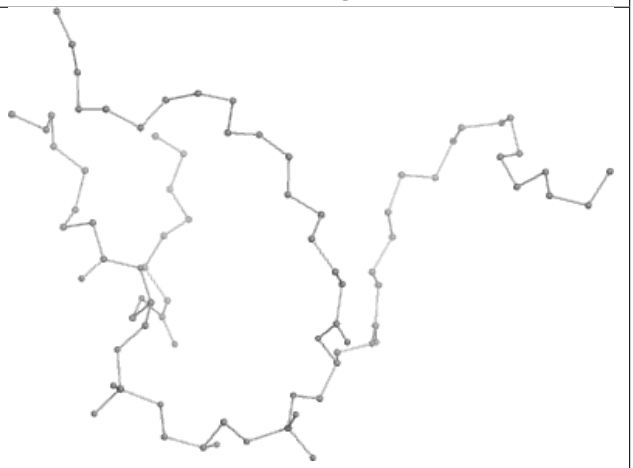
Bond lengths



Bond angles



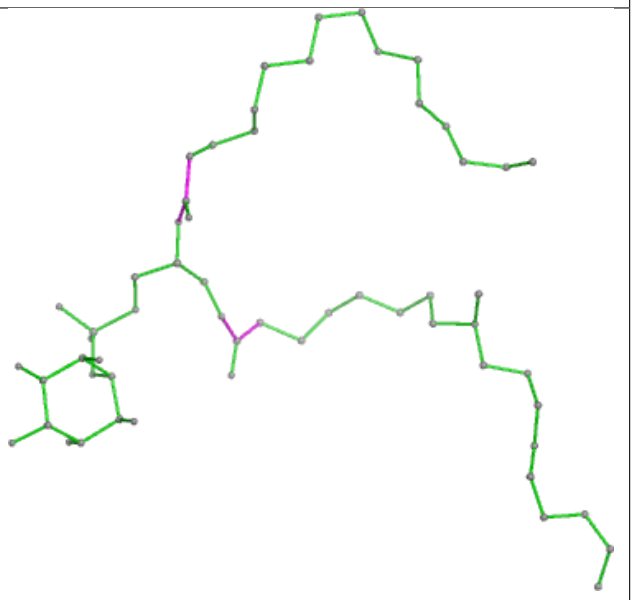
Torsions



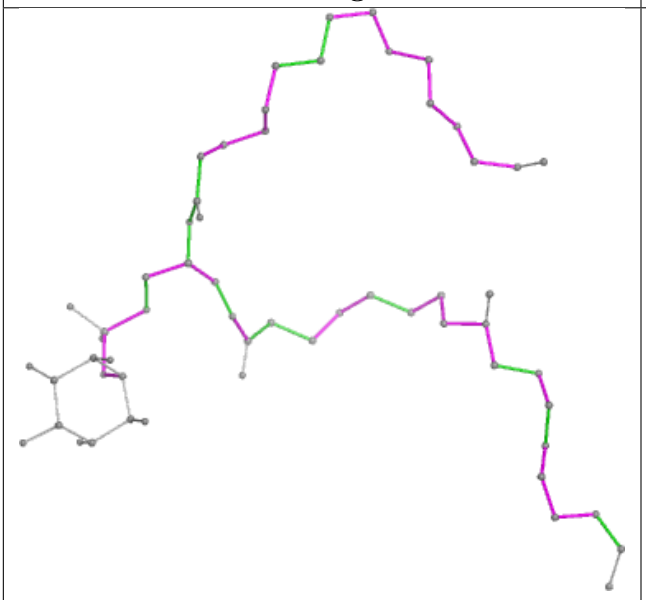
Rings

Ligand 9YF C 303

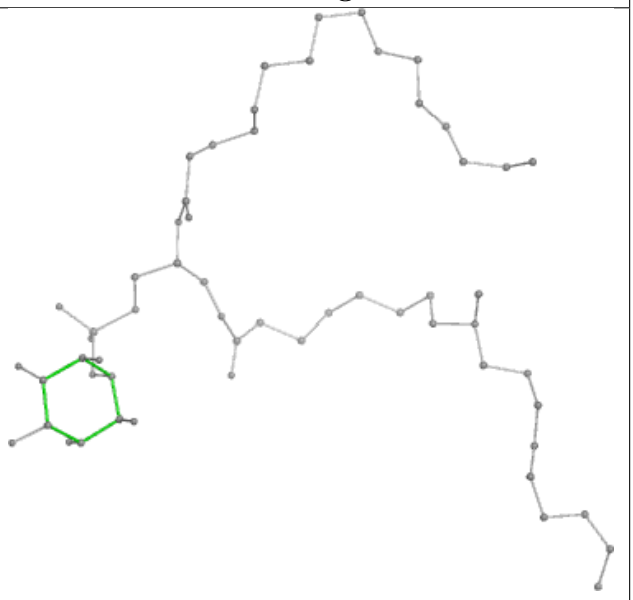
Bond lengths



Bond angles

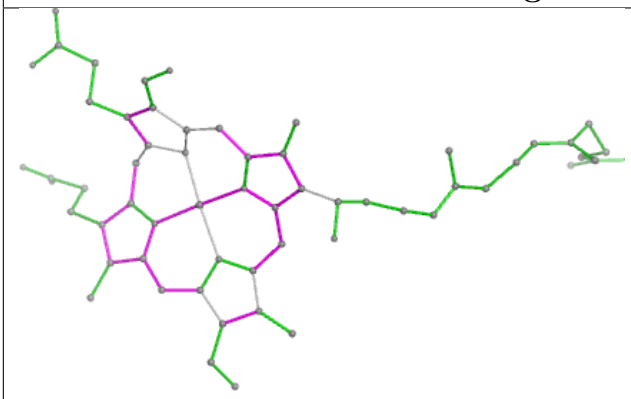


Torsions



Rings

Ligand HEA F 602



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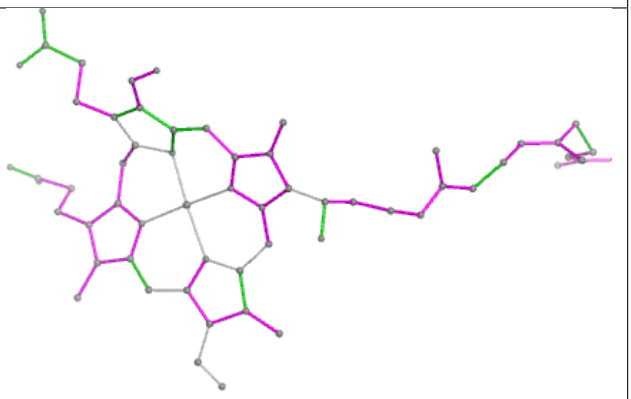
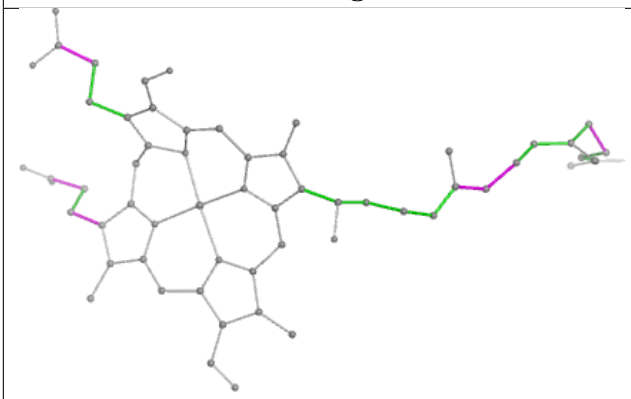


Bond angles



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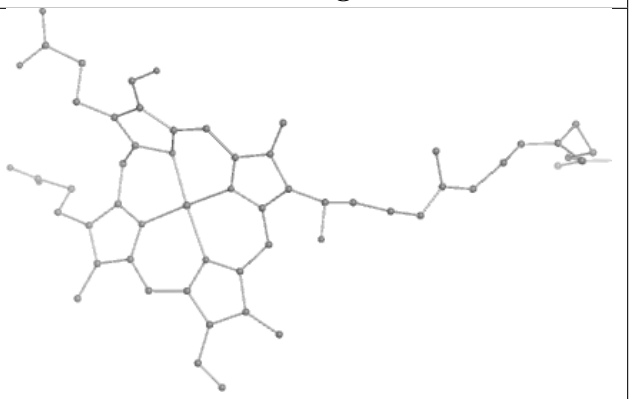
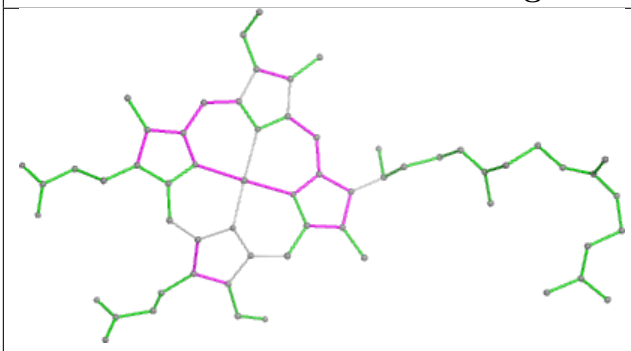


Rings

Ligand HEA F 601



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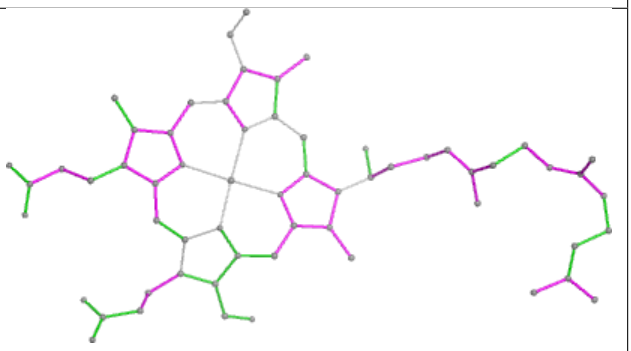
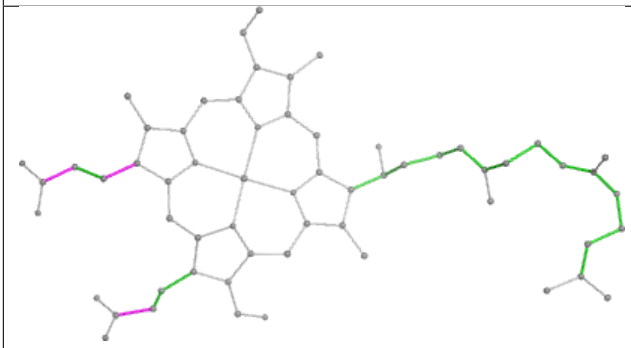
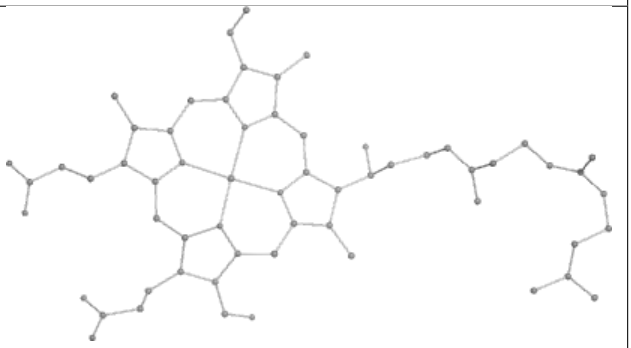


