Full wwPDB EM Validation Report ⓘ

Apr 22, 2024 – 05:42 pm BST

PDB ID	:	7NHQ
EMDB ID	:	EMD-12337
Title	:	Structure of PSII-I prime (PSII with Psb28, and Psb34)
Authors	:	Zabret, J.; Bohn, S.; Schuller, S.K.; Arnolds, O.; Chan, A.; Tajkhorshid, E.; Stoll, R.; Engel, B.D.; Rudack, T.; Schuller, J.M.; Nowaczyk, M.M.
Deposited on	:	2021-02-11
Resolution	:	2.68 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:

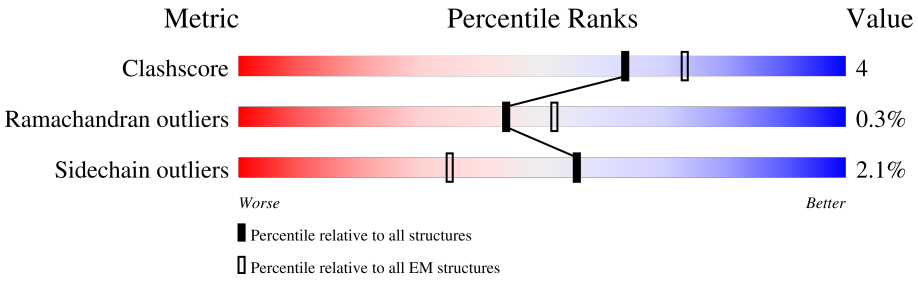
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.68 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	360	6% 86% 6% · 7%
2	B	510	· 94% · ·
3	C	461	5% 84% 9% · 6%
4	D	352	· 89% 8% · ·
5	E	84	17% 80% 11% · 8%
6	F	45	16% 71% 11% · 16%
7	H	66	· 94% · · ·
8	I	38	· 61% 5% · 32%

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Mol	Chain	Length	Quality of chain
9	K	46	7% 67% 13% 20%
10	L	37	86% 14%
11	M	36	11% 89% 6% 6%
12	T	32	84% 12%
13	X	41	83% 15%
14	y	46	22% 50% 11% 39%
15	Z	62	8% 85% 10%
16	2	116	5% 87% 7%
17	3	56	41% 93%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	PHO	A	404	X	-	-	-
21	PHO	D	406	X	-	-	-
22	CLA	A	405	X	-	-	-
22	CLA	A	406	X	-	-	-
22	CLA	B	601	X	-	-	-
22	CLA	B	602	X	-	-	-
22	CLA	B	603	X	-	-	-
22	CLA	B	604	X	-	-	-
22	CLA	B	605	X	-	-	-
22	CLA	B	606	X	-	-	-
22	CLA	B	607	X	-	-	-
22	CLA	B	609	X	-	-	-
22	CLA	B	610	X	-	-	-
22	CLA	B	611	X	-	-	-
22	CLA	B	612	X	-	-	-
22	CLA	B	613	X	-	-	-
22	CLA	B	614	X	-	-	-
22	CLA	B	615	X	-	-	-
22	CLA	B	616	X	-	-	-
22	CLA	C	504	X	-	-	-
22	CLA	C	505	X	-	-	-
22	CLA	C	506	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	C	507	X	-	-	-
22	CLA	C	508	X	-	-	-
22	CLA	C	509	X	-	-	-
22	CLA	C	510	X	-	-	-
22	CLA	C	511	X	-	-	-
22	CLA	C	512	X	-	-	-
22	CLA	C	513	X	-	-	-
22	CLA	C	514	X	-	-	-
22	CLA	C	517	X	-	-	-
22	CLA	D	402	X	-	-	-
22	CLA	D	407	X	-	-	-
22	CLA	D	408	X	-	-	-

2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 20946 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 Photosystem II protein D1 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	335	Total	C	N	O	S	0	0
			2627	1720	432	460	15		

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	496	Total	C	N	O	S	0	0
			3909	2569	649	678	13		

- Molecule 3 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	432	Total	C	N	O	S	0	0
			3345	2197	561	575	12		

- Molecule 4 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	341	Total	C	N	O	S	0	0
			2717	1800	444	461	12		

- Molecule 5 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	77	Total	C	N	O	0	0
			635	417	103	115		

- Molecule 6 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	38	Total	C	N	O	S	0	0
			307	207	50	49	1		

- Molecule 7 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	65	Total	C	N	O	S	0	0
			511	341	82	86	2		

- Molecule 8 is a protein called Photosystem II reaction center protein I.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	26	Total	C	N	O	S	0	0
			211	150	27	33	1		

- Molecule 9 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	K	37	Total	C	N	O	0	0
			293	204	43	46		

- Molecule 10 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	37	Total	C	N	O	S	0	0
			304	202	48	53	1		

- Molecule 11 is a protein called Photosystem II reaction center protein M.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	34	Total	C	N	O	S	0	0
			267	178	40	48	1		

- Molecule 12 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	T	28	Total	C	N	O	S	0	0
			241	170	34	35	2		

- Molecule 13 is a protein called Photosystem II reaction center X protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	X	35	Total	C	N	O	0	0
			254	172	38	44		

- Molecule 14 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	y	28	Total	C	N	O	S	0	0
			208	137	36	32	3		

- Molecule 15 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Z	60	Total	C	N	O	S	0	0
			463	318	70	74	1		

- Molecule 16 is a protein called Photosystem II reaction center Psb28 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	2	112	Total	C	N	O	S	0	0
			897	562	156	173	6		

- Molecule 17 is a protein called Tsl0063 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	3	56	Total	C	N	O	S	0	0
			419	269	74	75	1		

- Molecule 18 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
18	A	1	Total	Fe	0
			1	1	

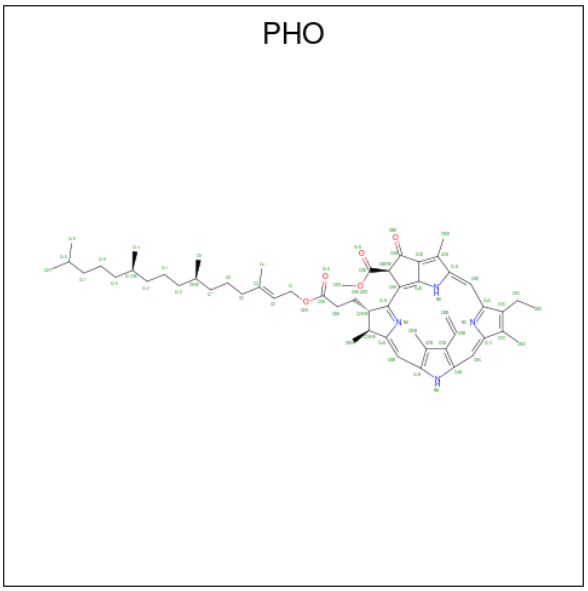
- Molecule 19 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		AltConf
19	A	1	Total	Mn	0
			1	1	

- Molecule 20 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

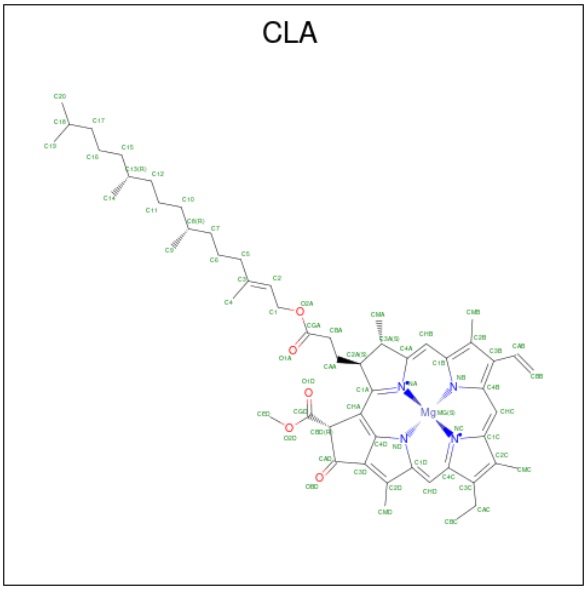
Mol	Chain	Residues	Atoms		AltConf
20	A	1	Total	Cl	0
			1	1	

- Molecule 21 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



Mol	Chain	Residues	Atoms				AltConf
21	A	1	Total	C	N	O	0
			64	55	4	5	
21	D	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 22 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0

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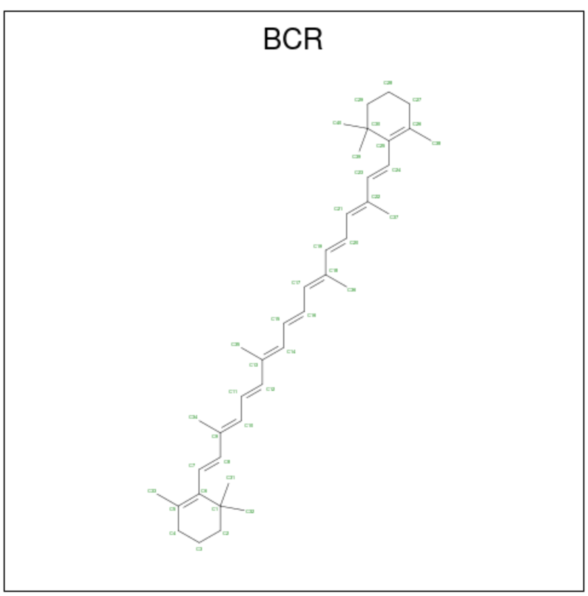
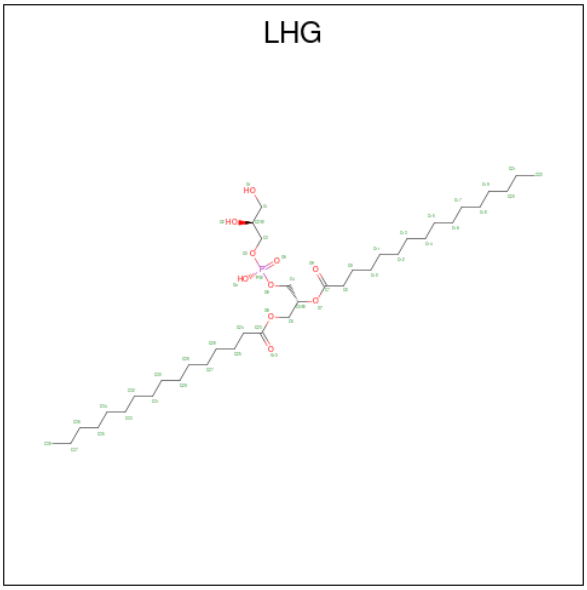
Mol	Chain	Residues	Atoms	AltConf
22	C	1	Total C Mg N O 65 55 1 4 5	0
22	C	1	Total C Mg N O 65 55 1 4 5	0
22	C	1	Total C Mg N O 65 55 1 4 5	0
22	C	1	Total C Mg N O 65 55 1 4 5	0
22	C	1	Total C Mg N O 65 55 1 4 5	0
22	C	1	Total C Mg N O 65 55 1 4 5	0
22	C	1	Total C Mg N O 65 55 1 4 5	0
22	C	1	Total C Mg N O 65 55 1 4 5	0
22	D	1	Total C Mg N O 65 55 1 4 5	0
22	D	1	Total C Mg N O 65 55 1 4 5	0
22	D	1	Total C Mg N O 65 55 1 4 5	0
22	D	1	Total C Mg N O 65 55 1 4 5	0

- Molecule 23 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



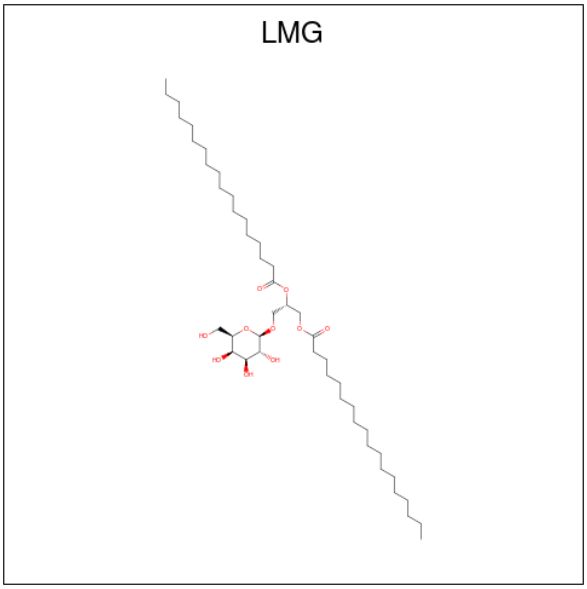
Mol	Chain	Residues	Atoms	AltConf
23	A	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	C	1	Total C 40 40	0
23	C	1	Total C 40 40	0
23	C	1	Total C 40 40	0
23	F	1	Total C 40 40	0
23	H	1	Total C 40 40	0
23	K	1	Total C 40 40	0

- Molecule 24 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



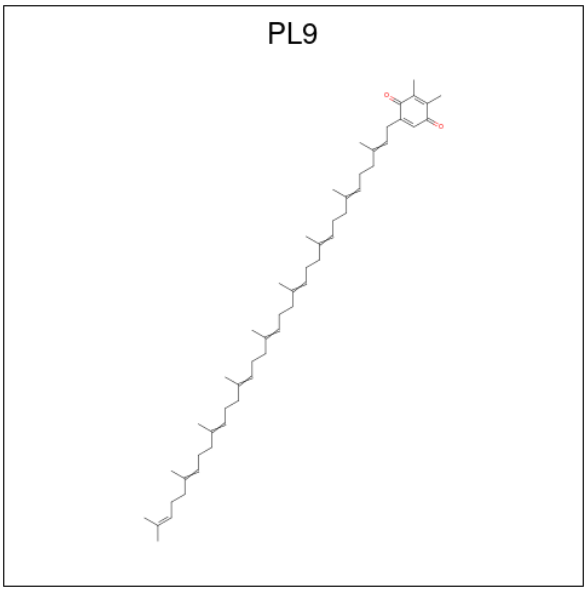
Mol	Chain	Residues	Atoms	AltConf
24	A	1	Total C O P 49 38 10 1	0

- Molecule 25 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



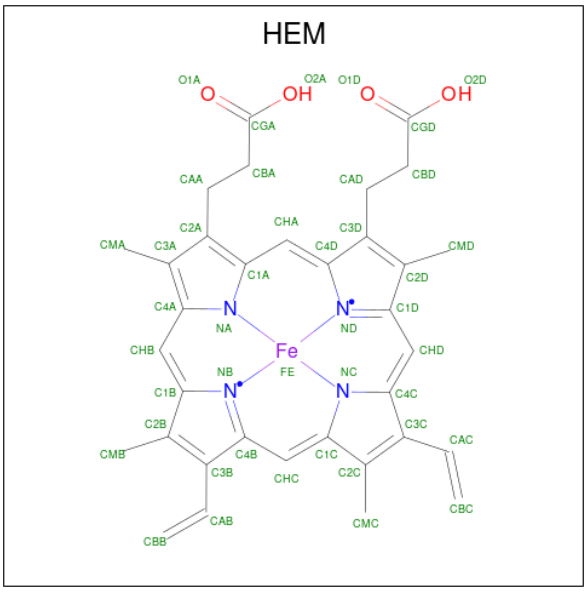
Mol	Chain	Residues	Atoms			AltConf
25	C	1	Total	C	O	0
			55	45	10	
25	C	1	Total	C	O	0
			55	45	10	
25	D	1	Total	C	O	0
			55	45	10	
25	D	1	Total	C	O	0
			55	45	10	
25	F	1	Total	C	O	0
			55	45	10	
25	I	1	Total	C	O	0
			55	45	10	
25	3	1	Total	C	O	0
			55	45	10	

- Molecule 26 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula: $C_{53}H_{80}O_2$).



Mol	Chain	Residues	Atoms			AltConf
26	D	1	Total	C	O	0
			55	53	2	

- Molecule 27 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

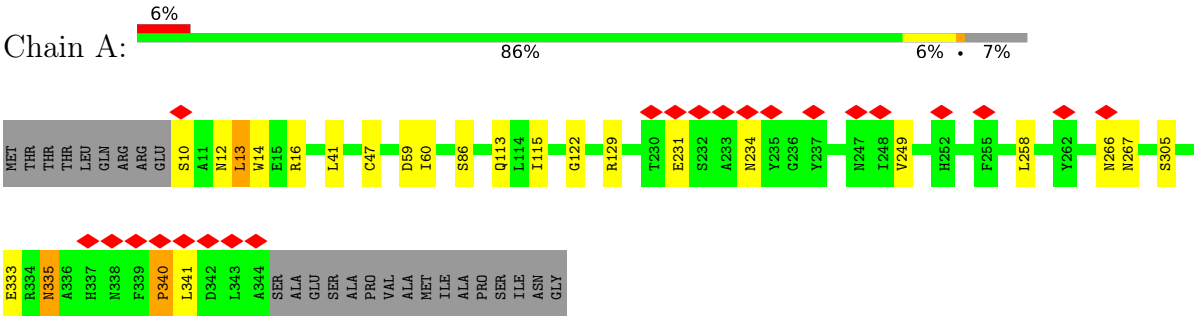


Mol	Chain	Residues	Atoms					AltConf
27	E	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

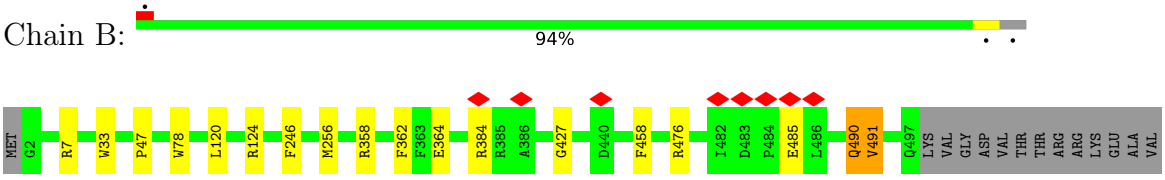
3 Residue-property plots (i)

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.

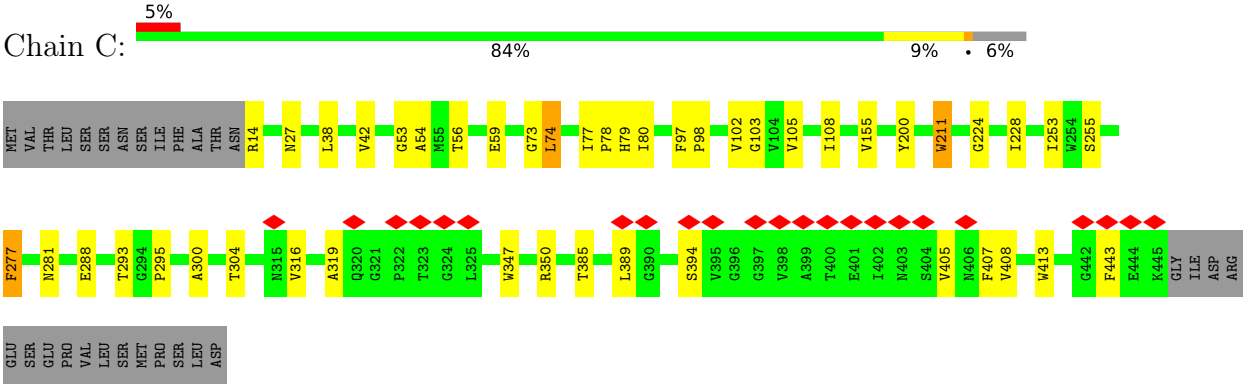
• Molecule 1: Photosystem II protein D1 1



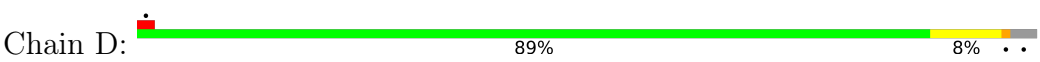
• Molecule 2: Photosystem II CP47 reaction center protein

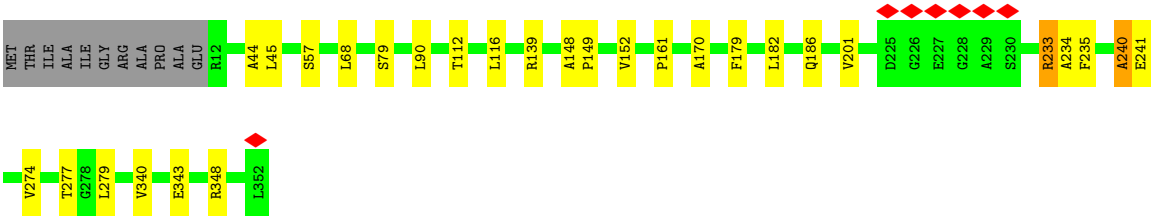


• Molecule 3: Photosystem II CP43 reaction center protein

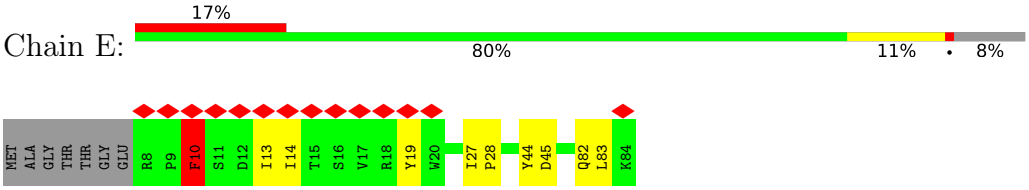


• Molecule 4: Photosystem II D2 protein

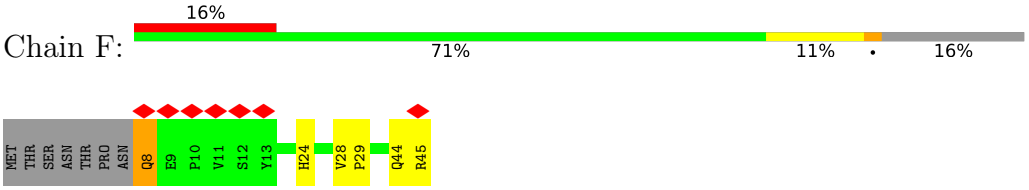




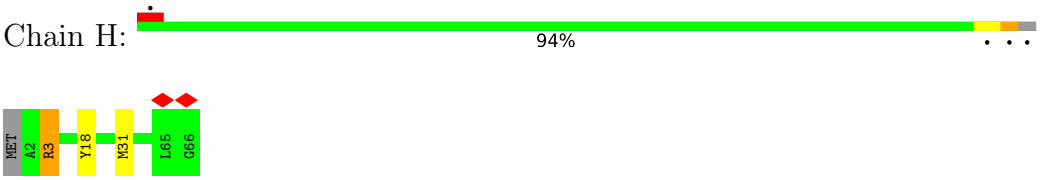
• Molecule 5: Cytochrome b559 subunit alpha



• Molecule 6: Cytochrome b559 subunit beta

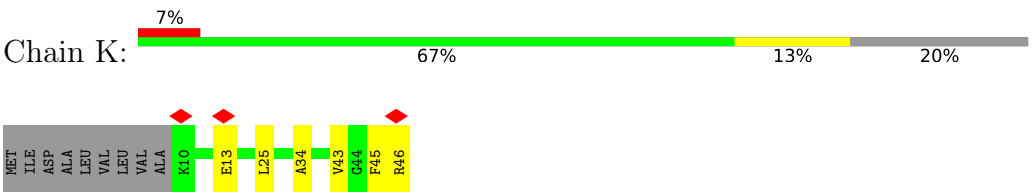


• Molecule 7: Photosystem II reaction center protein H

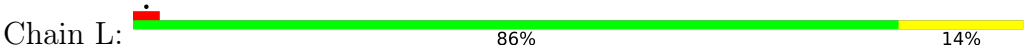


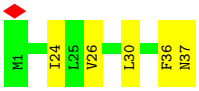
• Molecule 8: Photosystem II reaction center protein I

• Molecule 9: Photosystem II reaction center protein K



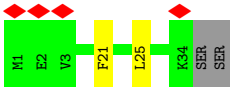
• Molecule 10: Photosystem II reaction center protein L





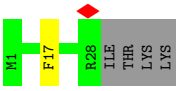
• Molecule 11: Photosystem II reaction center protein M

Chain M:



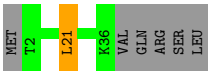
• Molecule 12: Photosystem II reaction center protein T

Chain T:



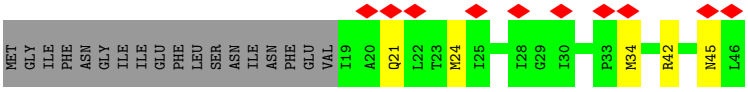
• Molecule 13: Photosystem II reaction center X protein

Chain X:



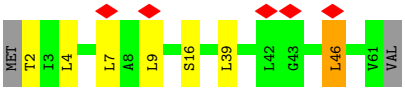
• Molecule 14: Photosystem II reaction center protein Ycf12

Chain y:



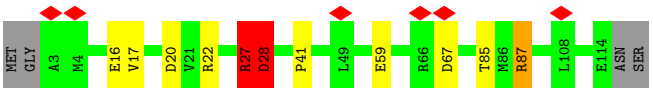
• Molecule 15: Photosystem II reaction center protein Z

Chain Z:



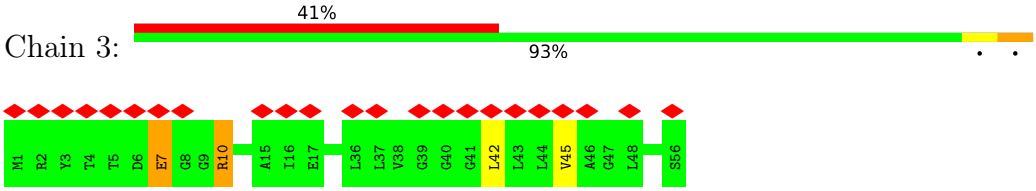
• Molecule 16: Photosystem II reaction center Psb28 protein

Chain 2:



• Molecule 17: Tsl0063 protein

Chain 3:


41%
93%
M1
R2
Y3
T4
T5
D6
E7
G8
G9
R10
A15
I16
E17
L36
L37
V38
G39
G40
G41
L42
L43
L44
V45
A46
G47
L48
S56

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	91479	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 ($e^-/Å^2$)	55	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.065	Depositor
Minimum map value	-0.030	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.006	Depositor
Map size (Å)	283.4, 283.4, 283.4	wwPDB
Map dimensions	260, 260, 260	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.09, 1.09, 1.09	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: BCR, PL9, CL, MN, PHO, LMG, CLA, HEM, LHG, FE

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	0.43	0/2712	0.75	1/3700 (0.0%)
2	B	0.45	0/4049	0.76	2/5519 (0.0%)
3	C	0.44	0/3456	0.75	5/4706 (0.1%)
4	D	0.43	0/2812	0.77	1/3832 (0.0%)
5	E	0.44	0/654	0.80	1/891 (0.1%)
6	F	0.57	0/317	0.96	1/433 (0.2%)
7	H	0.41	0/524	0.81	1/713 (0.1%)
8	I	0.52	0/216	0.91	0/292
9	K	0.50	0/303	0.72	0/416
10	L	0.43	0/311	0.79	0/422
11	M	0.46	0/270	0.83	0/367
12	T	0.55	0/250	0.84	1/338 (0.3%)
13	X	0.48	0/257	0.97	1/348 (0.3%)
14	y	0.52	0/209	1.01	1/279 (0.4%)
15	Z	0.48	0/474	0.99	3/649 (0.5%)
16	2	0.52	0/914	0.93	0/1231
17	3	0.57	1/426 (0.2%)	1.11	3/578 (0.5%)
All	All	0.45	1/18154 (0.0%)	0.80	21/24714 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	3
4	D	0	1
5	E	0	1
14	y	0	1
16	2	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	9

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	3	7	GLU	CB-CG	-5.73	1.41	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	3	7	GLU	CA-CB-CG	9.35	133.98	113.40
15	Z	46	LEU	CB-CG-CD1	7.83	124.31	111.00
1	A	249	VAL	CG1-CB-CG2	-7.13	99.49	110.90
4	D	45	LEU	CA-CB-CG	6.99	131.37	115.30
5	E	10	PHE	CB-CG-CD1	-6.88	115.98	120.80
17	3	7	GLU	CB-CA-C	-6.74	96.93	110.40
3	C	443	PHE	CB-CG-CD1	6.53	125.37	120.80
3	C	443	PHE	CB-CG-CD2	-6.41	116.31	120.80
7	H	3	ARG	NE-CZ-NH1	6.17	123.38	120.30
14	y	34	MET	CA-CB-CG	6.12	123.70	113.30
15	Z	9	LEU	CB-CG-CD1	-6.10	100.63	111.00
3	C	14	ARG	NE-CZ-NH2	-5.93	117.33	120.30
12	T	17	PHE	CB-CG-CD1	5.70	124.79	120.80
13	X	21	LEU	CB-CG-CD2	-5.62	101.44	111.00
15	Z	39	LEU	CA-CB-CG	5.60	128.18	115.30
2	B	490	GLN	CA-CB-CG	5.59	125.71	113.40
3	C	14	ARG	NE-CZ-NH1	5.50	123.05	120.30
17	3	7	GLU	CB-CG-CD	5.47	128.97	114.20
6	F	8	GLN	CA-CB-CG	5.44	125.36	113.40
2	B	491	VAL	N-CA-CB	-5.44	99.54	111.50
3	C	211	TRP	N-CA-C	5.12	124.83	111.00

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	2	27	ARG	Peptide
16	2	67	ASP	Sidechain
1	A	335	ASN	Sidechain
2	B	364	GLU	Sidechain
2	B	485	GLU	Sidechain

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Mol	Chain	Res	Type	Group
2	B	490	GLN	Mainchain
4	D	233	ARG	Peptide
5	E	10	PHE	Sidechain
14	y	45	ASN	Peptide

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	2627	0	2524	14	0
2	B	3909	0	3763	8	0
3	C	3345	0	3273	33	0
4	D	2717	0	2621	19	0
5	E	635	0	625	5	0
6	F	307	0	312	4	0
7	H	511	0	532	2	0
8	I	211	0	227	2	0
9	K	293	0	305	7	0
10	L	304	0	316	4	0
11	M	267	0	289	2	0
12	T	241	0	244	0	0
13	X	254	0	282	0	0
14	y	208	0	237	0	0
15	Z	463	0	495	2	0
16	2	897	0	859	4	0
17	3	419	0	438	4	0
18	A	1	0	0	0	0
19	A	1	0	0	0	0
20	A	1	0	0	0	0
21	A	64	0	73	2	0
21	D	64	0	73	3	0
22	A	130	0	140	2	0
22	B	1040	0	1121	32	0
22	C	845	0	909	22	0
22	D	260	0	279	10	0
23	A	40	0	56	1	0
23	B	120	0	168	3	0
23	C	120	0	168	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	F	40	0	56	1	0
23	H	40	0	56	15	0
23	K	40	0	56	11	0
24	A	49	0	74	0	0
25	3	55	0	86	2	0
25	C	110	0	172	0	0
25	D	110	0	172	2	0
25	F	55	0	86	0	0
25	I	55	0	86	2	0
26	D	55	0	80	4	0
27	E	43	0	30	3	0
All	All	20946	0	21283	181	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 4.

All (181) 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)
22:B:609:CLA:C4B	23:H:101:BCR:H333	1.79	1.12
23:C:515:BCR:H353	23:K:101:BCR:H332	1.25	1.08
22:B:609:CLA:C3B	23:H:101:BCR:H333	1.95	0.96
23:K:101:BCR:C38	23:K:101:BCR:H23C	2.02	0.90
23:H:101:BCR:C38	23:H:101:BCR:H23C	2.03	0.89
22:B:602:CLA:HED2	22:B:603:CLA:H43	1.57	0.87
23:C:515:BCR:C35	23:K:101:BCR:H332	2.05	0.86
1:A:341:LEU:HD13	3:C:385:THR:HA	1.62	0.82
23:C:515:BCR:H353	23:K:101:BCR:C33	2.08	0.80
4:D:116:LEU:HD13	22:D:408:CLA:HBA1	1.65	0.78
22:B:602:CLA:HBA2	22:B:602:CLA:HMA2	1.69	0.74
22:C:517:CLA:HMB1	22:C:517:CLA:HBB1	1.69	0.74
23:H:101:BCR:H23C	23:H:101:BCR:H382	1.69	0.74
22:B:607:CLA:H142	22:B:607:CLA:H101	1.71	0.72
23:K:101:BCR:H23C	23:K:101:BCR:H382	1.69	0.72
1:A:341:LEU:CD1	3:C:385:THR:HA	2.21	0.70
22:B:609:CLA:C3B	23:H:101:BCR:C33	2.69	0.69
6:F:45:ARG:OXT	6:F:45:ARG:HD2	1.92	0.69
27:E:101:HEM:HMB2	27:E:101:HEM:HBB2	1.75	0.69
9:K:34:ALA:HB1	23:K:101:BCR:H21C	1.75	0.69
3:C:59:GLU:HG3	3:C:74:LEU:HD12	1.75	0.67
22:C:511:CLA:HMA3	22:C:517:CLA:HMA1	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:D:402:CLA:H41	22:D:402:CLA:H92	1.78	0.65
22:C:503:CLA:HMA1	23:C:516:BCR:H401	1.82	0.62
3:C:408:VAL:HG13	3:C:413:TRP:HE1	1.64	0.61
22:B:601:CLA:HMA3	23:H:101:BCR:H382	1.83	0.60
26:D:405:PL9:H352	10:L:26:VAL:HG12	1.83	0.59
2:B:33:TRP:HE1	22:B:607:CLA:HBC2	1.67	0.59
22:B:609:CLA:NB	23:H:101:BCR:H333	2.18	0.59
21:A:404:PHO:HMB1	21:A:404:PHO:HBB1	1.84	0.59
22:C:504:CLA:H42	22:C:505:CLA:H172	1.85	0.59
16:2:85:THR:O	16:2:87:ARG:NH1	2.36	0.59
4:D:116:LEU:HD13	22:D:408:CLA:CBA	2.32	0.57
22:C:511:CLA:HAA2	22:C:517:CLA:HMB2	1.87	0.56
17:3:42:LEU:O	17:3:45:VAL:HG12	2.04	0.56
3:C:288:GLU:N	3:C:288:GLU:OE1	2.39	0.56
17:3:42:LEU:HA	17:3:45:VAL:HG12	1.86	0.56
22:B:603:CLA:HAB	22:B:605:CLA:H171	1.88	0.56
3:C:293:THR:HG22	3:C:295:PRO:HD2	1.87	0.54
3:C:102:VAL:HG21	22:C:505:CLA:HMA3	1.90	0.54
5:E:27:ILE:HB	5:E:28:PRO:HD3	1.89	0.54
22:C:505:CLA:HMD2	22:C:505:CLA:H191	1.89	0.54
3:C:108:ILE:HD11	23:C:518:BCR:H10C	1.90	0.53
22:C:509:CLA:H72	22:C:509:CLA:H41	1.90	0.53
23:K:101:BCR:H23C	23:K:101:BCR:H383	1.89	0.53
4:D:161:PRO:HG3	4:D:170:ALA:HB2	1.91	0.52
22:D:402:CLA:HAA1	22:D:402:CLA:CGD	2.40	0.52
9:K:34:ALA:HB1	23:K:101:BCR:C21	2.39	0.52
22:B:614:CLA:HAA1	22:B:614:CLA:CGD	2.39	0.52
1:A:231:GLU:HB2	1:A:234:ASN:OD1	2.10	0.52
22:A:406:CLA:HBB1	22:A:406:CLA:HMB1	1.91	0.52
22:C:510:CLA:CMA	22:C:511:CLA:HMC3	2.41	0.51
1:A:12:ASN:O	1:A:14:TRP:N	2.43	0.51
22:B:604:CLA:H72	22:B:604:CLA:H41	1.92	0.51
3:C:405:VAL:HG22	3:C:407:PHE:H	1.76	0.51
4:D:148:ALA:HB3	4:D:149:PRO:HD3	1.92	0.51
3:C:253:ILE:HG22	3:C:255:SER:H	1.76	0.51
4:D:233:ARG:HA	4:D:234:ALA:O	2.11	0.51
22:B:609:CLA:C2B	23:H:101:BCR:H333	2.38	0.51
25:D:403:LMG:H453	10:L:24:ILE:HD12	1.94	0.50
27:E:101:HEM:HBB2	27:E:101:HEM:CMB	2.41	0.50
9:K:25:LEU:CD2	23:K:101:BCR:H322	2.41	0.50
23:B:619:BCR:C8	23:B:619:BCR:H331	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:D:405:PL9:H202	26:D:405:PL9:H162	1.93	0.50
6:F:28:VAL:HG23	6:F:29:PRO:HD3	1.93	0.50
1:A:59:ASP:O	1:A:86:SER:HB3	2.11	0.49
4:D:234:ALA:HA	4:D:235:PHE:HB2	1.94	0.49
23:B:617:BCR:H392	23:B:617:BCR:H23C	1.95	0.49
4:D:240:ALA:O	4:D:241:GLU:HB2	2.12	0.49
22:C:503:CLA:H203	22:C:509:CLA:HMB3	1.95	0.49
1:A:341:LEU:CD1	3:C:385:THR:HG22	2.43	0.48
22:B:608:CLA:HBA1	22:B:608:CLA:HBD	1.95	0.48
3:C:389:LEU:O	3:C:408:VAL:HG23	2.13	0.48
21:D:406:PHO:HBB1	21:D:406:PHO:HMB1	1.95	0.48
9:K:43:VAL:HG12	9:K:43:VAL:O	2.13	0.48
22:B:609:CLA:H41	7:H:31:MET:SD	2.54	0.48
22:B:613:CLA:OBD	22:B:614:CLA:HHC	2.14	0.48
4:D:279:LEU:HD22	22:D:407:CLA:HBA2	1.96	0.48
22:D:408:CLA:HAA1	22:D:408:CLA:CGD	2.44	0.48
22:B:613:CLA:OBD	22:B:614:CLA:CAB	2.62	0.47
11:M:21:PHE:CE1	11:M:25:LEU:HD11	2.48	0.47
4:D:201:VAL:HG11	22:D:401:CLA:C3D	2.44	0.47
5:E:14:ILE:HD12	5:E:19:TYR:CZ	2.49	0.47
23:H:101:BCR:C8	23:H:101:BCR:H311	2.44	0.47
21:D:406:PHO:HMB1	21:D:406:PHO:CBB	2.45	0.47
3:C:316:VAL:HB	3:C:319:ALA:HB3	1.97	0.47
1:A:340:PRO:O	1:A:341:LEU:HG	2.15	0.47
23:K:101:BCR:C8	23:K:101:BCR:H311	2.42	0.47
22:B:609:CLA:HHC	22:B:609:CLA:HBB1	1.96	0.47
4:D:57:SER:HB3	4:D:79:SER:OG	2.15	0.47
22:B:609:CLA:O2A	22:B:610:CLA:HMC3	2.15	0.46
1:A:13:LEU:HA	1:A:16:ARG:HE	1.79	0.46
22:B:612:CLA:H93	22:B:612:CLA:CGA	2.45	0.46
3:C:77:ILE:N	3:C:78:PRO:CD	2.78	0.46
3:C:53:GLY:O	3:C:56:THR:HG22	2.16	0.46
4:D:343:GLU:H	4:D:343:GLU:CD	2.18	0.46
22:B:610:CLA:HAA1	22:B:610:CLA:CGD	2.46	0.46
22:C:510:CLA:HMA3	22:C:511:CLA:HMC3	1.97	0.46
1:A:341:LEU:HD12	3:C:385:THR:HG22	1.97	0.46
3:C:56:THR:CG2	3:C:103:GLY:HA2	2.45	0.46
23:H:101:BCR:H23C	23:H:101:BCR:H383	1.91	0.46
22:A:406:CLA:HMA2	22:A:406:CLA:HBA2	1.98	0.46
2:B:47:PRO:HG3	2:B:78:TRP:CD2	2.51	0.45
3:C:79:HIS:CE1	22:C:504:CLA:HAA2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:601:CLA:HMC3	23:H:101:BCR:H15C	1.98	0.45
3:C:42:VAL:HG23	22:C:513:CLA:HED1	1.97	0.45
5:E:10:PHE:HA	5:E:13:ILE:HB	1.99	0.45
26:D:405:PL9:H371	10:L:30:LEU:HB2	1.98	0.45
3:C:224:GLY:O	3:C:228:ILE:HG13	2.16	0.45
16:2:28:ASP:N	16:2:28:ASP:OD1	2.50	0.45
17:3:10:ARG:CZ	25:3:101:LMG:HC4	2.47	0.45
23:A:407:BCR:C8	23:A:407:BCR:H331	2.47	0.44
4:D:340:VAL:HG23	4:D:340:VAL:O	2.17	0.44
3:C:200:TYR:O	3:C:211:TRP:O	2.36	0.44
23:C:515:BCR:H371	23:C:515:BCR:H24C	1.78	0.44
8:I:11:VAL:HG12	25:I:101:LMG:H273	2.00	0.44
15:Z:4:LEU:HA	15:Z:7:LEU:HG	2.00	0.44
3:C:277:PHE:CE1	3:C:281:ASN:ND2	2.85	0.44
4:D:152:VAL:HG21	22:D:407:CLA:HBA1	1.98	0.44
5:E:82:GLN:O	5:E:83:LEU:HB2	2.17	0.44
22:C:503:CLA:CMB	22:C:503:CLA:H93	2.48	0.44
22:B:603:CLA:HMB1	22:B:603:CLA:CBB	2.48	0.44
3:C:155:VAL:HG21	22:C:513:CLA:HMA1	2.00	0.44
22:D:401:CLA:HMA2	25:3:101:LMG:H271	2.00	0.44
22:B:609:CLA:C1B	23:H:101:BCR:H333	2.48	0.43
1:A:41:LEU:CD1	1:A:122:GLY:HA3	2.48	0.43
1:A:60:ILE:HA	1:A:86:SER:HA	2.00	0.43
22:B:612:CLA:HAA2	22:B:613:CLA:HMB2	1.99	0.43
22:B:615:CLA:HBA1	22:B:615:CLA:HMA2	2.00	0.43
22:C:514:CLA:HAA1	22:C:514:CLA:CGD	2.48	0.43
22:C:517:CLA:HAA1	22:C:517:CLA:CGD	2.48	0.43
22:B:604:CLA:H93	22:B:606:CLA:HMB1	2.00	0.43
1:A:258:LEU:HD12	1:A:258:LEU:N	2.33	0.43
4:D:179:PHE:HA	4:D:182:LEU:HD12	2.01	0.43
11:M:21:PHE:CZ	11:M:25:LEU:HD11	2.53	0.43
2:B:458:PHE:CE1	22:B:613:CLA:H101	2.53	0.43
22:B:609:CLA:HMA2	22:B:609:CLA:HBA2	2.00	0.43
22:D:407:CLA:HBB1	22:D:407:CLA:HHC	2.01	0.43
9:K:45:PHE:C	9:K:46:ARG:O	2.57	0.43
2:B:120:LEU:HA	7:H:3:ARG:H	1.83	0.43
23:F:102:BCR:C8	23:F:102:BCR:H331	2.48	0.42
16:2:17:VAL:HG21	16:2:41:PRO:HA	2.01	0.42
23:H:101:BCR:HC31	23:H:101:BCR:H323	1.82	0.42
9:K:43:VAL:O	9:K:43:VAL:CG1	2.67	0.42
2:B:384:ARG:HH12	4:D:348:ARG:HH11	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:300:ALA:O	3:C:304:THR:HG22	2.20	0.42
23:H:101:BCR:C38	23:H:101:BCR:C23	2.82	0.42
22:B:603:CLA:H92	22:B:605:CLA:H122	2.01	0.42
3:C:77:ILE:HA	3:C:80:ILE:HD12	2.01	0.42
4:D:274:VAL:HG22	26:D:405:PL9:H253	2.01	0.42
3:C:73:GLY:HA3	22:C:506:CLA:HBA1	2.01	0.42
8:I:3:THR:HG21	25:I:101:LMG:HC1	2.02	0.42
3:C:102:VAL:HA	3:C:105:VAL:HG22	2.01	0.42
16:2:27:ARG:O	16:2:28:ASP:O	2.38	0.42
3:C:228:ILE:HD11	23:C:516:BCR:H392	2.02	0.42
1:A:47:CYS:SG	1:A:115:ILE:HG13	2.59	0.42
2:B:124:ARG:HH11	2:B:124:ARG:HG3	1.85	0.42
22:C:505:CLA:HMD2	22:C:505:CLA:C19	2.49	0.42
3:C:56:THR:HG21	3:C:103:GLY:HA2	2.03	0.41
3:C:347:TRP:CD1	3:C:347:TRP:N	2.89	0.41
4:D:68:LEU:HD11	5:E:44:TYR:CE2	2.55	0.41
2:B:7:ARG:HA	22:B:611:CLA:HBA1	2.01	0.41
10:L:36:PHE:O	10:L:37:ASN:O	2.38	0.41
23:B:617:BCR:C8	23:B:617:BCR:H331	2.51	0.41
22:C:511:CLA:H202	22:C:513:CLA:HMD2	2.02	0.41
4:D:44:ALA:HB1	21:D:406:PHO:H92	2.01	0.41
1:A:129:ARG:HH12	25:D:404:LMG:H441	1.86	0.41
23:C:516:BCR:H20C	23:C:516:BCR:H361	1.87	0.41
23:K:101:BCR:H331	23:K:101:BCR:HC7	1.50	0.41
17:3:42:LEU:HA	17:3:45:VAL:CG1	2.51	0.41
21:A:404:PHO:HMB1	21:A:404:PHO:CBB	2.51	0.41
2:B:358:ARG:CZ	2:B:427:GLY:HA2	2.51	0.41
22:B:609:CLA:C1B	23:H:101:BCR:HC42	2.51	0.41
27:E:101:HEM:C4D	6:F:24:HIS:HE1	2.39	0.41
15:Z:2:THR:CG2	15:Z:4:LEU:HD23	2.51	0.41
3:C:27:ASN:OD1	22:C:510:CLA:H42	2.21	0.40
3:C:97:PHE:HB3	3:C:98:PRO:HD3	2.03	0.40
22:C:503:CLA:H2	22:C:504:CLA:OBD	2.22	0.40
3:C:54:ALA:HB1	9:K:25:LEU:HB3	2.04	0.40
4:D:90:LEU:HD12	4:D:112:THR:HG21	2.04	0.40
6:F:44:GLN:CD	6:F:44:GLN:H	2.25	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	333/360 (92%)	314 (94%)	17 (5%)	2 (1%)	25 47
2	B	494/510 (97%)	470 (95%)	23 (5%)	1 (0%)	47 71
3	C	430/461 (93%)	405 (94%)	25 (6%)	0	100 100
4	D	339/352 (96%)	321 (95%)	17 (5%)	1 (0%)	41 64
5	E	75/84 (89%)	71 (95%)	4 (5%)	0	100 100
6	F	36/45 (80%)	32 (89%)	4 (11%)	0	100 100
7	H	63/66 (96%)	57 (90%)	5 (8%)	1 (2%)	9 22
8	I	24/38 (63%)	24 (100%)	0	0	100 100
9	K	35/46 (76%)	33 (94%)	2 (6%)	0	100 100
10	L	35/37 (95%)	34 (97%)	1 (3%)	0	100 100
11	M	32/36 (89%)	32 (100%)	0	0	100 100
12	T	26/32 (81%)	24 (92%)	2 (8%)	0	100 100
13	X	33/41 (80%)	32 (97%)	1 (3%)	0	100 100
14	y	26/46 (56%)	22 (85%)	4 (15%)	0	100 100
15	Z	58/62 (94%)	57 (98%)	1 (2%)	0	100 100
16	2	110/116 (95%)	102 (93%)	6 (6%)	2 (2%)	8 19
17	3	54/56 (96%)	53 (98%)	1 (2%)	0	100 100
All	All	2203/2388 (92%)	2083 (95%)	113 (5%)	7 (0%)	44 64

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	491	VAL
4	D	240	ALA
16	2	28	ASP
1	A	13	LEU
16	2	27	ARG

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Mol	Chain	Res	Type
1	A	340	PRO
7	H	18	TYR

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	271/291 (93%)	264 (97%)	7 (3%)	46 73
2	B	395/407 (97%)	391 (99%)	4 (1%)	76 90
3	C	335/362 (92%)	330 (98%)	5 (2%)	65 84
4	D	276/283 (98%)	273 (99%)	3 (1%)	73 89
5	E	69/73 (94%)	68 (99%)	1 (1%)	67 85
6	F	32/39 (82%)	31 (97%)	1 (3%)	40 67
7	H	54/55 (98%)	54 (100%)	0	100 100
8	I	24/35 (69%)	22 (92%)	2 (8%)	11 23
9	K	30/37 (81%)	29 (97%)	1 (3%)	38 64
10	L	35/35 (100%)	35 (100%)	0	100 100
11	M	31/33 (94%)	31 (100%)	0	100 100
12	T	25/29 (86%)	25 (100%)	0	100 100
13	X	28/34 (82%)	27 (96%)	1 (4%)	35 61
14	y	21/37 (57%)	18 (86%)	3 (14%)	3 7
15	Z	50/52 (96%)	48 (96%)	2 (4%)	31 57
16	2	94/97 (97%)	88 (94%)	6 (6%)	17 36
17	3	42/42 (100%)	40 (95%)	2 (5%)	25 49
All	All	1812/1941 (93%)	1774 (98%)	38 (2%)	56 78

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	SER

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Mol	Chain	Res	Type
1	A	113	GLN
1	A	266	ASN
1	A	267	ASN
1	A	305	SER
1	A	333	GLU
1	A	335	ASN
2	B	246	PHE
2	B	256	MET
2	B	362	PHE
2	B	476	ARG
3	C	38	LEU
3	C	74	LEU
3	C	277	PHE
3	C	350	ARG
3	C	394	SER
4	D	139	ARG
4	D	186	GLN
4	D	277	THR
5	E	45	ASP
6	F	8	GLN
8	I	3	THR
8	I	19	PHE
9	K	13	GLU
13	X	21	LEU
14	y	21	GLN
14	y	24	MET
14	y	42	ARG
15	Z	16	SER
15	Z	46	LEU
16	2	16	GLU
16	2	20	ASP
16	2	22	ARG
16	2	28	ASP
16	2	59	GLU
16	2	87	ARG
17	3	7	GLU
17	3	10	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 60 ligands modelled in this entry, 3 are monoatomic - leaving 57 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
23	BCR	K	101	-	41,41,41	2.83	10 (24%)	56,56,56	3.77	31 (55%)
22	CLA	B	607	-	65,73,73	1.58	9 (13%)	76,113,113	2.23	25 (32%)
23	BCR	H	101	-	41,41,41	3.05	11 (26%)	56,56,56	3.99	30 (53%)
25	LMG	C	502	-	55,55,55	1.06	3 (5%)	63,63,63	0.99	5 (7%)
23	BCR	C	516	-	41,41,41	0.93	1 (2%)	56,56,56	1.20	9 (16%)
22	CLA	D	402	-	65,73,73	1.62	10 (15%)	76,113,113	2.44	26 (34%)
22	CLA	B	604	-	65,73,73	1.61	9 (13%)	76,113,113	2.77	19 (25%)
22	CLA	B	614	-	65,73,73	1.73	12 (18%)	76,113,113	2.65	23 (30%)
22	CLA	D	401	-	65,73,73	1.55	9 (13%)	76,113,113	2.13	22 (28%)
22	CLA	C	513	-	65,73,73	1.65	9 (13%)	76,113,113	2.80	24 (31%)
23	BCR	A	407	-	41,41,41	0.91	2 (4%)	56,56,56	1.08	3 (5%)
24	LHG	A	408	-	48,48,48	0.82	1 (2%)	51,54,54	0.90	2 (3%)
25	LMG	C	501	-	55,55,55	0.91	0	63,63,63	1.13	5 (7%)
25	LMG	3	101	-	55,55,55	0.92	1 (1%)	63,63,63	1.08	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	LMG	I	101	-	55,55,55	0.98	2 (3%)	63,63,63	1.09	3 (4%)
22	CLA	B	606	-	65,73,73	1.57	11 (16%)	76,113,113	2.30	26 (34%)
22	CLA	C	505	-	65,73,73	1.58	10 (15%)	76,113,113	2.90	27 (35%)
27	HEM	E	101	6,5	41,50,50	1.45	3 (7%)	45,82,82	1.08	1 (2%)
21	PHO	D	406	-	51,69,69	1.08	5 (9%)	47,99,99	1.28	6 (12%)
22	CLA	B	608	-	65,73,73	1.72	11 (16%)	76,113,113	2.62	23 (30%)
22	CLA	C	514	-	65,73,73	1.77	10 (15%)	76,113,113	2.35	19 (25%)
22	CLA	B	612	-	65,73,73	1.66	15 (23%)	76,113,113	2.88	26 (34%)
22	CLA	B	601	-	65,73,73	1.66	10 (15%)	76,113,113	2.54	19 (25%)
22	CLA	A	405	-	65,73,73	1.62	9 (13%)	76,113,113	2.18	21 (27%)
22	CLA	C	512	-	65,73,73	1.79	11 (16%)	76,113,113	2.75	23 (30%)
22	CLA	C	510	22	65,73,73	1.79	13 (20%)	76,113,113	2.70	22 (28%)
22	CLA	C	503	-	65,73,73	1.69	11 (16%)	76,113,113	1.90	24 (31%)
23	BCR	B	619	-	41,41,41	0.92	2 (4%)	56,56,56	1.26	8 (14%)
22	CLA	C	504	-	65,73,73	1.59	12 (18%)	76,113,113	2.19	17 (22%)
25	LMG	D	404	-	55,55,55	0.97	2 (3%)	63,63,63	1.08	4 (6%)
23	BCR	B	618	-	41,41,41	1.00	1 (2%)	56,56,56	1.14	5 (8%)
22	CLA	C	517	22	65,73,73	1.76	12 (18%)	76,113,113	2.94	28 (36%)
23	BCR	C	515	-	41,41,41	1.01	2 (4%)	56,56,56	1.45	12 (21%)
22	CLA	B	613	-	65,73,73	1.72	10 (15%)	76,113,113	2.81	25 (32%)
22	CLA	B	603	-	65,73,73	1.54	8 (12%)	76,113,113	2.33	20 (26%)
23	BCR	B	617	-	41,41,41	0.98	2 (4%)	56,56,56	1.27	7 (12%)
23	BCR	C	518	-	41,41,41	0.99	2 (4%)	56,56,56	1.53	13 (23%)
22	CLA	B	602	-	65,73,73	1.62	9 (13%)	76,113,113	2.53	21 (27%)
22	CLA	B	609	-	65,73,73	1.79	9 (13%)	76,113,113	2.75	20 (26%)
22	CLA	B	615	-	65,73,73	1.71	8 (12%)	76,113,113	2.64	23 (30%)
22	CLA	B	616	-	65,73,73	1.80	12 (18%)	76,113,113	3.08	22 (28%)
22	CLA	A	406	-	65,73,73	1.57	9 (13%)	76,113,113	2.27	19 (25%)
22	CLA	C	508	-	65,73,73	1.78	12 (18%)	76,113,113	2.13	18 (23%)
22	CLA	C	507	-	65,73,73	1.83	13 (20%)	76,113,113	2.82	25 (32%)
22	CLA	C	511	-	65,73,73	1.64	9 (13%)	76,113,113	2.64	21 (27%)
23	BCR	F	102	-	41,41,41	0.84	0	56,56,56	1.18	8 (14%)
22	CLA	B	611	-	65,73,73	1.70	9 (13%)	76,113,113	2.42	23 (30%)
21	PHO	A	404	-	51,69,69	1.04	5 (9%)	47,99,99	1.22	5 (10%)
25	LMG	F	101	-	55,55,55	1.02	2 (3%)	63,63,63	1.00	3 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	C	506	-	65,73,73	1.57	12 (18%)	76,113,113	2.44	18 (23%)
22	CLA	B	610	-	65,73,73	1.67	13 (20%)	76,113,113	2.84	24 (31%)
22	CLA	D	407	-	65,73,73	1.62	10 (15%)	76,113,113	2.05	21 (27%)
25	LMG	D	403	-	55,55,55	0.96	2 (3%)	63,63,63	1.05	3 (4%)
22	CLA	B	605	-	65,73,73	1.50	11 (16%)	76,113,113	2.35	17 (22%)
26	PL9	D	405	-	55,55,55	1.12	3 (5%)	68,69,69	1.41	11 (16%)
22	CLA	D	408	-	65,73,73	1.67	9 (13%)	76,113,113	2.08	16 (21%)
22	CLA	C	509	-	65,73,73	1.61	11 (16%)	76,113,113	2.49	15 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	BCR	K	101	-	-	15/29/63/63	0/2/2/2
22	CLA	B	607	-	2/2/15/20	12/37/115/115	-
23	BCR	H	101	-	-	15/29/63/63	0/2/2/2
25	LMG	C	502	-	-	7/50/70/70	0/1/1/1
23	BCR	C	516	-	-	14/29/63/63	0/2/2/2
22	CLA	D	402	-	2/2/15/20	9/37/115/115	-
22	CLA	B	604	-	1/1/15/20	7/37/115/115	-
22	CLA	B	614	-	3/3/15/20	9/37/115/115	-
22	CLA	D	401	-	-	13/37/115/115	-
22	CLA	C	513	-	3/3/15/20	4/37/115/115	-
23	BCR	A	407	-	-	8/29/63/63	0/2/2/2
24	LHG	A	408	-	-	7/53/53/53	-
25	LMG	C	501	-	-	18/50/70/70	0/1/1/1
25	LMG	3	101	-	-	8/50/70/70	0/1/1/1
25	LMG	I	101	-	-	5/50/70/70	0/1/1/1
22	CLA	B	606	-	2/2/15/20	14/37/115/115	-
22	CLA	C	505	-	1/1/15/20	17/37/115/115	-
27	HEM	E	101	6,5	-	4/12/54/54	-
21	PHO	D	406	-	1/1/17/22	6/37/103/103	0/5/6/6
22	CLA	B	608	-	-	6/37/115/115	-
22	CLA	C	514	-	3/3/15/20	10/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	612	-	4/4/15/20	12/37/115/115	-
22	CLA	B	601	-	3/3/15/20	9/37/115/115	-
22	CLA	A	405	-	2/2/15/20	12/37/115/115	-
22	CLA	C	512	-	1/1/15/20	9/37/115/115	-
22	CLA	C	510	22	1/1/15/20	12/37/115/115	-
22	CLA	C	503	-	-	7/37/115/115	-
23	BCR	B	619	-	-	6/29/63/63	0/2/2/2
22	CLA	C	504	-	2/2/15/20	13/37/115/115	-
25	LMG	D	404	-	-	11/50/70/70	0/1/1/1
23	BCR	B	618	-	-	5/29/63/63	0/2/2/2
22	CLA	C	517	22	3/3/15/20	11/37/115/115	-
23	BCR	C	515	-	-	9/29/63/63	0/2/2/2
22	CLA	B	613	-	3/3/15/20	8/37/115/115	-
22	CLA	B	603	-	3/3/15/20	10/37/115/115	-
23	BCR	B	617	-	-	14/29/63/63	0/2/2/2
23	BCR	C	518	-	-	9/29/63/63	0/2/2/2
22	CLA	B	602	-	2/2/15/20	11/37/115/115	-
22	CLA	B	609	-	2/2/15/20	7/37/115/115	-
22	CLA	B	615	-	3/3/15/20	10/37/115/115	-
22	CLA	B	616	-	4/4/15/20	9/37/115/115	-
22	CLA	A	406	-	2/2/15/20	10/37/115/115	-
22	CLA	C	508	-	1/1/15/20	3/37/115/115	-
22	CLA	C	507	-	2/2/15/20	11/37/115/115	-
22	CLA	C	511	-	3/3/15/20	9/37/115/115	-
23	BCR	F	102	-	-	3/29/63/63	0/2/2/2
22	CLA	B	611	-	1/1/15/20	13/37/115/115	-
21	PHO	A	404	-	1/1/17/22	7/37/103/103	0/5/6/6
25	LMG	F	101	-	-	7/50/70/70	0/1/1/1
22	CLA	C	506	-	3/3/15/20	11/37/115/115	-
22	CLA	B	610	-	2/2/15/20	9/37/115/115	-
22	CLA	D	407	-	2/2/15/20	9/37/115/115	-
25	LMG	D	403	-	-	5/50/70/70	0/1/1/1
22	CLA	B	605	-	2/2/15/20	9/37/115/115	-
26	PL9	D	405	-	-	14/53/73/73	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	D	408	-	3/3/15/20	5/37/115/115	-
22	CLA	C	509	-	2/2/15/20	8/37/115/115	-

All (429) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	H	101	BCR	C1-C6	-9.89	1.40	1.53
23	H	101	BCR	C5-C6	-9.63	1.17	1.34
22	B	615	CLA	C4B-NB	9.42	1.43	1.35
22	C	514	CLA	C4B-NB	9.37	1.43	1.35
22	C	512	CLA	C4B-NB	9.23	1.43	1.35
23	K	101	BCR	C1-C6	-9.10	1.41	1.53
22	D	408	CLA	C4B-NB	9.08	1.43	1.35
22	B	609	CLA	C4B-NB	8.79	1.43	1.35
22	B	616	CLA	C4B-NB	8.75	1.43	1.35
22	C	508	CLA	C4B-NB	8.69	1.43	1.35
22	A	405	CLA	C4B-NB	8.66	1.42	1.35
22	C	511	CLA	C4B-NB	8.54	1.42	1.35
22	C	507	CLA	C4B-NB	8.46	1.42	1.35
22	B	601	CLA	C4B-NB	8.33	1.42	1.35
22	C	503	CLA	C4B-NB	8.32	1.42	1.35
22	B	607	CLA	C4B-NB	8.31	1.42	1.35
23	K	101	BCR	C5-C6	-8.27	1.20	1.34
22	C	513	CLA	C4B-NB	8.26	1.42	1.35
22	B	608	CLA	C4B-NB	8.24	1.42	1.35
22	B	604	CLA	C4B-NB	8.21	1.42	1.35
22	B	613	CLA	C4B-NB	8.09	1.42	1.35
22	C	517	CLA	C4B-NB	8.09	1.42	1.35
22	D	407	CLA	C4B-NB	8.06	1.42	1.35
22	D	401	CLA	C4B-NB	7.96	1.42	1.35
22	D	402	CLA	C4B-NB	7.90	1.42	1.35
22	C	509	CLA	C4B-NB	7.86	1.42	1.35
22	B	614	CLA	C4B-NB	7.86	1.42	1.35
22	B	611	CLA	C4B-NB	7.83	1.42	1.35
22	C	505	CLA	C4B-NB	7.83	1.42	1.35
22	B	610	CLA	C4B-NB	7.79	1.42	1.35
22	C	510	CLA	C4B-NB	7.76	1.42	1.35
22	B	606	CLA	C4B-NB	7.65	1.42	1.35
22	C	506	CLA	C4B-NB	7.56	1.42	1.35
23	H	101	BCR	C33-C5	-7.40	1.38	1.50
22	B	602	CLA	C4B-NB	7.38	1.41	1.35
22	C	504	CLA	C4B-NB	7.33	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	406	CLA	C4B-NB	7.16	1.41	1.35
22	B	612	CLA	C4B-NB	7.13	1.41	1.35
22	B	605	CLA	C4B-NB	6.83	1.41	1.35
22	B	603	CLA	C4B-NB	6.71	1.41	1.35
23	K	101	BCR	C33-C5	-6.55	1.40	1.50
23	H	101	BCR	C30-C25	-6.47	1.44	1.53
23	K	101	BCR	C30-C25	-6.33	1.45	1.53
23	H	101	BCR	C31-C1	-5.30	1.43	1.53
23	K	101	BCR	C31-C1	-4.96	1.44	1.53
27	E	101	HEM	C3C-C2C	-4.82	1.33	1.40
22	C	510	CLA	C3D-CAD	4.67	1.61	1.45
22	B	609	CLA	C3D-C4D	4.34	1.54	1.44
22	B	616	CLA	C3D-C4D	4.31	1.53	1.44
22	C	507	CLA	C3D-CAD	4.23	1.59	1.45
22	C	510	CLA	C3D-C4D	4.17	1.53	1.44
22	B	614	CLA	C3D-CAD	4.14	1.59	1.45
22	C	517	CLA	C3D-CAD	4.12	1.59	1.45
22	C	507	CLA	C3D-C4D	4.10	1.53	1.44
22	B	614	CLA	C3D-C4D	4.09	1.53	1.44
22	C	512	CLA	C3D-C4D	4.01	1.53	1.44
22	B	611	CLA	C3D-CAD	3.98	1.58	1.45
22	B	613	CLA	C3D-CAD	3.97	1.58	1.45
22	C	508	CLA	C3D-CAD	3.94	1.58	1.45
22	B	612	CLA	CMD-C2D	-3.86	1.42	1.50
22	B	608	CLA	C3D-CAD	3.86	1.58	1.45
22	B	609	CLA	C3D-CAD	3.85	1.58	1.45
22	B	602	CLA	CMD-C2D	-3.84	1.42	1.50
23	K	101	BCR	C37-C22	-3.81	1.43	1.50
23	H	101	BCR	C37-C22	-3.78	1.43	1.50
22	C	508	CLA	C3D-C4D	3.72	1.52	1.44
22	B	606	CLA	CMD-C2D	-3.68	1.43	1.50
22	C	512	CLA	C3D-CAD	3.63	1.57	1.45
22	B	608	CLA	C3D-C4D	3.61	1.52	1.44
22	B	610	CLA	C3D-C4D	3.59	1.52	1.44
22	C	517	CLA	C3D-C4D	3.58	1.52	1.44
22	B	605	CLA	C1D-ND	3.57	1.42	1.37
22	B	612	CLA	CHC-C1C	3.54	1.44	1.35
22	C	504	CLA	C1D-ND	3.53	1.42	1.37
22	C	508	CLA	CHC-C1C	3.53	1.44	1.35
22	B	603	CLA	C1D-ND	3.51	1.42	1.37
22	A	405	CLA	CHC-C1C	3.49	1.43	1.35
22	B	615	CLA	CHC-C1C	3.49	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	613	CLA	C3D-C4D	3.49	1.52	1.44
22	C	510	CLA	CHC-C1C	3.44	1.43	1.35
22	C	512	CLA	CHC-C1C	3.44	1.43	1.35
22	B	602	CLA	CAA-C2A	-3.42	1.47	1.54
22	C	514	CLA	C3D-C4D	3.41	1.51	1.44
22	B	603	CLA	C4D-ND	-3.41	1.33	1.37
22	B	615	CLA	C1D-ND	3.40	1.42	1.37
22	B	611	CLA	C3D-C4D	3.39	1.51	1.44
22	C	514	CLA	CHC-C1C	3.35	1.43	1.35
22	B	611	CLA	CHC-C1C	3.35	1.43	1.35
22	B	615	CLA	C3D-C4D	3.35	1.51	1.44
22	C	517	CLA	CHC-C1C	3.33	1.43	1.35
22	C	513	CLA	CMD-C2D	-3.33	1.43	1.50
22	B	604	CLA	C3D-C4D	3.31	1.51	1.44
22	C	514	CLA	C3D-CAD	3.31	1.56	1.45
22	D	401	CLA	CHC-C1C	3.28	1.43	1.35
22	C	509	CLA	C1D-ND	3.28	1.41	1.37
22	C	507	CLA	C1D-C2D	3.28	1.51	1.45
22	C	512	CLA	CMD-C2D	-3.28	1.43	1.50
22	B	616	CLA	CMD-C2D	-3.28	1.43	1.50
22	A	406	CLA	CHC-C1C	3.27	1.43	1.35
22	C	511	CLA	CHC-C1C	3.27	1.43	1.35
22	D	402	CLA	C1D-ND	3.27	1.41	1.37
22	B	604	CLA	CHC-C1C	3.26	1.43	1.35
22	C	506	CLA	C1D-ND	3.26	1.41	1.37
22	C	505	CLA	C1D-ND	3.26	1.41	1.37
22	B	601	CLA	CMD-C2D	-3.25	1.43	1.50
22	B	608	CLA	CHC-C1C	3.24	1.43	1.35
22	A	405	CLA	C1D-ND	3.23	1.41	1.37
22	B	616	CLA	CHC-C1C	3.22	1.43	1.35
22	B	609	CLA	CAA-C2A	-3.21	1.48	1.54
22	B	608	CLA	C1D-ND	3.20	1.41	1.37
22	B	614	CLA	CAA-C2A	-3.20	1.48	1.54
23	B	617	BCR	C1-C6	-3.19	1.49	1.53
22	C	510	CLA	C1D-C2D	3.19	1.51	1.45
22	D	408	CLA	CHC-C1C	3.17	1.43	1.35
22	B	610	CLA	CMD-C2D	-3.17	1.44	1.50
22	C	503	CLA	C1D-ND	3.17	1.41	1.37
22	B	604	CLA	CMD-C2D	-3.14	1.44	1.50
23	K	101	BCR	C32-C1	-3.14	1.47	1.53
22	B	603	CLA	CHC-C1C	3.14	1.43	1.35
22	C	507	CLA	CHC-C1C	3.13	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	E	101	HEM	C3C-CAC	3.13	1.54	1.47
22	A	406	CLA	C1D-ND	3.12	1.41	1.37
22	B	606	CLA	CHC-C1C	3.11	1.42	1.35
22	B	610	CLA	CHC-C1C	3.10	1.42	1.35
22	B	607	CLA	CHC-C1C	3.10	1.42	1.35
22	B	613	CLA	CMD-C2D	-3.09	1.44	1.50
22	C	503	CLA	CHC-C1C	3.08	1.42	1.35
22	B	605	CLA	C4D-ND	-3.08	1.33	1.37
22	B	602	CLA	C3D-C4D	3.08	1.51	1.44
22	D	408	CLA	C4D-ND	-3.06	1.33	1.37
22	B	611	CLA	C3B-C2B	-3.06	1.36	1.40
22	B	601	CLA	CHC-C1C	3.04	1.42	1.35
22	B	602	CLA	CHC-C1C	3.03	1.42	1.35
22	B	607	CLA	CMD-C2D	-3.02	1.44	1.50
22	C	505	CLA	C3D-C4D	3.02	1.51	1.44
22	C	503	CLA	C4D-ND	-3.02	1.33	1.37
22	D	402	CLA	CHC-C1C	3.02	1.42	1.35
22	C	505	CLA	CHC-C1C	3.02	1.42	1.35
22	C	503	CLA	CMB-C2B	-3.02	1.45	1.51
22	B	611	CLA	CMD-C2D	-3.01	1.44	1.50
22	C	509	CLA	CHC-C1C	3.01	1.42	1.35
22	C	509	CLA	CMD-C2D	-3.00	1.44	1.50
22	C	504	CLA	CMD-C2D	-2.99	1.44	1.50
22	C	513	CLA	CHC-C1C	2.99	1.42	1.35
22	D	402	CLA	CMB-C2B	-2.99	1.45	1.51
22	C	514	CLA	CAA-C2A	-2.98	1.48	1.54
22	C	511	CLA	C3D-C4D	2.98	1.50	1.44
22	C	507	CLA	C1D-ND	2.98	1.41	1.37
22	A	406	CLA	C4D-ND	-2.98	1.33	1.37
22	B	603	CLA	CMD-C2D	-2.97	1.44	1.50
22	C	503	CLA	C3B-C2B	-2.96	1.36	1.40
22	B	614	CLA	CMD-C2D	-2.96	1.44	1.50
22	C	509	CLA	C3D-C4D	2.96	1.50	1.44
22	B	612	CLA	C3B-CAB	-2.95	1.41	1.47
23	B	619	BCR	C1-C6	-2.94	1.49	1.53
22	B	613	CLA	CHC-C1C	2.94	1.42	1.35
22	C	506	CLA	CMB-C2B	-2.93	1.45	1.51
22	B	610	CLA	C1D-ND	2.93	1.41	1.37
22	B	605	CLA	CHC-C1C	2.93	1.42	1.35
23	B	618	BCR	C30-C25	-2.93	1.49	1.53
26	D	405	PL9	C3-C4	-2.92	1.44	1.49
22	D	408	CLA	CMD-C2D	-2.91	1.44	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	404	PHO	CAC-C3C	-2.90	1.47	1.52
22	B	607	CLA	C1D-ND	2.90	1.41	1.37
21	D	406	PHO	CAC-C3C	-2.89	1.47	1.52
22	C	503	CLA	CMD-C2D	-2.89	1.44	1.50
22	C	510	CLA	C1D-ND	2.89	1.41	1.37
22	D	407	CLA	CMB-C2B	-2.88	1.45	1.51
22	A	406	CLA	MG-ND	-2.87	2.00	2.05
22	C	509	CLA	C4D-ND	-2.86	1.33	1.37
22	B	601	CLA	C3D-C4D	2.85	1.50	1.44
22	B	609	CLA	CHC-C1C	2.85	1.42	1.35
22	B	616	CLA	C1D-ND	2.85	1.41	1.37
22	C	513	CLA	C3D-C4D	2.85	1.50	1.44
23	C	515	BCR	C1-C6	-2.84	1.49	1.53
22	C	506	CLA	C4D-ND	-2.84	1.33	1.37
22	D	401	CLA	CMD-C2D	-2.84	1.44	1.50
22	C	517	CLA	CMD-C2D	-2.84	1.44	1.50
22	C	511	CLA	CMB-C2B	-2.84	1.45	1.51
22	C	511	CLA	CMD-C2D	-2.83	1.44	1.50
22	C	505	CLA	C4D-ND	-2.83	1.33	1.37
22	C	508	CLA	C3B-C2B	-2.83	1.36	1.40
22	D	407	CLA	C3D-CAD	2.82	1.54	1.45
22	B	616	CLA	C3D-CAD	2.82	1.54	1.45
22	B	615	CLA	CMD-C2D	-2.82	1.44	1.50
22	C	517	CLA	C1D-C2D	2.81	1.50	1.45
22	C	513	CLA	CMB-C2B	-2.81	1.45	1.51
22	C	507	CLA	CMD-C2D	-2.80	1.44	1.50
22	B	614	CLA	CHC-C1C	2.80	1.42	1.35
24	A	408	LHG	P-O6	2.79	1.70	1.59
22	C	511	CLA	C3B-C2B	-2.79	1.36	1.40
22	C	508	CLA	CMB-C2B	-2.79	1.45	1.51
22	C	504	CLA	C4D-ND	-2.79	1.33	1.37
22	B	613	CLA	CMB-C2B	-2.78	1.45	1.51
25	F	101	LMG	C4-C5	2.77	1.58	1.53
22	B	604	CLA	C3B-C2B	-2.76	1.36	1.40
22	B	609	CLA	CMD-C2D	-2.76	1.44	1.50
22	B	611	CLA	CMB-C2B	-2.76	1.45	1.51
22	B	606	CLA	C3B-C2B	-2.76	1.36	1.40
22	B	610	CLA	MG-NC	2.76	2.12	2.06
22	D	407	CLA	CMD-C2D	-2.76	1.45	1.50
22	A	406	CLA	CMD-C2D	-2.75	1.45	1.50
22	C	508	CLA	CMD-C2D	-2.75	1.45	1.50
22	A	405	CLA	CMD-C2D	-2.75	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	511	CLA	C1D-ND	2.75	1.41	1.37
22	B	612	CLA	CMB-C2B	-2.74	1.45	1.51
22	B	605	CLA	CMD-C2D	-2.74	1.45	1.50
22	C	514	CLA	CMD-C2D	-2.74	1.45	1.50
22	C	504	CLA	C3D-C4D	2.73	1.50	1.44
22	C	510	CLA	CMD-C2D	-2.72	1.45	1.50
22	D	402	CLA	C1D-C2D	2.71	1.50	1.45
22	C	506	CLA	CMD-C2D	-2.70	1.45	1.50
22	B	610	CLA	C3B-C2B	-2.70	1.36	1.40
22	C	510	CLA	C3B-C2B	-2.69	1.36	1.40
22	C	506	CLA	CHC-C1C	2.68	1.41	1.35
22	C	507	CLA	C3B-C2B	-2.68	1.36	1.40
22	B	616	CLA	CMB-C2B	-2.68	1.46	1.51
26	D	405	PL9	C46-C44	2.68	1.56	1.51
22	B	614	CLA	CMB-C2B	-2.67	1.46	1.51
22	B	601	CLA	C3B-C2B	-2.65	1.36	1.40
22	C	505	CLA	CMD-C2D	-2.65	1.45	1.50
23	C	518	BCR	C1-C6	-2.64	1.50	1.53
22	C	517	CLA	CAA-C2A	-2.64	1.49	1.54
22	B	608	CLA	C1D-C2D	2.64	1.50	1.45
22	C	517	CLA	C1B-NB	2.63	1.37	1.35
22	B	601	CLA	CMB-C2B	-2.63	1.46	1.51
22	C	517	CLA	C1D-ND	2.63	1.41	1.37
22	A	406	CLA	CMB-C2B	-2.62	1.46	1.51
22	B	609	CLA	CMB-C2B	-2.62	1.46	1.51
22	D	408	CLA	C1D-ND	2.62	1.41	1.37
22	C	508	CLA	C1D-ND	2.62	1.41	1.37
22	B	611	CLA	C1D-C2D	2.60	1.50	1.45
22	B	612	CLA	MG-ND	-2.60	2.00	2.05
27	E	101	HEM	CAB-C3B	2.59	1.54	1.47
22	B	610	CLA	CMB-C2B	-2.58	1.46	1.51
22	C	503	CLA	MG-NA	2.58	2.12	2.06
22	D	408	CLA	CMB-C2B	-2.57	1.46	1.51
22	B	607	CLA	C4D-ND	-2.56	1.34	1.37
22	B	602	CLA	C1D-ND	2.56	1.40	1.37
21	A	404	PHO	CBD-CGD	-2.56	1.49	1.52
22	B	606	CLA	CMB-C2B	-2.56	1.46	1.51
22	B	612	CLA	C3D-C4D	2.55	1.49	1.44
22	B	603	CLA	CMB-C2B	-2.55	1.46	1.51
22	D	401	CLA	CMB-C2B	-2.54	1.46	1.51
22	B	608	CLA	C3B-C2B	-2.54	1.36	1.40
22	D	407	CLA	C1D-ND	2.54	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	616	CLA	C3B-C2B	-2.53	1.36	1.40
22	D	402	CLA	C3B-C2B	-2.53	1.36	1.40
23	H	101	BCR	C32-C1	-2.52	1.48	1.53
22	C	503	CLA	MG-ND	-2.52	2.00	2.05
22	C	504	CLA	CHC-C1C	2.52	1.41	1.35
22	C	517	CLA	CMA-C3A	-2.52	1.47	1.53
22	B	616	CLA	C1B-NB	2.51	1.37	1.35
22	B	602	CLA	CMB-C2B	-2.50	1.46	1.51
22	C	504	CLA	CMB-C2B	-2.50	1.46	1.51
22	B	609	CLA	C1D-ND	2.49	1.40	1.37
22	B	613	CLA	C1D-C2D	2.49	1.50	1.45
22	C	512	CLA	C1D-ND	2.49	1.40	1.37
22	B	614	CLA	C3B-C2B	-2.48	1.36	1.40
22	B	608	CLA	CMD-C2D	-2.47	1.45	1.50
22	D	402	CLA	C3D-C4D	2.47	1.49	1.44
22	B	601	CLA	C1D-ND	2.46	1.40	1.37
25	C	502	LMG	C9-C8	2.45	1.58	1.50
23	C	518	BCR	C30-C25	-2.45	1.50	1.53
22	C	504	CLA	MG-NA	2.45	2.12	2.06
22	B	613	CLA	C3B-C2B	-2.44	1.37	1.40
22	D	407	CLA	C3D-C4D	2.44	1.49	1.44
22	D	407	CLA	CHC-C1C	2.44	1.41	1.35
22	B	604	CLA	CMB-C2B	-2.43	1.46	1.51
22	B	606	CLA	MG-ND	-2.43	2.01	2.05
22	B	610	CLA	MG-NA	2.43	2.12	2.06
22	D	407	CLA	C3B-C2B	-2.42	1.37	1.40
22	B	604	CLA	C1D-ND	2.41	1.40	1.37
22	D	401	CLA	CMA-C3A	-2.41	1.48	1.53
22	C	509	CLA	C3B-C2B	-2.41	1.37	1.40
22	C	507	CLA	CMB-C2B	-2.40	1.46	1.51
22	B	604	CLA	CMC-C2C	-2.40	1.45	1.50
22	C	510	CLA	CMB-C2B	-2.40	1.46	1.51
22	C	511	CLA	C4D-ND	-2.40	1.34	1.37
22	B	605	CLA	C3D-C4D	2.39	1.49	1.44
22	C	517	CLA	C3A-C2A	-2.39	1.47	1.54
22	C	506	CLA	C3D-C4D	2.39	1.49	1.44
22	C	509	CLA	CMB-C2B	-2.38	1.46	1.51
22	B	612	CLA	C4D-ND	-2.38	1.34	1.37
22	B	607	CLA	CMB-C2B	-2.38	1.46	1.51
22	D	402	CLA	C3D-CAD	2.38	1.53	1.45
22	B	603	CLA	C3B-C2B	-2.38	1.37	1.40
22	B	605	CLA	C3B-C2B	-2.37	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	602	CLA	C4D-ND	-2.37	1.34	1.37
22	B	613	CLA	C1D-ND	2.37	1.40	1.37
22	B	611	CLA	C3B-CAB	-2.37	1.43	1.47
22	B	608	CLA	CMB-C2B	-2.36	1.46	1.51
22	B	612	CLA	CMA-C3A	-2.36	1.48	1.53
22	B	607	CLA	MG-ND	-2.36	2.01	2.05
22	A	405	CLA	C3D-C4D	2.36	1.49	1.44
22	B	612	CLA	C3A-C2A	-2.36	1.47	1.54
22	B	612	CLA	C3B-C2B	-2.36	1.37	1.40
23	C	516	BCR	C30-C25	-2.35	1.50	1.53
22	C	507	CLA	C4C-C3C	2.35	1.49	1.45
21	A	404	PHO	CMC-C2C	-2.35	1.46	1.51
22	B	605	CLA	CMB-C2B	-2.35	1.46	1.51
22	B	616	CLA	C3A-C2A	-2.35	1.47	1.54
22	C	514	CLA	C3B-C2B	-2.34	1.37	1.40
22	C	514	CLA	C1D-ND	2.34	1.40	1.37
22	B	601	CLA	C4D-ND	-2.32	1.34	1.37
22	C	513	CLA	C1D-ND	2.32	1.40	1.37
22	C	510	CLA	C3B-CAB	-2.32	1.43	1.47
21	D	406	PHO	CMB-C2B	-2.32	1.46	1.51
23	A	407	BCR	C30-C25	-2.32	1.50	1.53
22	C	505	CLA	CMC-C2C	-2.31	1.45	1.50
22	C	517	CLA	CMB-C2B	-2.31	1.46	1.51
22	D	402	CLA	CMD-C2D	-2.30	1.45	1.50
22	C	503	CLA	C3B-CAB	-2.30	1.43	1.47
25	C	502	LMG	C7-C8	2.30	1.57	1.50
22	C	505	CLA	C3B-C2B	-2.30	1.37	1.40
22	C	512	CLA	C1B-NB	2.30	1.37	1.35
22	A	405	CLA	CMC-C2C	-2.29	1.45	1.50
22	B	609	CLA	C1D-C2D	2.29	1.49	1.45
21	D	406	PHO	CMC-C2C	-2.28	1.46	1.51
22	B	615	CLA	CMB-C2B	-2.28	1.46	1.51
22	C	510	CLA	C3C-C2C	2.28	1.41	1.36
25	D	404	LMG	C3-C2	2.27	1.58	1.52
22	B	608	CLA	C3B-CAB	-2.27	1.43	1.47
22	C	514	CLA	C1D-C2D	2.27	1.49	1.45
22	D	401	CLA	C3B-C2B	-2.27	1.37	1.40
22	C	510	CLA	C1B-NB	2.26	1.37	1.35
22	D	408	CLA	C3B-C2B	-2.26	1.37	1.40
22	B	612	CLA	C3D-C2D	-2.26	1.32	1.39
22	B	614	CLA	C2A-C1A	-2.26	1.47	1.52
22	B	610	CLA	C3B-CAB	-2.25	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	607	CLA	CMC-C2C	-2.25	1.46	1.50
22	B	601	CLA	CAA-C2A	-2.24	1.49	1.54
25	D	403	LMG	C3-C2	2.24	1.58	1.52
22	B	614	CLA	C1D-ND	2.24	1.40	1.37
22	C	513	CLA	C1B-NB	2.23	1.37	1.35
22	A	406	CLA	CAA-C2A	-2.23	1.50	1.54
22	C	513	CLA	C3B-C2B	-2.22	1.37	1.40
22	C	504	CLA	MG-NC	2.22	2.11	2.06
22	C	505	CLA	C3D-C2D	-2.22	1.33	1.39
21	D	406	PHO	C3B-C2B	-2.22	1.37	1.40
22	B	606	CLA	C4D-ND	-2.22	1.34	1.37
22	C	512	CLA	C1D-C2D	2.21	1.49	1.45
22	C	504	CLA	C3B-CAB	-2.21	1.43	1.47
23	H	101	BCR	C27-C26	-2.20	1.46	1.51
22	B	612	CLA	CAA-C2A	-2.20	1.50	1.54
22	C	509	CLA	C3D-C2D	-2.20	1.33	1.39
25	3	101	LMG	O7-C8	-2.20	1.41	1.46
22	C	512	CLA	CMB-C2B	-2.20	1.47	1.51
22	D	401	CLA	C3B-CAB	-2.19	1.43	1.47
22	C	514	CLA	CMB-C2B	-2.19	1.47	1.51
22	B	614	CLA	C3B-CAB	-2.19	1.43	1.47
21	D	406	PHO	CBD-CGD	-2.19	1.49	1.52
22	C	507	CLA	MG-NC	2.19	2.11	2.06
25	D	404	LMG	C4-C3	2.19	1.57	1.52
22	D	402	CLA	C3B-CAB	-2.18	1.43	1.47
22	A	405	CLA	CMB-C2B	-2.18	1.47	1.51
23	K	101	BCR	C27-C26	-2.18	1.46	1.51
23	K	101	BCR	C21-C22	-2.17	1.32	1.35
22	C	503	CLA	MG-NC	2.17	2.11	2.06
22	C	506	CLA	O2D-CGD	2.17	1.38	1.33
22	B	604	CLA	C4D-ND	-2.17	1.34	1.37
22	C	506	CLA	MG-ND	-2.17	2.01	2.05
25	I	101	LMG	C3-C2	2.17	1.57	1.52
22	B	601	CLA	CMC-C2C	-2.16	1.46	1.50
22	D	407	CLA	C1D-C2D	2.16	1.49	1.45
22	B	602	CLA	C3D-C2D	-2.16	1.33	1.39
22	D	408	CLA	MG-ND	-2.16	2.01	2.05
22	B	610	CLA	CMC-C2C	-2.15	1.46	1.50
22	C	504	CLA	C2A-C1A	2.14	1.57	1.52
22	D	401	CLA	C3D-C4D	2.13	1.49	1.44
21	A	404	PHO	CMB-C2B	-2.13	1.46	1.51
22	B	610	CLA	C4C-C3C	2.13	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	515	BCR	C35-C13	-2.12	1.46	1.50
22	A	405	CLA	C3D-CAD	2.12	1.52	1.45
22	B	606	CLA	C1D-ND	2.12	1.40	1.37
21	A	404	PHO	CMD-C2D	-2.12	1.46	1.51
22	C	504	CLA	MG-ND	-2.12	2.01	2.05
22	B	605	CLA	C3B-CAB	-2.12	1.43	1.47
22	C	508	CLA	C1D-C2D	2.12	1.49	1.45
22	C	508	CLA	MG-NC	2.11	2.11	2.06
22	A	406	CLA	MG-NC	2.11	2.11	2.06
22	C	506	CLA	C3B-C2B	-2.11	1.37	1.40
22	C	508	CLA	C3B-CAB	-2.11	1.43	1.47
22	B	612	CLA	C1D-ND	2.11	1.40	1.37
22	C	510	CLA	C4C-C3C	2.11	1.48	1.45
22	B	606	CLA	CMC-C2C	-2.11	1.46	1.50
22	B	616	CLA	OBD-CAD	-2.10	1.18	1.22
22	C	505	CLA	CMB-C2B	-2.10	1.47	1.51
22	D	407	CLA	C4C-C3C	2.09	1.48	1.45
22	B	603	CLA	C3D-C4D	2.09	1.48	1.44
23	K	101	BCR	C36-C18	-2.09	1.46	1.50
22	B	608	CLA	C1B-NB	2.09	1.37	1.35
26	D	405	PL9	C52-C5	-2.09	1.46	1.50
22	B	607	CLA	C3D-C2D	-2.09	1.33	1.39
22	C	506	CLA	CAA-C2A	-2.09	1.50	1.54
22	C	512	CLA	C3B-C2B	-2.09	1.37	1.40
23	H	101	BCR	C29-C30	-2.08	1.49	1.54
23	B	619	BCR	C30-C25	-2.08	1.50	1.53
22	B	610	CLA	MG-ND	-2.08	2.01	2.05
22	D	401	CLA	C1D-ND	2.08	1.40	1.37
22	B	605	CLA	CMC-C2C	-2.08	1.46	1.50
25	F	101	LMG	C4-C3	2.08	1.57	1.52
23	H	101	BCR	C36-C18	-2.07	1.46	1.50
22	B	615	CLA	MG-NC	2.07	2.11	2.06
22	B	606	CLA	C3B-CAB	-2.06	1.43	1.47
25	C	502	LMG	C3-C2	2.06	1.57	1.52
22	C	508	CLA	C3C-C2C	2.05	1.41	1.36
23	B	617	BCR	C33-C5	-2.05	1.47	1.50
22	B	614	CLA	C1D-C2D	2.05	1.49	1.45
25	I	101	LMG	C4-C3	2.05	1.57	1.52
23	H	101	BCR	C21-C22	-2.04	1.33	1.35
23	A	407	BCR	C1-C6	-2.04	1.51	1.53
22	B	615	CLA	C3B-C2B	-2.04	1.37	1.40
22	C	509	CLA	C3B-CAB	-2.04	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	613	CLA	CAA-C2A	-2.03	1.50	1.54
22	B	606	CLA	C3D-C4D	2.03	1.48	1.44
22	B	605	CLA	C3D-C2D	-2.03	1.33	1.39
22	C	509	CLA	C3C-C2C	2.03	1.41	1.36
22	C	507	CLA	C3C-C2C	2.03	1.41	1.36
22	B	612	CLA	CMC-C2C	-2.02	1.46	1.50
25	D	403	LMG	C7-C8	2.02	1.56	1.50
22	C	512	CLA	OBD-CAD	-2.02	1.19	1.22
22	B	616	CLA	CMA-C3A	-2.01	1.48	1.53
22	C	507	CLA	CHD-C4C	2.01	1.43	1.39
22	A	405	CLA	C1D-C2D	2.01	1.49	1.45
22	D	408	CLA	C3B-CAB	-2.01	1.43	1.47
22	C	511	CLA	C3B-CAB	-2.00	1.43	1.47
22	C	506	CLA	C3B-CAB	-2.00	1.43	1.47
22	C	513	CLA	C3A-C2A	-2.00	1.48	1.54