Bond angles

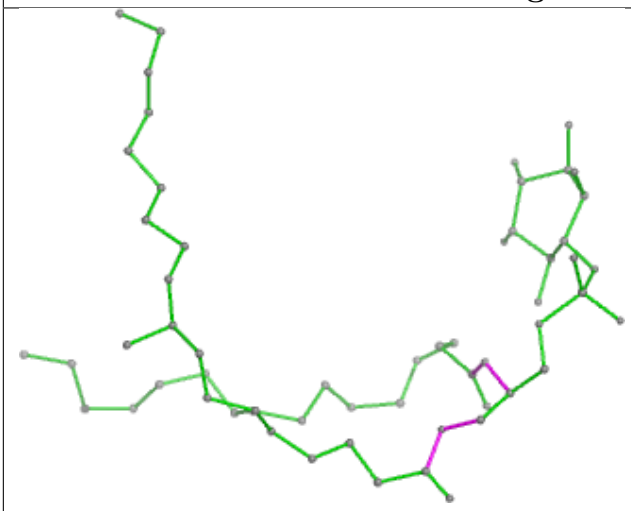


Torsions

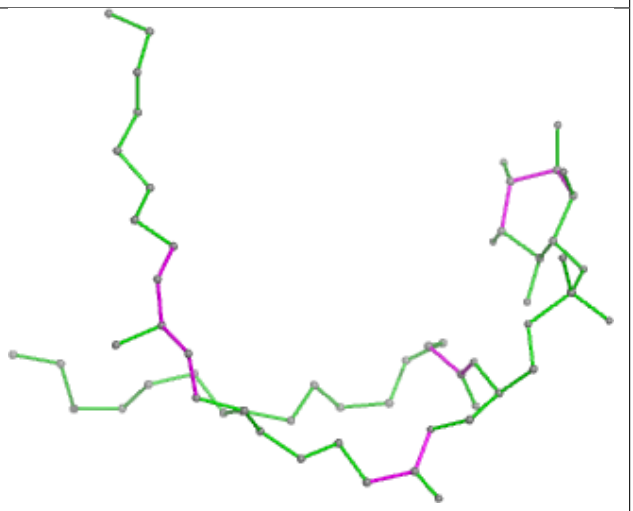


Rings

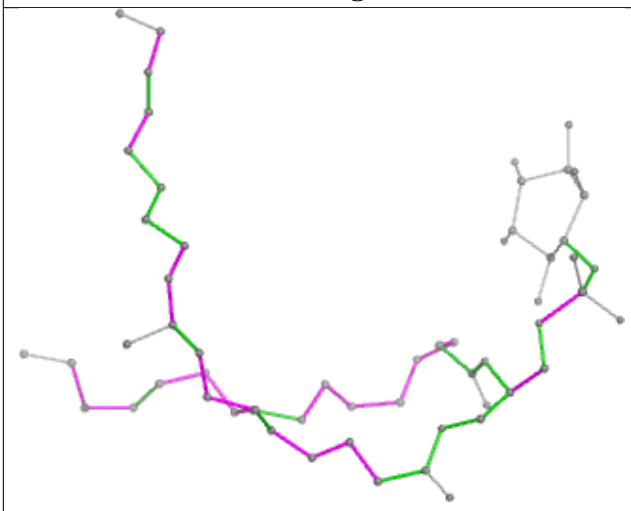
Ligand 9YF A 502



Bond lengths



Bond angles



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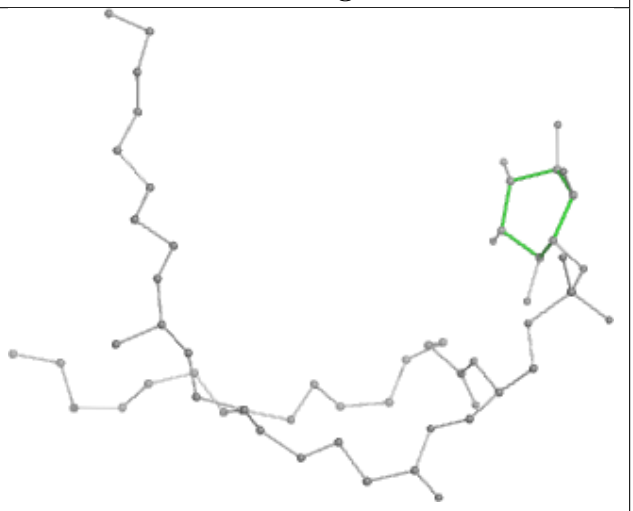
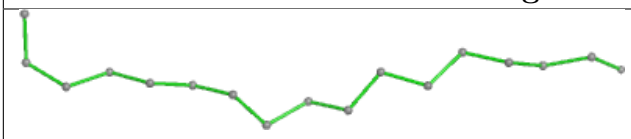
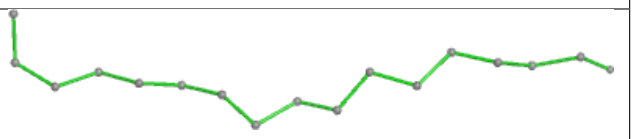


Rings

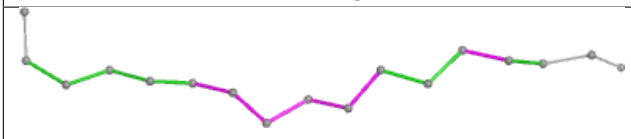
Ligand PLM T 201



Bond lengths



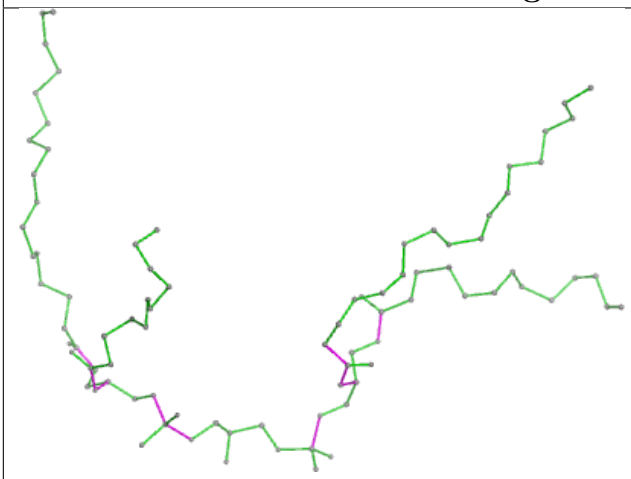
Bond angles



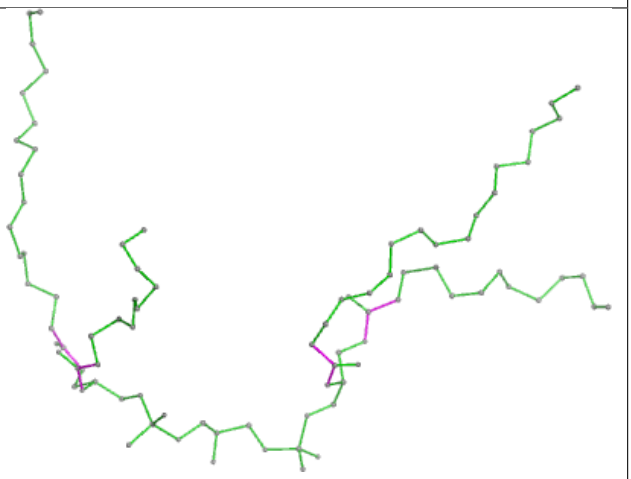
Torsions

Rings

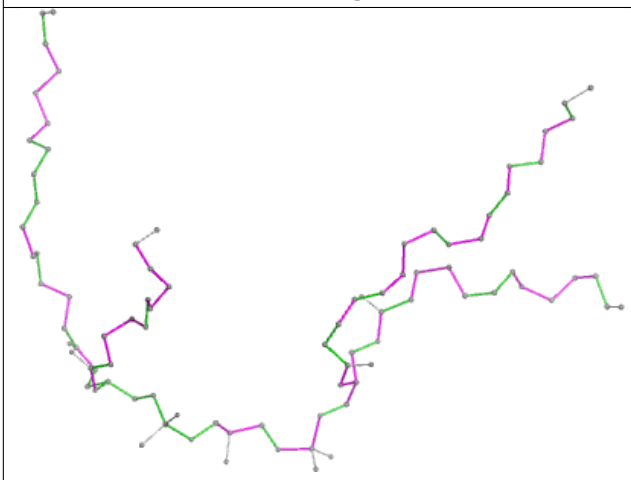
Ligand CDL D 101



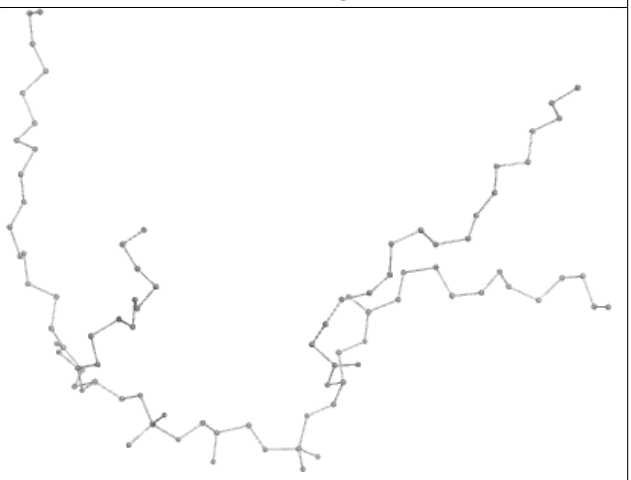
Bond lengths



Bond angles

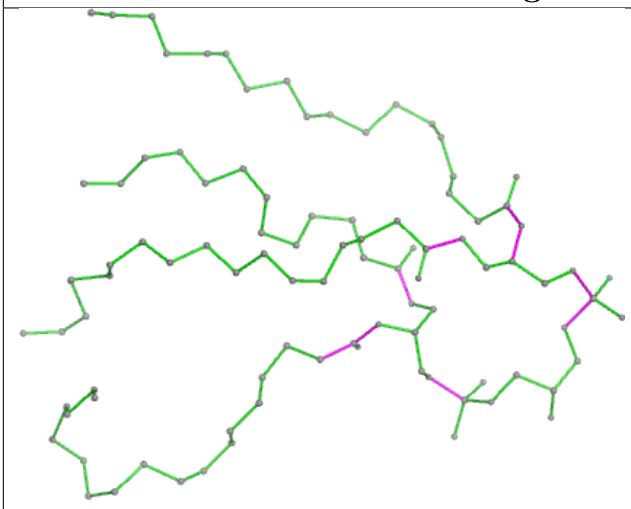


Torsions



Rings

Ligand CDL D 103



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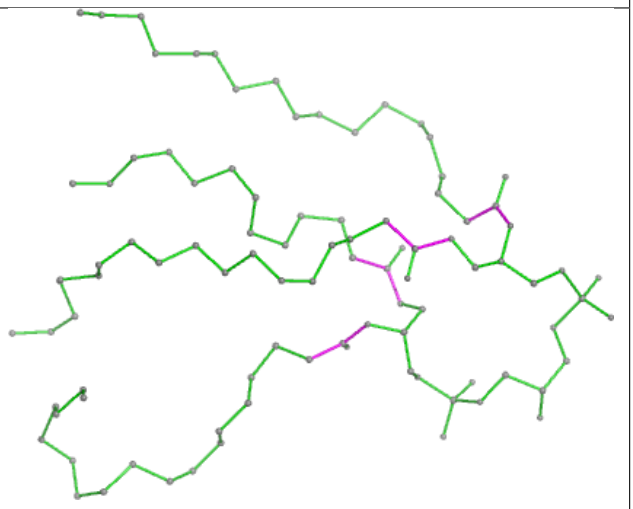
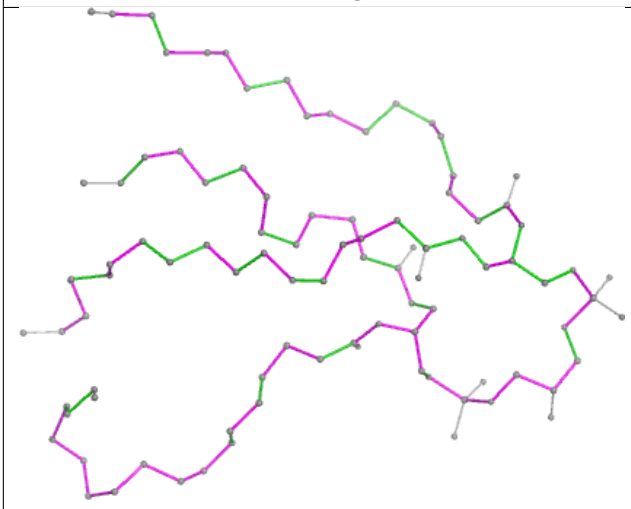


Bond angles



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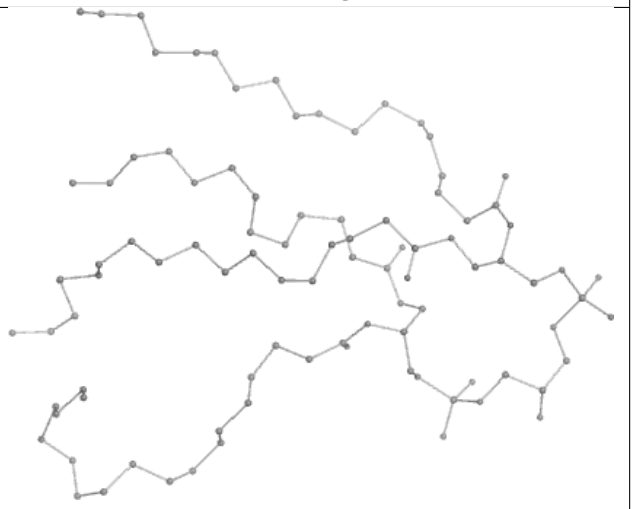
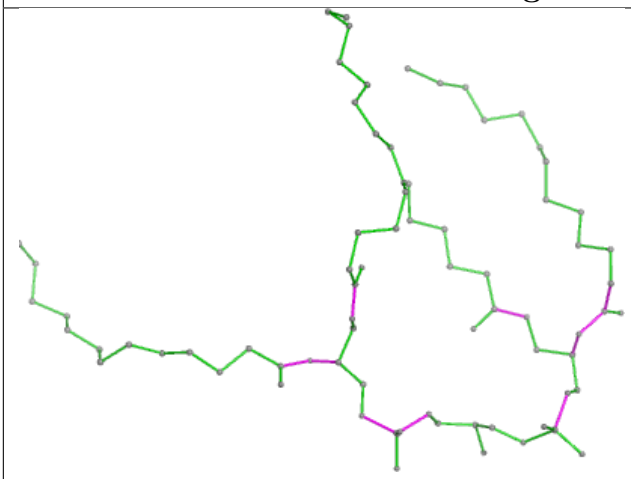