All (941) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	604	CLA	C4A-NA-C1A	15.59	113.71	106.71
22	C	505	CLA	C4A-NA-C1A	15.19	113.53	106.71
23	H	101	BCR	C33-C5-C6	-13.26	109.64	124.53
22	B	616	CLA	C4A-NA-C1A	13.21	112.64	106.71
22	B	605	CLA	C4A-NA-C1A	12.70	112.42	106.71
22	C	517	CLA	C4A-NA-C1A	12.57	112.36	106.71
22	B	603	CLA	C4A-NA-C1A	12.46	112.31	106.71
22	B	615	CLA	C4A-NA-C1A	12.10	112.14	106.71
22	C	513	CLA	C4A-NA-C1A	11.74	111.98	106.71
22	C	512	CLA	C4A-NA-C1A	11.64	111.94	106.71
22	B	609	CLA	C4A-NA-C1A	11.62	111.93	106.71
22	B	601	CLA	C4A-NA-C1A	11.58	111.91	106.71
22	B	616	CLA	C4D-C3D-CAD	11.55	121.71	108.10
22	C	511	CLA	C4A-NA-C1A	11.51	111.88	106.71
22	C	510	CLA	C4A-NA-C1A	11.33	111.80	106.71
23	K	101	BCR	C33-C5-C6	-11.23	111.92	124.53
22	C	512	CLA	C4D-C3D-CAD	11.16	121.25	108.10
22	B	613	CLA	C4A-NA-C1A	10.79	111.56	106.71
22	C	507	CLA	C4A-NA-C1A	10.73	111.53	106.71
22	B	608	CLA	C4A-NA-C1A	10.53	111.44	106.71
22	C	509	CLA	C4A-NA-C1A	10.53	111.44	106.71
22	B	614	CLA	C4A-NA-C1A	10.44	111.40	106.71
22	B	612	CLA	C4A-NA-C1A	10.40	111.38	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	602	CLA	C4A-NA-C1A	10.36	111.36	106.71
22	B	610	CLA	C4A-NA-C1A	10.01	111.21	106.71
22	C	507	CLA	C4D-C3D-CAD	9.93	119.80	108.10
22	B	606	CLA	C4A-NA-C1A	9.81	111.12	106.71
22	C	506	CLA	C4A-NA-C1A	9.75	111.09	106.71
22	C	513	CLA	CAA-C2A-C3A	9.73	139.43	112.78
22	B	607	CLA	C4A-NA-C1A	9.73	111.08	106.71
22	C	504	CLA	C4A-NA-C1A	9.62	111.03	106.71
22	D	402	CLA	C4A-NA-C1A	9.60	111.02	106.71
23	K	101	BCR	C37-C22-C21	-9.48	109.65	122.92
22	B	609	CLA	C3A-C2A-C1A	9.46	115.51	101.34
23	H	101	BCR	C37-C22-C23	-9.31	103.41	118.08
22	B	609	CLA	C4D-C3D-CAD	9.30	119.05	108.10
22	B	610	CLA	C3A-C2A-C1A	9.26	115.21	101.34
23	K	101	BCR	C37-C22-C23	-9.22	103.55	118.08
23	H	101	BCR	C37-C22-C21	-9.17	110.08	122.92
22	B	616	CLA	CAA-C2A-C3A	8.97	137.34	112.78
22	A	405	CLA	C4A-NA-C1A	8.97	110.74	106.71
22	B	602	CLA	C4D-C3D-CAD	8.77	118.44	108.10
22	B	613	CLA	C3A-C2A-C1A	8.75	114.45	101.34
22	B	614	CLA	C3A-C2A-C1A	8.75	114.44	101.34
22	B	610	CLA	C4D-C3D-CAD	8.68	118.33	108.10
22	B	602	CLA	C3A-C2A-C1A	8.48	114.05	101.34
23	H	101	BCR	C1-C6-C5	-8.48	110.67	122.61
22	D	408	CLA	C4A-NA-C1A	8.46	110.51	106.71
22	B	612	CLA	CAA-C2A-C3A	8.44	135.88	112.78
22	C	517	CLA	C4D-C3D-CAD	8.37	117.96	108.10
22	C	509	CLA	C4D-C3D-CAD	8.35	117.94	108.10
22	B	615	CLA	C4D-C3D-CAD	8.33	117.91	108.10
22	B	601	CLA	C4D-C3D-CAD	8.32	117.91	108.10
22	B	614	CLA	C4D-C3D-CAD	8.32	117.90	108.10
22	B	601	CLA	C3A-C2A-C1A	8.30	113.77	101.34
22	C	510	CLA	C4D-C3D-CAD	8.29	117.87	108.10
22	B	611	CLA	C4A-NA-C1A	8.29	110.43	106.71
22	A	406	CLA	C2A-C3A-C4A	-8.22	88.59	101.87
22	C	514	CLA	C4A-NA-C1A	8.22	110.40	106.71
23	K	101	BCR	C1-C6-C5	-8.19	111.08	122.61
22	D	401	CLA	C4A-NA-C1A	8.18	110.39	106.71
22	B	612	CLA	C4D-C3D-CAD	8.12	117.67	108.10
22	C	511	CLA	C3A-C2A-C1A	8.12	113.50	101.34
22	B	613	CLA	C4D-C3D-CAD	8.11	117.65	108.10
23	H	101	BCR	C2-C1-C6	8.07	122.90	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	506	CLA	C3A-C2A-C1A	7.84	113.08	101.34
22	B	604	CLA	C4D-C3D-CAD	7.84	117.33	108.10
22	C	517	CLA	CAA-C2A-C3A	7.80	134.13	112.78
22	C	505	CLA	C1D-ND-C4D	-7.77	100.82	106.33
22	D	407	CLA	C4A-NA-C1A	7.75	110.19	106.71
22	B	611	CLA	C4D-C3D-CAD	7.71	117.19	108.10
22	C	505	CLA	C4D-C3D-CAD	7.53	116.97	108.10
22	B	606	CLA	C4D-C3D-CAD	7.51	116.94	108.10
23	K	101	BCR	C2-C1-C6	7.51	122.04	110.48
22	C	508	CLA	C4A-NA-C1A	7.50	110.08	106.71
22	B	608	CLA	C4D-C3D-CAD	7.45	116.88	108.10
22	C	511	CLA	C4D-C3D-CAD	7.40	116.81	108.10
22	C	514	CLA	C3A-C2A-C1A	7.39	112.41	101.34
22	C	508	CLA	C4D-C3D-CAD	7.31	116.72	108.10
22	C	514	CLA	C4D-C3D-CAD	7.31	116.71	108.10
22	A	406	CLA	C2A-C1A-CHA	7.31	136.63	123.86
22	C	507	CLA	C3A-C2A-C1A	7.20	112.13	101.34
22	B	610	CLA	C2A-C1A-CHA	7.18	136.42	123.86
22	B	615	CLA	C3A-C2A-C1A	7.15	112.04	101.34
23	H	101	BCR	C32-C1-C6	-7.00	98.94	110.30
22	C	509	CLA	C3A-C2A-C1A	6.96	111.77	101.34
22	B	604	CLA	CAA-C2A-C3A	6.89	131.66	112.78
22	B	603	CLA	C3A-C2A-C1A	6.70	111.38	101.34
22	A	406	CLA	C3A-C2A-C1A	6.70	111.37	101.34
22	C	509	CLA	C2A-C1A-CHA	6.65	135.48	123.86
22	C	513	CLA	C4D-C3D-CAD	6.56	115.83	108.10
22	C	506	CLA	C2A-C1A-CHA	6.55	135.32	123.86
22	C	507	CLA	C3D-C2D-C1D	6.54	114.76	105.83
22	D	408	CLA	CAA-C2A-C3A	6.52	130.64	112.78
22	A	406	CLA	CAA-C2A-C3A	6.52	130.62	112.78
22	B	616	CLA	C2A-C1A-CHA	6.50	135.23	123.86
22	B	614	CLA	C6-C7-C8	-6.40	95.24	115.92
22	C	511	CLA	C2A-C1A-CHA	6.36	134.98	123.86
22	C	510	CLA	C3D-C2D-C1D	6.34	114.48	105.83
22	C	504	CLA	C4D-C3D-CAD	6.31	115.53	108.10
22	C	517	CLA	CHB-C4A-NA	6.25	133.15	124.51
22	B	613	CLA	C3D-C2D-C1D	6.23	114.33	105.83
22	C	512	CLA	C3A-C2A-C1A	6.21	110.64	101.34
22	B	612	CLA	C6-C7-C8	-6.18	95.96	115.92
22	B	610	CLA	C2A-C3A-C4A	-6.15	91.94	101.87
22	C	513	CLA	C2A-C1A-CHA	6.12	134.56	123.86
22	D	408	CLA	C3A-C2A-C1A	6.10	110.48	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	505	CLA	C3A-C2A-C1A	6.07	110.43	101.34
22	B	611	CLA	C3D-C2D-C1D	6.05	114.09	105.83
22	D	402	CLA	C3A-C2A-C1A	6.02	110.36	101.34
22	B	616	CLA	CMA-C3A-C4A	6.00	127.89	111.77
22	C	512	CLA	C3D-C2D-C1D	5.96	113.96	105.83
22	B	605	CLA	C4D-C3D-CAD	5.84	114.98	108.10
22	B	614	CLA	C3D-C2D-C1D	5.82	113.78	105.83
22	B	604	CLA	CHB-C4A-NA	5.80	132.53	124.51
22	B	604	CLA	CMA-C3A-C2A	5.80	137.22	113.83
22	B	608	CLA	C6-C7-C8	-5.79	97.19	115.92
22	C	508	CLA	CBA-CAA-C2A	5.77	130.91	113.86
22	B	612	CLA	C2A-C1A-CHA	5.77	133.94	123.86
22	C	517	CLA	C3D-C2D-C1D	5.75	113.68	105.83
22	B	613	CLA	C2A-C1A-CHA	5.73	133.88	123.86
22	B	601	CLA	C2A-C1A-CHA	5.73	133.87	123.86
22	B	610	CLA	CBA-CAA-C2A	5.70	130.70	113.86
22	C	517	CLA	CMA-C3A-C2A	5.68	136.74	113.83
22	C	514	CLA	C6-C7-C8	-5.68	97.56	115.92
22	D	402	CLA	CAA-C2A-C3A	5.66	128.28	112.78
23	H	101	BCR	C2-C3-C4	-5.66	98.74	111.38
23	K	101	BCR	C2-C3-C4	-5.65	98.76	111.38
22	B	602	CLA	C2A-C1A-CHA	5.63	133.70	123.86
22	C	507	CLA	C6-C7-C8	-5.60	97.83	115.92
22	B	609	CLA	C2A-C1A-CHA	5.59	133.63	123.86
22	C	506	CLA	C4D-C3D-CAD	5.58	114.68	108.10
22	C	504	CLA	CBA-CAA-C2A	5.58	130.32	113.86
22	C	510	CLA	C3D-C4D-ND	5.57	119.24	110.24
22	B	609	CLA	C3D-C2D-C1D	5.55	113.41	105.83
22	C	503	CLA	C4A-NA-C1A	5.51	109.18	106.71
23	H	101	BCR	C31-C1-C6	-5.50	101.38	110.30
22	B	610	CLA	CAC-C3C-C4C	5.49	131.93	124.81
23	K	101	BCR	C32-C1-C6	-5.48	101.42	110.30
22	D	407	CLA	C2D-C1D-ND	-5.47	106.08	110.10
23	K	101	BCR	C31-C1-C6	-5.45	101.46	110.30
22	C	513	CLA	CMA-C3A-C2A	5.44	135.77	113.83
22	B	613	CLA	C2D-C1D-ND	-5.39	106.13	110.10
22	B	612	CLA	CMA-C3A-C2A	5.38	135.54	113.83
22	C	507	CLA	C2D-C1D-ND	-5.37	106.15	110.10
22	C	509	CLA	C2A-C3A-C4A	-5.35	93.23	101.87
22	D	402	CLA	C2A-C3A-C4A	-5.34	93.24	101.87
22	D	401	CLA	C4D-C3D-CAD	5.33	114.38	108.10
22	C	503	CLA	C4D-C3D-CAD	5.31	114.35	108.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	D	408	CLA	CBA-CAA-C2A	5.29	129.49	113.86
22	B	611	CLA	C2D-C1D-ND	-5.29	106.20	110.10
22	B	610	CLA	OBD-CAD-C3D	5.24	141.13	128.52
22	B	607	CLA	C4D-C3D-CAD	5.21	114.23	108.10
22	B	615	CLA	O2A-C1-C2	-5.21	94.96	108.64
22	C	510	CLA	CHB-C4A-NA	5.20	131.71	124.51
22	C	517	CLA	C3D-C4D-ND	5.15	118.56	110.24
22	B	608	CLA	CMA-C3A-C2A	5.15	134.59	113.83
22	A	405	CLA	C3A-C2A-C1A	5.14	109.04	101.34
22	A	406	CLA	C4A-NA-C1A	5.13	109.01	106.71
22	D	402	CLA	CBA-CAA-C2A	5.12	128.99	113.86
22	B	616	CLA	OBD-CAD-C3D	5.07	140.73	128.52
22	B	602	CLA	OBD-CAD-C3D	5.04	140.65	128.52
22	C	510	CLA	CBA-CAA-C2A	5.03	128.72	113.86
22	A	405	CLA	C4D-C3D-CAD	5.01	114.01	108.10
22	C	508	CLA	C3D-C4D-ND	5.01	118.34	110.24
22	C	506	CLA	O2D-CGD-CBD	5.00	120.16	111.27
22	C	506	CLA	C2A-C3A-C4A	-5.00	93.80	101.87
22	B	615	CLA	C2A-C1A-CHA	4.99	132.59	123.86
22	A	405	CLA	CAA-C2A-C3A	4.98	126.41	112.78
23	H	101	BCR	C1-C6-C7	4.98	129.86	115.78
22	B	610	CLA	C6-C7-C8	-4.96	99.88	115.92
22	B	608	CLA	C3D-C2D-C1D	4.94	112.58	105.83
22	B	616	CLA	C3D-C2D-C1D	4.91	112.53	105.83
22	C	512	CLA	C3D-C4D-ND	4.90	118.16	110.24
22	B	614	CLA	C3D-C4D-ND	4.89	118.14	110.24
22	B	609	CLA	C2A-C3A-C4A	-4.87	94.00	101.87
22	C	507	CLA	C3D-C4D-ND	4.86	118.10	110.24
22	C	510	CLA	C2D-C1D-ND	-4.86	106.52	110.10
22	C	513	CLA	CMA-C3A-C4A	4.86	124.82	111.77
22	C	507	CLA	CAA-C2A-C3A	4.85	126.06	112.78
22	B	611	CLA	C3D-C4D-ND	4.84	118.06	110.24
22	C	514	CLA	C3D-C2D-C1D	4.83	112.42	105.83
22	B	603	CLA	C2A-C1A-CHA	4.81	132.27	123.86
22	C	510	CLA	C11-C10-C8	4.81	131.47	115.92
22	C	512	CLA	C1D-ND-C4D	-4.81	102.92	106.33
22	B	612	CLA	CHB-C4A-NA	4.79	131.14	124.51
22	C	513	CLA	CHB-C4A-NA	4.75	131.08	124.51
22	C	511	CLA	OBD-CAD-C3D	4.75	139.94	128.52
23	H	101	BCR	C23-C22-C21	4.71	126.17	118.94
22	C	511	CLA	C2A-C3A-C4A	-4.71	94.26	101.87
22	B	615	CLA	OBD-CAD-C3D	4.71	139.86	128.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	607	CLA	C2A-C1A-CHA	4.70	132.08	123.86
22	B	608	CLA	C3D-C4D-ND	4.68	117.81	110.24
22	D	407	CLA	C3D-C2D-C1D	4.66	112.19	105.83
22	C	508	CLA	C3D-C2D-C1D	4.66	112.19	105.83
23	K	101	BCR	C1-C6-C7	4.65	128.94	115.78
22	B	611	CLA	O2A-C1-C2	4.64	120.82	108.64
22	B	607	CLA	C3A-C2A-C1A	4.63	108.27	101.34
22	B	607	CLA	CAA-C2A-C1A	4.60	127.06	111.97
22	C	509	CLA	OBD-CAD-C3D	4.60	139.58	128.52
22	B	612	CLA	CMA-C3A-C4A	4.59	124.11	111.77
22	B	603	CLA	C4D-C3D-CAD	4.58	113.50	108.10
22	A	406	CLA	CBA-CAA-C2A	4.58	127.38	113.86
22	C	506	CLA	CAA-C2A-C3A	4.58	125.31	112.78
22	C	517	CLA	O2D-CGD-CBD	4.58	119.40	111.27
22	C	503	CLA	CBA-CAA-C2A	4.57	127.36	113.86
23	K	101	BCR	C23-C22-C21	4.55	125.93	118.94
22	B	616	CLA	CMA-C3A-C2A	4.54	132.14	113.83
22	D	407	CLA	C4D-C3D-CAD	4.52	113.42	108.10
22	C	513	CLA	OBD-CAD-C3D	4.52	139.40	128.52
22	B	601	CLA	CAA-C2A-C3A	4.52	125.15	112.78
22	C	506	CLA	O2D-CGD-O1D	-4.51	115.02	123.84
22	D	401	CLA	CHB-C4A-NA	4.51	130.75	124.51
22	B	610	CLA	CAA-C2A-C3A	4.47	125.03	112.78
22	C	509	CLA	CAA-C2A-C3A	4.46	124.99	112.78
22	B	612	CLA	OBD-CAD-C3D	4.46	139.24	128.52
22	C	504	CLA	O2D-CGD-O1D	-4.45	115.13	123.84
22	D	402	CLA	C2A-C1A-CHA	4.45	131.63	123.86
22	B	605	CLA	C3A-C2A-C1A	4.39	107.91	101.34
22	C	505	CLA	OBD-CAD-C3D	4.38	139.05	128.52
22	C	514	CLA	C3D-C4D-ND	4.36	117.30	110.24
22	B	616	CLA	C1D-ND-C4D	-4.35	103.25	106.33
22	B	608	CLA	CAA-C2A-C3A	4.34	124.67	112.78
22	B	613	CLA	C3D-C4D-ND	4.33	117.25	110.24
22	C	507	CLA	CBA-CAA-C2A	4.30	126.55	113.86
22	B	616	CLA	CHB-C4A-NA	4.29	130.44	124.51
23	H	101	BCR	C33-C5-C4	4.29	121.86	113.62
23	K	101	BCR	C36-C18-C17	-4.26	116.96	122.92
22	B	601	CLA	CBA-CAA-C2A	4.26	126.43	113.86
23	H	101	BCR	C36-C18-C17	-4.25	116.98	122.92
22	B	604	CLA	C2A-C1A-CHA	4.22	131.24	123.86
22	B	608	CLA	CAA-C2A-C1A	4.19	125.71	111.97
22	C	508	CLA	C1D-ND-C4D	-4.18	103.36	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	608	CLA	CHB-C4A-NA	4.17	130.28	124.51
22	C	510	CLA	CMA-C3A-C2A	4.17	130.66	113.83
22	C	510	CLA	CBC-CAC-C3C	4.14	123.84	112.43
22	B	603	CLA	CAA-C2A-C3A	4.12	124.05	112.78
22	B	613	CLA	C2A-C3A-C4A	-4.11	95.23	101.87
22	C	513	CLA	C11-C10-C8	4.11	129.21	115.92
22	C	505	CLA	C2D-C1D-ND	4.09	113.12	110.10
22	C	514	CLA	CAA-C2A-C3A	4.09	123.97	112.78
22	B	605	CLA	CAA-C2A-C1A	4.08	125.34	111.97
22	C	517	CLA	C2A-C1A-CHA	4.08	130.99	123.86
22	B	604	CLA	OBD-CAD-C3D	4.07	138.31	128.52
22	B	609	CLA	C3D-C4D-ND	4.06	116.81	110.24
23	K	101	BCR	C20-C21-C22	-4.06	121.52	127.31
22	B	608	CLA	C9-C8-C10	4.05	125.95	111.29
22	B	614	CLA	C2A-C1A-CHA	4.04	130.93	123.86
26	D	405	PL9	C7-C3-C4	4.03	120.16	116.88
22	C	511	CLA	CAA-C2A-C3A	4.03	123.81	112.78
22	C	504	CLA	C2A-C1A-CHA	4.01	130.87	123.86
26	D	405	PL9	C36-C34-C33	-4.01	113.00	121.12
22	B	612	CLA	CBA-CAA-C2A	4.00	125.67	113.86
22	D	401	CLA	C2A-C3A-C4A	4.00	108.33	101.87
22	B	611	CLA	C6-C7-C8	-3.99	103.02	115.92
22	C	506	CLA	CBA-CAA-C2A	3.99	125.64	113.86
22	B	613	CLA	O2A-C1-C2	-3.98	98.17	108.64
22	C	517	CLA	C2D-C1D-ND	-3.98	107.17	110.10
22	B	606	CLA	C3A-C2A-C1A	3.97	107.29	101.34
22	C	517	CLA	C6-C7-C8	-3.97	103.09	115.92
23	H	101	BCR	C4-C5-C6	3.96	128.48	122.73
22	B	609	CLA	CGD-CBD-CAD	-3.96	97.92	110.73
22	C	504	CLA	C3A-C2A-C1A	3.95	107.26	101.34
23	K	101	BCR	C39-C30-C25	-3.95	103.89	110.30
22	B	616	CLA	C11-C10-C8	3.94	128.66	115.92
23	B	618	BCR	C2-C1-C6	3.94	116.54	110.48
22	C	505	CLA	C2A-C1A-CHA	3.93	130.73	123.86
22	C	505	CLA	C6-C5-C3	3.92	123.74	113.45
23	H	101	BCR	C7-C8-C9	-3.92	120.32	126.23
22	D	408	CLA	C2A-C1A-CHA	3.91	130.70	123.86
22	B	615	CLA	CAA-C2A-C3A	3.91	123.47	112.78
23	H	101	BCR	C39-C30-C25	-3.88	104.00	110.30
22	B	615	CLA	C11-C10-C8	-3.88	103.38	115.92
22	B	608	CLA	C2A-C1A-CHA	3.88	130.64	123.86
22	B	611	CLA	CMA-C3A-C2A	-3.87	98.20	113.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	612	CLA	O2D-CGD-O1D	-3.87	116.27	123.84
22	C	513	CLA	O2D-CGD-O1D	-3.87	116.27	123.84
22	C	506	CLA	OBD-CAD-C3D	3.87	137.83	128.52
22	B	609	CLA	CAA-C2A-C3A	3.87	123.37	112.78
22	D	407	CLA	CAA-C2A-C3A	3.87	123.36	112.78
22	C	505	CLA	CMD-C2D-C1D	3.84	131.49	124.71
22	B	616	CLA	C3D-C4D-ND	3.84	116.46	110.24
22	B	603	CLA	CAA-C2A-C1A	3.84	124.54	111.97
22	C	507	CLA	CGD-CBD-CAD	-3.83	98.32	110.73
22	C	512	CLA	CAA-C2A-C3A	3.83	123.26	112.78
22	B	606	CLA	CBA-CAA-C2A	3.83	125.16	113.86
22	B	611	CLA	CAC-C3C-C4C	3.82	129.76	124.81
22	B	614	CLA	C11-C10-C8	3.81	128.23	115.92
22	B	615	CLA	CAA-C2A-C1A	3.80	124.44	111.97
22	D	407	CLA	CAA-C2A-C1A	3.79	124.39	111.97
23	H	101	BCR	C20-C21-C22	-3.77	121.94	127.31
22	C	510	CLA	C1B-CHB-C4A	-3.76	122.66	130.12
22	C	514	CLA	CGD-CBD-CAD	-3.75	98.59	110.73
22	B	605	CLA	OBD-CAD-C3D	3.74	137.53	128.52
22	B	612	CLA	C3B-C4B-NB	-3.74	104.37	109.21
22	C	513	CLA	CBA-CAA-C2A	3.74	124.91	113.86
22	B	608	CLA	CBA-CAA-C2A	3.74	124.90	113.86
22	C	504	CLA	OBD-CAD-C3D	3.73	137.51	128.52
22	C	517	CLA	CMA-C3A-C4A	3.73	121.80	111.77
22	C	504	CLA	O2D-CGD-CBD	3.73	117.89	111.27
24	A	408	LHG	O4-P-O5	3.73	130.68	112.24
22	C	503	CLA	C11-C10-C8	3.73	127.97	115.92
22	D	407	CLA	CMA-C3A-C2A	-3.73	98.79	113.83
22	B	604	CLA	C1D-ND-C4D	-3.72	103.69	106.33
22	B	608	CLA	CMB-C2B-C1B	-3.71	122.76	128.46
22	B	605	CLA	O2D-CGD-O1D	-3.71	116.58	123.84
22	D	402	CLA	C4D-C3D-CAD	3.71	112.47	108.10
22	B	606	CLA	O2D-CGD-O1D	-3.70	116.60	123.84
22	A	405	CLA	C2D-C1D-ND	-3.70	107.38	110.10
23	K	101	BCR	C4-C5-C6	3.69	128.09	122.73
22	B	601	CLA	OBD-CAD-C3D	3.69	137.40	128.52
23	K	101	BCR	C7-C8-C9	-3.68	120.67	126.23
22	B	602	CLA	CAC-C3C-C4C	3.68	129.59	124.81
22	B	602	CLA	C2A-C3A-C4A	-3.68	95.92	101.87
22	D	402	CLA	C2D-C1D-ND	-3.67	107.40	110.10
22	C	511	CLA	CAC-C3C-C4C	3.66	129.56	124.81
22	B	605	CLA	CMA-C3A-C2A	-3.66	99.06	113.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	512	CLA	CMD-C2D-C3D	-3.65	119.21	127.61
22	B	616	CLA	CMD-C2D-C3D	-3.65	119.21	127.61
22	D	401	CLA	CBA-CAA-C2A	3.65	124.63	113.86
22	B	602	CLA	CAA-C2A-C3A	3.64	122.73	112.78
22	B	613	CLA	C4D-CHA-C1A	-3.63	116.83	121.25
21	D	406	PHO	C9-C8-C7	3.62	124.39	111.29
22	B	612	CLA	CAA-C2A-C1A	3.62	123.83	111.97
22	B	612	CLA	O2A-C1-C2	-3.60	99.18	108.64
21	A	404	PHO	CMB-C2B-C3B	3.60	131.41	124.68
22	C	503	CLA	CMB-C2B-C1B	-3.60	122.94	128.46
22	B	609	CLA	C2D-C1D-ND	-3.59	107.45	110.10
22	A	405	CLA	C3D-C2D-C1D	3.59	110.73	105.83
22	D	402	CLA	C6-C7-C8	-3.58	104.34	115.92
22	C	503	CLA	CAA-C2A-C3A	3.58	122.57	112.78
22	A	406	CLA	CMB-C2B-C1B	-3.56	122.98	128.46
23	K	101	BCR	C16-C17-C18	-3.56	122.23	127.31
23	C	515	BCR	C35-C13-C14	-3.56	117.94	122.92
22	D	401	CLA	O2A-C1-C2	-3.56	99.29	108.64
23	H	101	BCR	C16-C17-C18	-3.55	122.24	127.31
23	H	101	BCR	C23-C24-C25	-3.54	117.25	127.20
22	D	401	CLA	CMA-C3A-C2A	3.54	128.11	113.83
22	C	514	CLA	C2A-C1A-CHA	3.54	130.05	123.86
22	B	605	CLA	CMD-C2D-C1D	3.53	130.93	124.71
22	D	401	CLA	C3D-C4D-ND	3.53	115.94	110.24
22	C	513	CLA	C1B-CHB-C4A	-3.52	123.14	130.12
22	B	608	CLA	CMA-C3A-C4A	3.52	121.24	111.77
22	A	405	CLA	CAC-C3C-C4C	3.52	129.37	124.81
23	K	101	BCR	C23-C24-C25	-3.50	117.36	127.20
22	A	405	CLA	CAA-C2A-C1A	3.50	123.46	111.97
22	B	607	CLA	CAA-C2A-C3A	3.50	122.37	112.78
22	B	608	CLA	C1B-CHB-C4A	-3.50	123.18	130.12
22	B	601	CLA	C2A-C3A-C4A	-3.49	96.24	101.87
22	C	512	CLA	CAA-C2A-C1A	3.48	123.39	111.97
22	B	603	CLA	OBD-CAD-C3D	3.48	136.90	128.52
22	B	616	CLA	C1B-CHB-C4A	-3.48	123.22	130.12
23	C	518	BCR	C37-C22-C21	-3.48	118.05	122.92
22	C	511	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
22	C	514	CLA	C11-C10-C8	3.47	127.13	115.92
22	C	508	CLA	CMA-C3A-C2A	-3.47	99.84	113.83
22	B	612	CLA	C1B-CHB-C4A	-3.46	123.26	130.12
23	B	619	BCR	C32-C1-C6	-3.45	104.70	110.30
22	B	606	CLA	C2A-C1A-CHA	3.45	129.89	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	D	408	CLA	C2A-C3A-C4A	-3.45	96.30	101.87
22	B	606	CLA	C6-C5-C3	3.44	122.47	113.45
22	C	509	CLA	CAA-C2A-C1A	3.44	123.24	111.97
22	B	612	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
22	D	401	CLA	CAA-C2A-C1A	3.43	123.22	111.97
22	B	616	CLA	CBA-CAA-C2A	3.43	123.98	113.86
22	C	512	CLA	OBD-CAD-C3D	3.43	136.77	128.52
22	B	605	CLA	C2A-C1A-CHA	3.42	129.84	123.86
22	D	401	CLA	C3D-C2D-C1D	3.42	110.50	105.83
22	B	607	CLA	O2D-CGD-O1D	-3.41	117.16	123.84
23	C	518	BCR	C35-C13-C14	-3.41	118.14	122.92
22	C	504	CLA	C6-C7-C8	3.41	126.95	115.92
22	B	601	CLA	C11-C10-C8	3.41	126.95	115.92
22	C	511	CLA	O2A-C1-C2	-3.41	99.67	108.64
22	C	514	CLA	CBA-CAA-C2A	3.40	123.91	113.86
22	D	402	CLA	O2D-CGD-O1D	-3.40	117.19	123.84
22	B	613	CLA	CAA-C2A-C3A	3.40	122.08	112.78
22	C	507	CLA	C2A-C1A-CHA	3.40	129.80	123.86
23	C	515	BCR	C30-C25-C26	-3.39	117.84	122.61
22	B	614	CLA	C2A-C3A-C4A	-3.38	96.41	101.87
22	B	607	CLA	C6-C7-C8	3.38	126.84	115.92
22	B	605	CLA	CHB-C4A-NA	3.38	129.19	124.51
22	B	602	CLA	C3D-C2D-C1D	3.37	110.43	105.83
22	D	401	CLA	CMA-C3A-C4A	3.36	120.81	111.77
22	C	503	CLA	C3A-C2A-C1A	3.36	106.37	101.34
22	B	606	CLA	CAA-C2A-C1A	3.34	122.90	111.97
22	D	407	CLA	C3D-C4D-ND	3.33	115.62	110.24
22	B	613	CLA	CAC-C3C-C4C	3.32	129.12	124.81
23	K	101	BCR	C33-C5-C4	3.32	119.99	113.62
22	C	517	CLA	O2D-CGD-O1D	-3.32	117.35	123.84
22	C	517	CLA	C1B-CHB-C4A	-3.31	123.55	130.12
22	B	615	CLA	C1-O2A-CGA	3.31	125.12	116.44
23	K	101	BCR	C16-C15-C14	-3.30	116.70	123.47
22	D	402	CLA	CMB-C2B-C1B	-3.30	123.39	128.46
22	B	604	CLA	O2D-CGD-O1D	-3.30	117.39	123.84
23	H	101	BCR	C38-C26-C25	3.30	128.23	124.53
22	D	402	CLA	C3D-C4D-ND	3.29	115.56	110.24
23	H	101	BCR	C16-C15-C14	-3.28	116.75	123.47
22	B	611	CLA	C11-C10-C8	3.28	126.53	115.92
22	C	517	CLA	CAA-C2A-C1A	3.28	122.72	111.97
22	C	511	CLA	CAA-C2A-C1A	3.27	122.68	111.97
22	B	612	CLA	O2D-CGD-CBD	3.27	117.07	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	D	408	CLA	C6-C7-C8	3.26	126.47	115.92
22	C	503	CLA	CAA-C2A-C1A	3.26	122.67	111.97
22	B	613	CLA	C9-C8-C10	3.25	123.08	111.29
23	H	101	BCR	C29-C28-C27	-3.25	104.11	111.38
22	C	511	CLA	C4-C3-C5	3.25	120.74	115.27
22	C	505	CLA	CHB-C4A-NA	3.25	129.00	124.51
22	B	606	CLA	OBD-CAD-C3D	3.24	136.33	128.52
22	C	512	CLA	C2A-C1A-CHA	3.24	129.53	123.86
22	C	512	CLA	C11-C10-C8	3.24	126.40	115.92
23	B	617	BCR	C1-C6-C5	-3.24	118.05	122.61
22	C	508	CLA	C3A-C2A-C1A	3.24	106.19	101.34
22	C	506	CLA	CMB-C2B-C1B	-3.24	123.49	128.46
22	C	505	CLA	CAA-C2A-C3A	3.23	121.63	112.78
23	K	101	BCR	C29-C28-C27	-3.23	104.16	111.38
22	C	504	CLA	CAA-C2A-C1A	3.23	122.55	111.97
21	A	404	PHO	C9-C8-C7	3.22	122.97	111.29
22	C	503	CLA	CMD-C2D-C1D	3.22	130.40	124.71
22	B	606	CLA	C7-C6-C5	-3.22	104.61	113.36
22	B	614	CLA	C1D-ND-C4D	-3.22	104.05	106.33
22	B	614	CLA	C2D-C1D-ND	-3.22	107.73	110.10
22	C	517	CLA	C1D-ND-C4D	-3.22	104.05	106.33
25	C	501	LMG	C3-C4-C5	-3.21	104.51	110.24
22	C	508	CLA	CAA-C2A-C3A	3.21	121.56	112.78
23	H	101	BCR	C38-C26-C27	-3.21	107.46	113.62
22	B	612	CLA	CMB-C2B-C3B	3.20	130.67	124.68
22	D	402	CLA	CHD-C1D-ND	-3.20	121.51	124.45
22	B	608	CLA	C2D-C1D-ND	-3.20	107.74	110.10
22	C	507	CLA	C2A-C3A-C4A	-3.20	96.70	101.87
22	C	509	CLA	CMD-C2D-C1D	3.19	130.34	124.71
22	B	616	CLA	C6-C7-C8	3.19	126.23	115.92
23	K	101	BCR	C38-C26-C27	-3.19	107.49	113.62
22	D	402	CLA	C4-C3-C2	-3.19	115.50	123.68
22	C	505	CLA	C6-C7-C8	-3.19	105.62	115.92
22	B	610	CLA	C3D-C2D-C1D	3.19	110.18	105.83
22	B	607	CLA	OBD-CAD-C3D	3.18	136.17	128.52
23	K	101	BCR	C38-C26-C25	3.17	128.09	124.53
22	B	612	CLA	C3D-C2D-C1D	3.15	110.13	105.83
22	A	405	CLA	C9-C8-C10	3.15	122.71	111.29
23	C	518	BCR	C12-C13-C14	3.15	123.78	118.94
22	D	408	CLA	C3B-C4B-NB	-3.14	105.16	109.21
22	C	505	CLA	O2A-C1-C2	3.13	116.86	108.64
22	B	614	CLA	CAA-C2A-C3A	3.12	121.33	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	608	CLA	C1D-ND-C4D	-3.11	104.13	106.33
22	B	611	CLA	C3A-C2A-C1A	3.11	105.99	101.34
22	C	510	CLA	O1D-CGD-CBD	3.10	130.84	124.48
22	C	514	CLA	C1D-ND-C4D	-3.10	104.14	106.33
22	D	401	CLA	C9-C8-C7	3.09	122.49	111.29
22	B	611	CLA	C1-C2-C3	3.09	131.39	126.04
22	D	401	CLA	C1D-ND-C4D	-3.09	104.14	106.33
22	C	507	CLA	C4D-CHA-C1A	-3.09	117.49	121.25
22	B	615	CLA	CMD-C2D-C1D	3.08	130.15	124.71
22	D	408	CLA	C9-C8-C7	3.08	122.45	111.29
22	C	512	CLA	CBA-CAA-C2A	3.07	122.94	113.86
22	C	511	CLA	CBA-CAA-C2A	3.07	122.92	113.86
22	D	401	CLA	C1B-CHB-C4A	-3.06	124.05	130.12
22	B	602	CLA	CBA-CAA-C2A	3.06	122.89	113.86
22	D	402	CLA	C3D-C2D-C1D	3.06	110.01	105.83
22	B	604	CLA	C6-C7-C8	3.05	125.79	115.92
22	B	604	CLA	CBA-CAA-C2A	3.05	122.86	113.86
22	B	615	CLA	CBA-CAA-C2A	3.05	122.85	113.86
22	B	614	CLA	CMD-C2D-C1D	-3.04	119.35	124.71
22	C	510	CLA	C2A-C3A-C4A	3.04	106.78	101.87
22	B	612	CLA	C9-C8-C10	3.04	122.30	111.29
22	B	606	CLA	CMA-C3A-C4A	3.04	119.94	111.77
23	B	617	BCR	C39-C30-C25	3.04	115.22	110.30
22	D	408	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
22	B	608	CLA	CMB-C2B-C3B	3.03	130.35	124.68
22	D	408	CLA	C4D-C3D-CAD	3.03	111.67	108.10
22	D	407	CLA	CAC-C3C-C4C	3.03	128.74	124.81