Rings

Ligand CDL N 603



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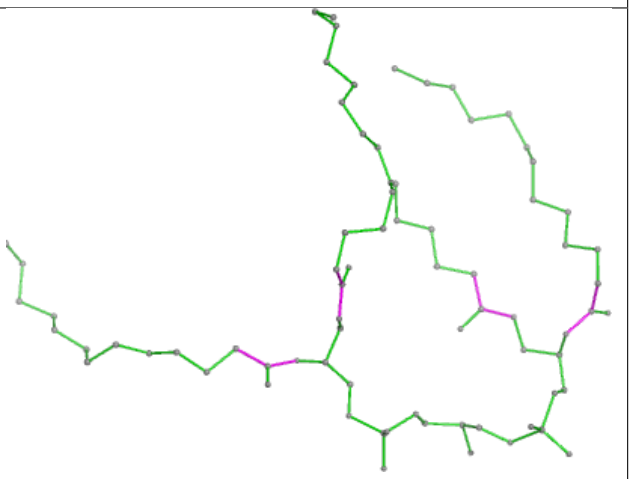
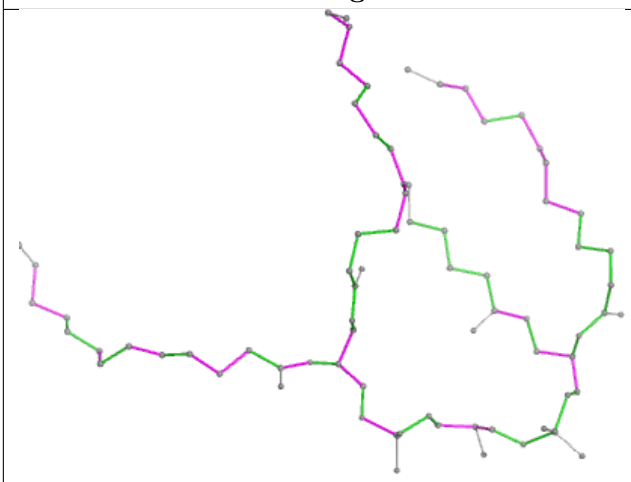
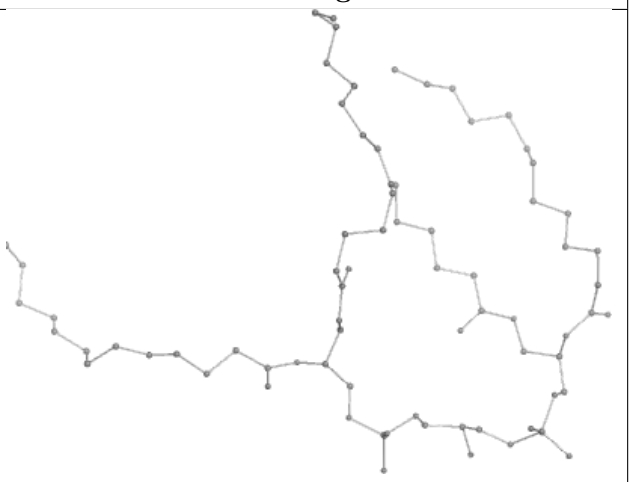


Bond angles

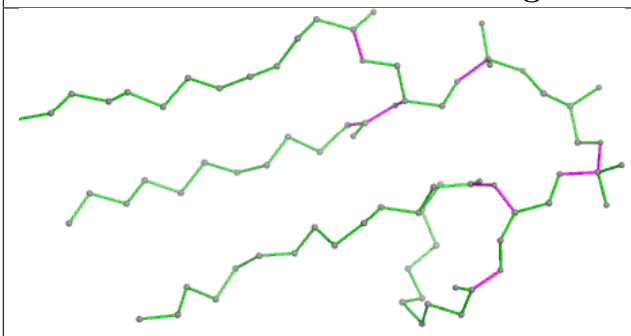


Torsions



Rings

Ligand CDL N 604



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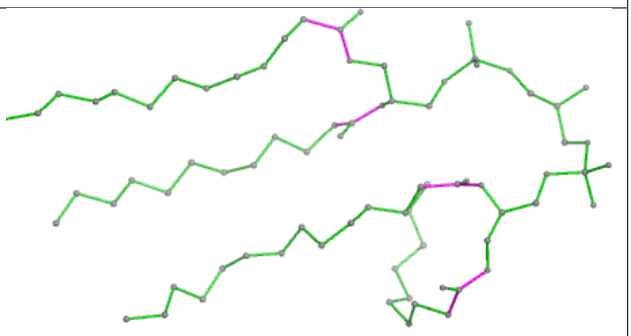
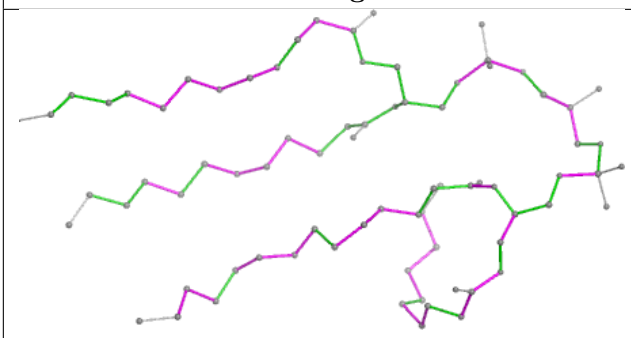


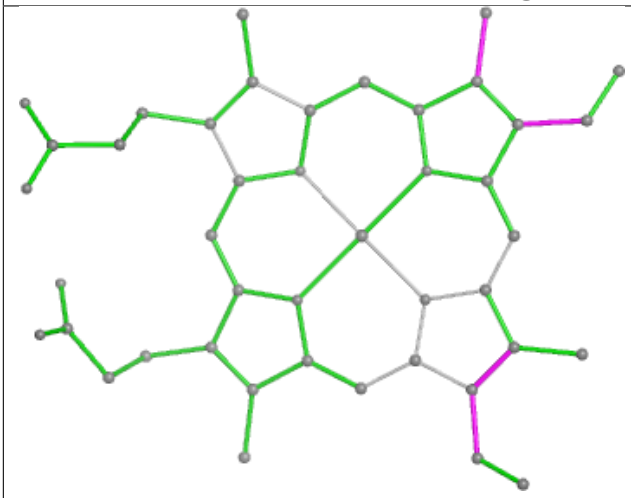
Bond angles



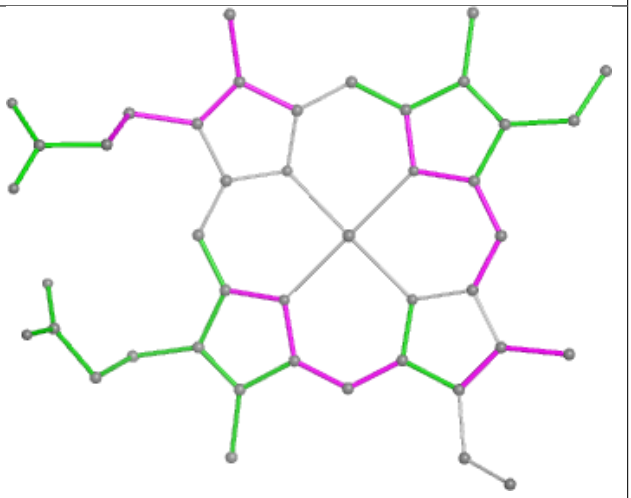
Torsions

Rings

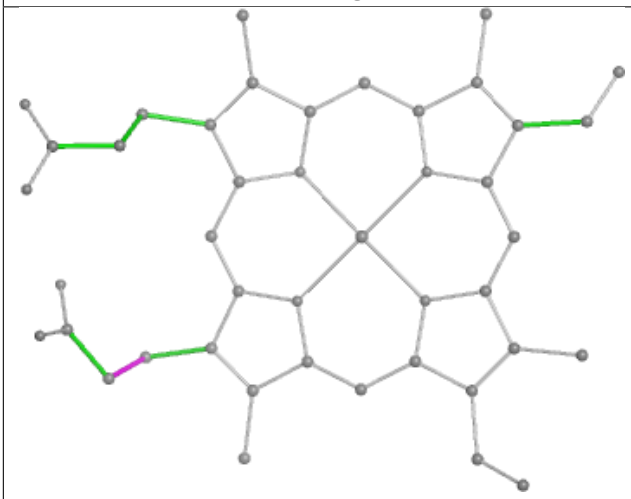
Ligand HEM N 602



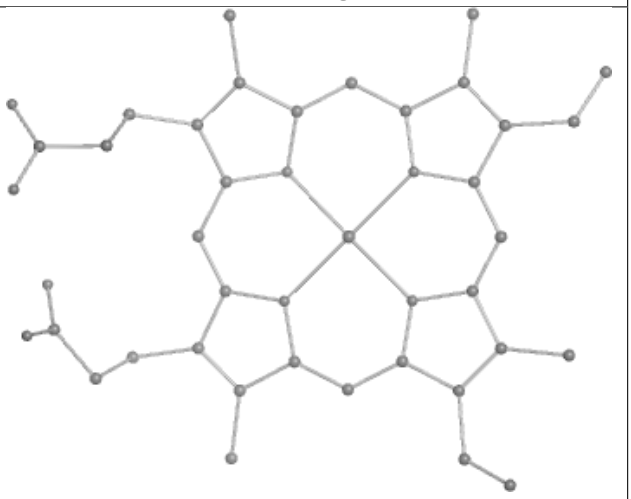
Bond lengths



Bond angles

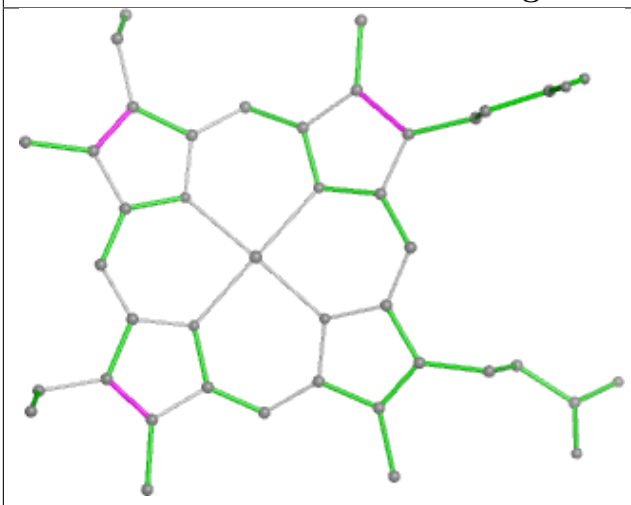


Torsions

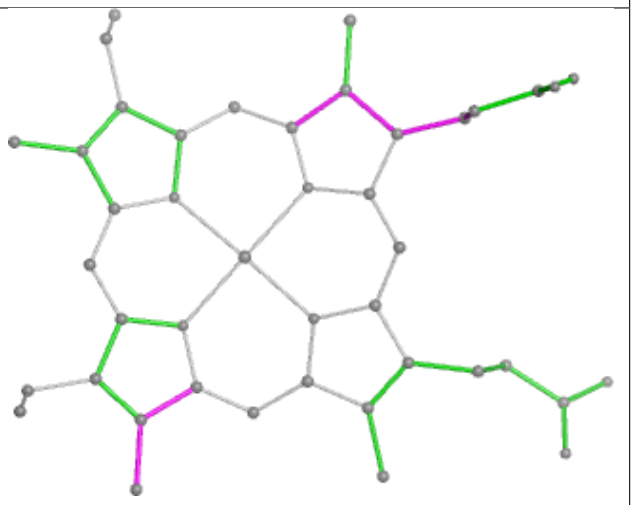


Rings

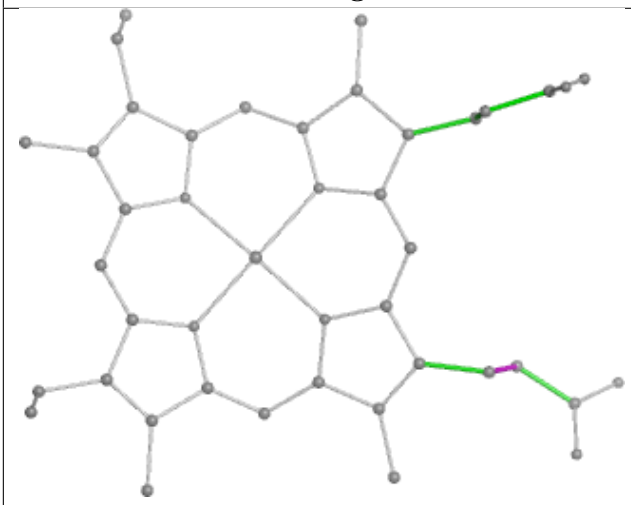
Ligand HEC O 303



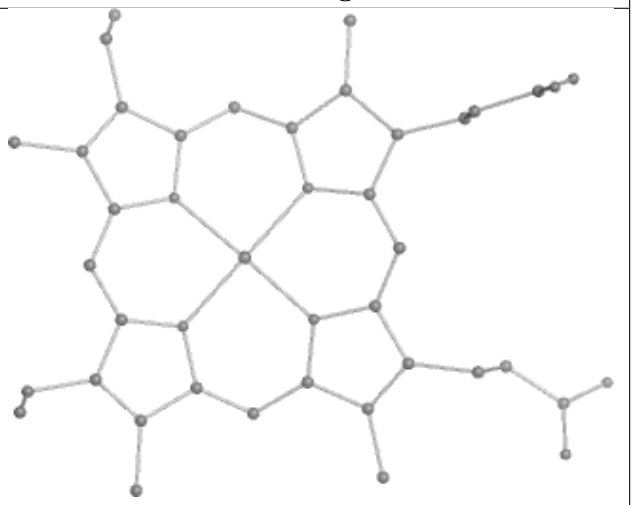
Bond lengths



Bond angles

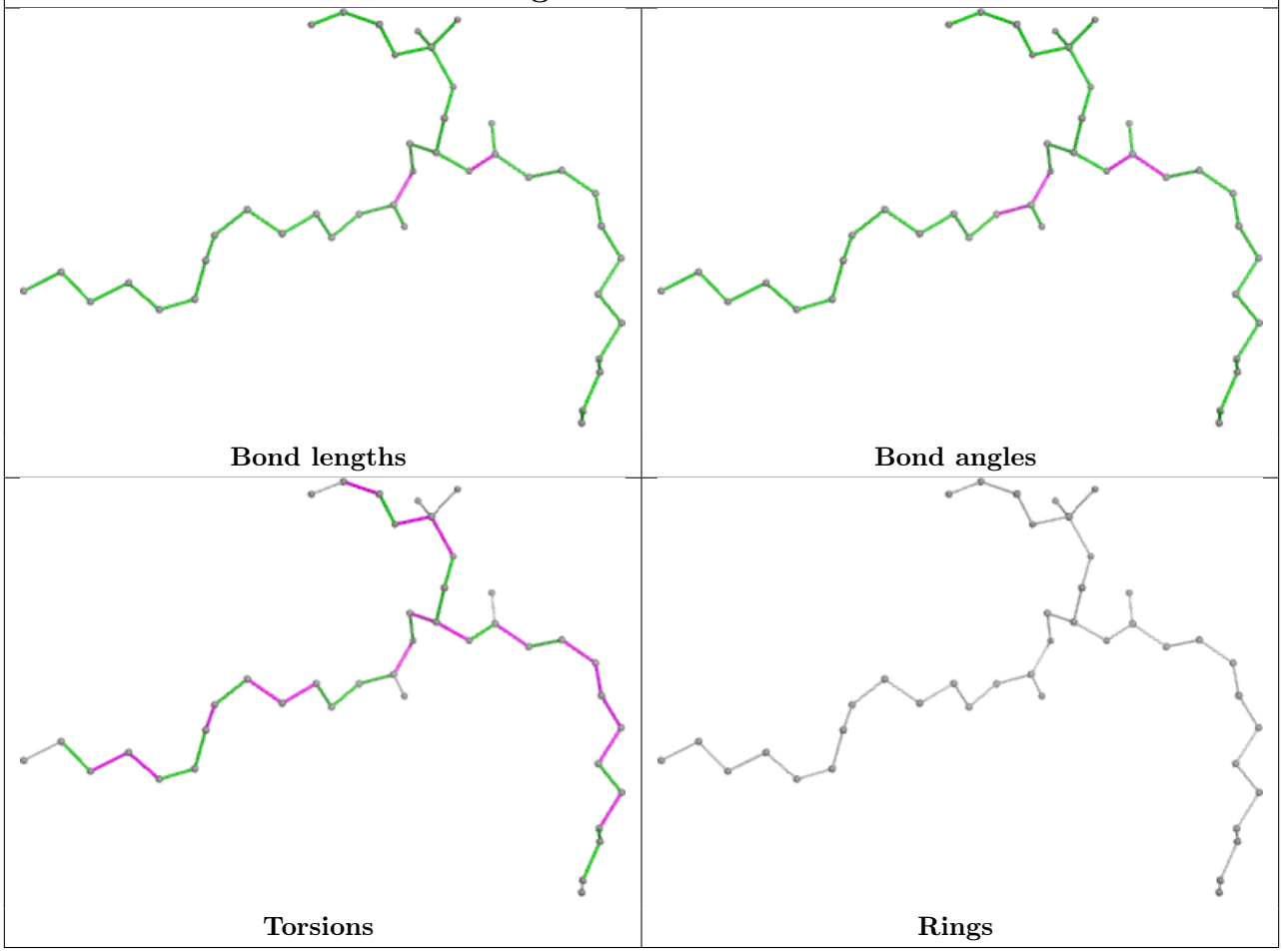


Torsions

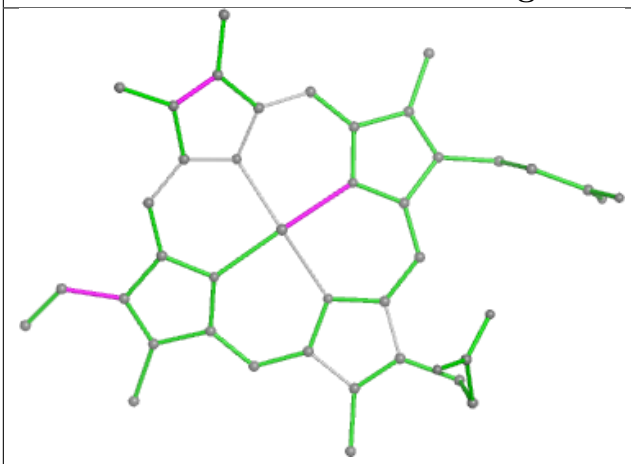


Rings

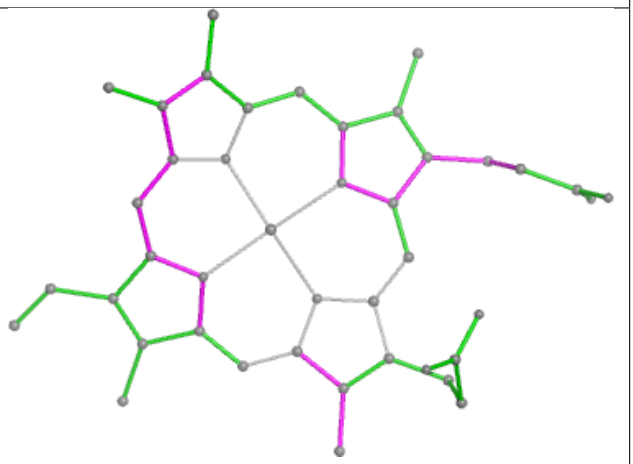
Ligand 9Y0 P 102



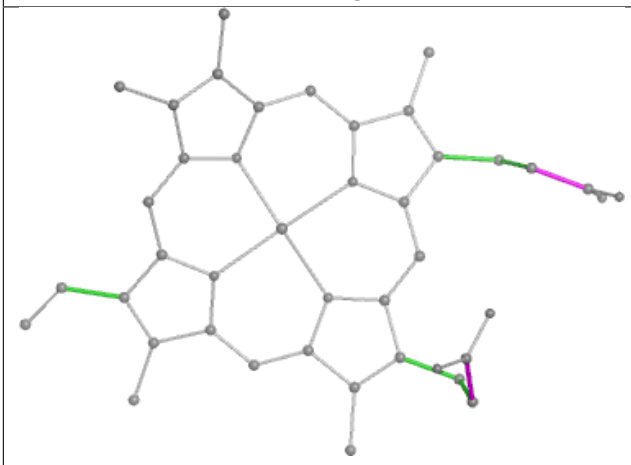
Ligand HEM N 601



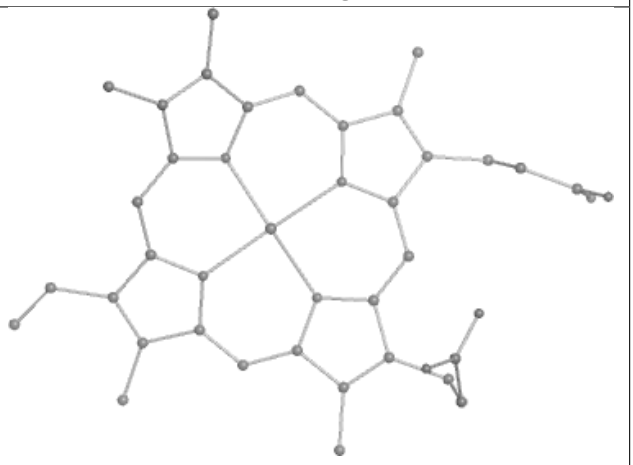
Bond lengths



Bond angles