22	B	601	CLA	C9-C8-C10	3.03	122.26	111.29
22	B	612	CLA	CAC-C3C-C4C	3.03	128.74	124.81
25	3	101	LMG	C1-C2-C3	-3.03	103.69	110.00
22	B	602	CLA	CMB-C2B-C1B	-3.02	123.82	128.46
23	C	518	BCR	C30-C25-C26	-3.01	118.37	122.61
22	B	607	CLA	C11-C10-C8	3.01	125.64	115.92
22	B	603	CLA	C1B-CHB-C4A	-3.00	124.17	130.12
22	B	608	CLA	C11-C10-C8	3.00	125.62	115.92
22	B	606	CLA	CHB-C4A-NA	3.00	128.66	124.51
22	C	510	CLA	C1D-ND-C4D	-2.99	104.21	106.33
22	B	613	CLA	CHD-C4C-C3C	2.99	129.23	124.84
22	C	504	CLA	CMA-C3A-C4A	2.98	119.79	111.77
22	C	513	CLA	O2D-CGD-CBD	2.97	116.55	111.27
23	K	101	BCR	C24-C23-C22	-2.97	121.75	126.23
22	A	405	CLA	C3D-C4D-ND	2.97	115.04	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	406	CLA	O2A-C1-C2	-2.96	100.85	108.64
22	C	512	CLA	O1D-CGD-CBD	2.96	130.54	124.48
22	C	517	CLA	C4D-CHA-C1A	-2.96	117.65	121.25
23	C	515	BCR	C33-C5-C6	-2.95	121.21	124.53
22	A	406	CLA	C2D-C1D-ND	-2.95	107.93	110.10
22	D	401	CLA	CMB-C2B-C1B	-2.95	123.93	128.46
23	H	101	BCR	C24-C23-C22	-2.94	121.79	126.23
22	C	513	CLA	CMB-C2B-C1B	-2.94	123.94	128.46
22	B	603	CLA	CMD-C2D-C1D	2.94	129.89	124.71
22	A	405	CLA	O2A-C1-C2	-2.93	100.92	108.64
22	B	613	CLA	CHB-C4A-NA	2.93	128.57	124.51
22	B	605	CLA	C6-C7-C8	2.93	125.39	115.92
22	D	402	CLA	O2A-C1-C2	-2.93	100.94	108.64
25	3	101	LMG	C1-O6-C5	-2.93	107.94	113.69
22	B	611	CLA	CBA-CAA-C2A	2.93	122.51	113.86
22	B	607	CLA	C9-C8-C7	2.93	121.89	111.29
23	C	518	BCR	C2-C1-C6	2.93	114.98	110.48
22	B	606	CLA	CAC-C3C-C4C	2.93	128.61	124.81
22	B	616	CLA	CAA-C2A-C1A	2.92	121.56	111.97
22	B	605	CLA	C11-C10-C8	2.92	125.36	115.92
22	D	401	CLA	C6-C7-C8	2.92	125.35	115.92
22	C	517	CLA	CHD-C1D-ND	-2.91	121.78	124.45
22	B	604	CLA	C9-C8-C7	2.90	121.81	111.29
23	F	102	BCR	C31-C1-C6	2.90	115.01	110.30
22	B	615	CLA	C9-C8-C7	2.90	121.80	111.29
22	B	614	CLA	O2A-C1-C2	-2.90	101.01	108.64
22	B	614	CLA	C10-C8-C7	2.89	127.34	112.13
22	C	511	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
22	C	503	CLA	C9-C8-C7	2.88	121.72	111.29
22	C	503	CLA	O2A-C1-C2	2.87	116.18	108.64
26	D	405	PL9	C35-C34-C36	2.87	120.10	115.27
22	D	402	CLA	CAA-C2A-C1A	2.86	121.35	111.97
22	C	513	CLA	C4D-CHA-C1A	-2.86	117.77	121.25
22	B	602	CLA	C4-C3-C5	2.86	120.08	115.27
22	C	506	CLA	CAA-C2A-C1A	2.85	121.32	111.97
22	C	513	CLA	C3D-C2D-C1D	2.85	109.72	105.83
23	B	619	BCR	C39-C30-C25	2.85	114.92	110.30
22	C	512	CLA	C4D-CHA-C1A	-2.84	117.79	121.25
22	C	507	CLA	CMD-C2D-C3D	-2.83	121.10	127.61
22	B	609	CLA	CBA-CAA-C2A	2.83	122.22	113.86
25	C	502	LMG	C6-C5-C4	-2.83	106.38	113.00
22	B	606	CLA	C3D-C2D-C1D	2.83	109.69	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	503	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
22	D	407	CLA	CGD-CBD-CAD	-2.82	101.59	110.73
22	B	604	CLA	O1D-CGD-CBD	2.82	130.25	124.48
21	D	406	PHO	C6-C7-C8	2.81	125.01	115.92
22	B	613	CLA	C4-C3-C5	2.81	120.00	115.27
22	B	602	CLA	C9-C8-C10	2.81	121.45	111.29
23	H	101	BCR	C21-C20-C19	-2.81	114.46	123.22
22	B	611	CLA	CAA-C2A-C3A	2.80	120.45	112.78
27	E	101	HEM	C4B-CHC-C1C	2.80	126.25	122.56
23	K	101	BCR	C21-C20-C19	-2.79	114.51	123.22
22	C	512	CLA	C2A-C3A-C4A	-2.79	97.36	101.87
22	B	613	CLA	CAA-C2A-C1A	2.79	121.12	111.97
23	H	101	BCR	C8-C9-C10	-2.79	114.66	118.94
25	C	501	LMG	C1-C2-C3	-2.79	104.19	110.00
22	C	511	CLA	CAA-CBA-CGA	-2.78	105.13	113.25
22	C	513	CLA	C10-C8-C7	2.78	126.74	112.13
22	C	507	CLA	CAA-C2A-C1A	2.78	121.07	111.97
22	C	504	CLA	C9-C8-C7	2.77	121.33	111.29
22	B	615	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
23	C	515	BCR	C40-C30-C25	2.77	114.79	110.30
22	D	407	CLA	C3A-C2A-C1A	2.76	105.47	101.34
22	C	514	CLA	C2D-C1D-ND	-2.76	108.07	110.10
22	B	601	CLA	C6-C5-C3	2.76	120.68	113.45
22	A	405	CLA	C4D-CHA-C1A	-2.75	117.90	121.25
22	B	611	CLA	CHB-C4A-NA	2.75	128.32	124.51
22	B	606	CLA	C9-C8-C7	2.75	121.25	111.29
23	F	102	BCR	C35-C13-C14	-2.75	119.08	122.92
23	K	101	BCR	C8-C9-C10	-2.74	114.73	118.94
22	C	509	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
22	C	508	CLA	C9-C8-C10	2.73	121.19	111.29
22	A	406	CLA	C9-C8-C7	2.73	121.18	111.29
22	B	609	CLA	CHB-C4A-NA	2.73	128.29	124.51
23	H	101	BCR	C32-C1-C31	2.72	116.89	108.53
22	D	401	CLA	C9-C8-C10	2.72	121.14	111.29
22	C	505	CLA	C3D-C4D-ND	2.72	114.64	110.24
22	C	509	CLA	CMD-C2D-C3D	-2.72	121.36	127.61
22	C	512	CLA	C2D-C1D-ND	-2.72	108.10	110.10
22	B	609	CLA	OBD-CAD-C3D	2.71	135.04	128.52
22	C	507	CLA	CHD-C1D-C2D	2.71	131.16	125.48
22	B	607	CLA	C2D-C1D-ND	-2.71	108.11	110.10
22	C	513	CLA	CAA-C2A-C1A	2.71	120.84	111.97
23	H	101	BCR	C3-C4-C5	2.70	118.91	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	K	101	BCR	C3-C4-C5	2.70	118.90	114.08
22	B	612	CLA	C4D-CHA-C1A	-2.70	117.96	121.25
22	B	611	CLA	C9-C8-C7	2.70	121.06	111.29
23	B	617	BCR	C7-C6-C5	2.69	127.99	121.46
22	D	407	CLA	CBA-CAA-C2A	2.69	121.81	113.86
22	B	601	CLA	C6-C7-C8	2.69	124.61	115.92
22	B	615	CLA	CMD-C2D-C3D	-2.69	121.43	127.61
22	B	616	CLA	C10-C8-C7	2.69	126.27	112.13
22	B	607	CLA	CMB-C2B-C1B	-2.69	124.33	128.46
26	D	405	PL9	C46-C44-C43	2.68	126.54	121.12
22	A	406	CLA	C11-C10-C8	2.68	124.59	115.92
22	B	601	CLA	C9-C8-C7	2.68	121.00	111.29
22	C	503	CLA	CMA-C3A-C4A	2.67	118.96	111.77
22	B	610	CLA	C3B-C4B-NB	-2.67	105.75	109.21
22	D	402	CLA	C3C-C4C-NC	-2.67	107.57	110.57
22	D	402	CLA	C4-C3-C5	2.67	119.77	115.27
22	C	505	CLA	C5-C3-C2	2.67	126.52	121.12
22	C	504	CLA	CMB-C2B-C1B	-2.67	124.36	128.46
21	D	406	PHO	C1B-NB-C4B	2.67	112.57	107.09
23	B	618	BCR	C12-C13-C14	2.67	123.03	118.94
22	C	512	CLA	CMA-C3A-C4A	2.66	118.93	111.77
23	C	515	BCR	C15-C14-C13	-2.66	123.52	127.31
22	C	507	CLA	C9-C8-C10	2.66	120.91	111.29
22	C	505	CLA	CMD-C2D-C3D	-2.65	121.51	127.61
22	A	406	CLA	CMB-C2B-C3B	2.65	129.63	124.68
22	B	610	CLA	CMB-C2B-C1B	-2.65	124.40	128.46
22	D	407	CLA	CHD-C4C-C3C	2.64	128.72	124.84
22	C	509	CLA	CBA-CAA-C2A	2.64	121.66	113.86
22	B	602	CLA	CMD-C2D-C3D	-2.64	121.54	127.61
22	C	507	CLA	CBC-CAC-C3C	2.64	119.70	112.43
22	B	613	CLA	O1D-CGD-CBD	2.64	129.88	124.48
22	A	405	CLA	CGD-CBD-CAD	-2.64	102.20	110.73
22	C	504	CLA	CMD-C2D-C1D	2.63	129.35	124.71
23	B	619	BCR	C2-C1-C6	2.63	114.53	110.48
22	A	405	CLA	O1D-CGD-CBD	2.63	129.86	124.48
22	B	609	CLA	C11-C10-C8	2.61	124.37	115.92
22	C	507	CLA	CHB-C4A-NA	2.61	128.13	124.51
22	A	405	CLA	C6-C7-C8	2.61	124.36	115.92
22	B	613	CLA	CMB-C2B-C1B	-2.61	124.45	128.46
22	B	609	CLA	C4D-CHA-C1A	-2.61	118.07	121.25
22	B	615	CLA	CHB-C4A-NA	2.60	128.11	124.51
22	C	517	CLA	CMD-C2D-C3D	-2.60	121.64	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	603	CLA	CHB-C4A-NA	2.60	128.10	124.51
22	B	610	CLA	CBC-CAC-C3C	2.59	119.58	112.43
22	B	603	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
22	B	615	CLA	C1D-ND-C4D	-2.59	104.49	106.33
22	C	512	CLA	C9-C8-C7	2.59	120.67	111.29
23	B	619	BCR	C33-C5-C6	-2.59	121.62	124.53
22	C	503	CLA	C3B-C4B-NB	-2.58	105.87	109.21
22	B	615	CLA	O2D-CGD-CBD	2.58	115.86	111.27
22	C	505	CLA	C1B-CHB-C4A	-2.58	125.01	130.12
22	B	609	CLA	CAC-C3C-C4C	2.58	128.16	124.81
23	H	101	BCR	C24-C25-C26	2.58	127.71	121.46
22	C	505	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
23	K	101	BCR	C32-C1-C31	2.58	116.44	108.53
23	B	619	BCR	C27-C26-C25	2.57	126.47	122.73
22	C	508	CLA	C3B-C4B-NB	-2.57	105.89	109.21
22	D	408	CLA	C6-C5-C3	2.57	120.20	113.45
22	B	613	CLA	C11-C10-C8	2.57	124.21	115.92
22	B	611	CLA	CHD-C1D-C2D	2.57	130.86	125.48
22	C	503	CLA	OBD-CAD-C3D	2.56	134.68	128.52
23	B	619	BCR	C31-C1-C6	2.56	114.45	110.30
22	C	505	CLA	O1D-CGD-CBD	2.56	129.72	124.48
22	B	607	CLA	CMD-C2D-C1D	2.56	129.22	124.71
22	C	506	CLA	CMD-C2D-C1D	2.56	129.22	124.71
22	C	510	CLA	C6-C7-C8	2.55	124.17	115.92
22	B	606	CLA	C6-C7-C8	2.55	124.16	115.92
22	C	517	CLA	C9-C8-C10	2.54	120.50	111.29
22	A	406	CLA	C3B-C4B-NB	-2.54	105.92	109.21
22	A	405	CLA	C4-C3-C2	-2.54	117.16	123.68
22	D	402	CLA	CHD-C1D-C2D	2.54	130.81	125.48
22	B	612	CLA	C2D-C1D-ND	-2.54	108.23	110.10
22	C	514	CLA	C2A-C3A-C4A	-2.53	97.78	101.87
23	B	618	BCR	C27-C26-C25	2.53	126.40	122.73
22	C	509	CLA	C6-C7-C8	2.52	124.08	115.92
22	B	610	CLA	CHD-C4C-NC	-2.52	120.23	124.20
22	A	405	CLA	CHB-C4A-NA	2.52	128.00	124.51
22	D	407	CLA	C9-C8-C10	2.52	120.41	111.29
22	C	514	CLA	C4D-CHA-C1A	-2.52	118.19	121.25
22	B	607	CLA	O1D-CGD-CBD	2.51	129.63	124.48
22	B	609	CLA	C9-C8-C10	2.51	120.39	111.29
22	D	401	CLA	C2D-C1D-ND	-2.51	108.25	110.10
23	K	101	BCR	C24-C25-C26	2.51	127.54	121.46
22	D	407	CLA	C2C-C1C-NC	2.50	112.31	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	518	BCR	C15-C14-C13	-2.50	123.75	127.31
25	D	403	LMG	O6-C1-O1	-2.49	104.07	109.97
22	B	603	CLA	C5-C3-C2	-2.49	116.08	121.12
22	B	602	CLA	CMB-C2B-C3B	2.49	129.34	124.68
25	D	404	LMG	C1-O6-C5	-2.49	108.81	113.69
22	D	402	CLA	C9-C8-C7	2.49	120.29	111.29
22	B	614	CLA	CHB-C4A-NA	2.49	127.95	124.51
22	C	505	CLA	O2A-CGA-O1A	-2.48	117.33	123.59
22	C	505	CLA	CHD-C1D-ND	-2.48	122.18	124.45
22	C	517	CLA	CMB-C2B-C1B	-2.48	124.66	128.46
23	C	516	BCR	C27-C26-C25	2.47	126.31	122.73
22	C	508	CLA	CMB-C2B-C1B	-2.46	124.68	128.46
22	B	602	CLA	O2D-CGD-O1D	-2.46	119.02	123.84
22	C	507	CLA	CHD-C4C-C3C	2.46	128.46	124.84
22	B	606	CLA	CMA-C3A-C2A	-2.46	103.91	113.83
22	C	512	CLA	O2D-CGD-CBD	-2.45	106.91	111.27
22	B	612	CLA	C9-C8-C7	2.45	120.17	111.29
22	C	510	CLA	C10-C8-C7	2.45	125.01	112.13
22	B	607	CLA	C4D-CHA-C1A	-2.45	118.27	121.25
23	C	516	BCR	C8-C7-C6	-2.45	120.33	127.20
23	C	515	BCR	C27-C26-C25	2.44	126.28	122.73
22	A	406	CLA	C1D-ND-C4D	2.44	108.07	106.33
23	A	407	BCR	C29-C30-C25	2.44	114.24	110.48
23	B	617	BCR	C24-C23-C22	-2.44	122.55	126.23
22	C	510	CLA	CHD-C1D-C2D	2.43	130.59	125.48
22	C	517	CLA	CHD-C1D-C2D	2.43	130.58	125.48
25	D	403	LMG	C1-O6-C5	-2.43	108.91	113.69
22	B	601	CLA	CBC-CAC-C3C	2.43	119.14	112.43
23	C	518	BCR	C8-C9-C10	2.43	122.67	118.94
22	B	603	CLA	C6-C5-C3	2.43	119.83	113.45
23	C	516	BCR	C39-C30-C25	2.43	114.24	110.30
25	F	101	LMG	O2-C2-C1	-2.43	104.15	110.05
22	C	503	CLA	CMB-C2B-C3B	2.43	129.22	124.68
22	C	510	CLA	CAA-CBA-CGA	2.42	120.34	113.25
22	B	612	CLA	CMD-C2D-C3D	-2.42	122.05	127.61
22	C	510	CLA	CMA-C3A-C4A	2.42	118.28	111.77
22	B	604	CLA	C1B-CHB-C4A	-2.42	125.33	130.12
22	C	511	CLA	C6-C7-C8	2.42	123.73	115.92
25	C	502	LMG	O6-C1-O1	-2.41	104.26	109.97
22	D	407	CLA	O1D-CGD-CBD	2.41	129.42	124.48
23	C	516	BCR	C19-C18-C17	2.41	122.64	118.94
22	B	611	CLA	CMA-C3A-C4A	2.41	118.24	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	3	101	LMG	O6-C5-C6	2.40	112.41	106.44
22	C	513	CLA	C2A-C3A-C4A	-2.40	97.99	101.87
26	D	405	PL9	O1-C4-C3	-2.40	118.08	120.72
22	B	615	CLA	O2A-CGA-O1A	-2.40	117.53	123.59
22	C	509	CLA	C1B-CHB-C4A	-2.40	125.37	130.12
22	C	514	CLA	C9-C8-C7	2.39	119.96	111.29
22	B	606	CLA	CMD-C2D-C3D	-2.39	122.11	127.61
22	B	605	CLA	CBA-CAA-C2A	2.39	120.92	113.86
22	C	505	CLA	CGD-CBD-CAD	2.39	118.47	110.73
22	B	608	CLA	CBC-CAC-C3C	2.39	119.01	112.43
22	B	606	CLA	O1D-CGD-CBD	2.38	129.36	124.48
22	C	509	CLA	C9-C8-C7	2.38	119.92	111.29
22	A	406	CLA	O1D-CGD-CBD	2.38	129.36	124.48
23	A	407	BCR	C2-C1-C6	2.38	114.14	110.48
22	A	405	CLA	CMA-C3A-C2A	-2.38	104.24	113.83
22	B	603	CLA	CMA-C3A-C2A	-2.37	104.28	113.83
22	B	605	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
23	C	516	BCR	C36-C18-C17	-2.37	119.61	122.92
22	B	603	CLA	C9-C8-C7	2.36	119.84	111.29
22	A	405	CLA	C9-C8-C7	2.36	119.83	111.29
25	C	501	LMG	O6-C1-O1	-2.36	104.39	109.97
26	D	405	PL9	C45-C44-C46	-2.35	111.31	115.27
23	C	516	BCR	C31-C1-C6	2.34	114.10	110.30
22	B	610	CLA	CHD-C1D-ND	2.34	126.61	124.45
23	F	102	BCR	C27-C26-C25	2.34	126.13	122.73
22	B	611	CLA	C3B-C4B-NB	-2.34	106.19	109.21
26	D	405	PL9	C37-C38-C39	-2.33	122.05	127.66
22	B	605	CLA	C1D-ND-C4D	-2.33	104.68	106.33
22	C	506	CLA	C6-C5-C3	2.33	119.57	113.45
22	B	611	CLA	CBC-CAC-C3C	2.33	118.84	112.43
22	C	503	CLA	CMD-C2D-C3D	-2.32	122.27	127.61
23	B	617	BCR	C15-C16-C17	-2.32	118.71	123.47
25	D	404	LMG	O1-C7-C8	-2.32	105.29	110.90
22	C	514	CLA	C10-C8-C7	2.32	124.34	112.13
22	B	604	CLA	C3D-C2D-C1D	2.32	109.00	105.83
22	B	613	CLA	CHD-C1D-C2D	2.32	130.34	125.48
22	C	514	CLA	CHB-C4A-NA	2.31	127.71	124.51
22	B	610	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
25	F	101	LMG	O6-C1-O1	-2.31	104.50	109.97
22	C	503	CLA	C1-C2-C3	2.31	130.04	126.04
22	A	405	CLA	CBA-CAA-C2A	2.31	120.68	113.86
22	C	511	CLA	CMB-C2B-C3B	2.31	128.99	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	C	501	LMG	C8-O7-C10	2.31	123.47	117.79
23	A	407	BCR	C30-C25-C26	-2.30	119.37	122.61
22	B	610	CLA	C4C-C3C-C2C	-2.30	103.54	106.90
22	B	605	CLA	CMD-C2D-C3D	-2.30	122.32	127.61
22	C	513	CLA	C6-C7-C8	2.29	123.33	115.92
22	C	513	CLA	CAC-C3C-C4C	2.29	127.78	124.81
22	C	508	CLA	CAA-C2A-C1A	2.29	119.47	111.97
22	B	616	CLA	CMB-C2B-C1B	-2.29	124.95	128.46
22	B	610	CLA	C2D-C1D-ND	-2.29	108.42	110.10
22	B	604	CLA	C6-C5-C3	2.28	119.45	113.45
22	C	508	CLA	CMA-C3A-C4A	2.28	117.91	111.77
25	I	101	LMG	C1-O6-C5	-2.28	109.21	113.69
22	B	615	CLA	C9-C8-C10	2.28	119.55	111.29
22	C	517	CLA	CAA-CBA-CGA	-2.28	106.59	113.25
22	D	402	CLA	CAC-C3C-C4C	2.28	127.76	124.81
23	F	102	BCR	C39-C30-C25	2.28	113.99	110.30
25	C	502	LMG	O2-C2-C1	-2.27	104.53	110.05
22	C	513	CLA	CBC-CAC-C3C	-2.27	106.18	112.43
22	B	614	CLA	CMB-C2B-C1B	-2.27	124.98	128.46
22	C	510	CLA	OBD-CAD-C3D	2.26	133.96	128.52
22	D	402	CLA	CMB-C2B-C3B	2.26	128.91	124.68
22	B	613	CLA	CAC-C3C-C2C	-2.26	123.67	127.53
23	B	618	BCR	C1-C6-C5	-2.26	119.43	122.61
25	C	501	LMG	C1-O6-C5	-2.26	109.26	113.69
23	C	518	BCR	C38-C26-C25	-2.25	122.00	124.53
22	C	513	CLA	CGD-CBD-CAD	2.25	118.04	110.73
22	D	401	CLA	CMB-C2B-C3B	2.25	128.89	124.68
22	C	510	CLA	C9-C8-C10	2.25	119.43	111.29
22	B	603	CLA	C9-C8-C10	2.25	119.43	111.29
23	C	516	BCR	C30-C25-C26	-2.24	119.45	122.61
23	C	515	BCR	C29-C30-C25	2.24	113.93	110.48
24	A	408	LHG	O8-C23-C24	2.24	118.94	111.91
23	C	518	BCR	C36-C18-C17	-2.24	119.79	122.92
22	B	613	CLA	CMA-C3A-C4A	-2.24	105.76	111.77
22	D	402	CLA	C1B-CHB-C4A	-2.23	125.69	130.12
22	D	401	CLA	CAC-C3C-C4C	2.23	127.71	124.81
22	B	610	CLA	CMB-C2B-C3B	2.23	128.85	124.68
23	F	102	BCR	C8-C7-C6	-2.23	120.94	127.20
22	B	601	CLA	CMD-C2D-C1D	2.23	128.64	124.71
23	C	518	BCR	C27-C26-C25	2.23	125.96	122.73
22	C	503	CLA	O1D-CGD-CBD	2.23	129.04	124.48
22	C	517	CLA	CMB-C2B-C3B	2.22	128.83	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	614	CLA	CGD-CBD-CAD	-2.22	103.55	110.73
22	B	607	CLA	C5-C3-C2	-2.22	116.63	121.12
22	B	616	CLA	C9-C8-C7	2.22	119.32	111.29
25	I	101	LMG	C32-C31-C30	-2.22	103.18	114.42
22	B	611	CLA	C1B-CHB-C4A	-2.21	125.73	130.12
22	B	607	CLA	O2A-C1-C2	-2.21	102.82	108.64
22	D	407	CLA	CMD-C2D-C1D	-2.21	120.82	124.71
22	B	601	CLA	O2D-CGD-O1D	-2.21	119.52	123.84
22	B	610	CLA	CAA-C2A-C1A	2.21	119.21	111.97
22	A	406	CLA	C6-C7-C8	2.21	123.05	115.92
22	C	506	CLA	CMB-C2B-C3B	2.21	128.81	124.68
22	B	607	CLA	C2A-C3A-C4A	-2.21	98.31	101.87
22	B	607	CLA	CAC-C3C-C4C	2.20	127.67	124.81
22	B	603	CLA	C2A-C3A-C4A	-2.20	98.31	101.87
22	C	512	CLA	CGD-CBD-CAD	-2.20	103.62	110.73
22	B	604	CLA	O2A-CGA-O1A	-2.20	118.05	123.59
22	A	405	CLA	CBC-CAC-C3C	2.20	118.48	112.43
22	B	609	CLA	CMA-C3A-C4A	-2.19	105.88	111.77
22	B	601	CLA	CMD-C2D-C3D	-2.19	122.57	127.61
26	D	405	PL9	C8-C7-C3	2.19	118.17	111.98
26	D	405	PL9	C40-C39-C41	2.19	118.95	115.27
21	A	404	PHO	C9-C8-C10	2.19	119.22	111.29
23	C	518	BCR	C33-C5-C6	-2.18	122.08	124.53
22	C	512	CLA	CHB-C4A-NA	2.18	127.53	124.51
23	C	515	BCR	C1-C6-C5	-2.18	119.54	122.61
22	C	508	CLA	C2D-C1D-ND	-2.18	108.50	110.10
22	C	507	CLA	OBD-CAD-C3D	2.18	133.76	128.52
22	B	606	CLA	C4D-CHA-C1A	-2.18	118.60	121.25
22	C	513	CLA	CMB-C2B-C3B	2.18	128.75	124.68
22	B	605	CLA	O1D-CGD-CBD	2.17	128.93	124.48
22	C	517	CLA	C9-C8-C7	2.17	119.16	111.29
22	C	510	CLA	CMD-C2D-C1D	-2.17	120.89	124.71
22	B	606	CLA	C1D-ND-C4D	-2.17	104.79	106.33
22	A	406	CLA	CHA-C4D-ND	2.17	137.04	132.50
22	C	505	CLA	O2A-CGA-CBA	2.17	118.71	111.91
22	B	601	CLA	C3D-C2D-C1D	2.17	108.79	105.83
22	C	503	CLA	C2A-C1A-CHA	2.16	127.64	123.86
23	C	518	BCR	C34-C9-C8	-2.16	114.67	118.08
22	B	606	CLA	CAA-C2A-C3A	2.16	118.70	112.78
25	D	403	LMG	O2-C2-C1	-2.16	104.80	110.05
22	C	508	CLA	CGD-CBD-CAD	-2.16	103.74	110.73
22	B	606	CLA	C5-C3-C2	-2.16	116.75	121.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	607	CLA	CBA-CAA-C2A	2.16	120.23	113.86
22	B	614	CLA	CMA-C3A-C4A	-2.15	105.99	111.77
22	B	608	CLA	CAC-C3C-C4C	2.15	127.60	124.81
22	C	511	CLA	C10-C8-C7	2.15	123.44	112.13
21	D	406	PHO	C11-C10-C8	2.15	122.85	115.92
22	B	608	CLA	O1D-CGD-CBD	2.14	128.87	124.48
23	C	515	BCR	C2-C1-C6	2.14	113.78	110.48
23	C	516	BCR	C29-C30-C25	2.14	113.78	110.48
22	B	612	CLA	C4C-C3C-C2C	-2.14	103.78	106.90
22	C	505	CLA	CED-O2D-CGD	2.14	120.78	115.94
22	C	507	CLA	C1D-ND-C4D	-2.14	104.82	106.33
22	D	407	CLA	CHD-C1D-C2D	2.14	129.96	125.48
22	C	512	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
23	B	619	BCR	C37-C22-C21	-2.14	119.93	122.92
22	B	603	CLA	CMB-C2B-C1B	-2.14	125.18	128.46
22	C	504	CLA	CMB-C2B-C3B	2.14	128.67	124.68
22	B	610	CLA	O2A-C1-C2	-2.14	103.02	108.64
25	D	404	LMG	C8-O7-C10	2.14	123.05	117.79
22	D	407	CLA	C6-C7-C8	2.13	122.82	115.92
25	3	101	LMG	C6-C5-C4	-2.13	108.00	113.00
22	C	514	CLA	C4-C3-C5	2.13	118.86	115.27
23	K	101	BCR	C34-C9-C8	2.13	121.44	118.08
22	C	508	CLA	C1B-CHB-C4A	-2.13	125.89	130.12
21	A	404	PHO	O2D-CGD-O1D	-2.13	119.67	123.84
22	B	615	CLA	C4D-CHA-C1A	-2.13	118.66	121.25
22	C	508	CLA	C6-C7-C8	2.13	122.81	115.92
22	B	613	CLA	CMD-C2D-C3D	-2.13	122.72	127.61
22	B	606	CLA	C9-C8-C10	2.13	118.99	111.29
22	B	606	CLA	O2A-CGA-O1A	-2.13	118.23	123.59
22	C	517	CLA	CBA-CAA-C2A	2.12	120.14	113.86
22	B	616	CLA	C2A-C3A-C4A	-2.12	98.44	101.87
22	B	604	CLA	C3D-C4D-ND	2.12	113.67	110.24
22	D	401	CLA	C3A-C2A-C1A	-2.12	98.16	101.34
22	C	506	CLA	C9-C8-C7	2.12	118.97	111.29
22	C	517	CLA	C3A-C2A-C1A	-2.12	98.17	101.34
22	B	614	CLA	C4D-CHA-C1A	-2.12	118.67	121.25
22	C	506	CLA	C9-C8-C10	2.12	118.96	111.29
22	B	614	CLA	C1B-CHB-C4A	-2.12	125.93	130.12
22	C	507	CLA	C1B-CHB-C4A	-2.11	125.93	130.12
22	D	408	CLA	O1D-CGD-CBD	2.11	128.81	124.48
22	C	505	CLA	C9-C8-C7	2.11	118.95	111.29
22	B	607	CLA	CHB-C4A-NA	2.11	127.43	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	D	405	PL9	C7-C3-C2	-2.11	120.52	123.30
22	B	616	CLA	O1D-CGD-CBD	2.11	128.81	124.48
23	C	515	BCR	C39-C30-C25	-2.11	106.88	110.30
22	C	504	CLA	CMD-C2D-C3D	-2.11	122.77	127.61
22	D	408	CLA	CAA-C2A-C1A	2.11	118.88	111.97
22	B	607	CLA	CMB-C2B-C3B	2.11	128.62	124.68
22	C	511	CLA	CMD-C2D-C1D	2.10	128.42	124.71
22	B	606	CLA	C4-C3-C5	2.10	118.81	115.27
22	B	602	CLA	CHB-C4A-NA	2.10	127.42	124.51
22	C	503	CLA	CMA-C3A-C2A	-2.10	105.35	113.83
22	B	611	CLA	CMD-C2D-C1D	-2.10	121.01	124.71
22	B	614	CLA	OBD-CAD-C3D	2.10	133.57	128.52
23	H	101	BCR	C34-C9-C8	2.10	121.39	118.08
23	C	515	BCR	C38-C26-C27	-2.10	109.58	113.62
22	B	607	CLA	CHA-C4D-ND	2.10	136.88	132.50
22	A	406	CLA	C1B-CHB-C4A	-2.10	125.97	130.12
21	A	404	PHO	C1B-NB-C4B	2.09	111.39	107.09
22	D	407	CLA	CAC-C3C-C2C	-2.09	123.95	127.53
22	B	609	CLA	C1D-ND-C4D	-2.09	104.85	106.33
22	B	607	CLA	CED-O2D-CGD	2.09	120.67	115.94
22	B	610	CLA	C10-C8-C7	2.09	123.12	112.13
25	I	101	LMG	C1-C2-C3	-2.09	105.64	110.00
22	C	503	CLA	C1B-CHB-C4A	-2.09	125.98	130.12
22	C	507	CLA	O1D-CGD-CBD	2.09	128.76	124.48
22	B	614	CLA	CBC-CAC-C3C	2.09	118.19	112.43
22	B	611	CLA	CAC-C3C-C2C	-2.09	123.96	127.53
23	B	618	BCR	C35-C13-C14	-2.08	120.00	122.92
22	B	613	CLA	C3C-C4C-NC	-2.08	108.24	110.57
22	C	511	CLA	C9-C8-C7	2.08	118.81	111.29
21	D	406	PHO	CMC-C2C-C3C	2.07	128.85	124.94
23	C	516	BCR	C23-C24-C25	-2.07	121.39	127.20
22	C	511	CLA	C3B-C4B-NB	-2.07	106.54	109.21
22	C	503	CLA	C9-C8-C10	2.06	118.76	111.29
22	D	402	CLA	O1D-CGD-CBD	2.06	128.70	124.48
22	D	408	CLA	C9-C8-C10	2.06	118.75	111.29
23	B	617	BCR	C8-C9-C10	2.06	122.10	118.94
22	B	603	CLA	CMA-C3A-C4A	-2.06	106.24	111.77
22	D	408	CLA	C4D-CHA-C1A	-2.06	118.75	121.25
22	C	517	CLA	C3D-C4D-CHA	-2.05	108.03	112.72
26	D	405	PL9	O2-C1-C6	2.05	124.14	120.59
22	B	602	CLA	C1B-CHB-C4A	-2.05	126.06	130.12
22	B	609	CLA	CMD-C2D-C1D	-2.05	121.10	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	615	CLA	CMB-C2B-C1B	-2.05	125.32	128.46
22	B	601	CLA	O2D-CGD-CBD	2.05	114.90	111.27
23	B	619	BCR	C1-C6-C5	-2.05	119.73	122.61
22	B	602	CLA	O2D-CGD-CBD	2.05	114.90	111.27
23	K	101	BCR	C28-C27-C26	-2.04	110.43	114.08
22	D	402	CLA	CHB-C4A-NA	2.04	127.34	124.51
22	C	505	CLA	CBA-CAA-C2A	2.04	119.89	113.86
25	D	404	LMG	O6-C1-O1	-2.04	105.15	109.97
23	K	101	BCR	C11-C10-C9	-2.04	124.40	127.31
25	C	502	LMG	C1-C2-C3	-2.03	105.76	110.00
23	F	102	BCR	C16-C15-C14	-2.03	119.31	123.47
23	C	518	BCR	C11-C10-C9	-2.03	124.41	127.31
25	F	101	LMG	O3-C3-C2	-2.03	105.66	110.35
22	B	610	CLA	O2D-CGD-O1D	-2.03	119.87	123.84
22	C	505	CLA	CMA-C3A-C2A	-2.03	105.65	113.83
22	D	401	CLA	O2D-CGD-O1D	-2.02	119.88	123.84
23	H	101	BCR	C28-C27-C26	-2.02	110.46	114.08
22	C	506	CLA	CHB-C4A-NA	2.02	127.31	124.51
22	B	602	CLA	C2D-C1D-ND	-2.02	108.61	110.10
23	F	102	BCR	C2-C1-C6	2.02	113.59	110.48
22	B	608	CLA	C3B-C4B-NB	-2.02	106.60	109.21
21	D	406	PHO	O2D-CGD-O1D	-2.02	119.89	123.84
22	D	407	CLA	CHB-C4A-NA	2.02	127.30	124.51
22	C	507	CLA	C11-C10-C8	2.02	122.43	115.92
22	C	504	CLA	C2C-C1C-NC	2.02	111.86	109.97
23	C	515	BCR	C35-C13-C12	2.02	121.25	118.08
22	B	604	CLA	C10-C8-C7	2.01	122.71	112.13
22	B	615	CLA	C2A-C3A-C4A	-2.01	98.62	101.87
22	B	603	CLA	CMD-C2D-C3D	-2.01	122.99	127.61
25	C	502	LMG	O6-C5-C6	2.01	111.43	106.44
22	C	503	CLA	CHA-C4D-ND	2.01	136.70	132.50
22	A	406	CLA	C4D-C3D-CAD	2.01	110.46	108.10
23	B	617	BCR	C34-C9-C10	-2.00	120.11	122.92
22	B	602	CLA	CAC-C3C-C2C	-2.00	124.10	127.53
25	3	101	LMG	O6-C1-O1	-2.00	105.23	109.97
23	F	102	BCR	C37-C22-C21	-2.00	120.12	122.92