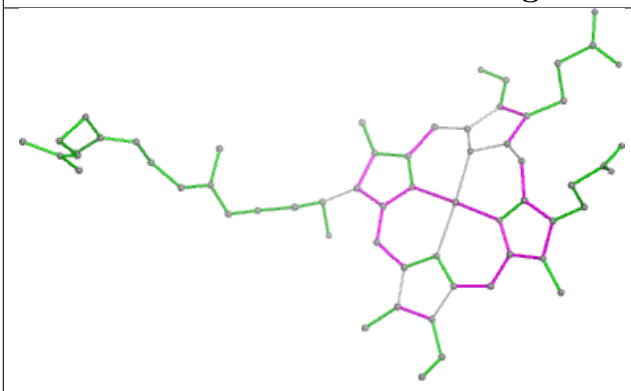


Torsions

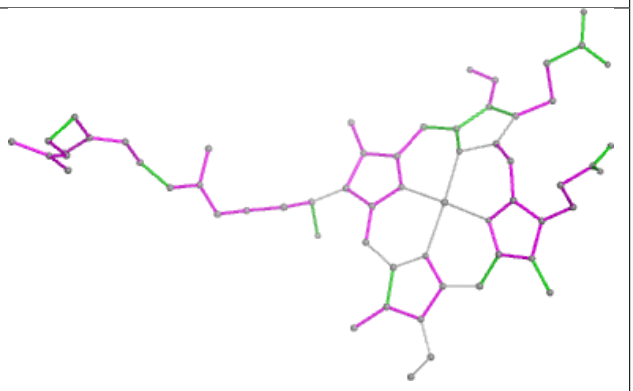


Rings

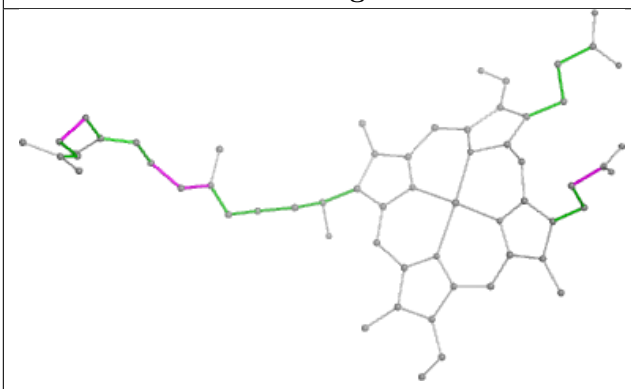
Ligand HEA R 602



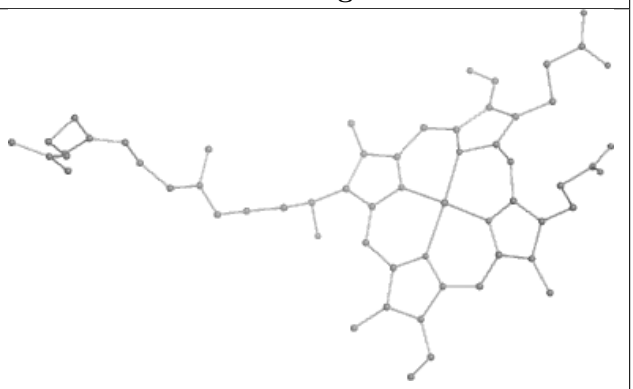
Bond lengths



Bond angles

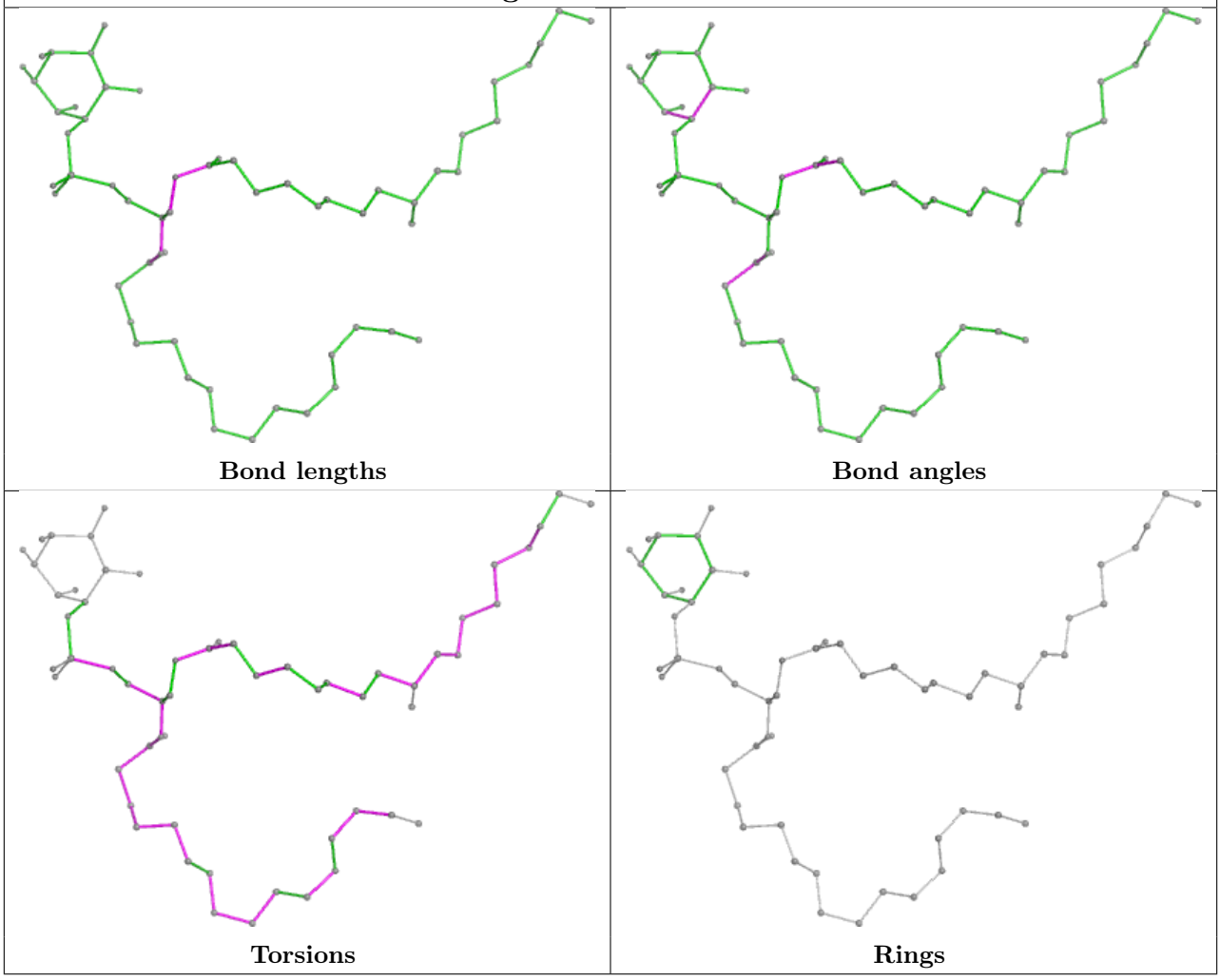


Torsions

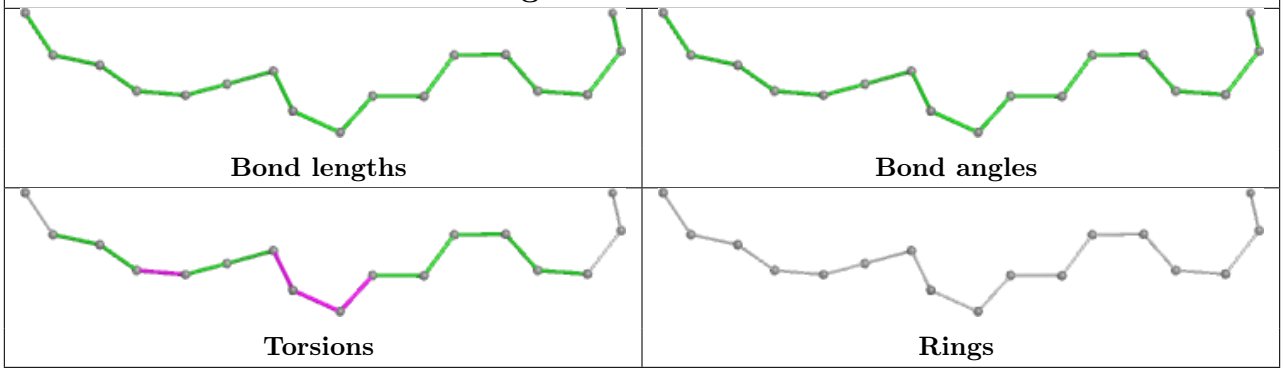


Rings

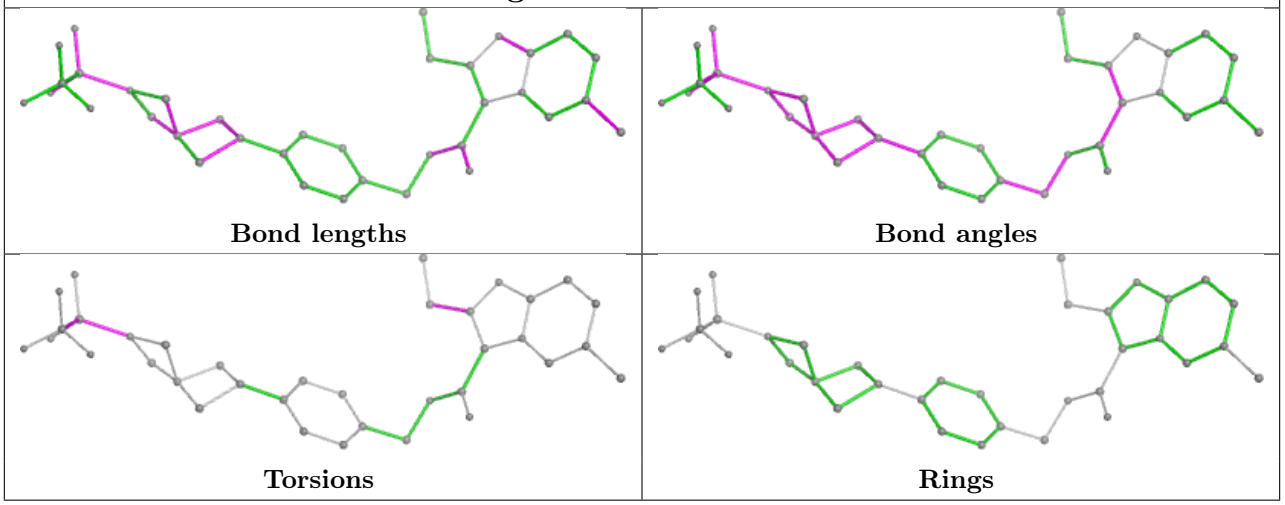
Ligand 9YF O 304



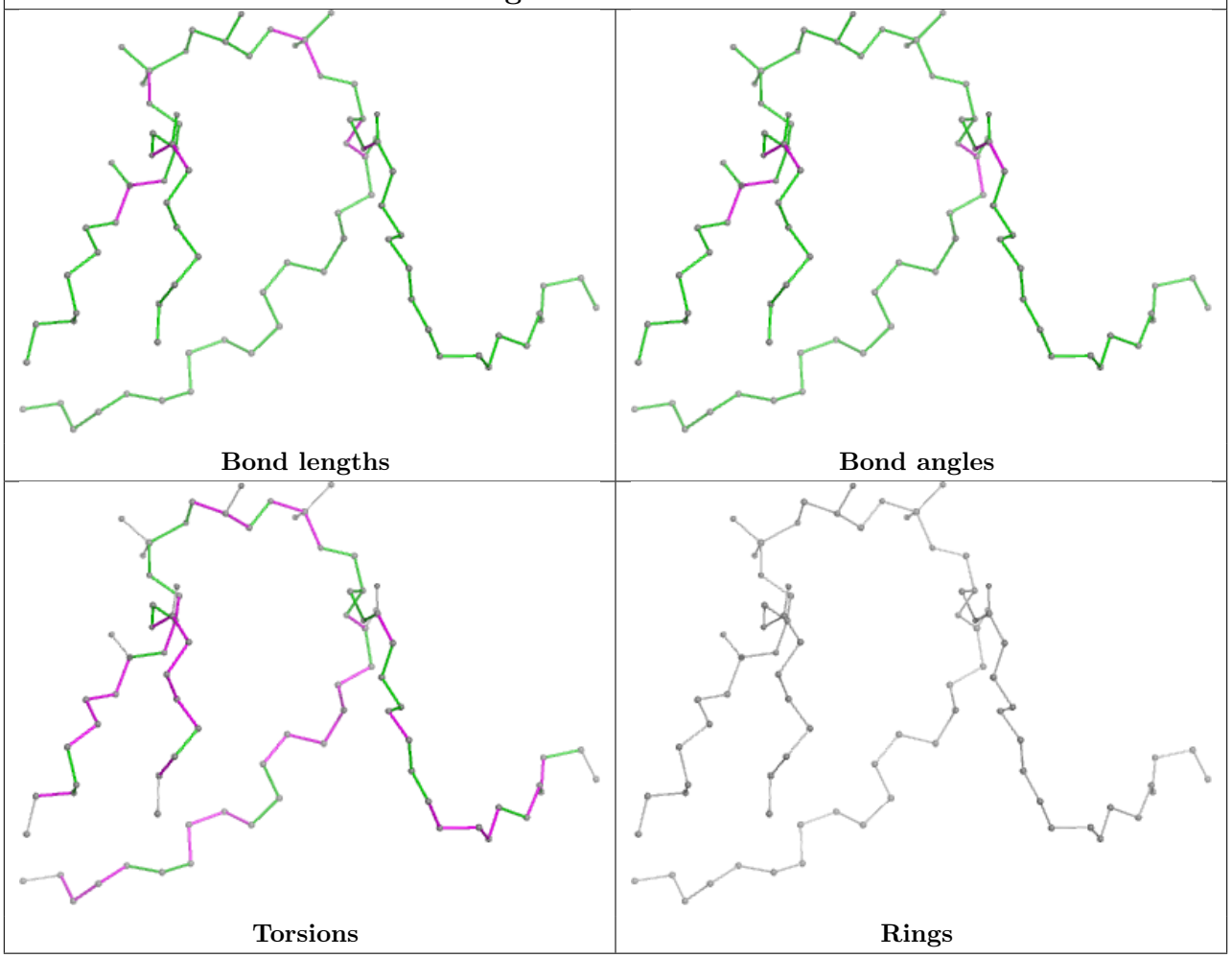
Ligand PLM G 302



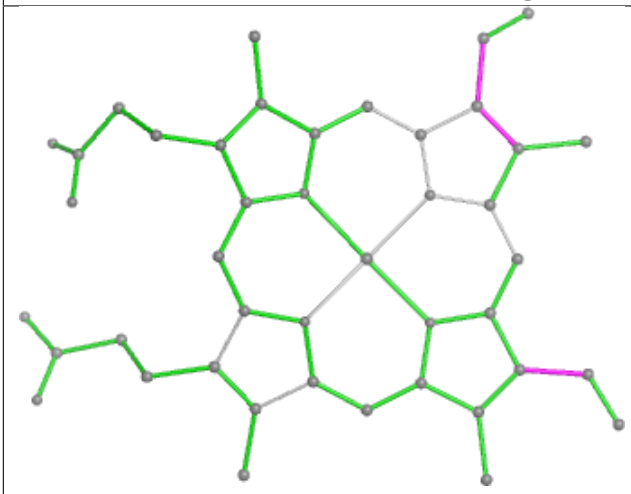
Ligand A1IRE N 606



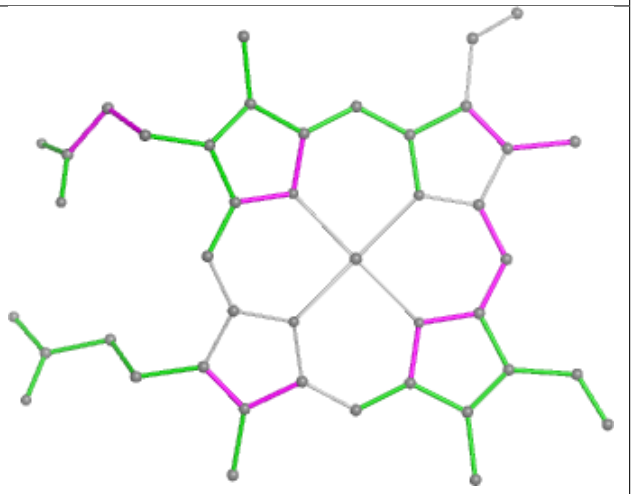
Ligand CDL F 606



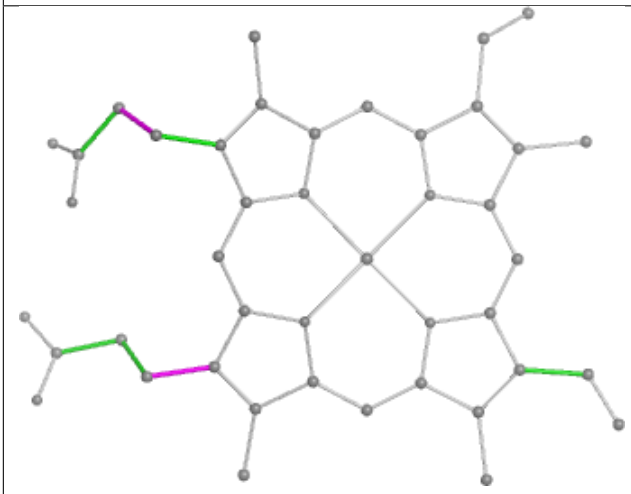
Ligand HEM B 602



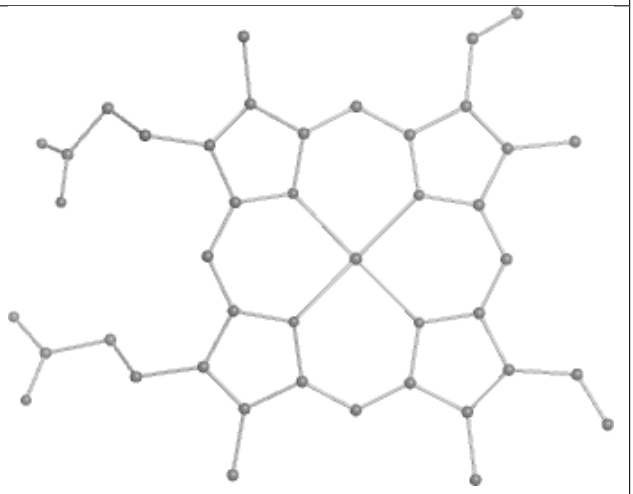
Bond lengths



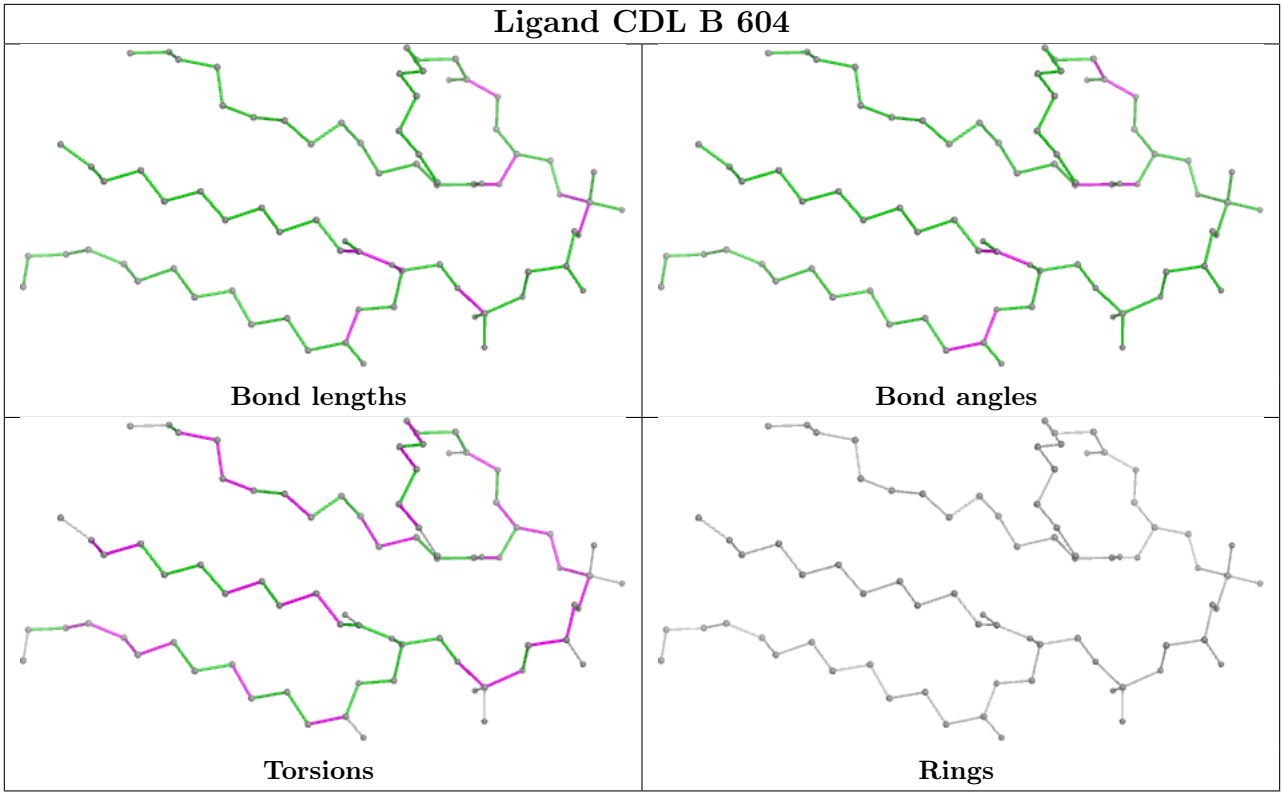
Bond angles



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.