All (75) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
21	A	404	PHO	C8
21	D	406	PHO	C8

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Mol	Chain	Res	Type	Atom
22	A	405	CLA	ND
22	A	405	CLA	C2A
22	A	406	CLA	ND
22	A	406	CLA	C2A
22	B	601	CLA	ND
22	B	601	CLA	C8
22	B	601	CLA	C2A
22	B	602	CLA	ND
22	B	602	CLA	C2A
22	B	603	CLA	ND
22	B	603	CLA	C8
22	B	603	CLA	C2A
22	B	604	CLA	ND
22	B	605	CLA	ND
22	B	605	CLA	C8
22	B	606	CLA	ND
22	B	606	CLA	C8
22	B	607	CLA	ND
22	B	607	CLA	C8
22	B	609	CLA	ND
22	B	609	CLA	C2A
22	B	610	CLA	ND
22	B	610	CLA	C2A
22	B	611	CLA	ND
22	B	612	CLA	ND
22	B	612	CLA	C3A
22	B	612	CLA	C8
22	B	612	CLA	C2A
22	B	613	CLA	ND
22	B	613	CLA	C8
22	B	613	CLA	C2A
22	B	614	CLA	ND
22	B	614	CLA	C8
22	B	614	CLA	C2A
22	B	615	CLA	ND
22	B	615	CLA	C8
22	B	615	CLA	C2A
22	B	616	CLA	ND
22	B	616	CLA	C8
22	B	616	CLA	C3A
22	B	616	CLA	C2A
22	C	504	CLA	ND

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Mol	Chain	Res	Type	Atom
22	C	504	CLA	C8
22	C	505	CLA	C8
22	C	506	CLA	ND
22	C	506	CLA	C8
22	C	506	CLA	C2A
22	C	507	CLA	ND
22	C	507	CLA	C2A
22	C	508	CLA	C8
22	C	509	CLA	ND
22	C	509	CLA	C2A
22	C	510	CLA	C8
22	C	511	CLA	ND
22	C	511	CLA	C8
22	C	511	CLA	C2A
22	C	512	CLA	ND
22	C	513	CLA	ND
22	C	513	CLA	C3A
22	C	513	CLA	C2A
22	C	514	CLA	ND
22	C	514	CLA	C8
22	C	514	CLA	C2A
22	C	517	CLA	ND
22	C	517	CLA	C8
22	C	517	CLA	C3A
22	D	402	CLA	ND
22	D	402	CLA	C2A
22	D	407	CLA	ND
22	D	407	CLA	C8
22	D	408	CLA	ND
22	D	408	CLA	C8
22	D	408	CLA	C2A

All (535) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	A	404	PHO	O2A-C1-C2-C3
22	A	405	CLA	C3A-C2A-CAA-CBA
22	A	406	CLA	C3A-C2A-CAA-CBA
22	A	406	CLA	C11-C10-C8-C7
22	B	601	CLA	C11-C10-C8-C9
22	B	602	CLA	CHA-CBD-CGD-O1D
22	B	602	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	B	603	CLA	C1A-C2A-CAA-CBA
22	B	603	CLA	C2-C3-C5-C6
22	B	603	CLA	C4-C3-C5-C6
22	B	603	CLA	C11-C10-C8-C9
22	B	604	CLA	C3A-C2A-CAA-CBA
22	B	605	CLA	C1A-C2A-CAA-CBA
22	B	606	CLA	C1A-C2A-CAA-CBA
22	B	610	CLA	C1A-C2A-CAA-CBA
22	B	611	CLA	C3A-C2A-CAA-CBA
22	B	611	CLA	O2A-C1-C2-C3
22	B	613	CLA	C1A-C2A-CAA-CBA
22	B	615	CLA	C3A-C2A-CAA-CBA
22	B	616	CLA	C3A-C2A-CAA-CBA
22	C	503	CLA	O2A-C1-C2-C3
22	C	504	CLA	C1A-C2A-CAA-CBA
22	C	504	CLA	CHA-CBD-CGD-O1D
22	C	504	CLA	CHA-CBD-CGD-O2D
22	C	505	CLA	C1A-C2A-CAA-CBA
22	C	505	CLA	C3A-C2A-CAA-CBA
22	C	505	CLA	O2A-C1-C2-C3
22	C	506	CLA	C1A-C2A-CAA-CBA
22	C	507	CLA	C1A-C2A-CAA-CBA
22	C	513	CLA	C3A-C2A-CAA-CBA
22	C	514	CLA	O2A-C1-C2-C3
22	C	517	CLA	C1A-C2A-CAA-CBA
22	C	517	CLA	C3A-C2A-CAA-CBA
22	D	401	CLA	C1A-C2A-CAA-CBA
22	D	402	CLA	C1A-C2A-CAA-CBA
22	D	407	CLA	C3A-C2A-CAA-CBA
22	D	407	CLA	O2A-C1-C2-C3
22	D	407	CLA	C11-C10-C8-C9
22	D	408	CLA	C3A-C2A-CAA-CBA
23	A	407	BCR	C21-C22-C23-C24
23	A	407	BCR	C37-C22-C23-C24
23	B	617	BCR	C7-C8-C9-C10
23	B	617	BCR	C9-C10-C11-C12
23	B	617	BCR	C11-C12-C13-C14
23	B	617	BCR	C11-C12-C13-C35
23	B	617	BCR	C15-C16-C17-C18
23	B	617	BCR	C17-C18-C19-C20
23	B	617	BCR	C21-C22-C23-C24
23	B	617	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
23	B	618	BCR	C36-C18-C19-C20
23	B	619	BCR	C13-C14-C15-C16
23	B	619	BCR	C36-C18-C19-C20
23	C	515	BCR	C7-C8-C9-C10
23	C	515	BCR	C7-C8-C9-C34
23	C	515	BCR	C11-C12-C13-C14
23	C	515	BCR	C11-C12-C13-C35
23	C	515	BCR	C17-C18-C19-C20
23	C	515	BCR	C36-C18-C19-C20
23	C	516	BCR	C11-C12-C13-C14
23	C	516	BCR	C11-C12-C13-C35
23	C	516	BCR	C23-C24-C25-C30
23	C	518	BCR	C7-C8-C9-C10
23	C	518	BCR	C7-C8-C9-C34
23	C	518	BCR	C15-C16-C17-C18
23	C	518	BCR	C36-C18-C19-C20
23	C	518	BCR	C37-C22-C23-C24
23	F	102	BCR	C21-C22-C23-C24
23	F	102	BCR	C37-C22-C23-C24
23	H	101	BCR	C5-C6-C7-C8
23	H	101	BCR	C17-C18-C19-C20
23	H	101	BCR	C20-C21-C22-C37
23	H	101	BCR	C23-C24-C25-C26
23	H	101	BCR	C23-C24-C25-C30
23	K	101	BCR	C7-C8-C9-C10
23	K	101	BCR	C17-C18-C19-C20
23	K	101	BCR	C20-C21-C22-C37
23	K	101	BCR	C23-C24-C25-C26
23	K	101	BCR	C23-C24-C25-C30
26	D	405	PL9	C35-C34-C36-C37
22	B	616	CLA	CBD-CGD-O2D-CED
22	C	507	CLA	CBD-CGD-O2D-CED
22	C	517	CLA	CBD-CGD-O2D-CED
22	B	602	CLA	C4-C3-C5-C6
22	B	601	CLA	CBD-CGD-O2D-CED
22	C	504	CLA	C2A-CAA-CBA-CGA
22	C	507	CLA	C2A-CAA-CBA-CGA
22	C	510	CLA	C2A-CAA-CBA-CGA
23	C	515	BCR	C19-C20-C21-C22
23	C	516	BCR	C13-C14-C15-C16
23	C	518	BCR	C13-C14-C15-C16
22	B	609	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
26	D	405	PL9	C33-C34-C36-C37
22	B	616	CLA	O1D-CGD-O2D-CED
23	A	407	BCR	C19-C20-C21-C22
23	C	515	BCR	C13-C14-C15-C16
23	C	515	BCR	C15-C16-C17-C18
23	C	516	BCR	C15-C16-C17-C18
21	D	406	PHO	C8-C10-C11-C12
22	B	602	CLA	C2-C3-C5-C6
22	A	405	CLA	C6-C7-C8-C9
22	A	405	CLA	C11-C10-C8-C9
22	A	406	CLA	C6-C7-C8-C9
22	B	601	CLA	C6-C7-C8-C9
22	B	602	CLA	C11-C10-C8-C9
22	B	604	CLA	C6-C7-C8-C9
22	B	608	CLA	C11-C10-C8-C9
22	B	609	CLA	C6-C7-C8-C9
22	B	612	CLA	C11-C10-C8-C9
22	B	613	CLA	C6-C7-C8-C9
22	C	503	CLA	C6-C7-C8-C9
22	C	506	CLA	C11-C10-C8-C9
22	C	507	CLA	C11-C10-C8-C9
22	C	508	CLA	C11-C10-C8-C9
22	C	509	CLA	C6-C7-C8-C9
22	C	512	CLA	C6-C7-C8-C9
22	C	512	CLA	C11-C10-C8-C9
22	D	401	CLA	C6-C7-C8-C9
22	D	401	CLA	C11-C10-C8-C9
22	D	408	CLA	C11-C10-C8-C9
23	A	407	BCR	C36-C18-C19-C20
23	B	617	BCR	C7-C8-C9-C34
23	B	617	BCR	C36-C18-C19-C20
23	B	619	BCR	C11-C12-C13-C35
23	C	516	BCR	C37-C22-C23-C24
23	H	101	BCR	C11-C12-C13-C35
23	H	101	BCR	C37-C22-C23-C24
23	K	101	BCR	C11-C12-C13-C35
23	K	101	BCR	C37-C22-C23-C24
23	A	407	BCR	C17-C18-C19-C20
23	C	516	BCR	C7-C8-C9-C10
23	H	101	BCR	C7-C8-C9-C10
23	H	101	BCR	C11-C12-C13-C14
23	K	101	BCR	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
22	B	615	CLA	CBA-CGA-O2A-C1
22	B	612	CLA	C5-C6-C7-C8
22	B	605	CLA	C3-C5-C6-C7
22	B	602	CLA	C6-C7-C8-C10
22	B	604	CLA	C11-C10-C8-C7
22	B	610	CLA	C11-C10-C8-C7
22	B	614	CLA	C11-C10-C8-C7
22	C	504	CLA	C11-C10-C8-C7
22	C	509	CLA	C11-C10-C8-C7
22	C	510	CLA	C6-C7-C8-C10
22	C	513	CLA	C6-C7-C8-C10
22	C	514	CLA	C11-C10-C8-C7
22	D	402	CLA	C11-C10-C8-C7
22	B	614	CLA	C3-C5-C6-C7
22	B	615	CLA	O1A-CGA-O2A-C1
23	A	407	BCR	C9-C10-C11-C12
23	A	407	BCR	C13-C14-C15-C16
23	C	516	BCR	C9-C10-C11-C12
23	F	102	BCR	C19-C20-C21-C22
23	H	101	BCR	C19-C20-C21-C22
23	K	101	BCR	C19-C20-C21-C22
22	C	517	CLA	O1D-CGD-O2D-CED
22	B	614	CLA	C2A-CAA-CBA-CGA
23	B	617	BCR	C13-C14-C15-C16
22	A	405	CLA	C3-C5-C6-C7
22	C	507	CLA	O1D-CGD-O2D-CED
24	A	408	LHG	C32-C33-C34-C35
21	D	406	PHO	C4-C3-C5-C6
22	C	504	CLA	C11-C10-C8-C9
22	C	505	CLA	C11-C10-C8-C9
22	C	505	CLA	C14-C13-C15-C16
22	C	506	CLA	C11-C12-C13-C14
23	B	619	BCR	C37-C22-C23-C24
23	C	516	BCR	C7-C8-C9-C34
23	H	101	BCR	C7-C8-C9-C34
23	K	101	BCR	C7-C8-C9-C34
23	B	619	BCR	C21-C22-C23-C24
24	A	408	LHG	C11-C12-C13-C14
25	D	403	LMG	C37-C38-C39-C40
25	D	404	LMG	O6-C1-O1-C7
25	3	101	LMG	C32-C33-C34-C35
22	B	601	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	B	608	CLA	C3A-C2A-CAA-CBA
22	C	507	CLA	C3A-C2A-CAA-CBA
22	B	605	CLA	C5-C6-C7-C8
25	C	502	LMG	C15-C16-C17-C18
25	3	101	LMG	C37-C38-C39-C40
22	B	601	CLA	C4-C3-C5-C6
22	B	616	CLA	C4-C3-C5-C6
22	B	616	CLA	C2-C3-C5-C6
26	D	405	PL9	C13-C14-C16-C17
22	C	509	CLA	C3-C5-C6-C7
23	B	617	BCR	C23-C24-C25-C30
23	H	101	BCR	C1-C6-C7-C8
23	K	101	BCR	C1-C6-C7-C8
23	K	101	BCR	C5-C6-C7-C8
25	I	101	LMG	C39-C40-C41-C42
22	B	606	CLA	CBA-CGA-O2A-C1
25	C	501	LMG	C22-C23-C24-C25
26	D	405	PL9	C47-C48-C49-C50
26	D	405	PL9	C47-C48-C49-C51
21	D	406	PHO	C2-C3-C5-C6
22	B	608	CLA	C6-C7-C8-C10
22	B	611	CLA	C6-C7-C8-C10
22	B	615	CLA	C12-C13-C15-C16
22	B	616	CLA	C6-C7-C8-C10
22	C	505	CLA	C12-C13-C15-C16
22	C	514	CLA	C6-C7-C8-C10
22	C	517	CLA	C11-C10-C8-C7
22	B	606	CLA	O1A-CGA-O2A-C1
23	H	101	BCR	C9-C10-C11-C12
25	I	101	LMG	C16-C17-C18-C19
22	B	602	CLA	C5-C6-C7-C8
25	C	501	LMG	C11-C10-O7-C8
22	D	401	CLA	CBD-CGD-O2D-CED
25	D	404	LMG	C13-C14-C15-C16
26	D	405	PL9	C15-C14-C16-C17
21	D	406	PHO	C11-C10-C8-C9
22	B	603	CLA	C6-C7-C8-C9
22	B	603	CLA	C11-C12-C13-C14
22	B	607	CLA	C11-C10-C8-C9
22	B	613	CLA	C11-C10-C8-C9
22	B	616	CLA	C6-C7-C8-C9
22	B	604	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	B	607	CLA	C1A-C2A-CAA-CBA
22	B	611	CLA	C1A-C2A-CAA-CBA
22	B	612	CLA	C1A-C2A-CAA-CBA
22	C	509	CLA	C1A-C2A-CAA-CBA
22	C	511	CLA	C1A-C2A-CAA-CBA
22	C	512	CLA	C1A-C2A-CAA-CBA
22	D	407	CLA	C1A-C2A-CAA-CBA
22	D	408	CLA	C1A-C2A-CAA-CBA
23	K	101	BCR	C9-C10-C11-C12
22	C	505	CLA	C4-C3-C5-C6
25	D	404	LMG	O1-C7-C8-C9
24	A	408	LHG	C27-C28-C29-C30
26	D	405	PL9	C46-C47-C48-C49
23	B	618	BCR	C16-C17-C18-C36
25	I	101	LMG	O6-C5-C6-O5
22	A	406	CLA	C4-C3-C5-C6
22	C	505	CLA	CBA-CGA-O2A-C1
22	C	517	CLA	C8-C10-C11-C12
22	B	611	CLA	C5-C6-C7-C8
25	C	501	LMG	O9-C10-O7-C8
22	A	406	CLA	C2-C3-C5-C6
22	B	605	CLA	C6-C7-C8-C10
22	B	606	CLA	C11-C12-C13-C15
22	B	607	CLA	C6-C7-C8-C10
22	B	607	CLA	C11-C10-C8-C7
22	B	612	CLA	C6-C7-C8-C10
22	C	506	CLA	C6-C7-C8-C10
22	C	507	CLA	C6-C7-C8-C10
22	C	510	CLA	C11-C10-C8-C7
21	A	404	PHO	C6-C7-C8-C9
22	A	406	CLA	C11-C10-C8-C9
22	B	605	CLA	C11-C10-C8-C9
22	B	609	CLA	C11-C10-C8-C9
22	B	615	CLA	C14-C13-C15-C16
22	B	616	CLA	C11-C10-C8-C9
22	C	507	CLA	C14-C13-C15-C16
22	C	513	CLA	C11-C10-C8-C9
22	D	402	CLA	C6-C7-C8-C9
22	D	407	CLA	C6-C7-C8-C9
23	H	101	BCR	C21-C22-C23-C24
23	K	101	BCR	C21-C22-C23-C24
25	3	101	LMG	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
22	B	610	CLA	C4-C3-C5-C6
22	B	601	CLA	C2-C3-C5-C6
26	D	405	PL9	C43-C44-C46-C47
25	D	403	LMG	C22-C23-C24-C25
22	B	603	CLA	C3A-C2A-CAA-CBA
22	B	606	CLA	C3A-C2A-CAA-CBA
22	B	607	CLA	C3A-C2A-CAA-CBA
22	B	612	CLA	C3A-C2A-CAA-CBA
22	D	401	CLA	C3A-C2A-CAA-CBA
25	D	403	LMG	C12-C13-C14-C15
22	B	604	CLA	CBA-CGA-O2A-C1
22	B	610	CLA	CBA-CGA-O2A-C1
22	D	401	CLA	CBA-CGA-O2A-C1
22	B	602	CLA	C8-C10-C11-C12
25	C	502	LMG	C18-C19-C20-C21
25	F	101	LMG	C15-C16-C17-C18
22	B	610	CLA	C2-C3-C5-C6
22	C	505	CLA	C2-C3-C5-C6
22	C	511	CLA	C2A-CAA-CBA-CGA
22	C	505	CLA	O1A-CGA-O2A-C1
25	D	404	LMG	O1-C7-C8-O7
25	F	101	LMG	O1-C7-C8-O7
22	B	606	CLA	C11-C10-C8-C9
22	B	611	CLA	C11-C10-C8-C9
22	C	508	CLA	C6-C7-C8-C9
22	D	407	CLA	C2C-C3C-CAC-CBC
24	A	408	LHG	C5-C4-O6-P
22	D	401	CLA	O1A-CGA-O2A-C1
22	C	514	CLA	C2A-CAA-CBA-CGA
23	B	617	BCR	C23-C24-C25-C26
23	B	618	BCR	C23-C24-C25-C26
23	B	618	BCR	C23-C24-C25-C30
23	C	516	BCR	C1-C6-C7-C8
23	C	516	BCR	C23-C24-C25-C26
25	C	501	LMG	C40-C41-C42-C43
23	B	619	BCR	C17-C18-C19-C20
22	B	610	CLA	C2C-C3C-CAC-CBC
25	C	501	LMG	C29-C30-C31-C32
21	A	404	PHO	C11-C10-C8-C7
22	A	405	CLA	C6-C7-C8-C10
22	A	405	CLA	C12-C13-C15-C16
22	B	601	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
22	B	602	CLA	C12-C13-C15-C16
22	B	610	CLA	C6-C7-C8-C10
22	C	504	CLA	C6-C7-C8-C10
22	C	507	CLA	C11-C10-C8-C7
22	C	507	CLA	C12-C13-C15-C16
22	C	510	CLA	C11-C12-C13-C15
22	B	609	CLA	O1D-CGD-O2D-CED
23	H	101	BCR	C13-C14-C15-C16
23	K	101	BCR	C13-C14-C15-C16
22	D	407	CLA	C4C-C3C-CAC-CBC
22	B	613	CLA	C5-C6-C7-C8
21	D	406	PHO	CAD-CBD-CGD-O2D
22	A	406	CLA	CAD-CBD-CGD-O2D
22	B	609	CLA	CAD-CBD-CGD-O2D
22	C	503	CLA	CAD-CBD-CGD-O2D
22	C	511	CLA	CAD-CBD-CGD-O2D
25	D	404	LMG	C9-C8-O7-C10
23	C	518	BCR	C6-C7-C8-C9
26	D	405	PL9	C44-C46-C47-C48
25	F	101	LMG	O1-C7-C8-C9
22	B	604	CLA	O1A-CGA-O2A-C1
22	B	610	CLA	O1A-CGA-O2A-C1
22	B	612	CLA	C8-C10-C11-C12
22	B	605	CLA	CHA-CBD-CGD-O1D
22	B	605	CLA	CHA-CBD-CGD-O2D
22	C	517	CLA	CHA-CBD-CGD-O1D
22	C	517	CLA	CHA-CBD-CGD-O2D
22	B	603	CLA	C3-C5-C6-C7
22	C	505	CLA	C8-C10-C11-C12
25	D	404	LMG	C22-C23-C24-C25
22	B	614	CLA	C6-C7-C8-C9
22	C	514	CLA	C11-C10-C8-C9
22	C	517	CLA	C6-C7-C8-C9
25	3	101	LMG	C29-C30-C31-C32
22	C	514	CLA	C1A-C2A-CAA-CBA
25	C	502	LMG	C28-C29-C30-C31
25	C	501	LMG	O6-C1-O1-C7
25	3	101	LMG	C13-C14-C15-C16
22	B	605	CLA	CAD-CBD-CGD-O1D
25	D	404	LMG	C39-C40-C41-C42
25	D	404	LMG	C14-C15-C16-C17
22	A	405	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
22	B	601	CLA	C6-C7-C8-C10
22	B	601	CLA	C11-C10-C8-C7
22	B	604	CLA	C6-C7-C8-C10
22	B	615	CLA	C6-C7-C8-C10
22	C	511	CLA	C6-C7-C8-C10
22	C	512	CLA	C11-C10-C8-C7
22	D	401	CLA	C6-C7-C8-C10
22	B	602	CLA	C2A-CAA-CBA-CGA
22	C	505	CLA	C16-C17-C18-C20
25	F	101	LMG	C10-C11-C12-C13
25	D	404	LMG	C8-C7-O1-C1
22	C	504	CLA	C3-C5-C6-C7
22	C	511	CLA	C4-C3-C5-C6
22	A	405	CLA	C14-C13-C15-C16
22	C	504	CLA	C6-C7-C8-C9
22	C	510	CLA	C11-C12-C13-C14
22	C	511	CLA	C11-C10-C8-C9
23	B	618	BCR	C17-C18-C19-C20
22	C	510	CLA	C8-C10-C11-C12
25	F	101	LMG	C7-C8-O7-C10
22	C	503	CLA	C2A-CAA-CBA-CGA
22	B	607	CLA	C2-C1-O2A-CGA
22	C	505	CLA	C2-C1-O2A-CGA
22	C	509	CLA	C2-C1-O2A-CGA
22	B	606	CLA	C4-C3-C5-C6
22	B	611	CLA	C4-C3-C5-C6
23	C	516	BCR	C5-C6-C7-C8
22	B	606	CLA	C2-C3-C5-C6
25	D	404	LMG	C2-C1-O1-C7
22	C	504	CLA	C10-C11-C12-C13
22	C	511	CLA	C10-C11-C12-C13
25	C	501	LMG	C12-C13-C14-C15
25	C	501	LMG	C15-C16-C17-C18
22	B	609	CLA	C11-C10-C8-C7
22	B	612	CLA	C11-C12-C13-C15
22	B	613	CLA	C11-C10-C8-C7
22	C	506	CLA	C11-C12-C13-C15
22	B	608	CLA	C6-C7-C8-C9
22	B	611	CLA	C6-C7-C8-C9
22	B	612	CLA	C11-C12-C13-C14
22	C	505	CLA	C6-C7-C8-C9
22	C	514	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
22	C	510	CLA	O1A-CGA-O2A-C1
22	B	616	CLA	C8-C10-C11-C12
25	D	404	LMG	C40-C41-C42-C43
21	A	404	PHO	C16-C17-C18-C19
22	D	402	CLA	C8-C10-C11-C12
22	B	613	CLA	C2-C1-O2A-CGA
22	C	512	CLA	C3A-C2A-CAA-CBA
22	B	607	CLA	C4-C3-C5-C6
22	B	603	CLA	C2C-C3C-CAC-CBC
22	C	511	CLA	C2-C3-C5-C6
22	B	614	CLA	C11-C10-C8-C9
22	D	408	CLA	C6-C7-C8-C9
22	B	615	CLA	C5-C6-C7-C8
27	E	101	HEM	CAD-CBD-CGD-O2D
25	C	501	LMG	C7-C8-O7-C10
25	C	501	LMG	C9-C8-O7-C10
22	A	405	CLA	C1A-C2A-CAA-CBA
22	B	609	CLA	C1A-C2A-CAA-CBA
22	C	513	CLA	C1A-C2A-CAA-CBA
22	C	505	CLA	CAA-CBA-CGA-O2A
22	B	606	CLA	C6-C7-C8-C10
22	B	612	CLA	C12-C13-C15-C16
22	C	509	CLA	C6-C7-C8-C10
27	E	101	HEM	CAD-CBD-CGD-O1D
22	C	517	CLA	C2A-CAA-CBA-CGA
24	A	408	LHG	O6-C4-C5-O7
22	B	607	CLA	CBA-CGA-O2A-C1
22	C	506	CLA	C13-C15-C16-C17
22	B	611	CLA	C2-C3-C5-C6
25	C	502	LMG	C23-C24-C25-C26
22	B	607	CLA	O1A-CGA-O2A-C1
23	C	518	BCR	C1-C6-C7-C8
22	B	607	CLA	C2-C3-C5-C6
22	C	509	CLA	C2A-CAA-CBA-CGA
25	D	403	LMG	C40-C41-C42-C43
24	A	408	LHG	O6-C4-C5-C6
22	D	401	CLA	O1D-CGD-O2D-CED
26	D	405	PL9	C29-C31-C32-C33
22	A	405	CLA	C11-C10-C8-C7
22	C	511	CLA	C11-C10-C8-C7
22	D	402	CLA	C6-C7-C8-C10
22	D	408	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
22	C	505	CLA	C10-C11-C12-C13
25	C	501	LMG	C2-C1-O1-C7
22	C	505	CLA	CBD-CGD-O2D-CED
21	A	404	PHO	C16-C17-C18-C20
23	A	407	BCR	C11-C10-C9-C34
22	B	612	CLA	CAA-CBA-CGA-O2A
21	D	406	PHO	C6-C7-C8-C9
22	B	606	CLA	C6-C7-C8-C9
22	B	606	CLA	C11-C12-C13-C14
22	B	615	CLA	C11-C10-C8-C9
22	C	503	CLA	C11-C10-C8-C9
22	C	507	CLA	C6-C7-C8-C9
22	C	504	CLA	C3A-C2A-CAA-CBA
22	D	402	CLA	C3A-C2A-CAA-CBA
22	B	613	CLA	CAA-CBA-CGA-O2A
22	D	402	CLA	CAA-CBA-CGA-O2A
21	A	404	PHO	CAD-CBD-CGD-O2D
25	F	101	LMG	C9-C8-O7-C10
21	A	404	PHO	C10-C11-C12-C13
22	C	504	CLA	CAA-CBA-CGA-O2A
22	D	401	CLA	C2-C3-C5-C6
26	D	405	PL9	C39-C41-C42-C43
25	3	101	LMG	C40-C41-C42-C43
22	D	402	CLA	C13-C15-C16-C17
22	B	614	CLA	CAA-CBA-CGA-O2A
23	B	617	BCR	C10-C11-C12-C13
22	B	608	CLA	O2A-C1-C2-C3
22	C	509	CLA	O2A-C1-C2-C3
22	B	611	CLA	CBA-CGA-O2A-C1
25	C	501	LMG	C42-C43-C44-C45
22	B	606	CLA	CHA-CBD-CGD-O1D
22	B	606	CLA	CHA-CBD-CGD-O2D
22	C	506	CLA	CHA-CBD-CGD-O1D
22	C	506	CLA	CHA-CBD-CGD-O2D
22	C	514	CLA	CHA-CBD-CGD-O1D
22	C	514	CLA	CHA-CBD-CGD-O2D
27	E	101	HEM	CAA-CBA-CGA-O2A
25	C	501	LMG	O8-C28-C29-C30
23	C	516	BCR	C12-C13-C14-C15
25	C	501	LMG	O1-C7-C8-O7
22	B	611	CLA	O1A-CGA-O2A-C1
25	I	101	LMG	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
22	C	510	CLA	CBA-CGA-O2A-C1
22	B	611	CLA	CAA-CBA-CGA-O2A
22	A	406	CLA	C6-C7-C8-C10
22	B	613	CLA	C6-C7-C8-C10
22	B	614	CLA	C11-C12-C13-C15
22	C	510	CLA	C16-C17-C18-C19
22	A	405	CLA	C11-C12-C13-C14
22	B	615	CLA	C6-C7-C8-C9
22	C	506	CLA	C6-C7-C8-C9
22	C	510	CLA	C6-C7-C8-C9
22	D	407	CLA	CAA-CBA-CGA-O2A
25	C	502	LMG	O8-C28-C29-C30
22	C	512	CLA	C2A-CAA-CBA-CGA
26	D	405	PL9	C16-C17-C18-C19
26	D	405	PL9	C26-C27-C28-C29
22	B	612	CLA	CAA-CBA-CGA-O1A
22	B	614	CLA	C1A-C2A-CAA-CBA
22	B	615	CLA	C1A-C2A-CAA-CBA
22	C	508	CLA	C1A-C2A-CAA-CBA
22	B	603	CLA	C15-C16-C17-C18
25	F	101	LMG	O6-C5-C6-O5
22	D	402	CLA	CAA-CBA-CGA-O1A
25	C	501	LMG	O10-C28-C29-C30
25	3	101	LMG	C30-C31-C32-C33
25	C	501	LMG	O1-C7-C8-C9
22	B	614	CLA	CAA-CBA-CGA-O1A
25	C	502	LMG	O10-C28-C29-C30
25	I	101	LMG	C15-C16-C17-C18
27	E	101	HEM	CAA-CBA-CGA-O1A
22	C	514	CLA	C16-C17-C18-C20
22	D	407	CLA	CAA-CBA-CGA-O1A
25	C	501	LMG	O9-C10-C11-C12
22	A	406	CLA	CAA-CBA-CGA-O2A
25	C	501	LMG	O7-C10-C11-C12
23	C	518	BCR	C5-C6-C7-C8
25	3	101	LMG	C14-C15-C16-C17
22	C	504	CLA	CAA-CBA-CGA-O1A
22	C	512	CLA	C5-C6-C7-C8
25	C	502	LMG	C38-C39-C40-C41
22	C	510	CLA	CAA-CBA-CGA-O2A
22	B	606	CLA	CAD-CBD-CGD-O1D
22	C	506	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
22	B	602	CLA	C14-C13-C15-C16
22	B	612	CLA	C6-C7-C8-C9
22	B	611	CLA	CAA-CBA-CGA-O1A
22	C	503	CLA	CAA-CBA-CGA-O2A
22	B	607	CLA	CAA-CBA-CGA-O2A
22	C	510	CLA	CAA-CBA-CGA-O1A
25	D	403	LMG	C24-C25-C26-C27
22	B	605	CLA	C11-C10-C8-C7
22	B	608	CLA	C11-C10-C8-C7
22	C	503	CLA	C6-C7-C8-C10
22	C	517	CLA	C11-C12-C13-C15
22	D	401	CLA	C12-C13-C15-C16
22	C	512	CLA	CAA-CBA-CGA-O2A
23	C	516	BCR	C21-C22-C23-C24
22	B	607	CLA	CAA-CBA-CGA-O1A
22	C	506	CLA	CAA-CBA-CGA-O1A
22	C	512	CLA	CAA-CBA-CGA-O1A
22	A	405	CLA	CAA-CBA-CGA-O2A
24	A	408	LHG	C29-C30-C31-C32
22	B	610	CLA	C4C-C3C-CAC-CBC
22	D	401	CLA	C4C-C3C-CAC-CBC
22	A	406	CLA	CAA-CBA-CGA-O1A
22	D	401	CLA	C4-C3-C5-C6
26	D	405	PL9	C45-C44-C46-C47

There are no ring outliers.

47 monomers are involved in 109 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	K	101	BCR	11	0
22	B	607	CLA	2	0
23	H	101	BCR	15	0
23	C	516	BCR	3	0
22	D	402	CLA	2	0
22	B	604	CLA	2	0
22	B	614	CLA	3	0
22	D	401	CLA	2	0
22	C	513	CLA	3	0
23	A	407	BCR	1	0
25	3	101	LMG	2	0
25	I	101	LMG	2	0
22	B	606	CLA	1	0

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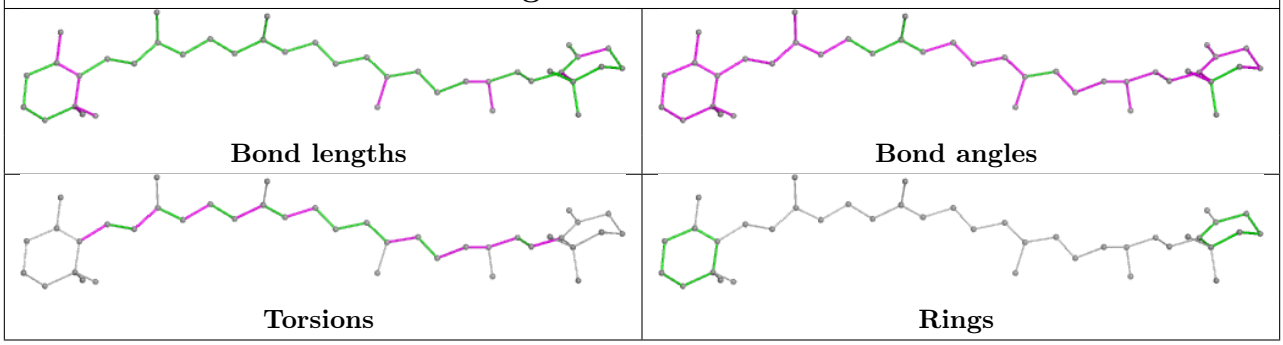
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	C	505	CLA	4	0
27	E	101	HEM	3	0
21	D	406	PHO	3	0
22	B	608	CLA	1	0
22	C	514	CLA	1	0
22	B	612	CLA	2	0
22	B	601	CLA	2	0
22	C	510	CLA	3	0
22	C	503	CLA	4	0
23	B	619	BCR	1	0
22	C	504	CLA	3	0
25	D	404	LMG	1	0
22	C	517	CLA	4	0
23	C	515	BCR	4	0
22	B	613	CLA	4	0
22	B	603	CLA	4	0
23	B	617	BCR	2	0
23	C	518	BCR	1	0
22	B	602	CLA	2	0
22	B	609	CLA	11	0
22	B	615	CLA	1	0
22	A	406	CLA	2	0
22	C	511	CLA	5	0
23	F	102	BCR	1	0
22	B	611	CLA	1	0
21	A	404	PHO	2	0
22	C	506	CLA	1	0
22	B	610	CLA	2	0
22	D	407	CLA	3	0
25	D	403	LMG	1	0
22	B	605	CLA	2	0
26	D	405	PL9	4	0
22	D	408	CLA	3	0
22	C	509	CLA	2	0

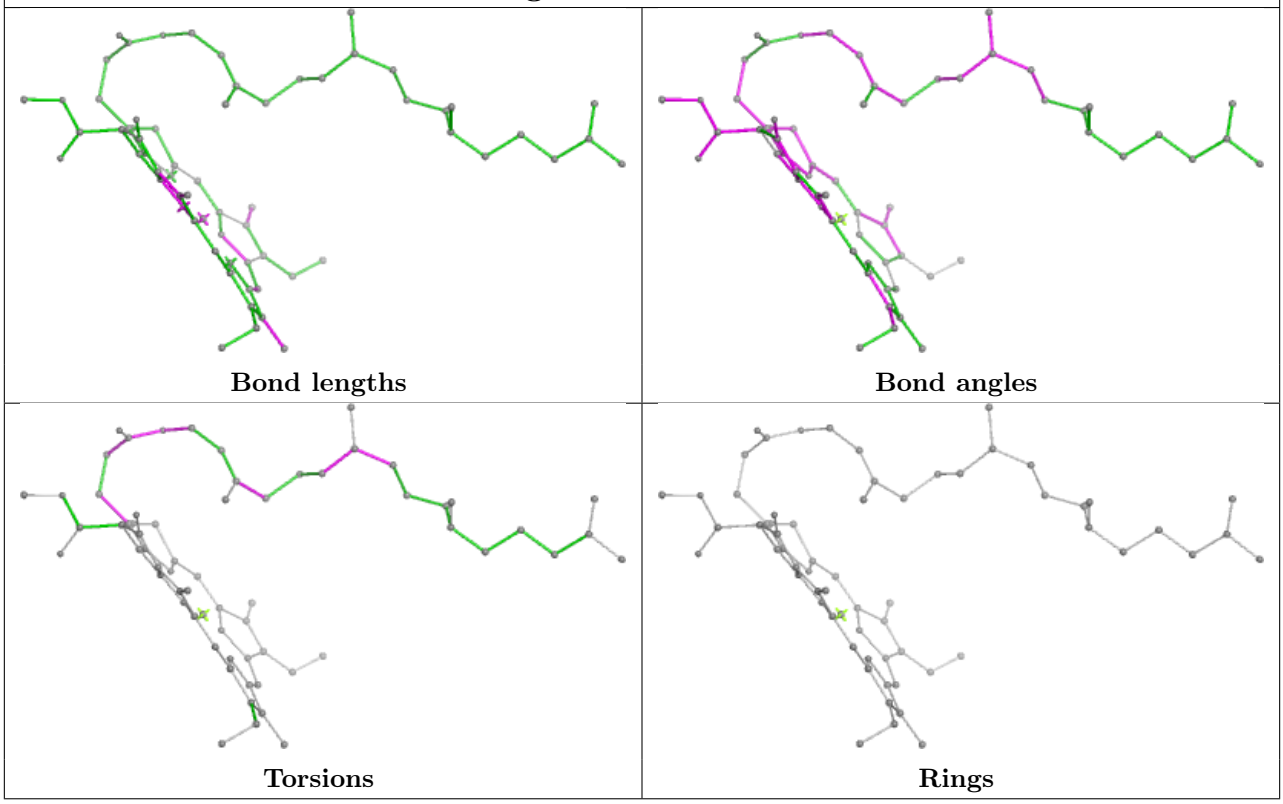
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