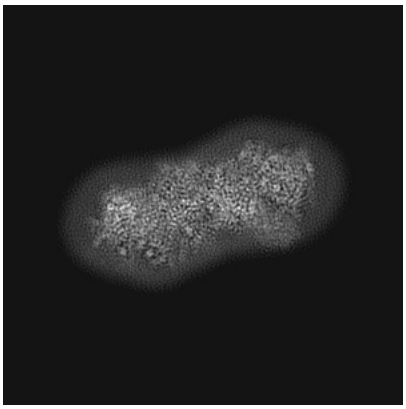
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-51689. These allow visual inspection of the internal detail of the map and identification of artifacts.

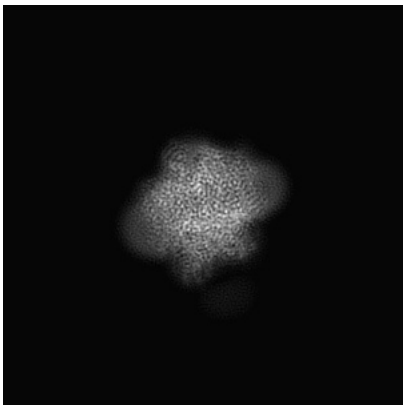
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

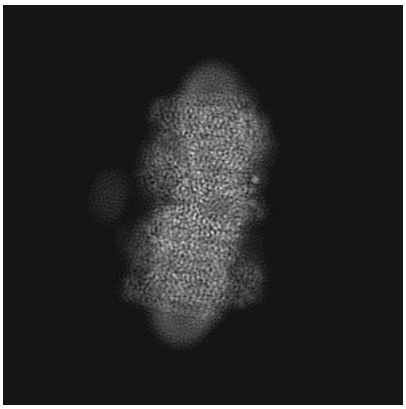
6.1.1 Primary map



X

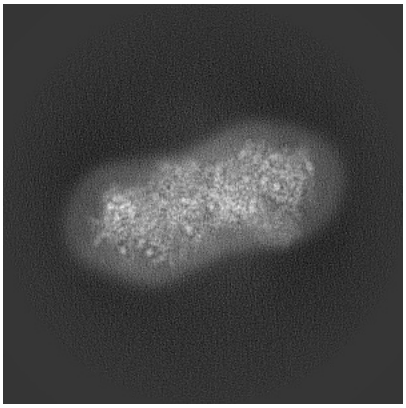


Y

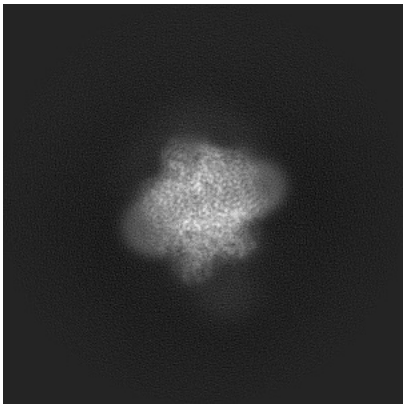


Z

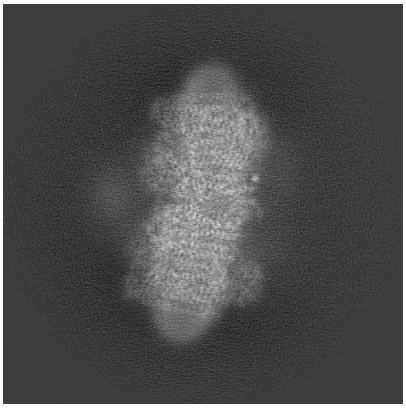
6.1.2 Raw map



X



Y

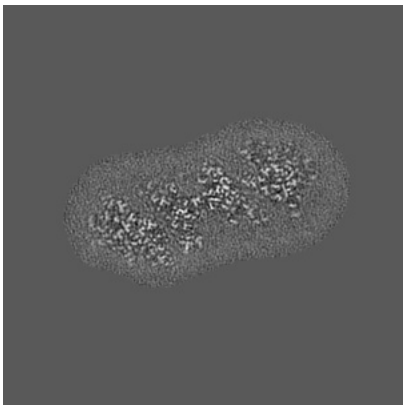


Z

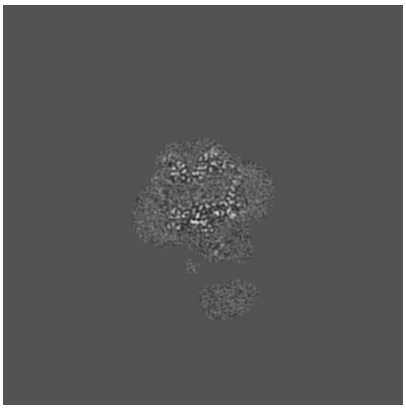
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

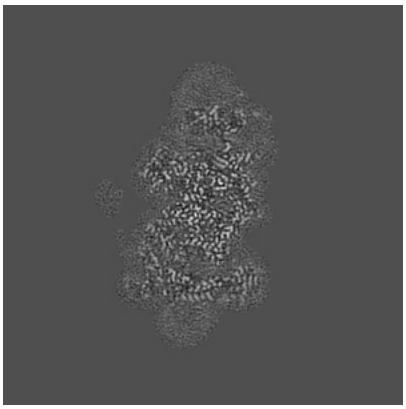
6.2.1 Primary map



X Index: 210

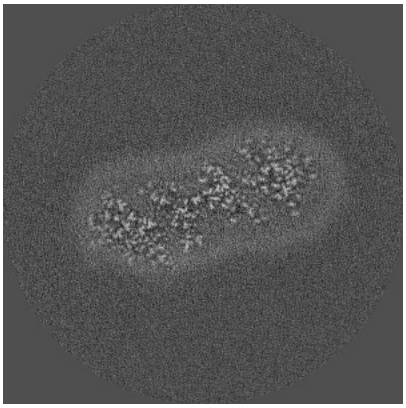


Y Index: 210

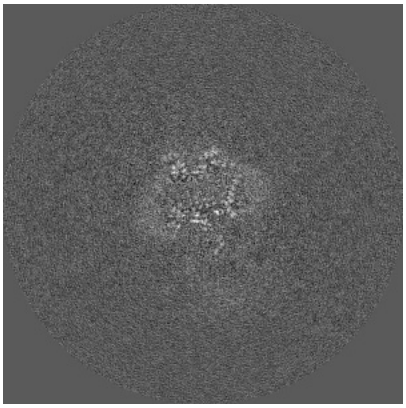


Z Index: 210

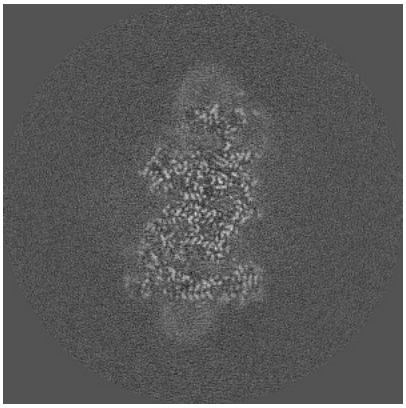
6.2.2 Raw map



X Index: 210



Y Index: 210

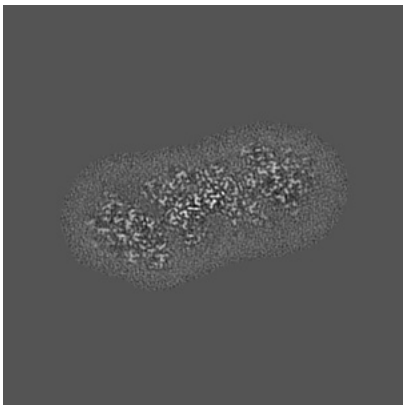


Z Index: 210

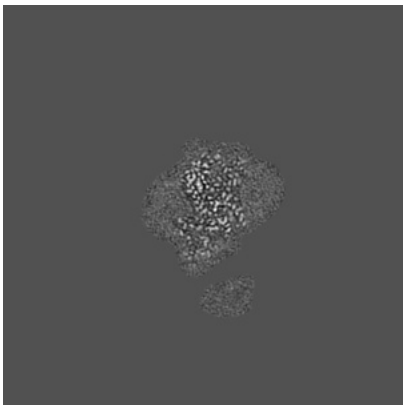
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

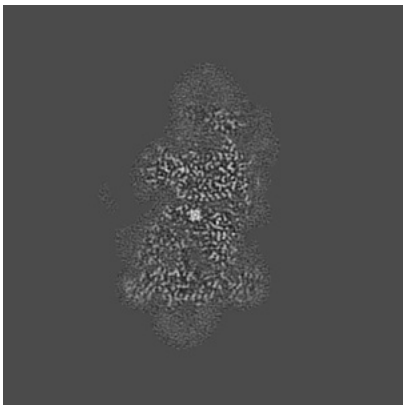
6.3.1 Primary map



X Index: 204

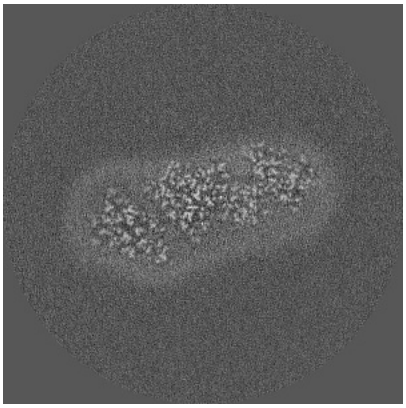


Y Index: 230

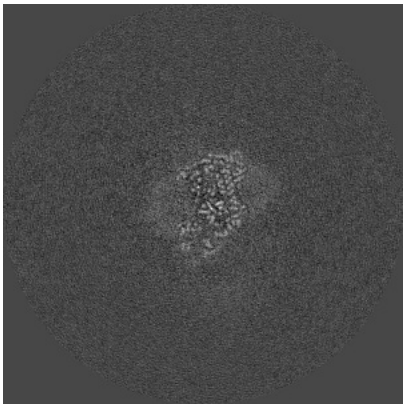


Z Index: 206

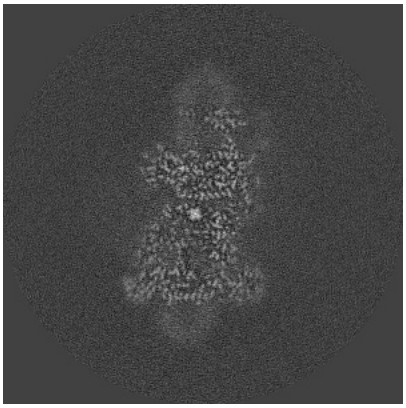
6.3.2 Raw map



X Index: 199



Y Index: 225

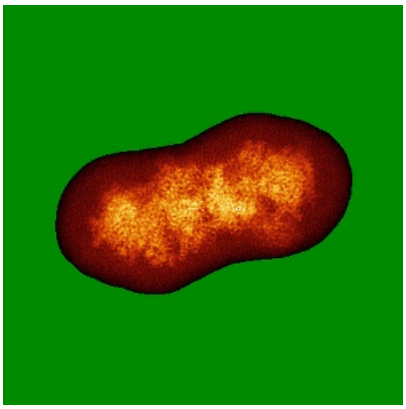


Z Index: 206

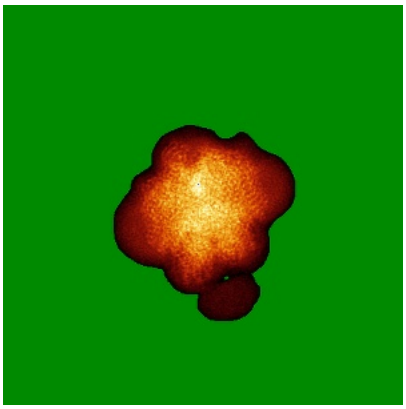
The images above show the largest variance slices of the map in three orthogonal directions.