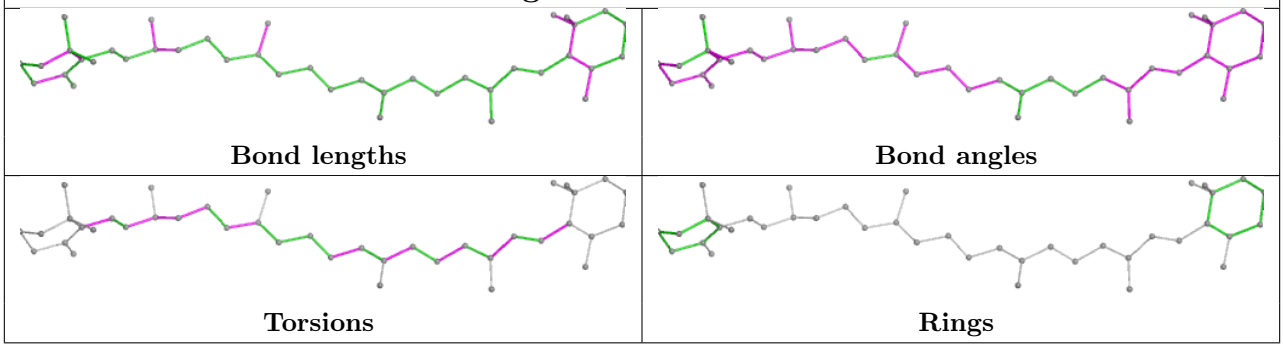
Ligand BCR K 101



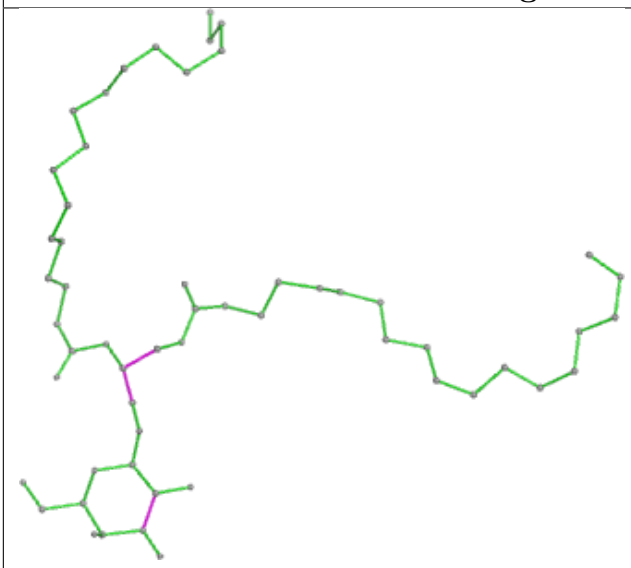
Ligand CLA B 607



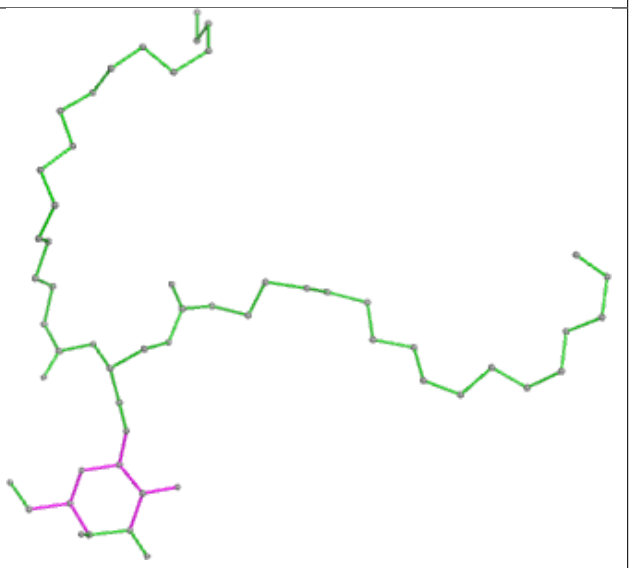
Ligand BCR H 101



Ligand LMG C 502

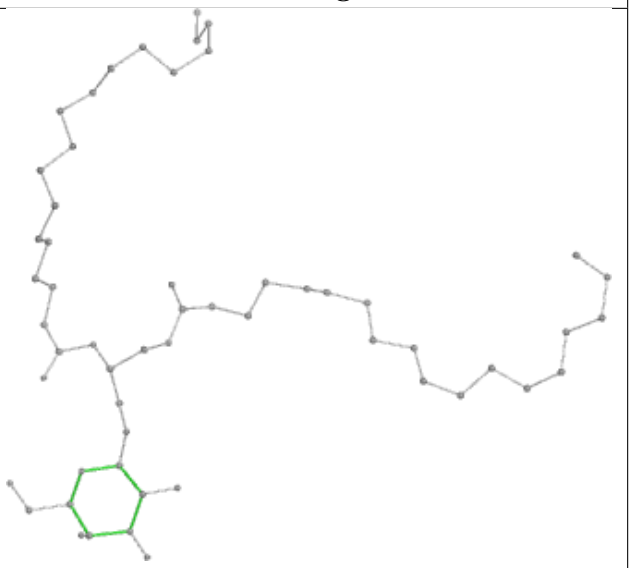


Bond lengths



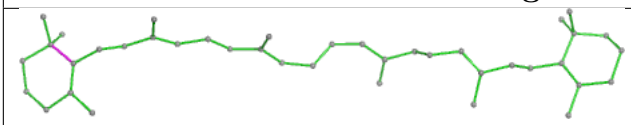
Bond angles

Torsions

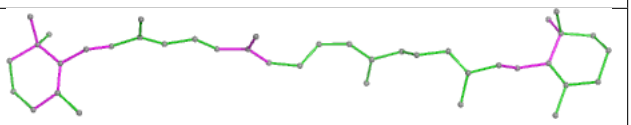


Rings

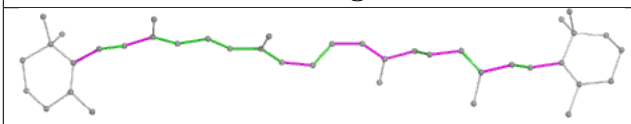
Ligand BCR C 516



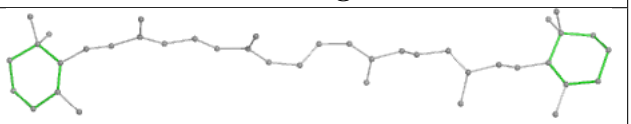
Bond lengths



Bond angles

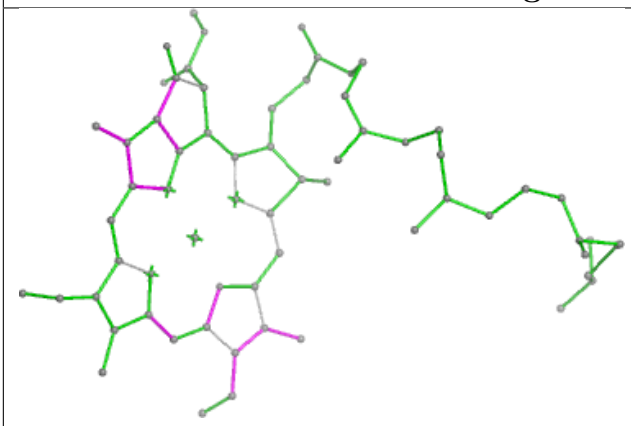


Torsions

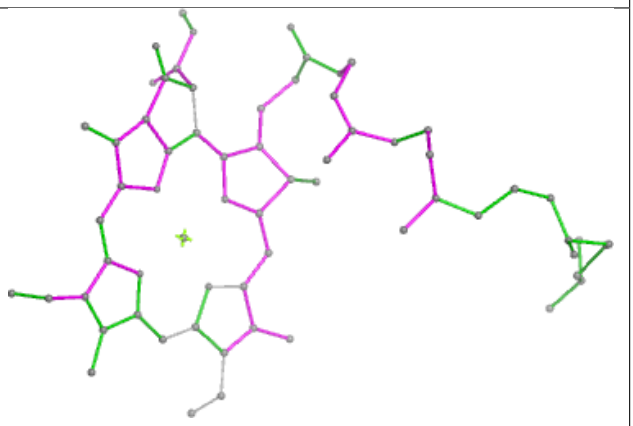


Rings

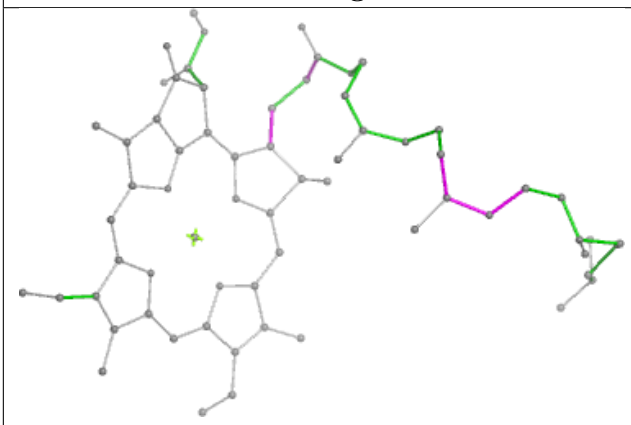
Ligand CLA D 402



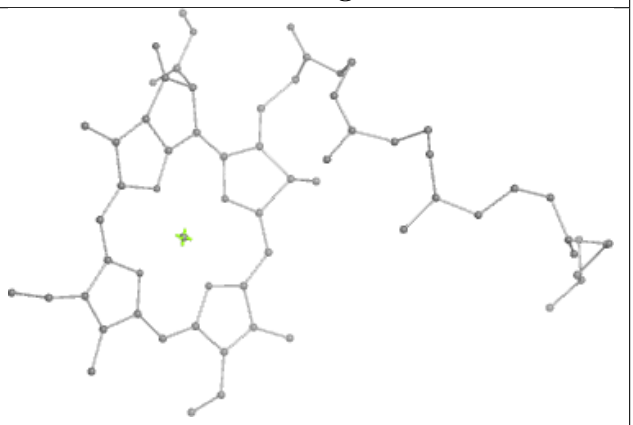
Bond lengths



Bond angles

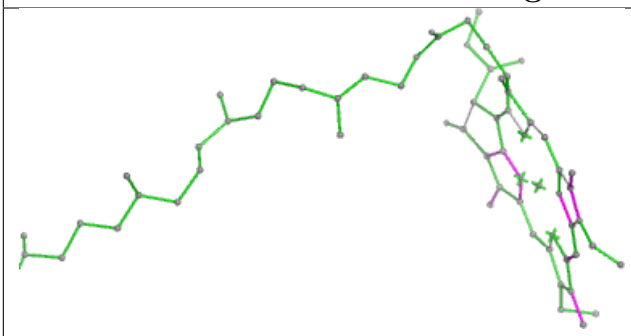


Torsions

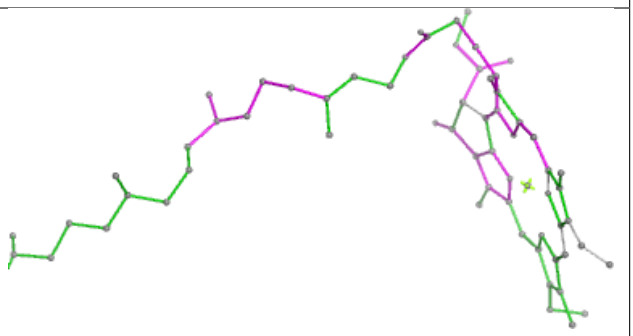


Rings

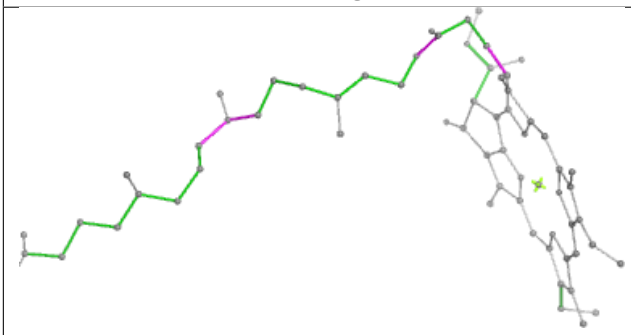
Ligand CLA B 604



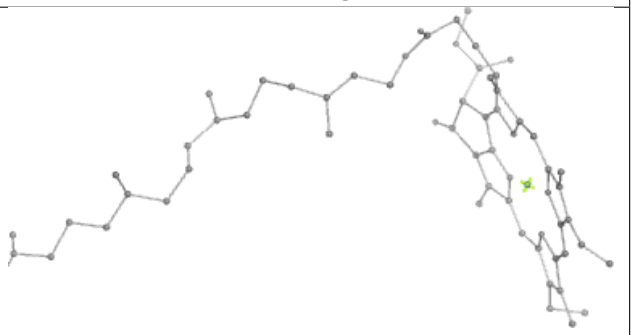
Bond lengths



Bond angles

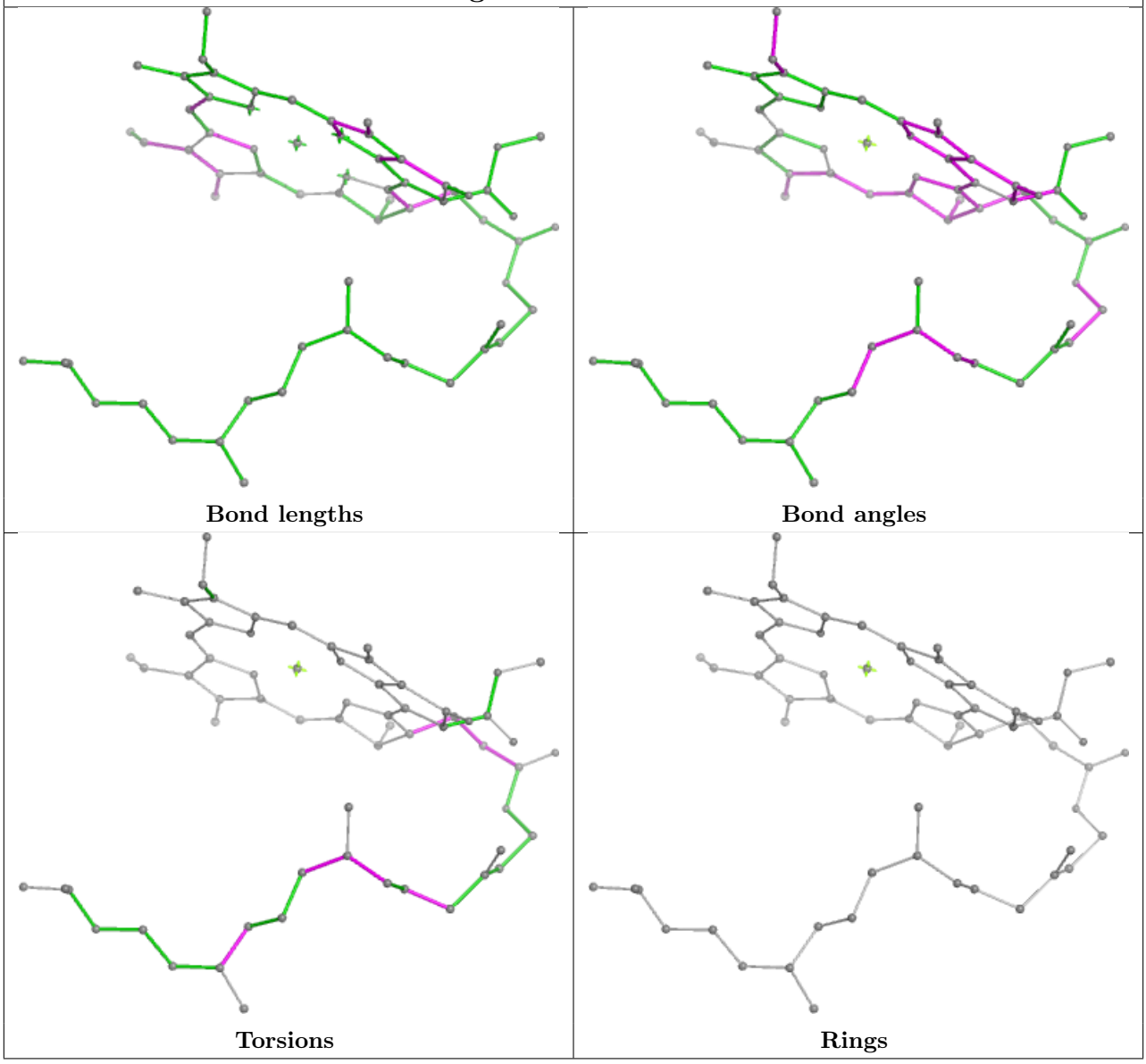


Torsions

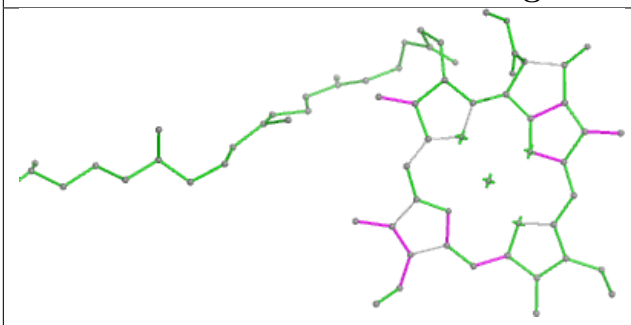


Rings

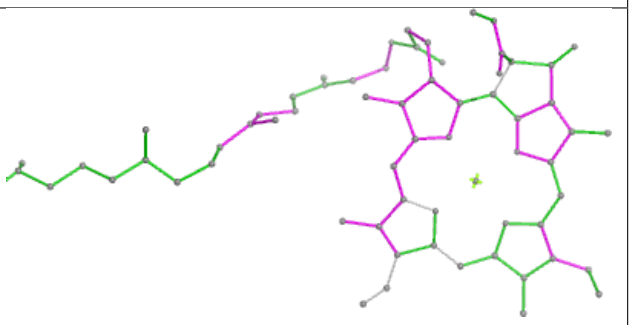
Ligand CLA B 614



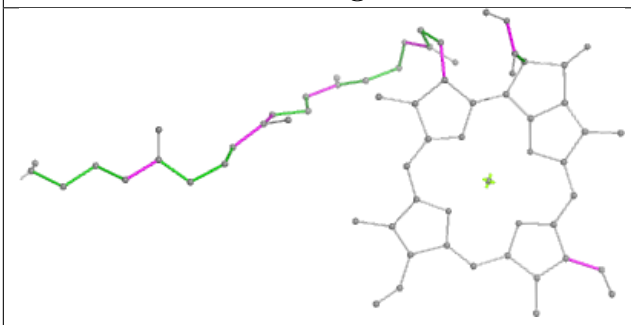
Ligand CLA D 401



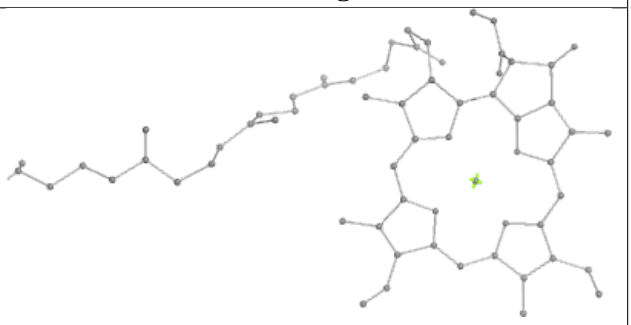
Bond lengths



Bond angles

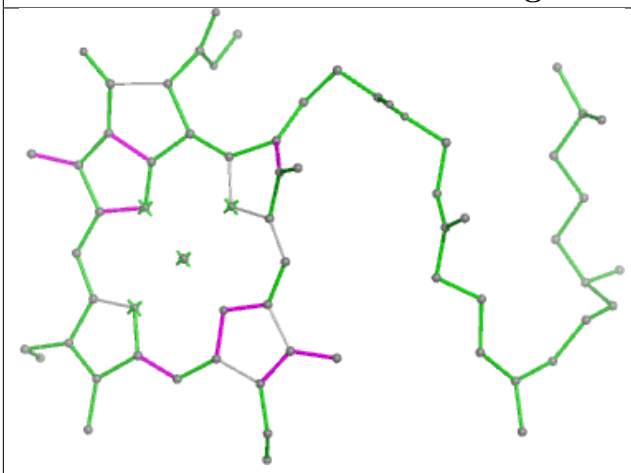


Torsions

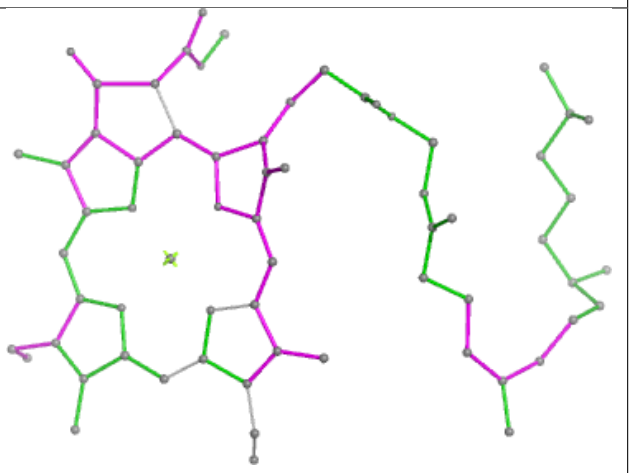


Rings

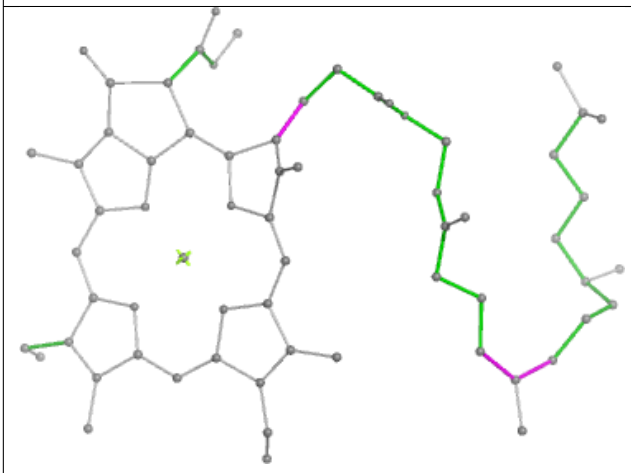
Ligand CLA C 513



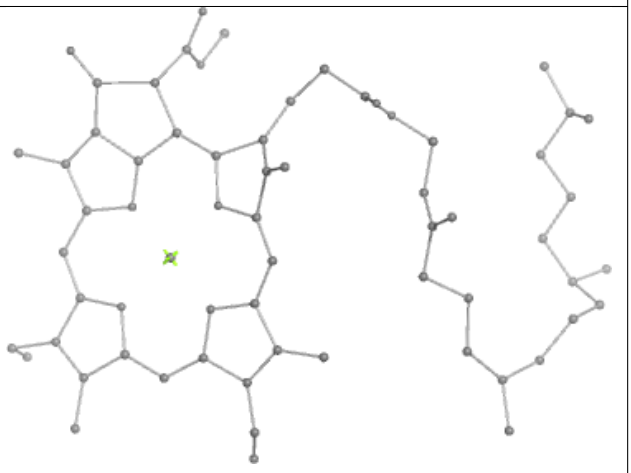
Bond lengths



Bond angles

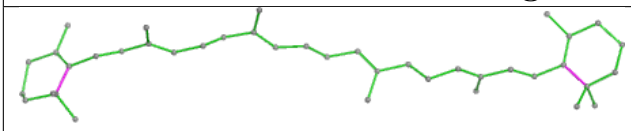


Torsions

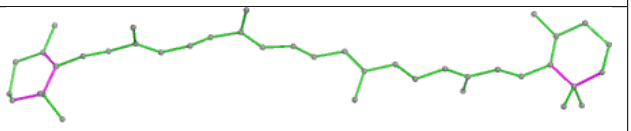


Rings

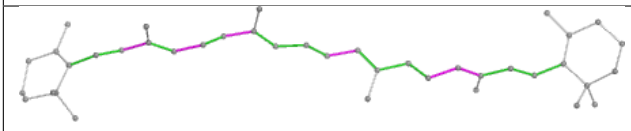
Ligand BCR A 407



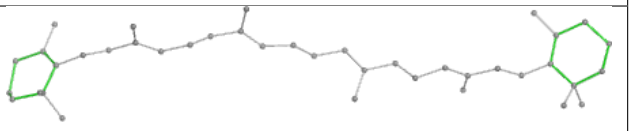
Bond lengths



Bond angles



Torsions

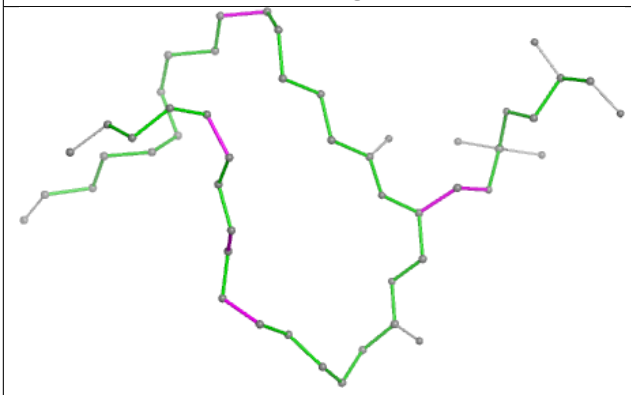


Rings

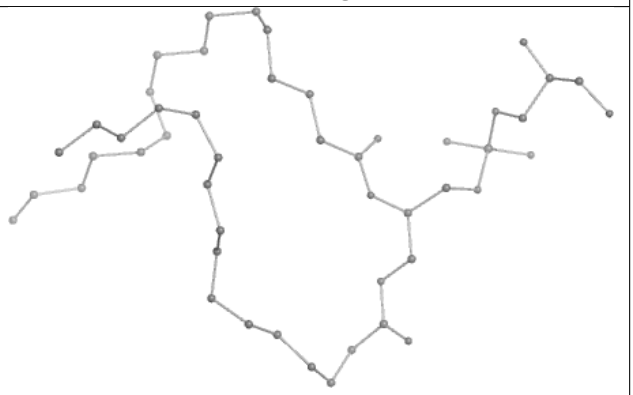
Ligand LHG A 408

Bond lengths

Bond angles



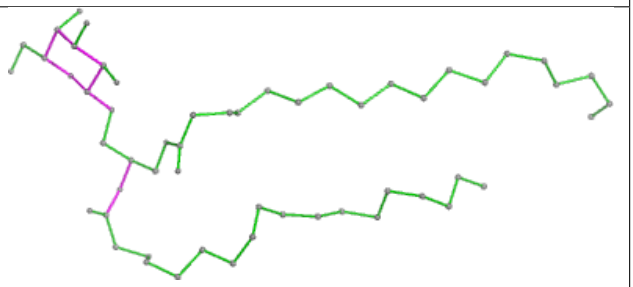
Torsions



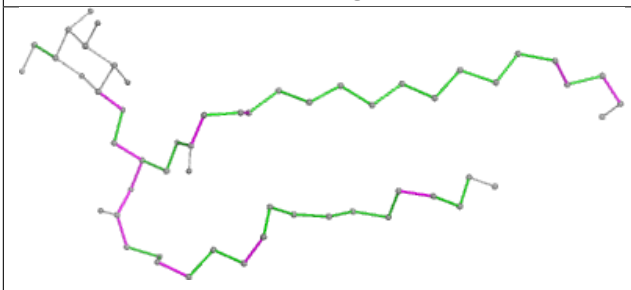
Rings

Ligand LMG C 501

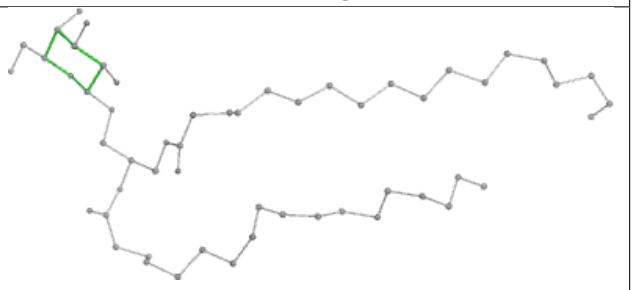
Bond lengths



Bond angles

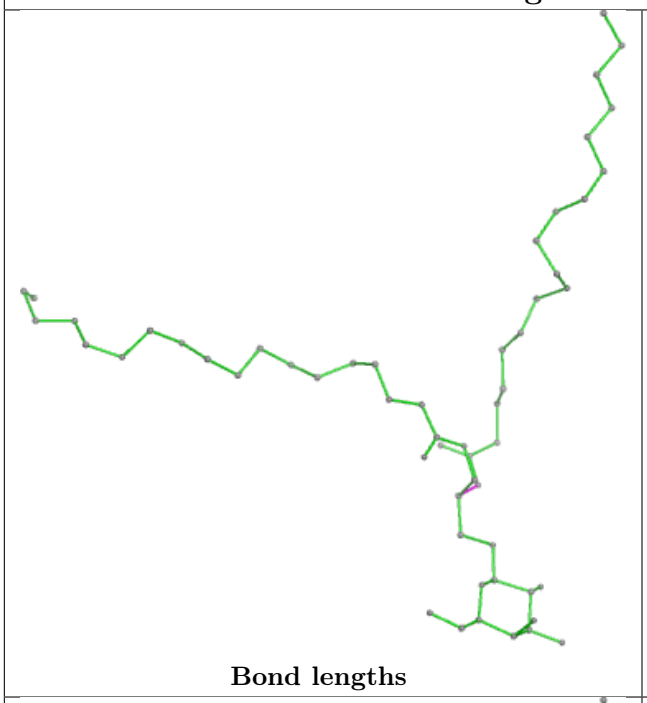


Torsions

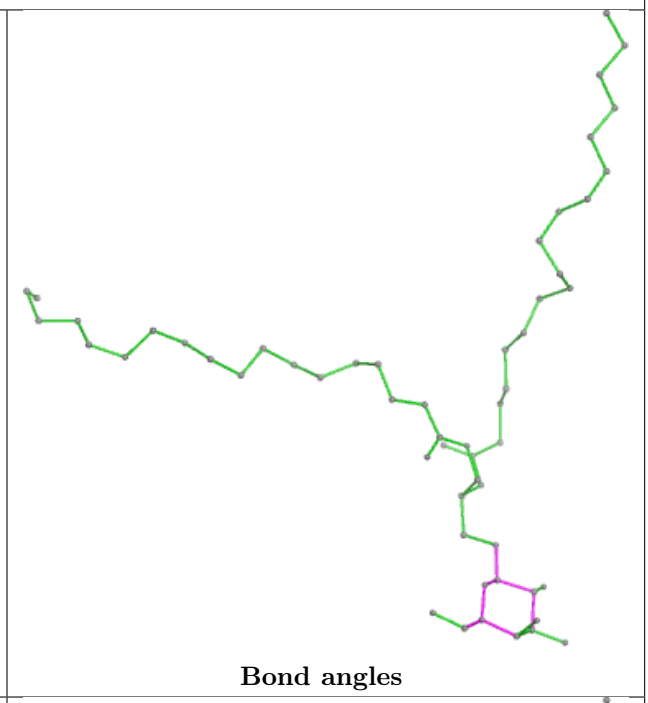


Rings

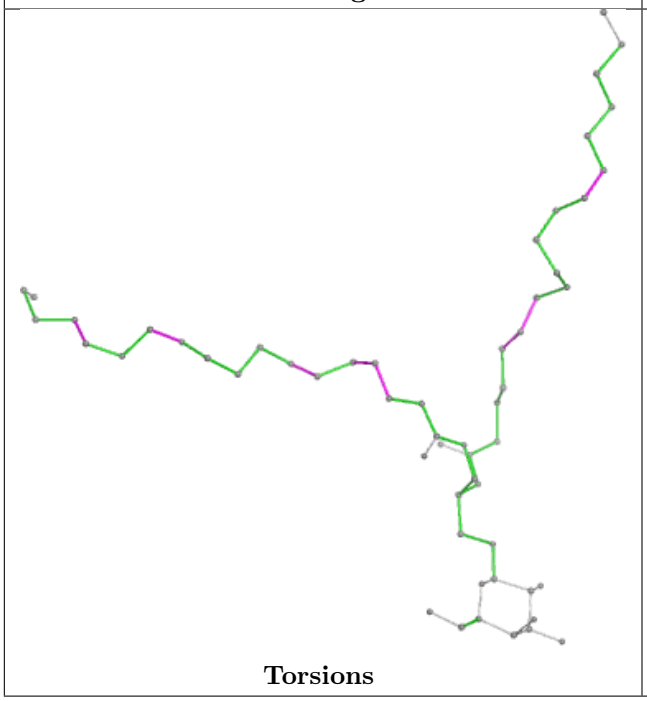
Ligand LMG 3 101



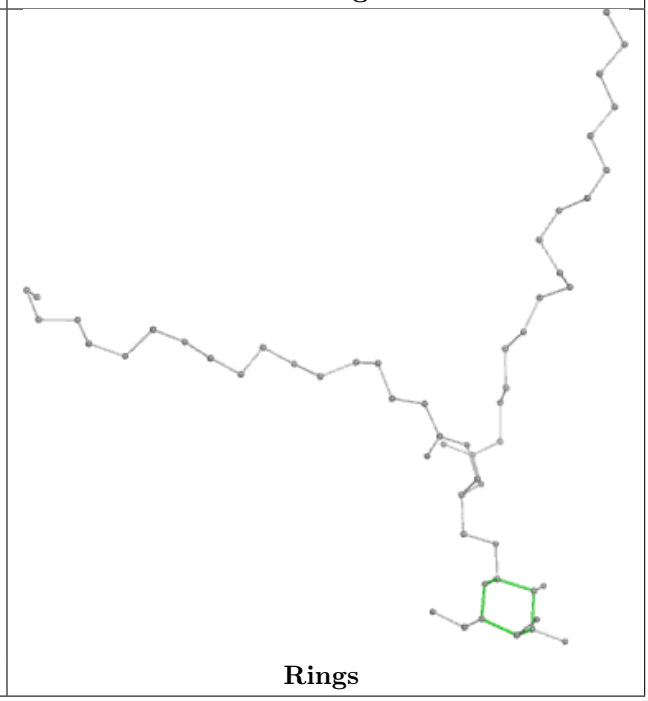
Bond lengths



Bond angles

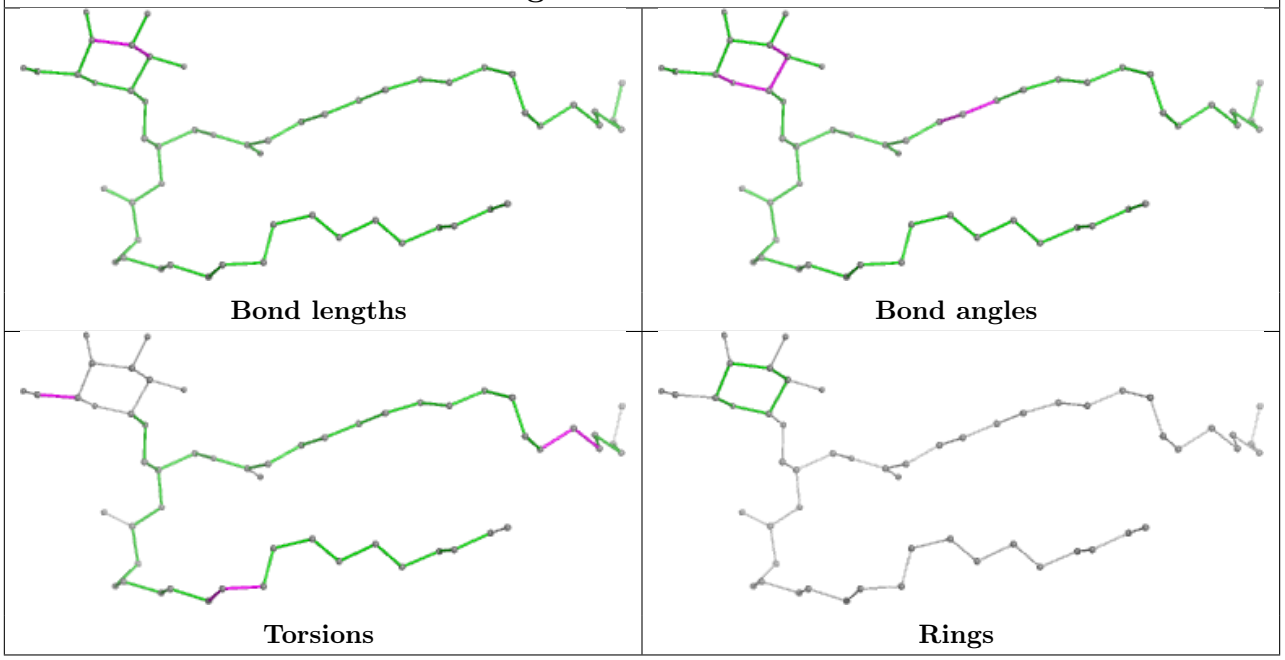


Torsions

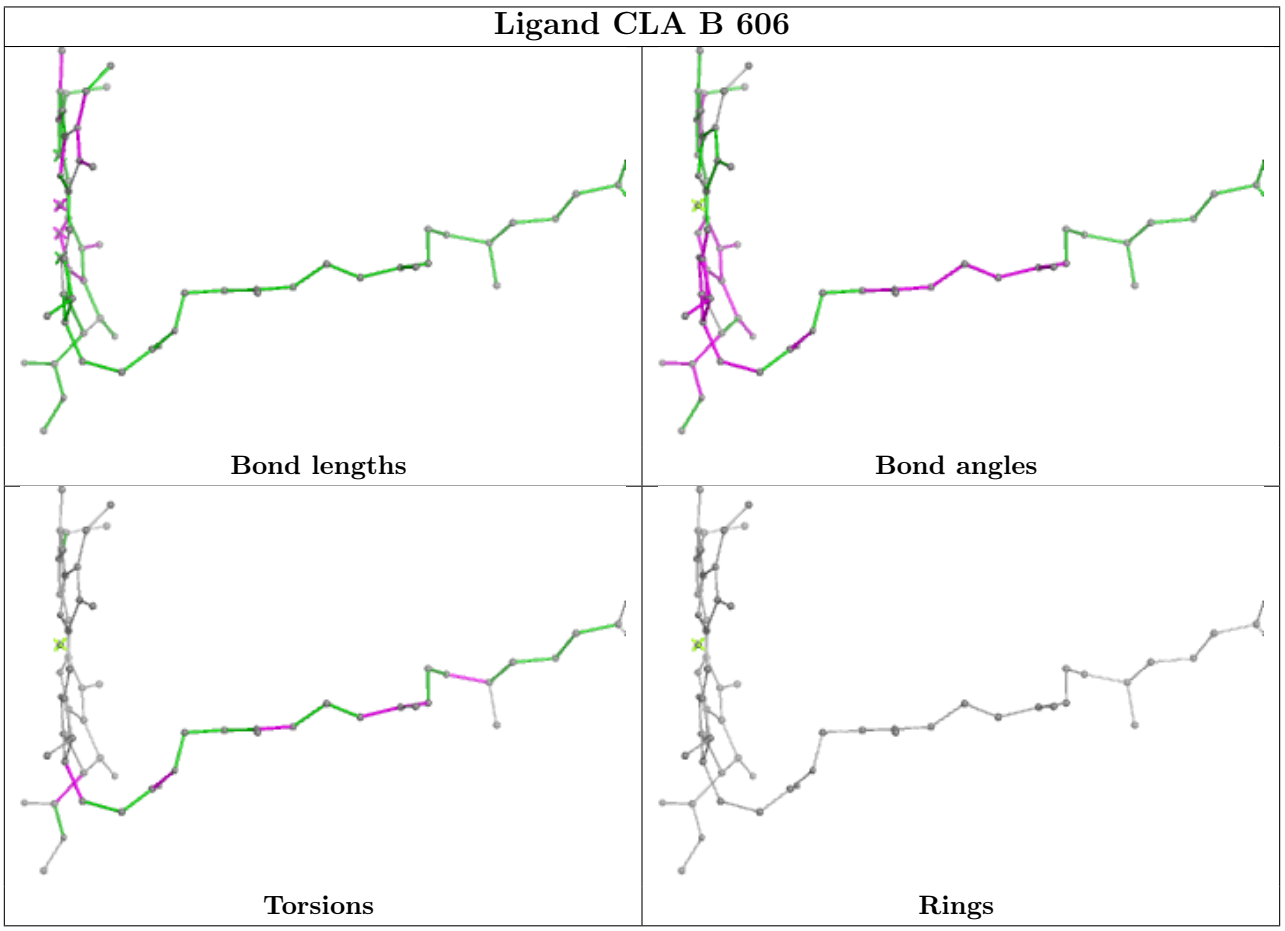


Rings

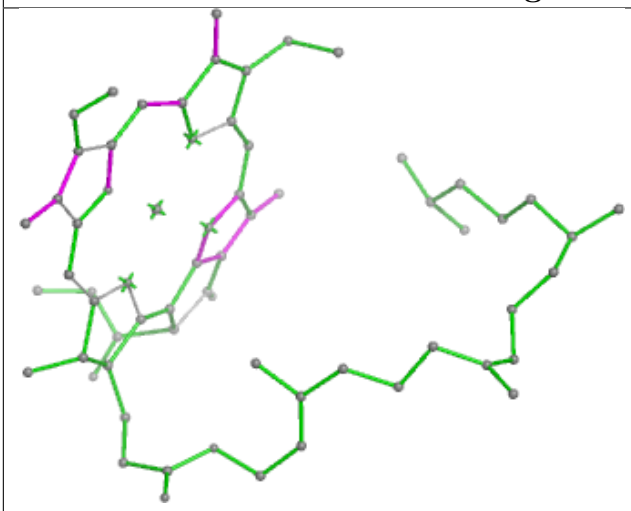
Ligand LMG I 101



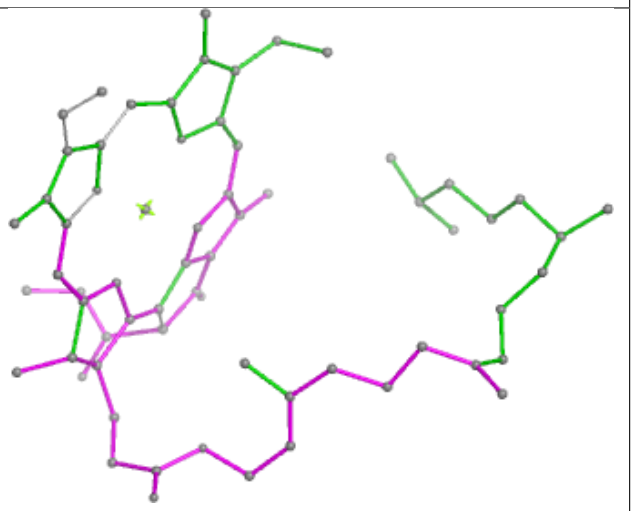
Ligand CLA B 606



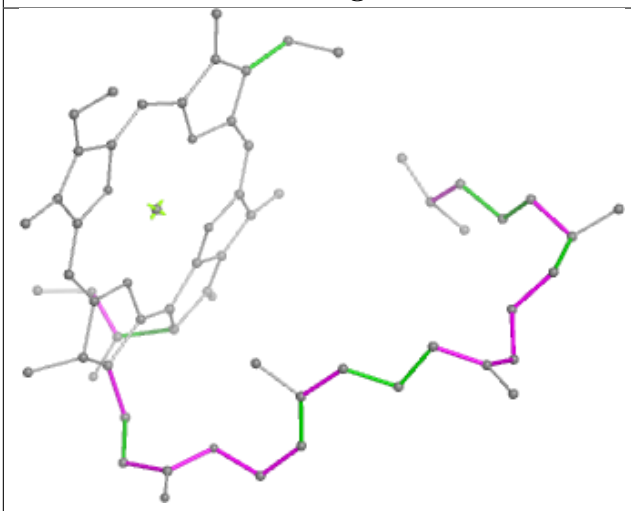
Ligand CLA C 505



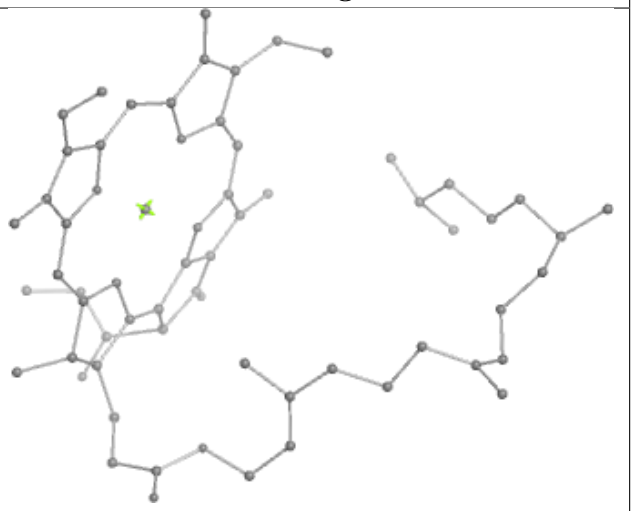
Bond lengths



Bond angles

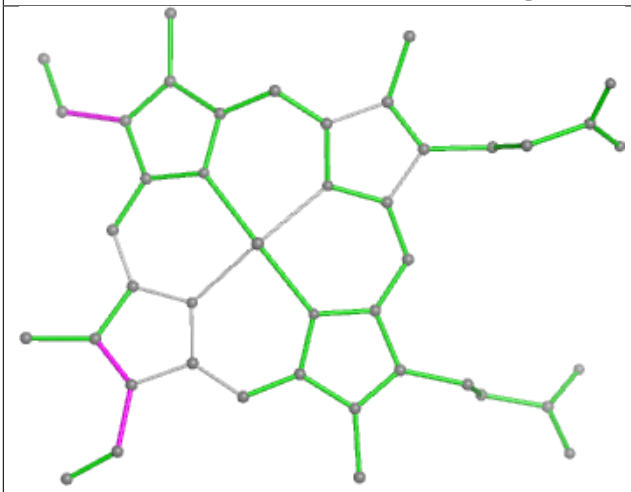


Torsions

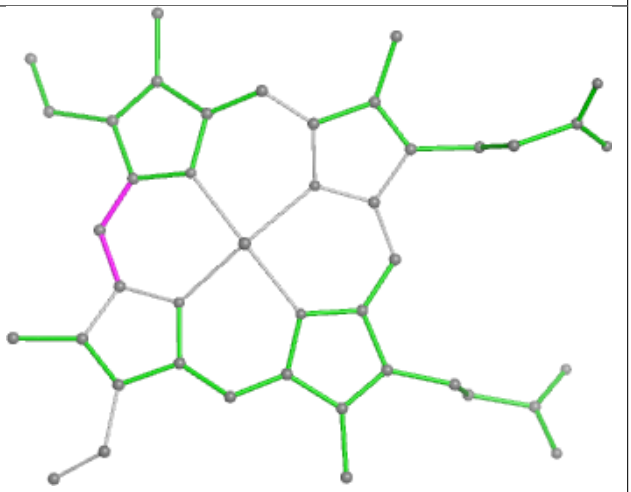


Rings

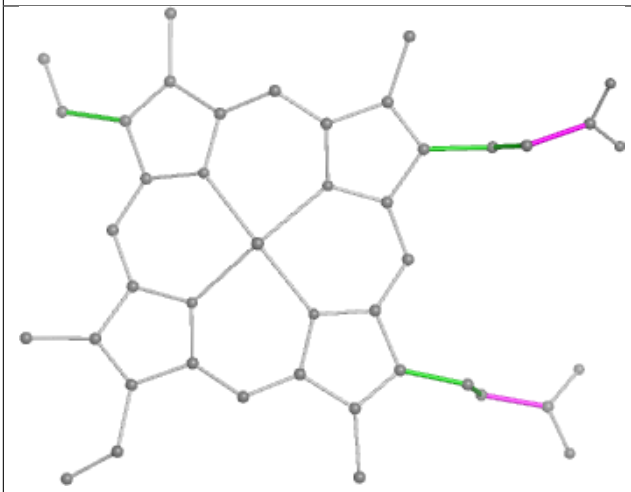
Ligand HEM E 101



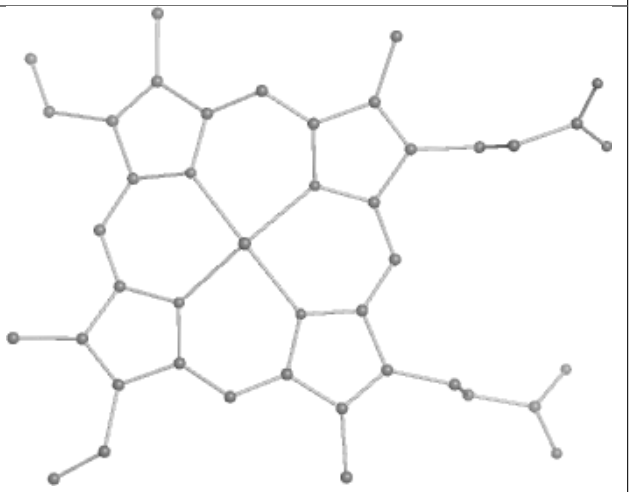
Bond lengths



Bond angles

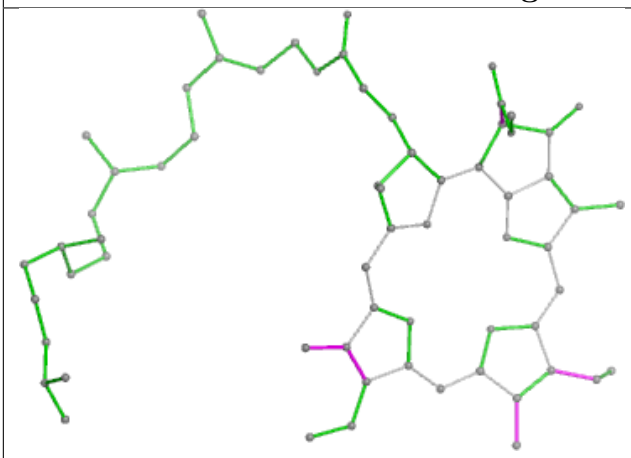


Torsions

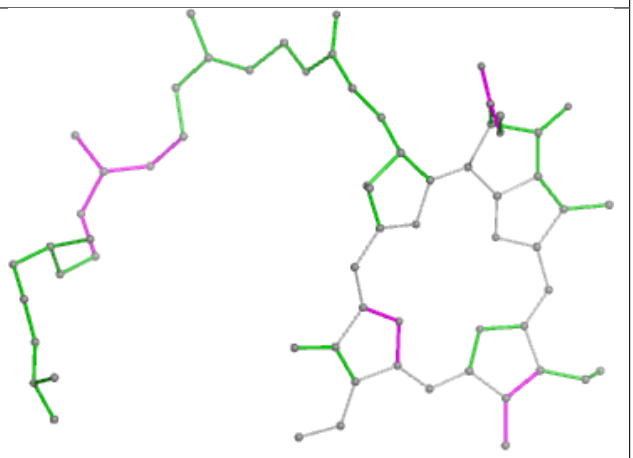


Rings

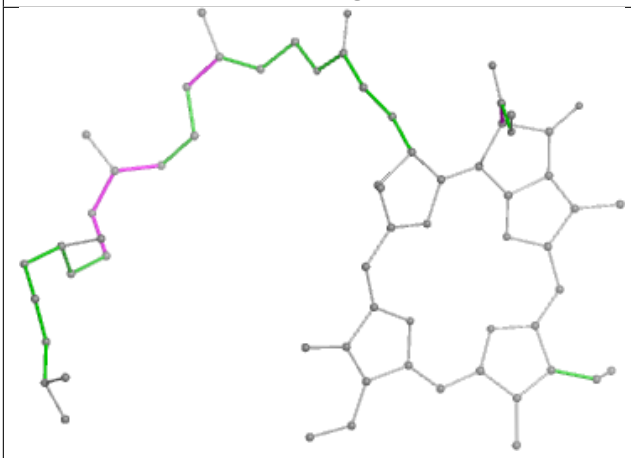
Ligand PHO D 406



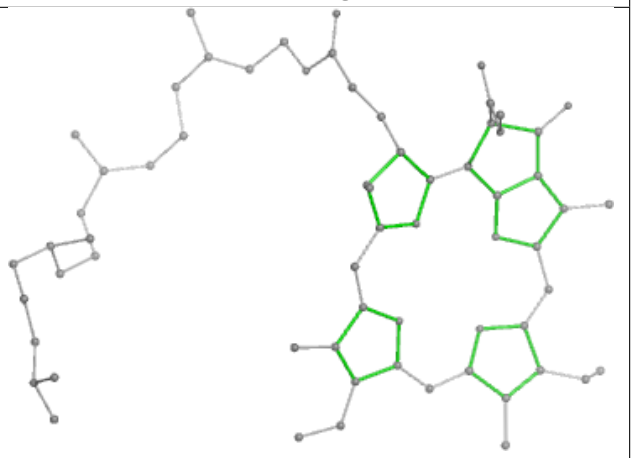
Bond lengths



Bond angles

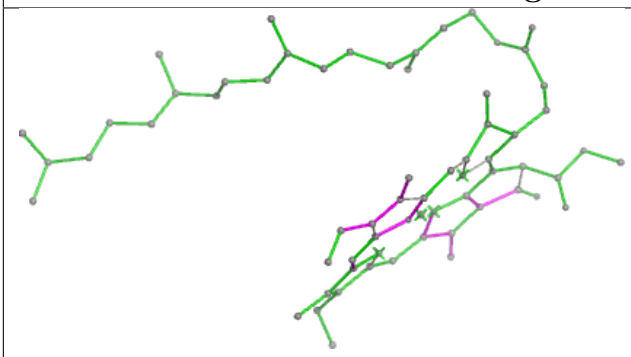


Torsions

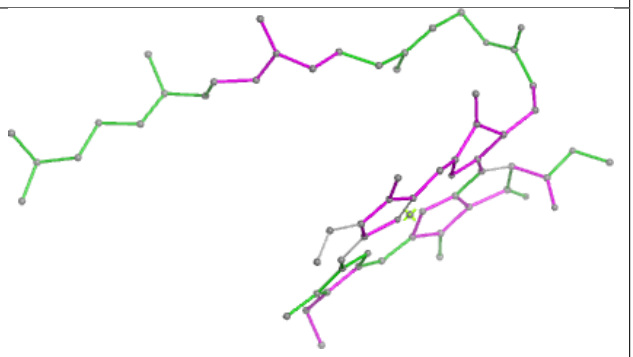


Rings

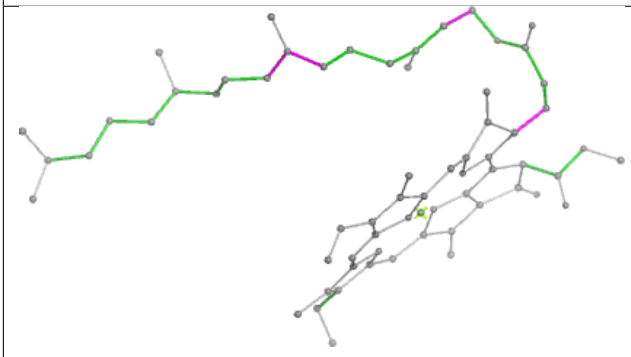
Ligand CLA B 608



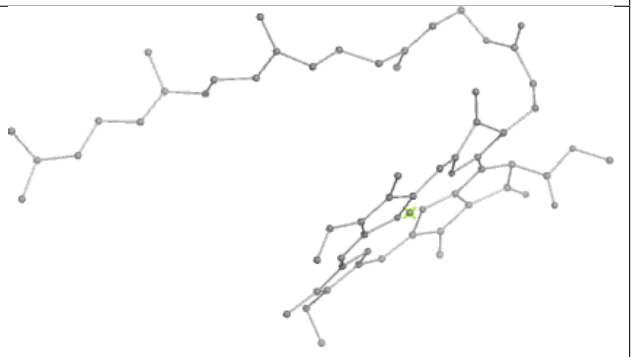
Bond lengths



Bond angles

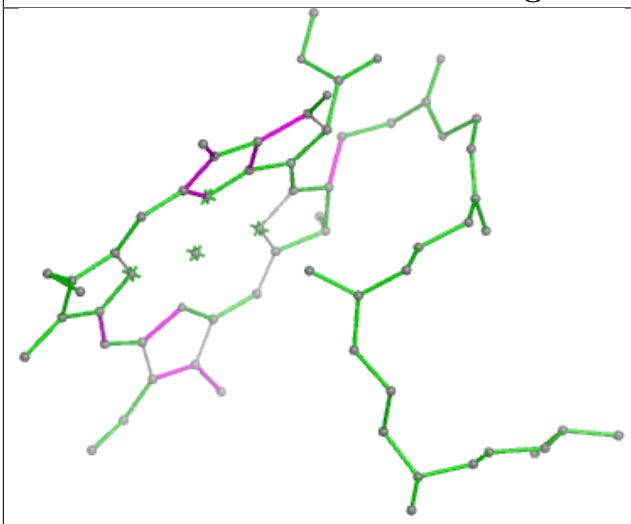


Torsions

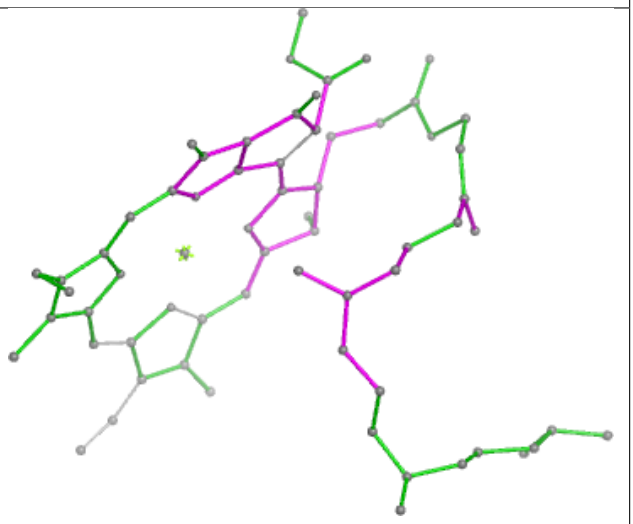


Rings

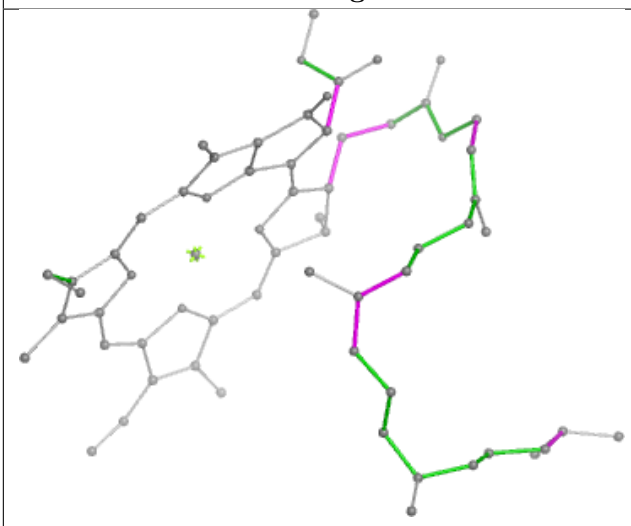
Ligand CLA C 514



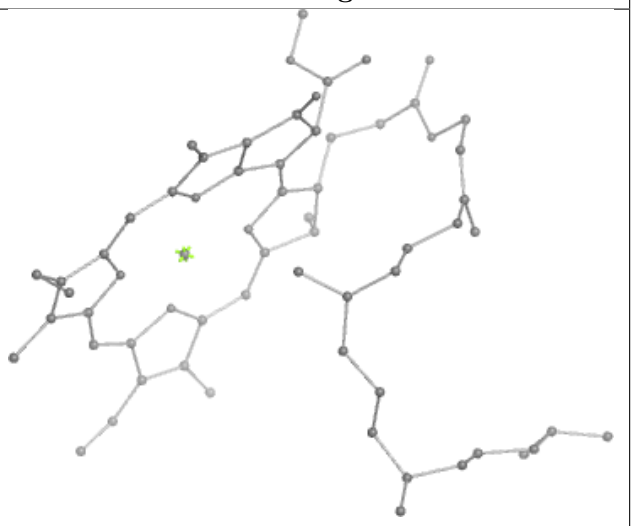