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

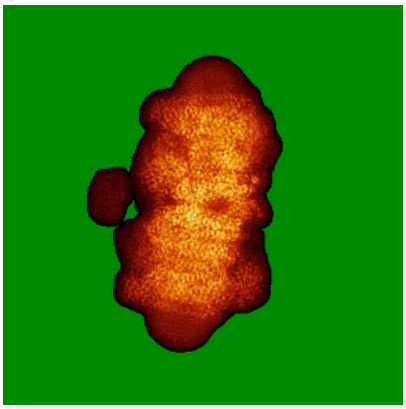
6.4.1 Primary map



X

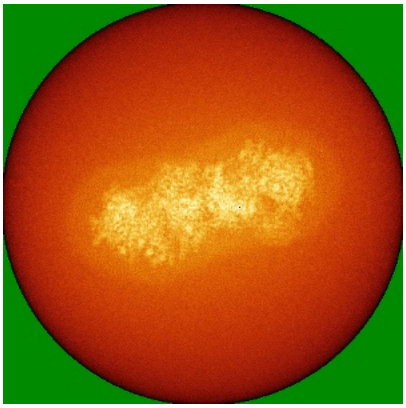


Y

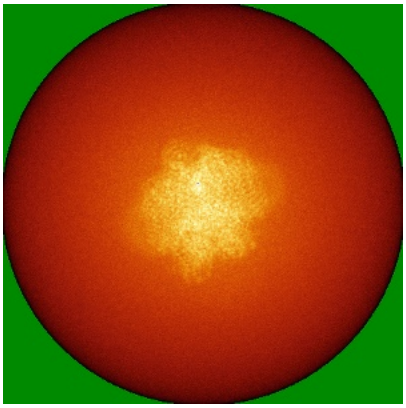


Z

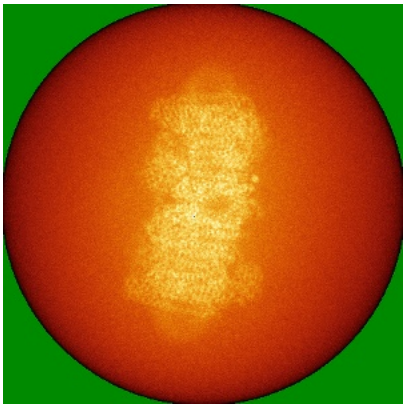
6.4.2 Raw map



X



Y



Z

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

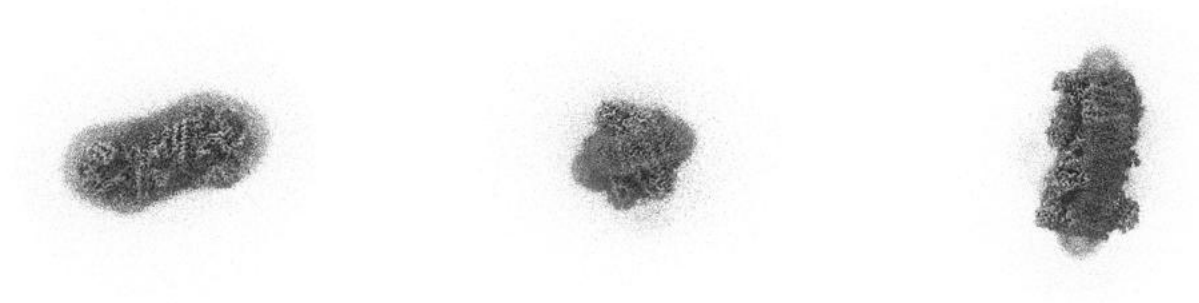
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.009. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

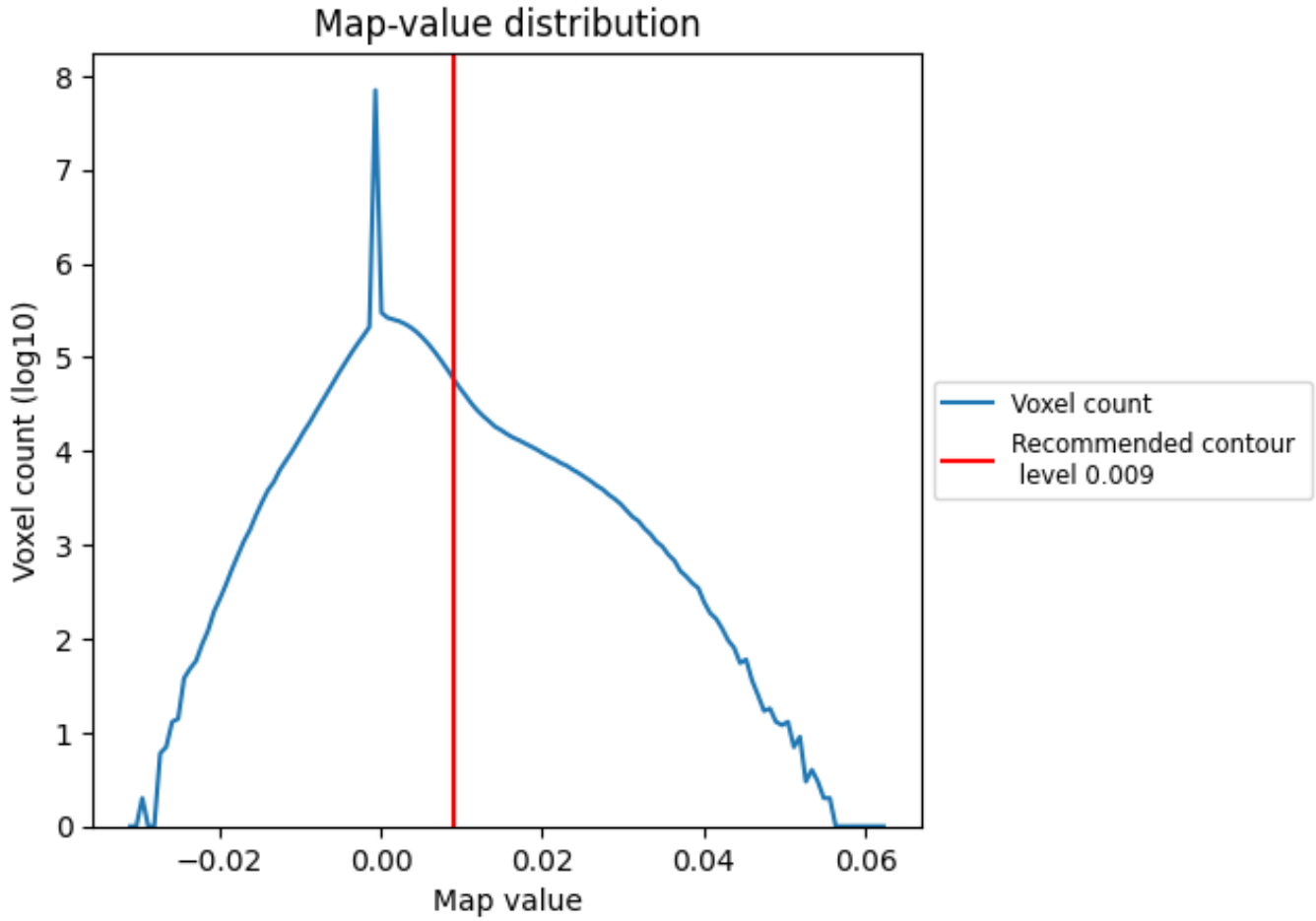
6.6 Mask visualisation (i)

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

7 Map analysis

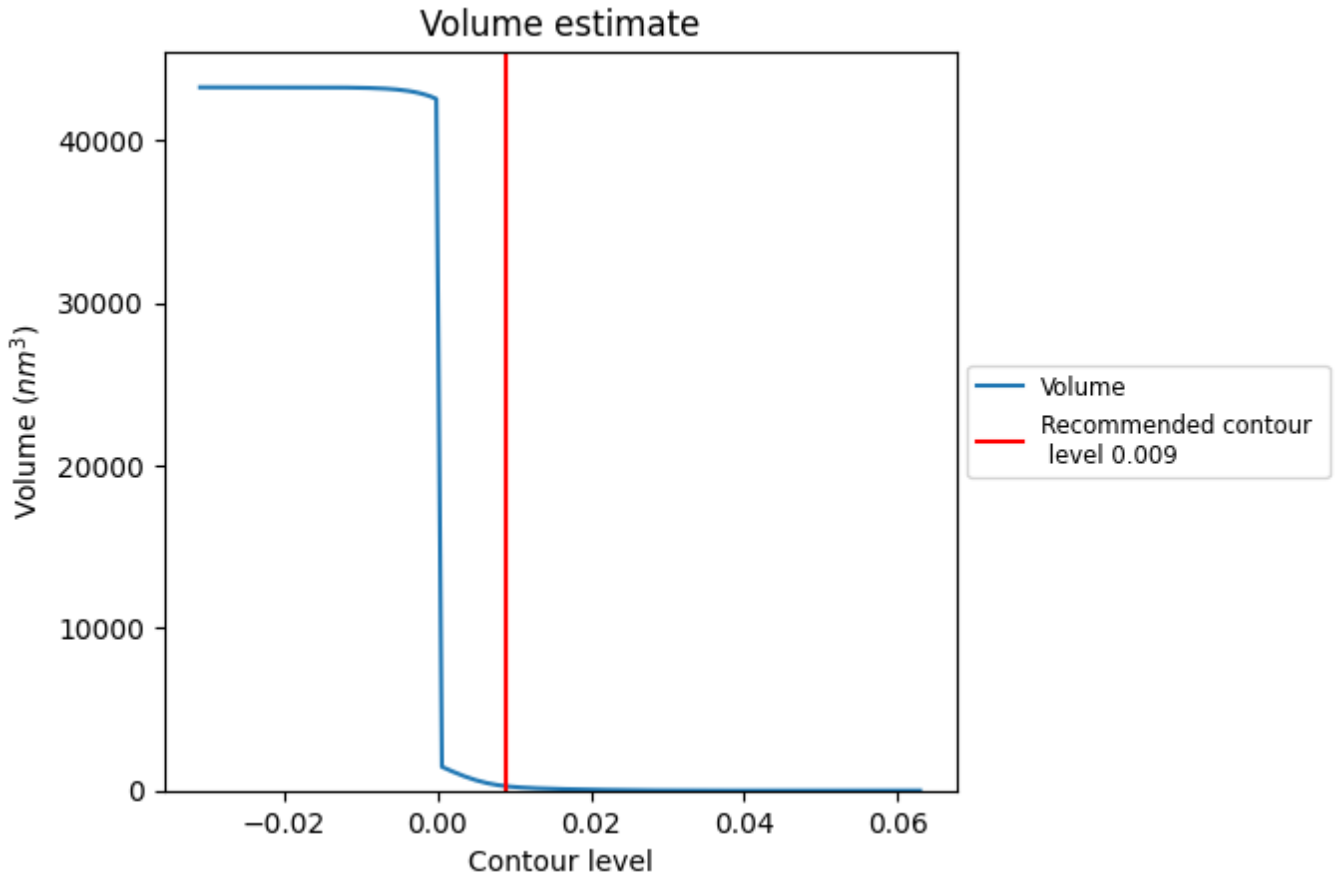
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

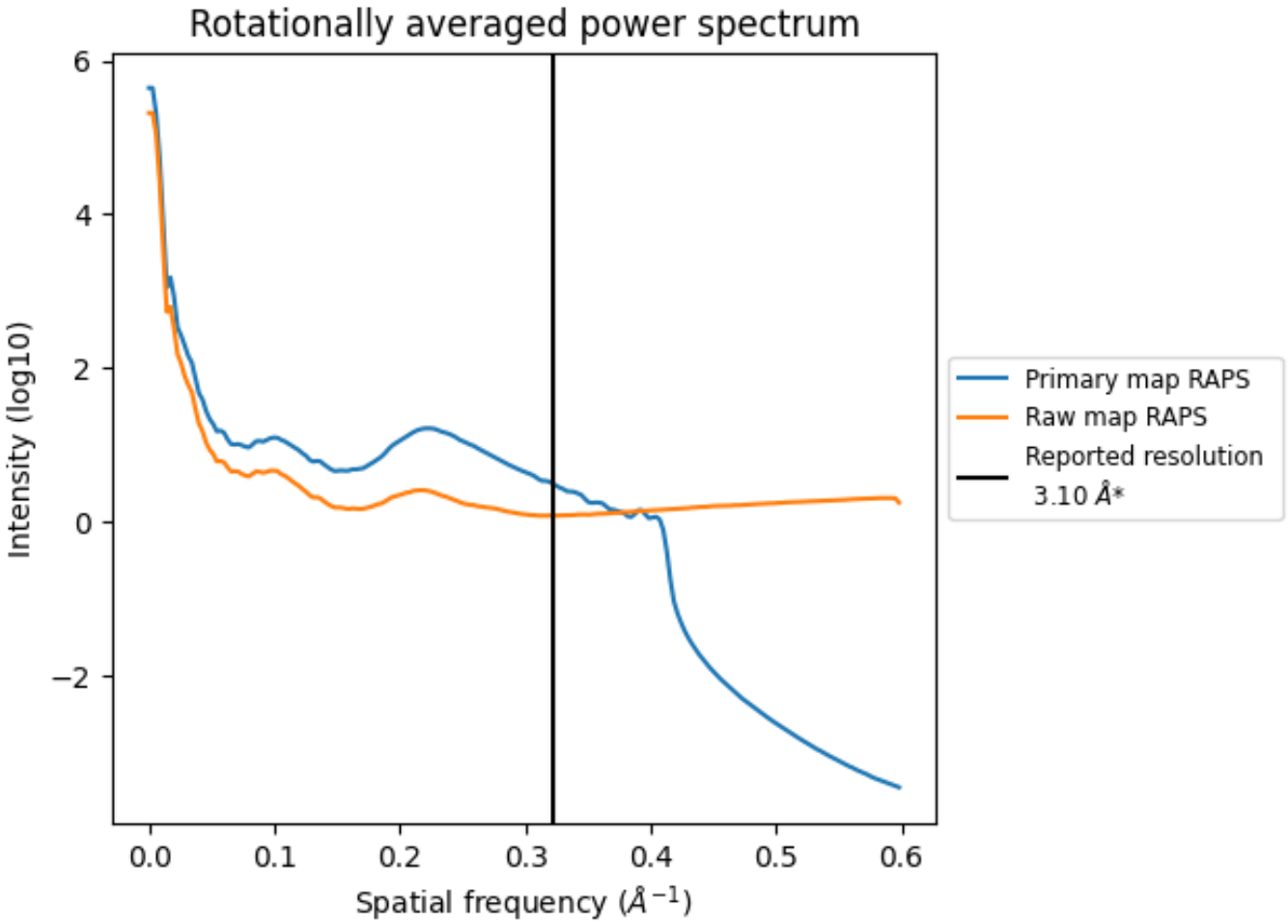
7.2 Volume estimate



The volume at the recommended contour level is 268 nm^3; this corresponds to an approximate mass of 242 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)

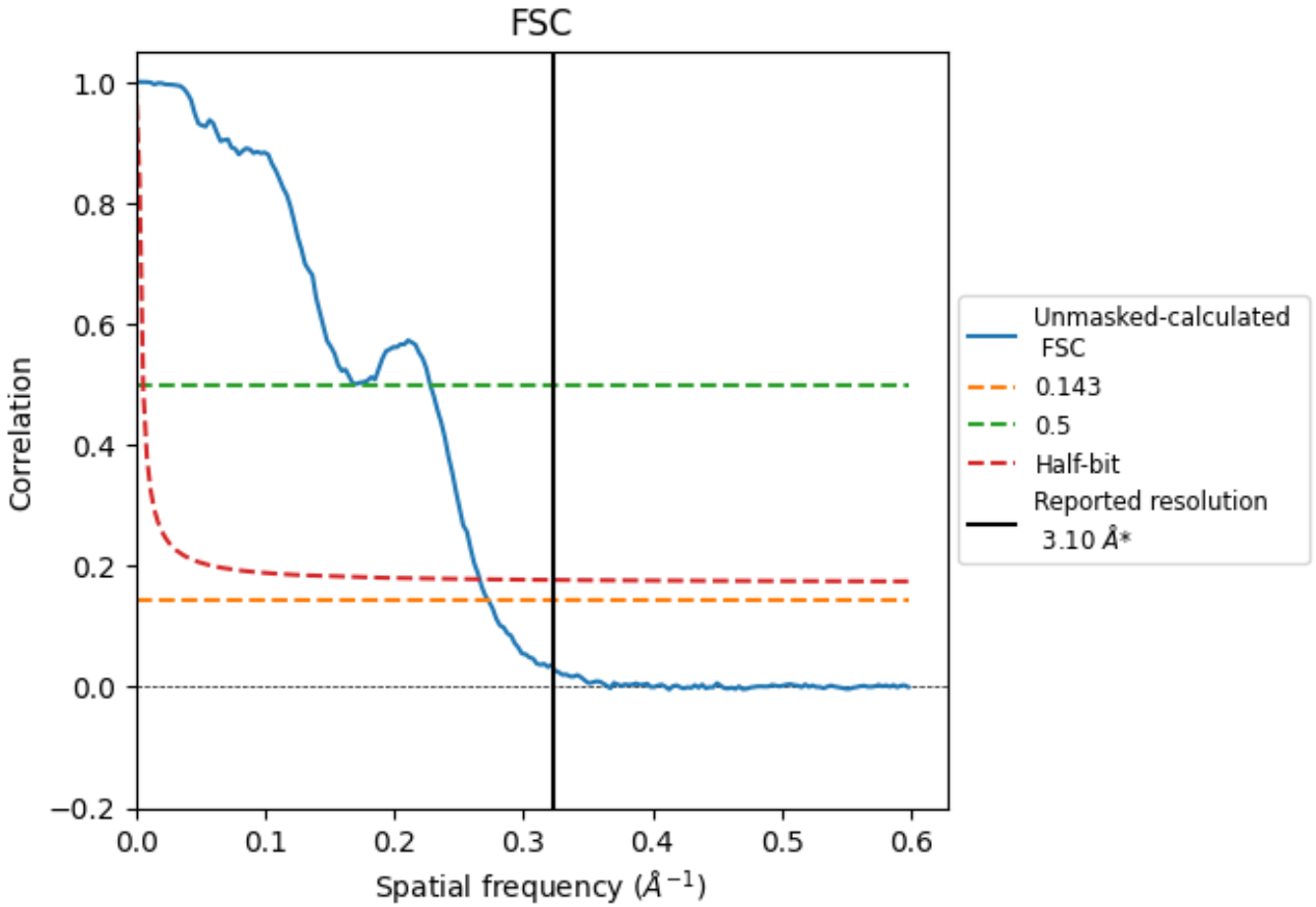


*Reported resolution corresponds to spatial frequency of 0.323 $Å^{-1}$

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8.2 Resolution estimates (i)

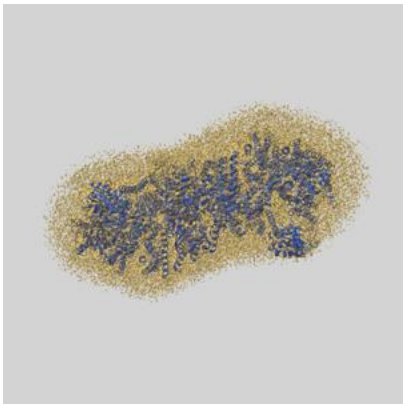
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.66	4.39	3.76

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.66 differs from the reported value 3.1 by more than 10 %

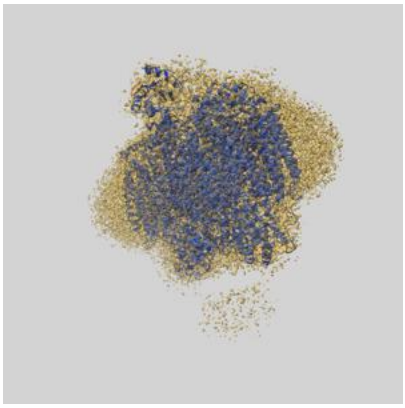
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-51689 and PDB model 9GY6. Per-residue inclusion information can be found in section 3 on page 18.

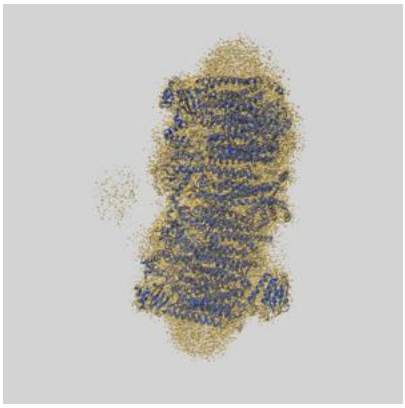
9.1 Map-model overlay



X



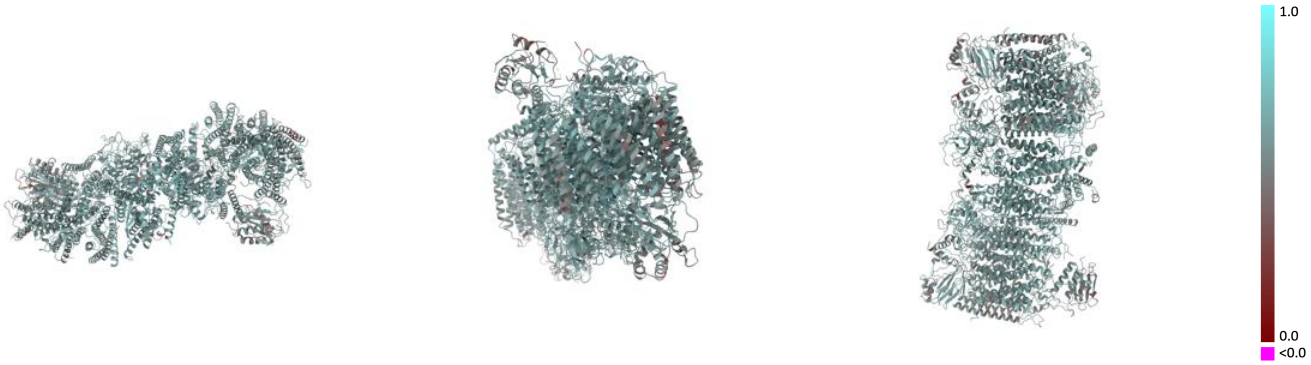
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.009 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

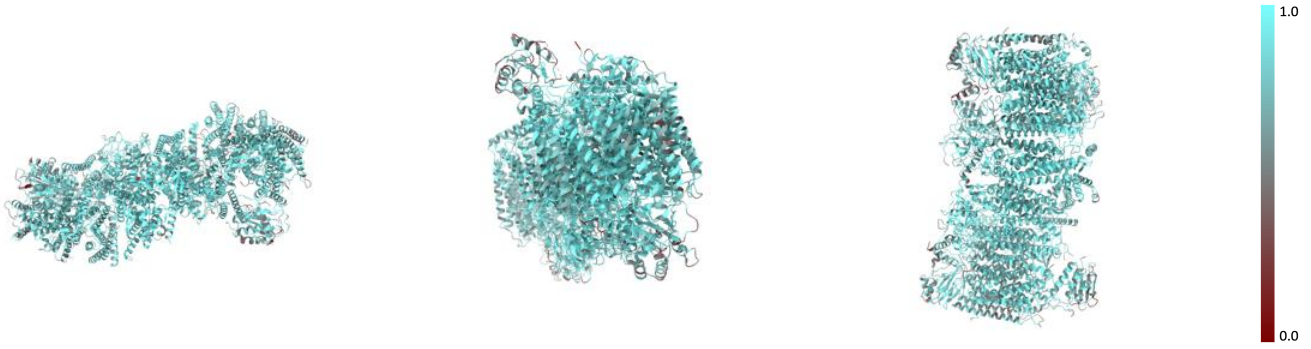
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

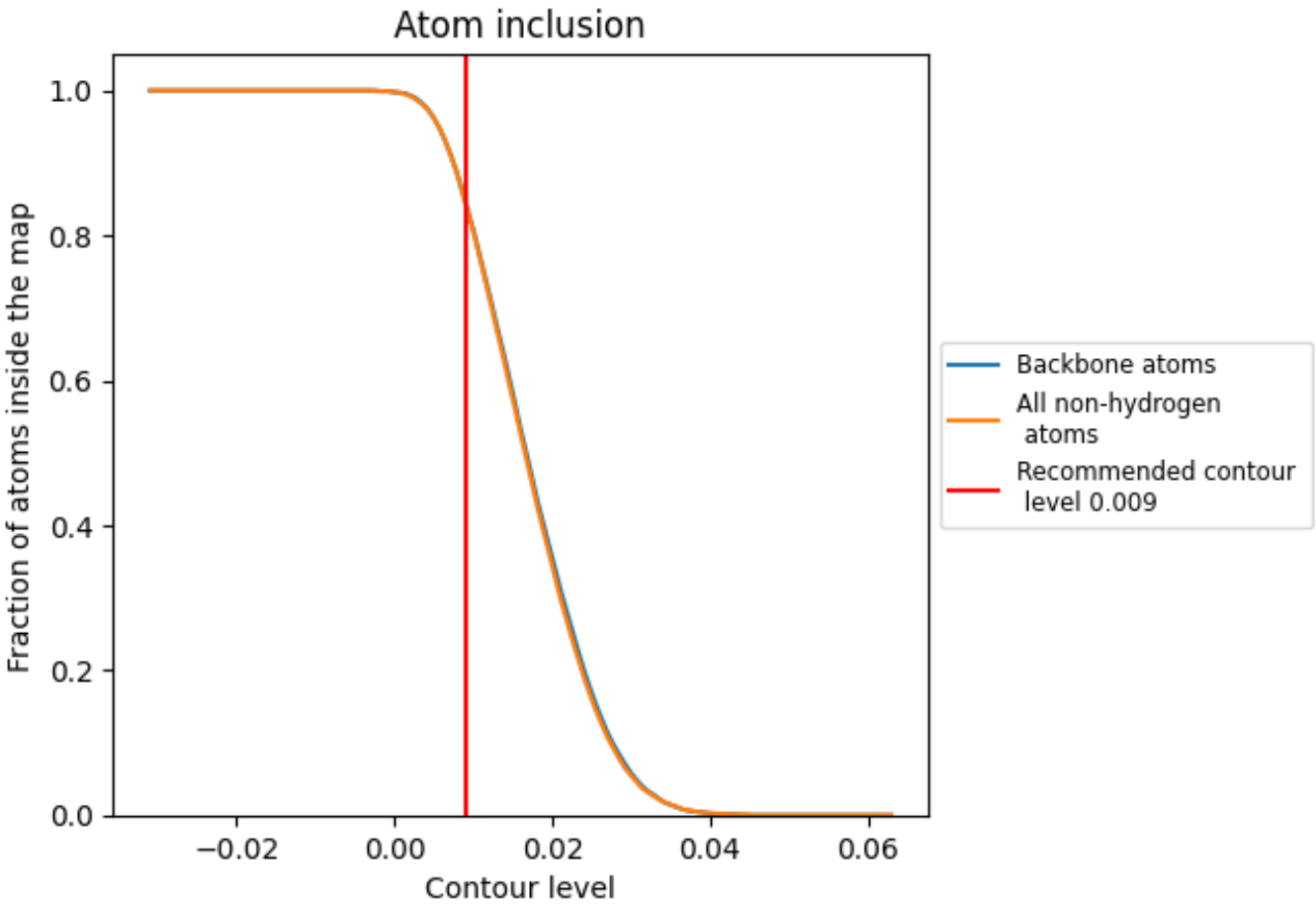
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.009).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.009) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8440	0.5920
A	0.8950	0.6120
B	0.9240	0.6310
C	0.8130	0.5800
D	0.7510	0.5750
E	0.7310	0.5460
F	0.8890	0.6030
G	0.8380	0.5810
H	0.8240	0.5900
I	0.7140	0.5200
J	0.7010	0.5140
L	0.7660	0.5490
M	0.8730	0.6080
N	0.9180	0.6270
O	0.7950	0.5790
P	0.7360	0.5710
Q	0.7310	0.5410
R	0.8980	0.6040
S	0.8580	0.5840
T	0.8450	0.5870
U	0.7000	0.5330
V	0.7110	0.5240
X	0.7010	0.5420