Bond lengths



Bond angles

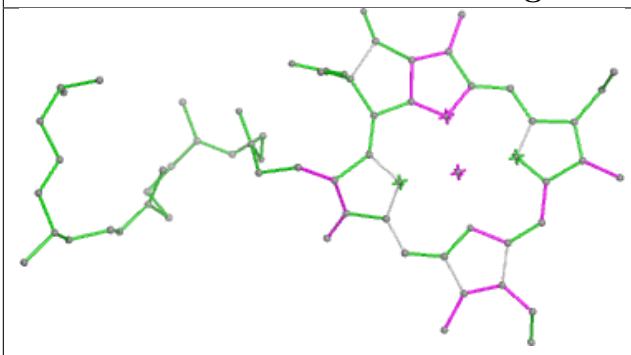


Torsions

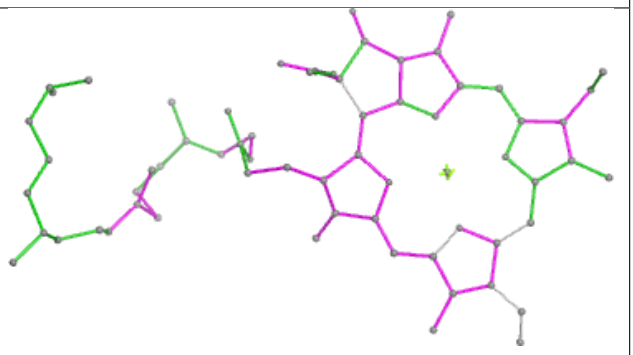


Rings

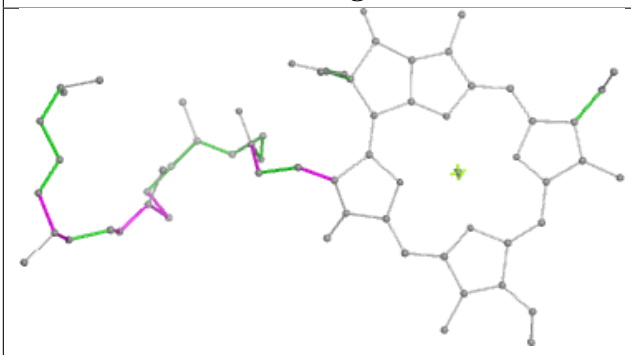
Ligand CLA B 612



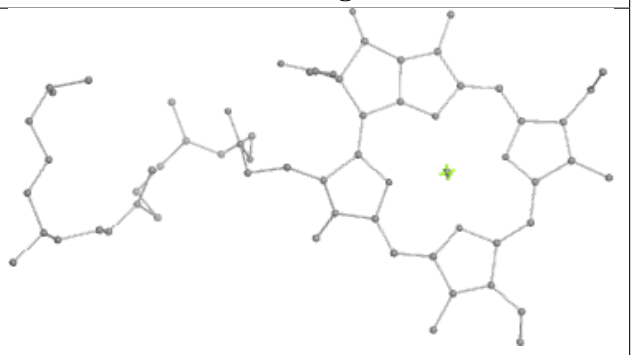
Bond lengths



Bond angles

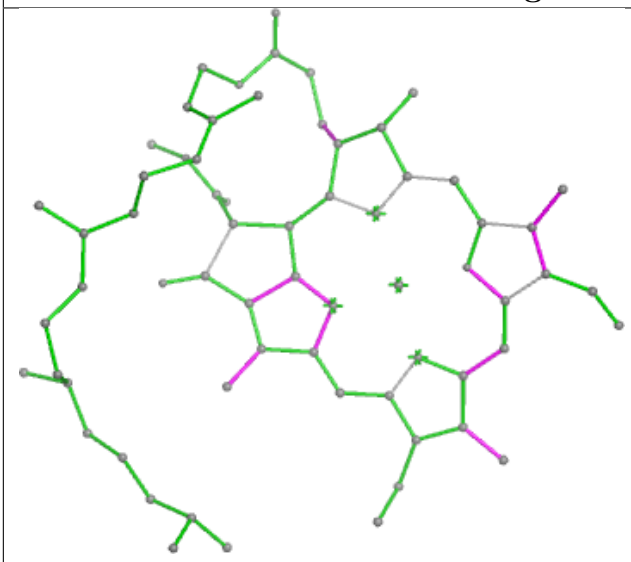


Torsions

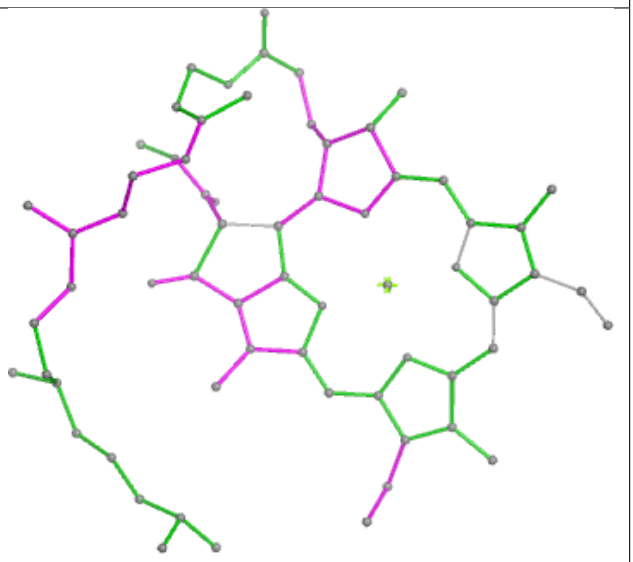


Rings

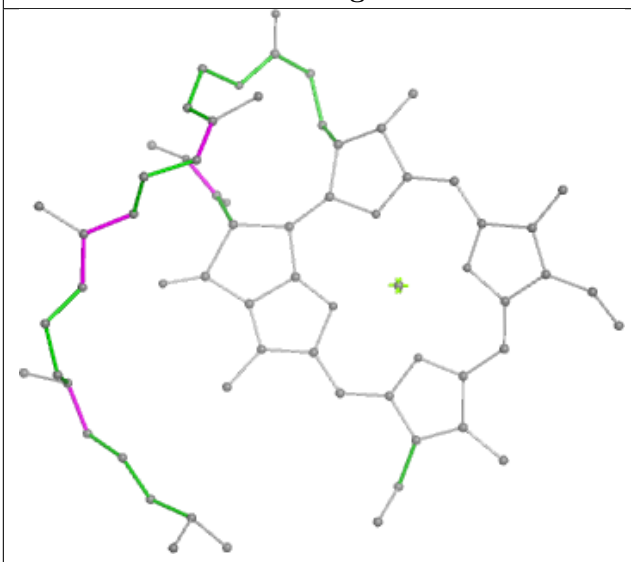
Ligand CLA B 601



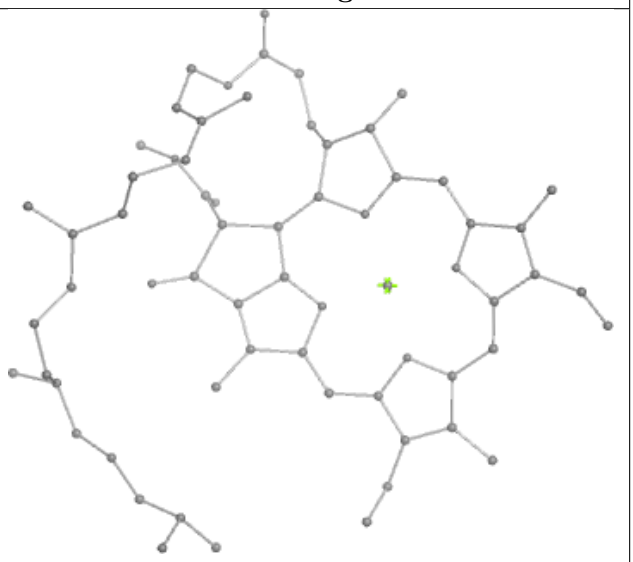
Bond lengths



Bond angles

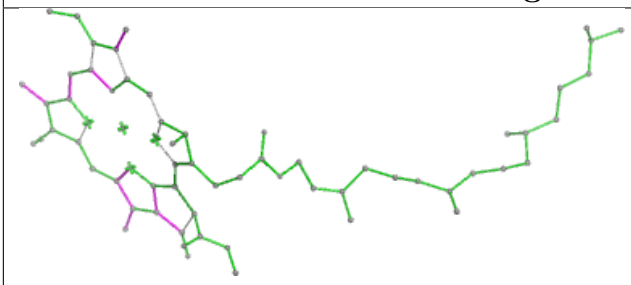


Torsions

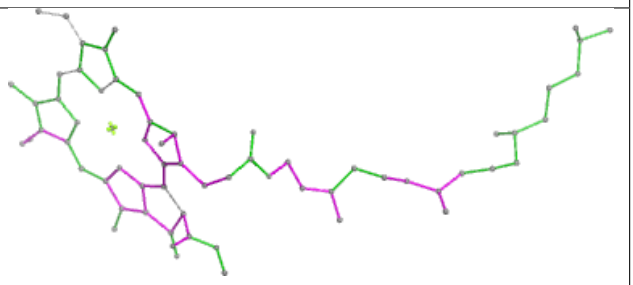


Rings

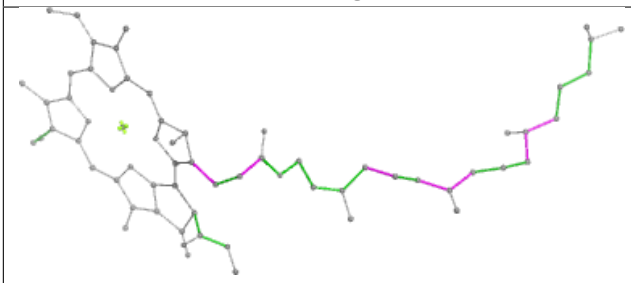
Ligand CLA A 405



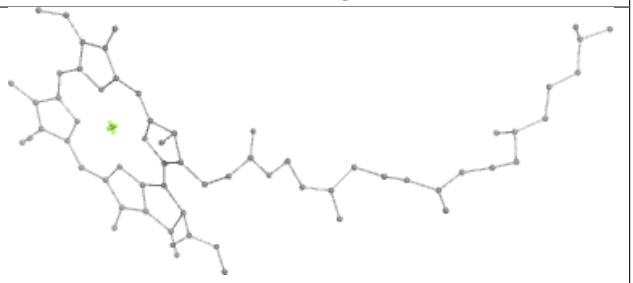
Bond lengths



Bond angles

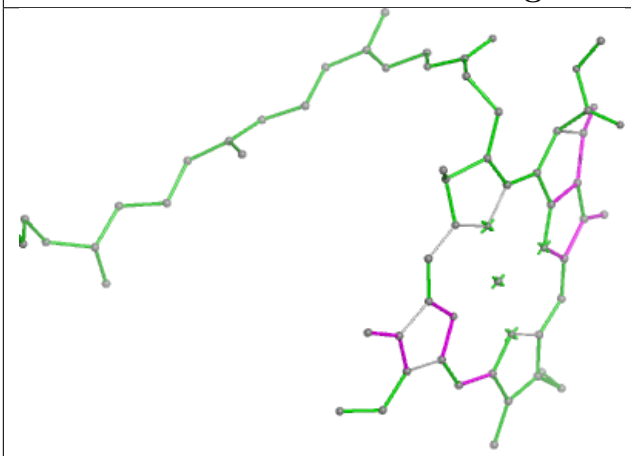


Torsions

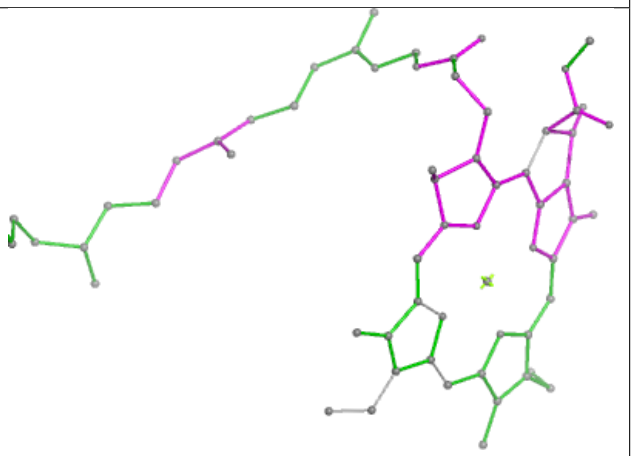


Rings

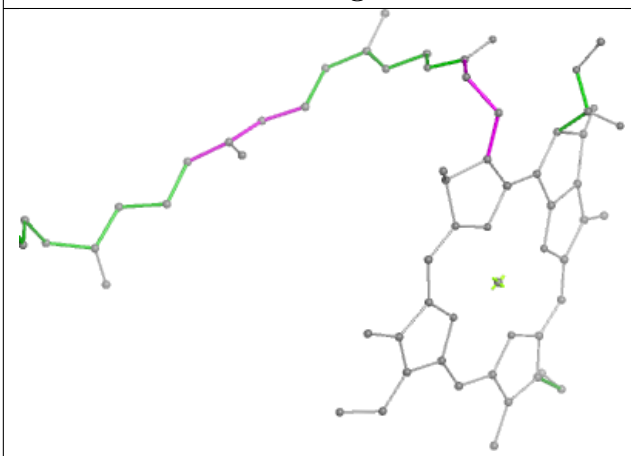
Ligand CLA C 512



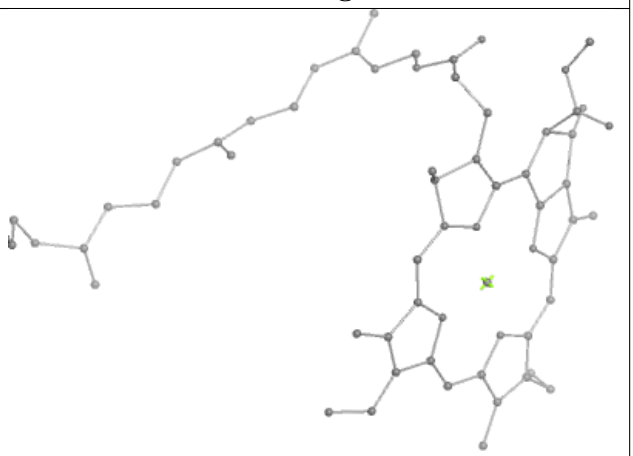
Bond lengths



Bond angles

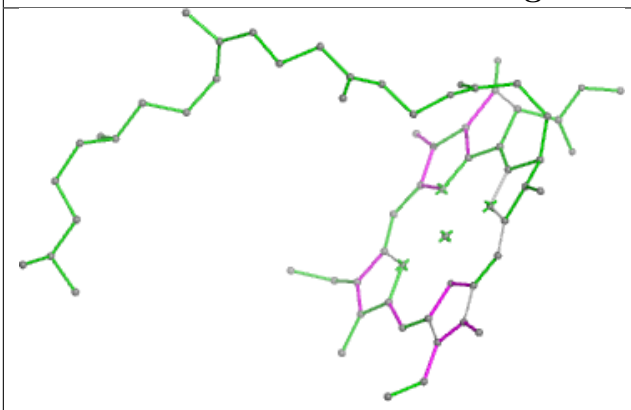


Torsions

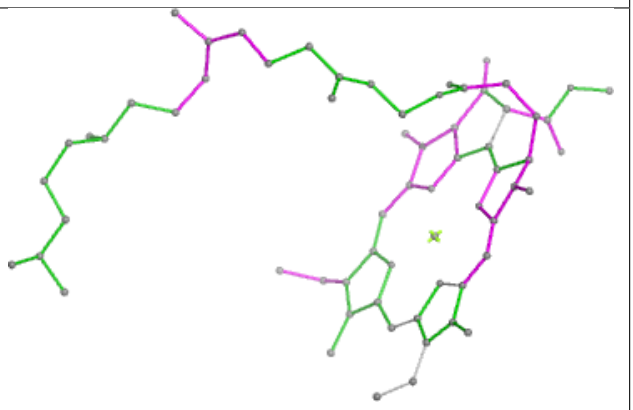


Rings

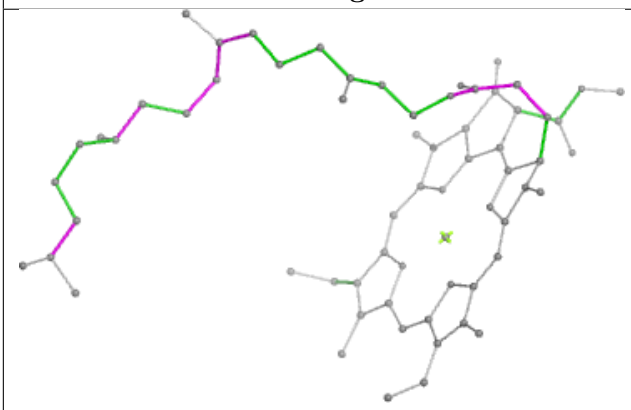
Ligand CLA C 510



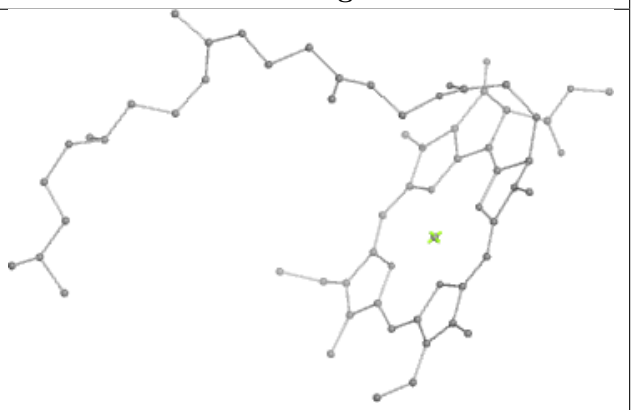
Bond lengths



Bond angles

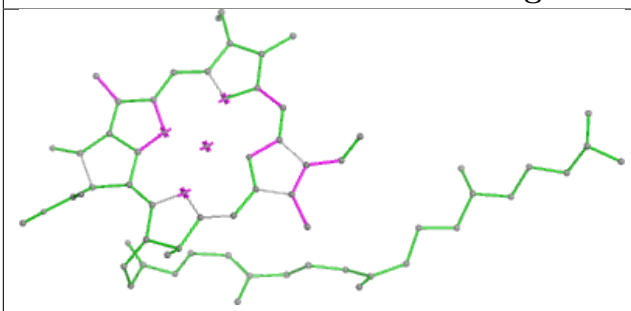


Torsions

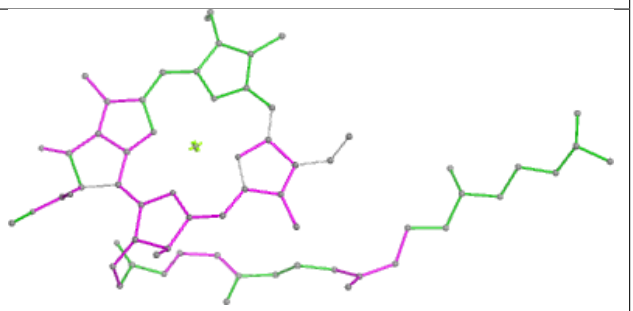


Rings

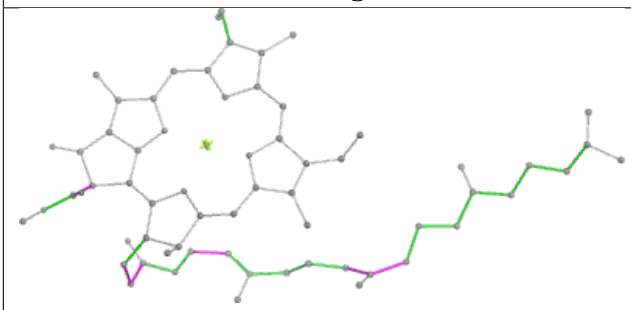
Ligand CLA C 503



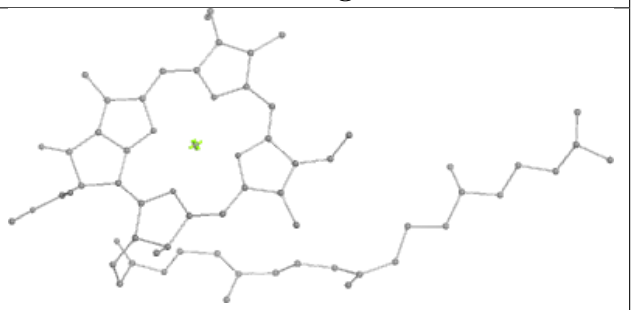
Bond lengths



Bond angles

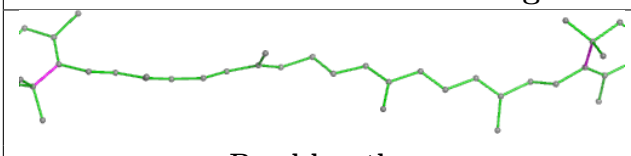


Torsions

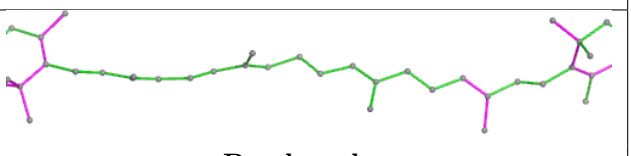


Rings

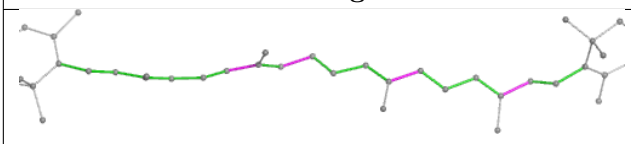
Ligand BCR B 619



Bond lengths



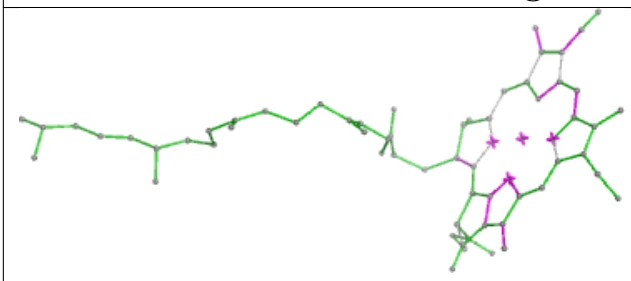
Bond angles



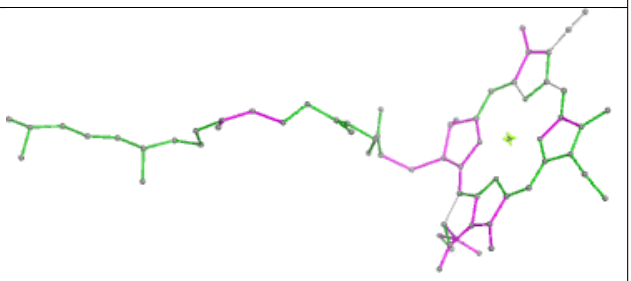
Torsions

Rings

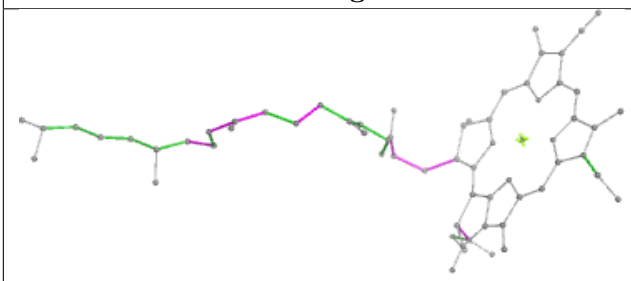
Ligand CLA C 504



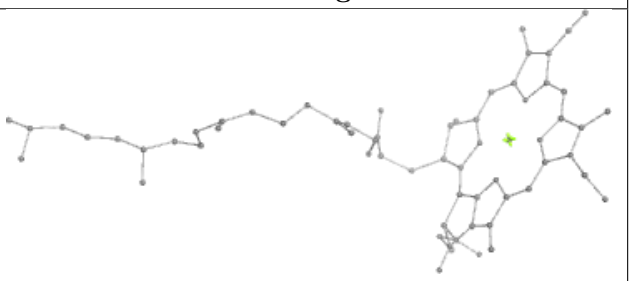
Bond lengths



Bond angles

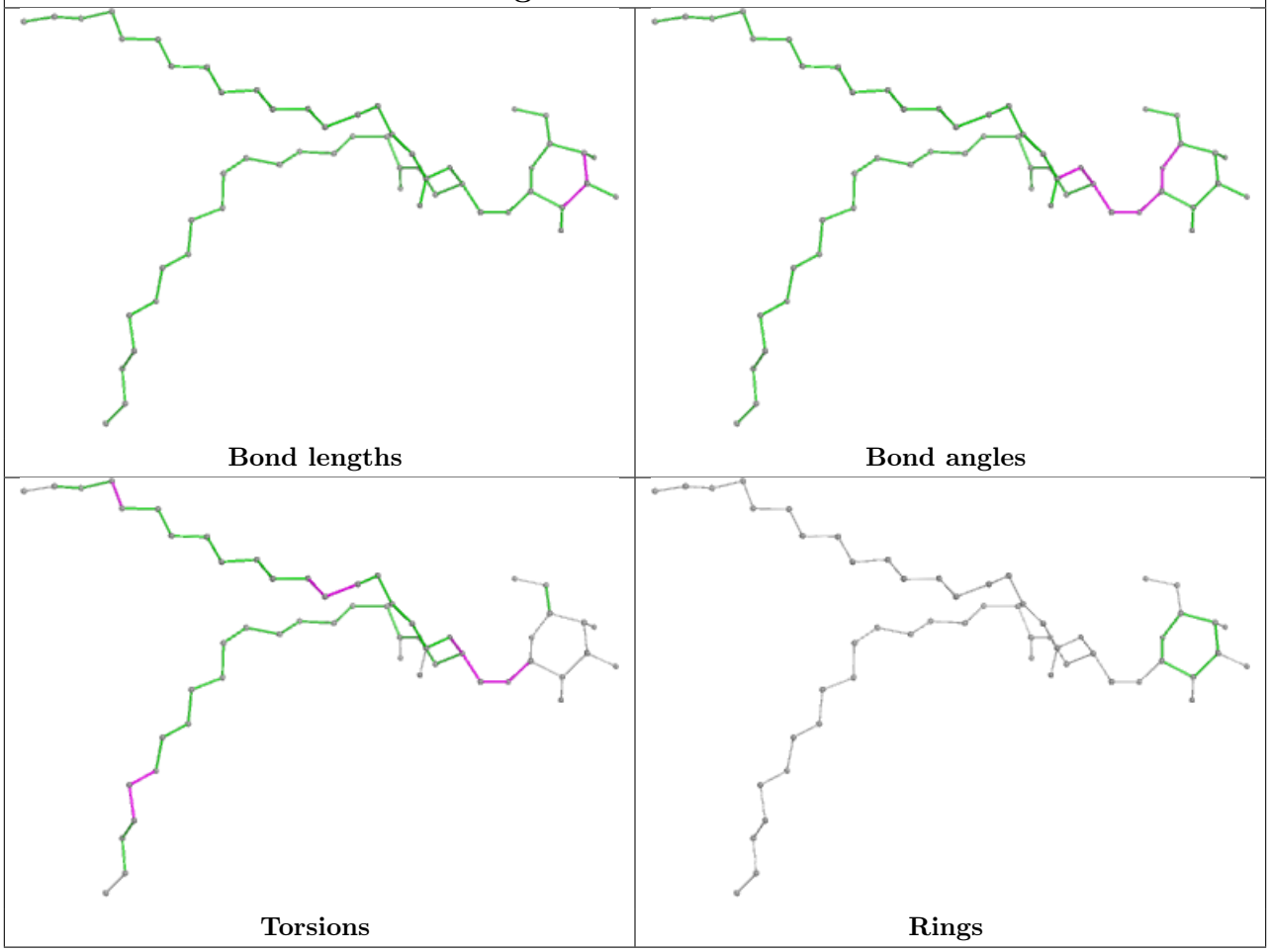


Torsions

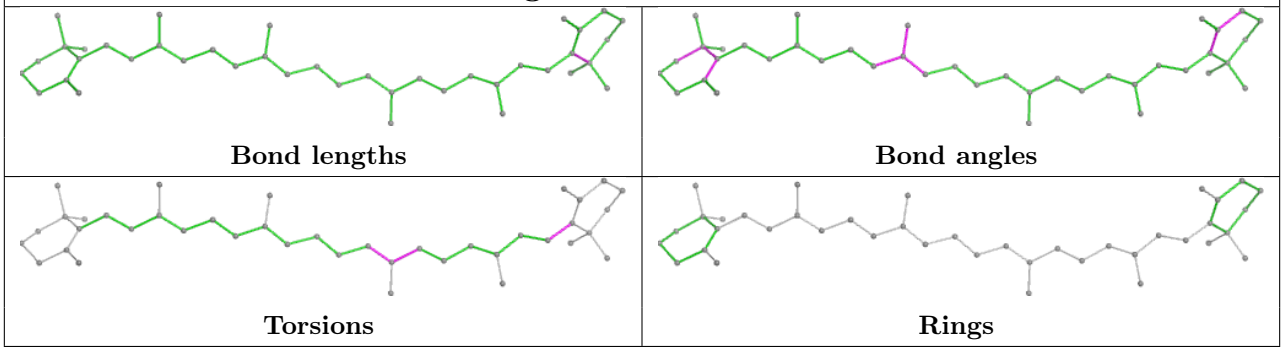


Rings

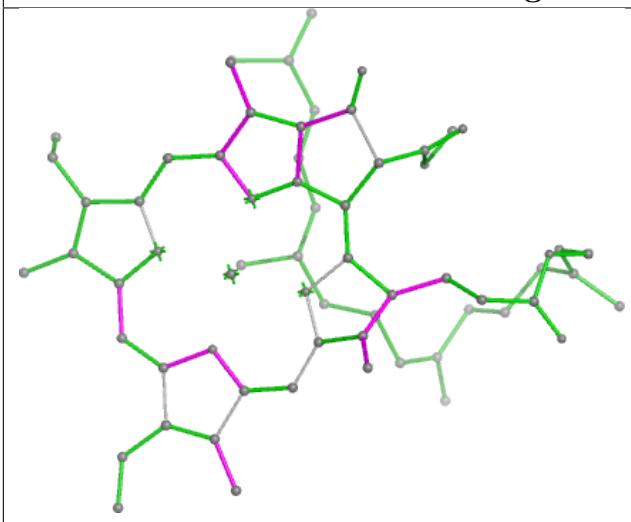
Ligand LMG D 404



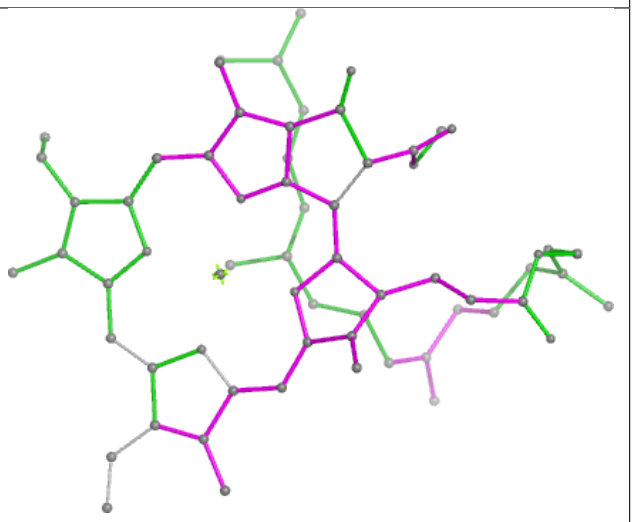
Ligand BCR B 618



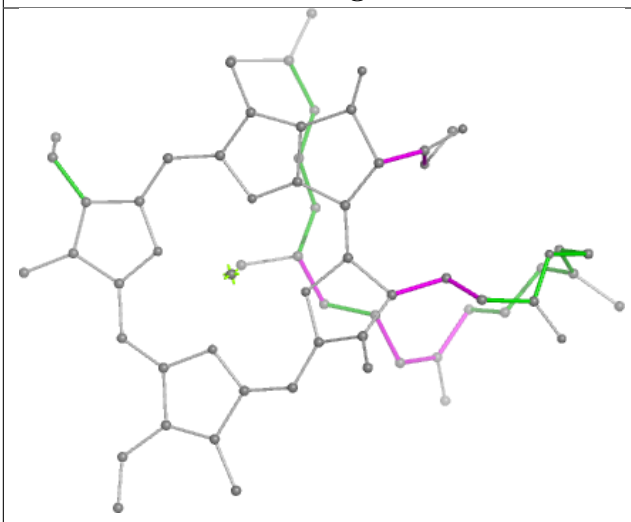
Ligand CLA C 517



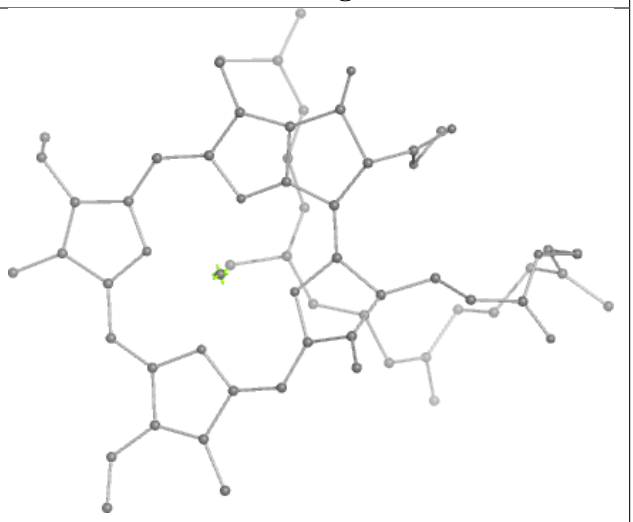
Bond lengths



Bond angles

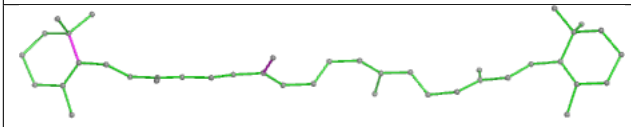


Torsions



Rings

Ligand BCR C 515



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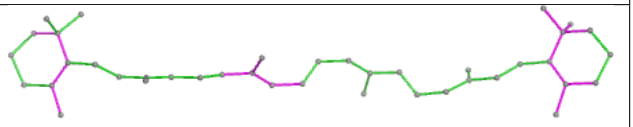
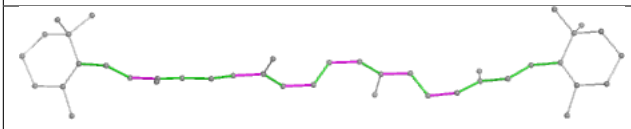
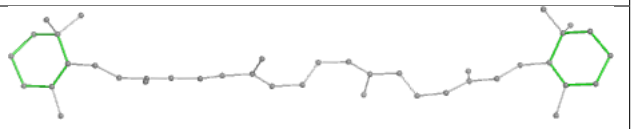


Bond angles

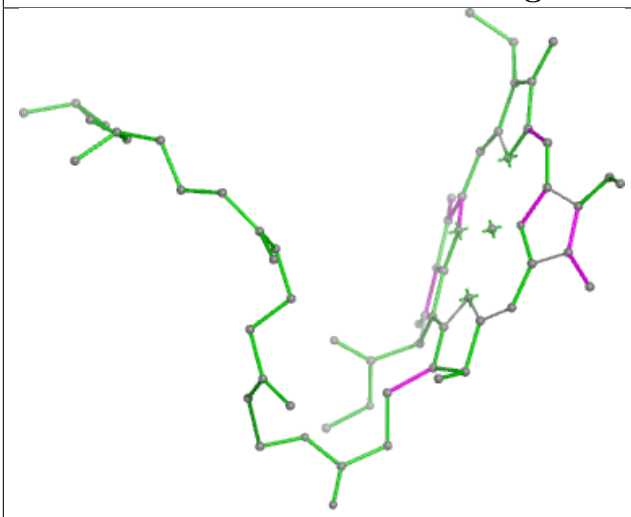


Torsions

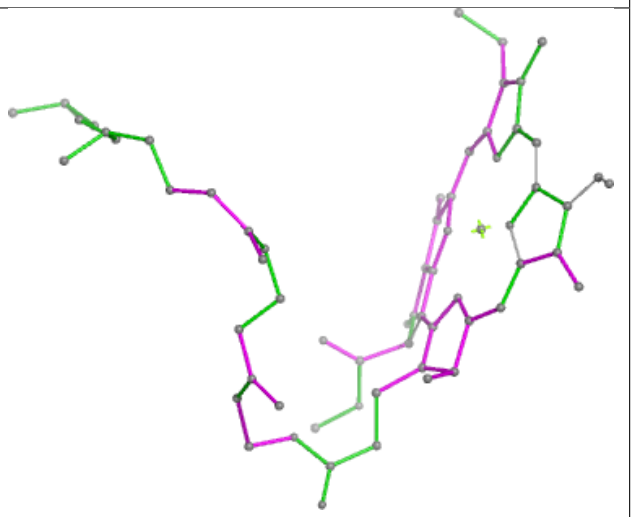


Rings

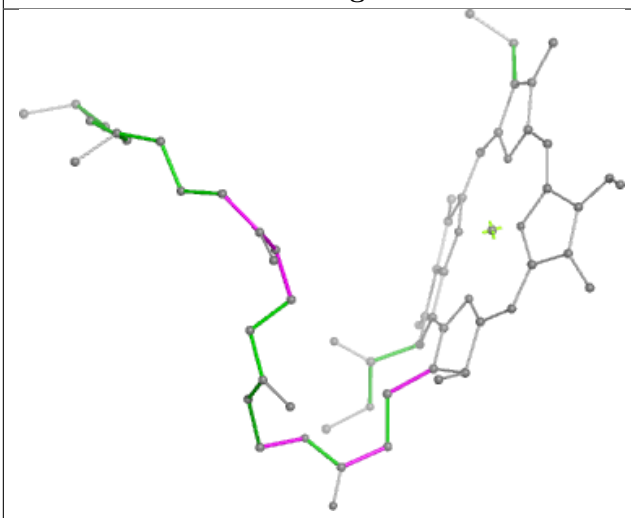
Ligand CLA B 613



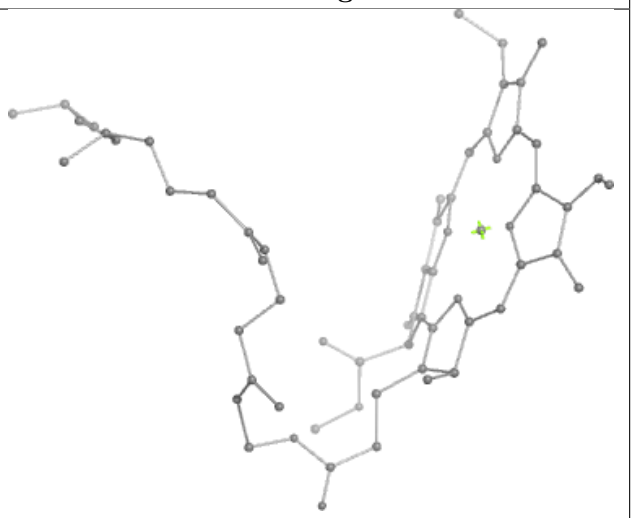
Bond lengths



Bond angles

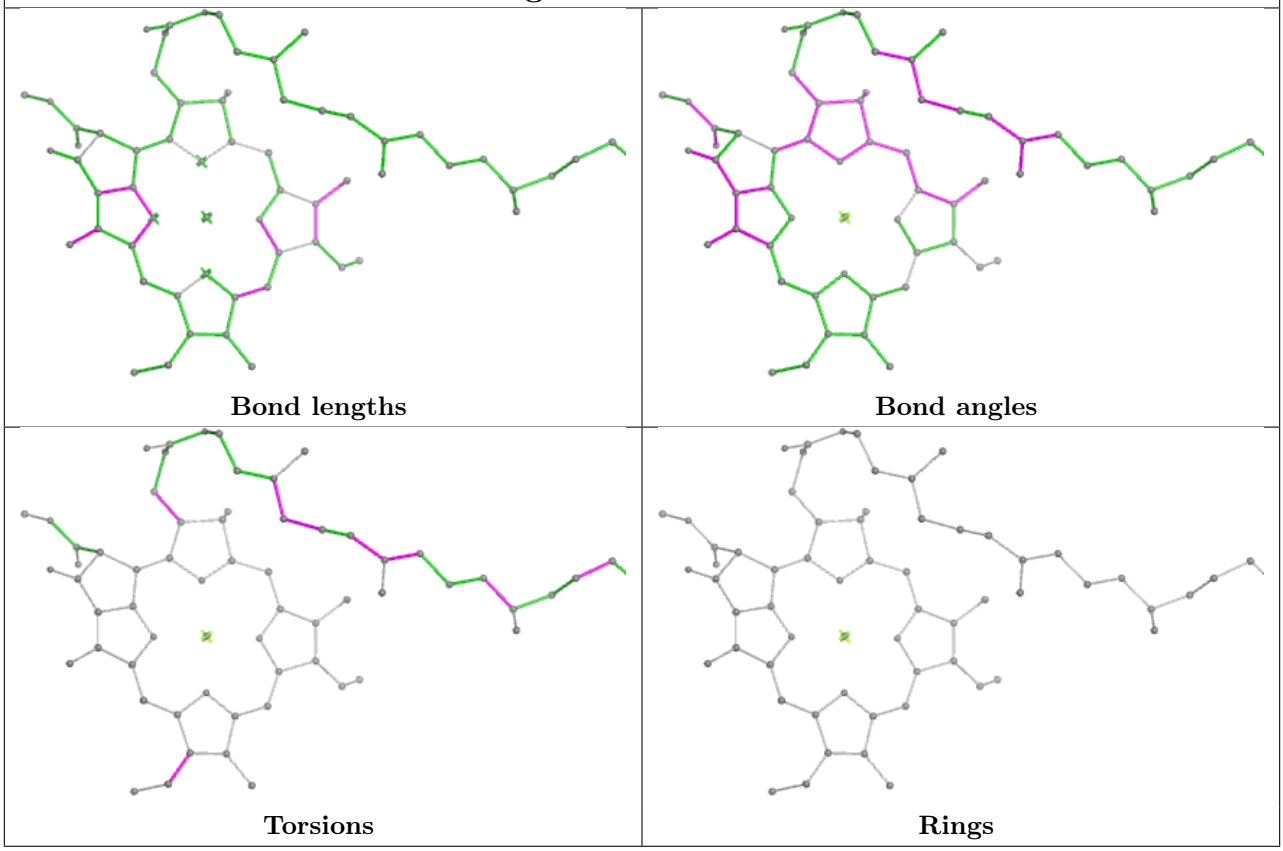


Torsions

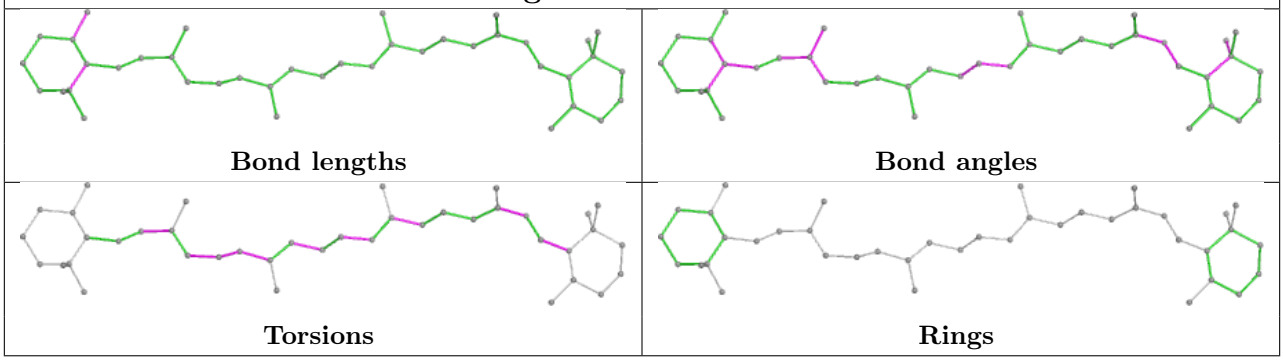


Rings

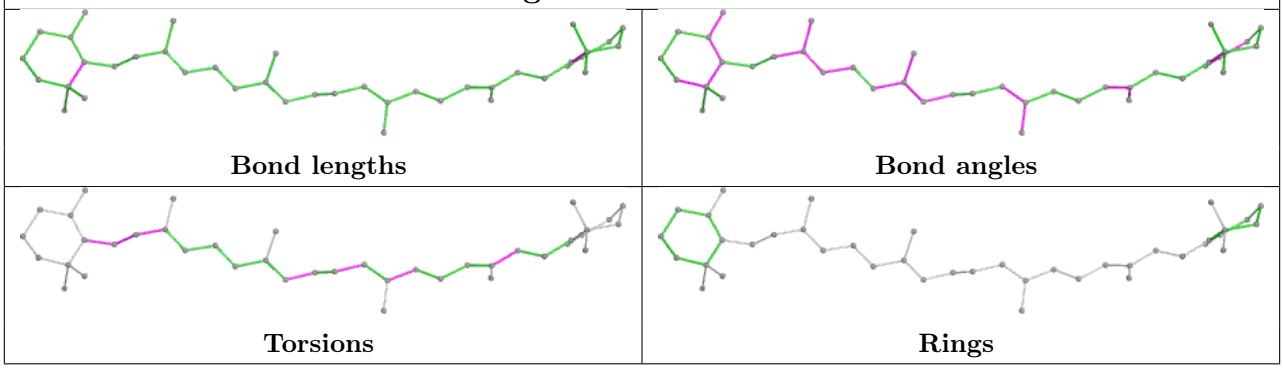
Ligand CLA B 603



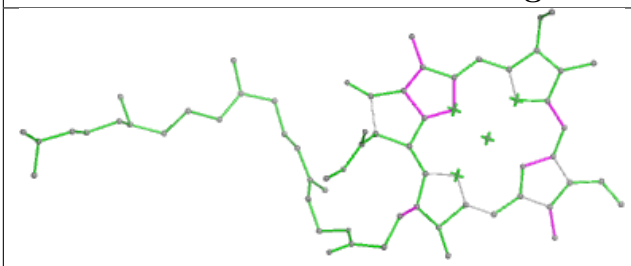
Ligand BCR B 617



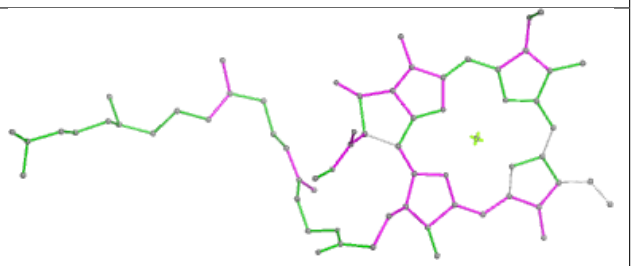
Ligand BCR C 518



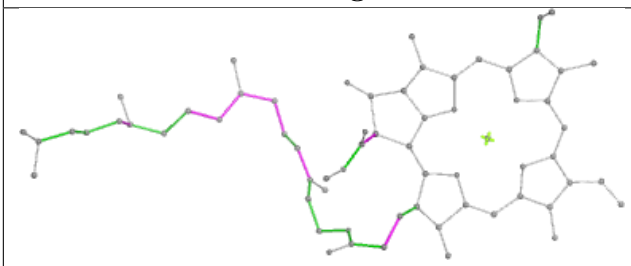
Ligand CLA B 602



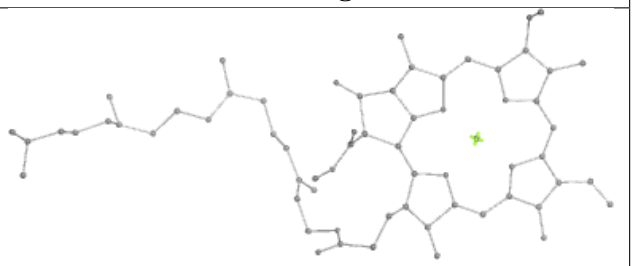
Bond lengths



Bond angles

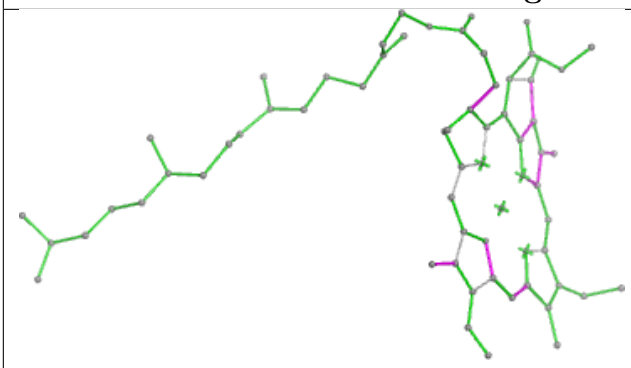


Torsions

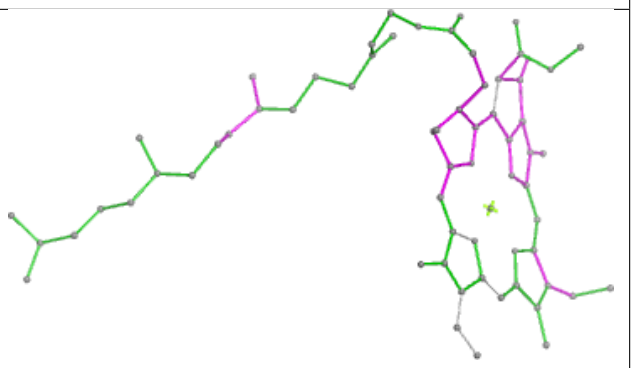


Rings

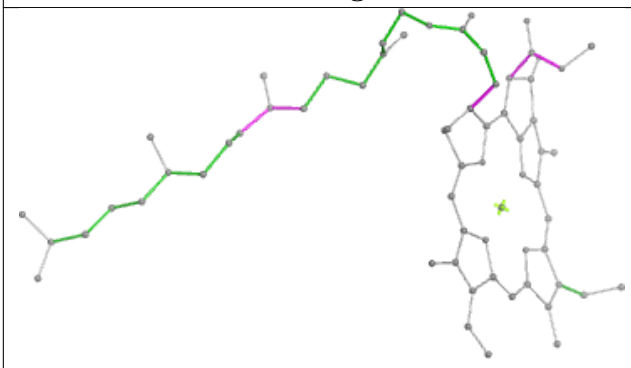
Ligand CLA B 609



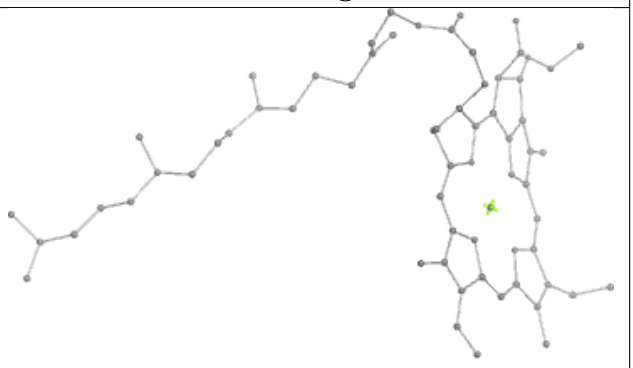
Bond lengths



Bond angles

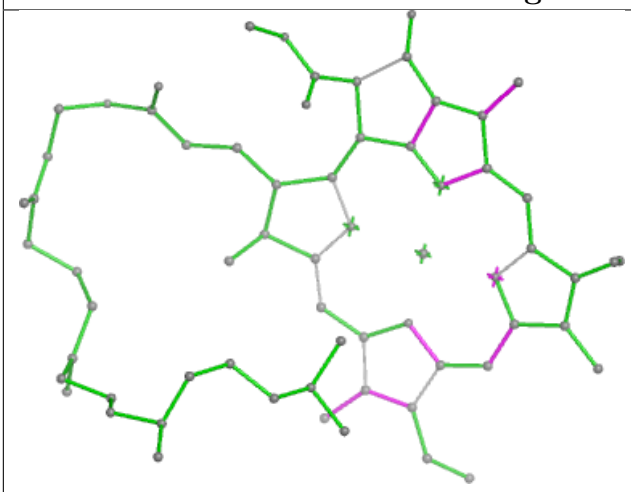


Torsions



Rings

Ligand CLA B 615



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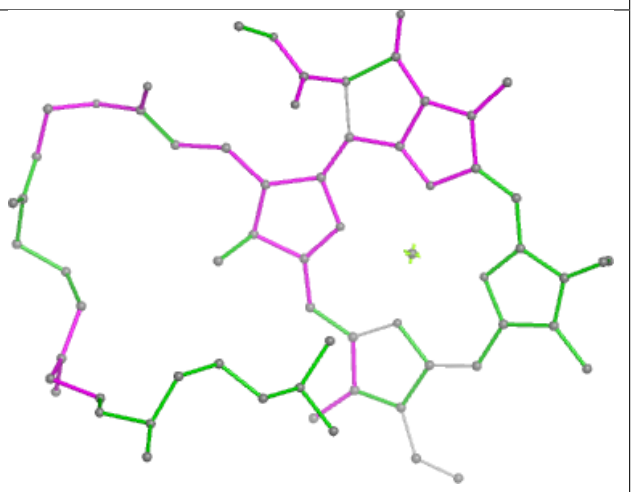
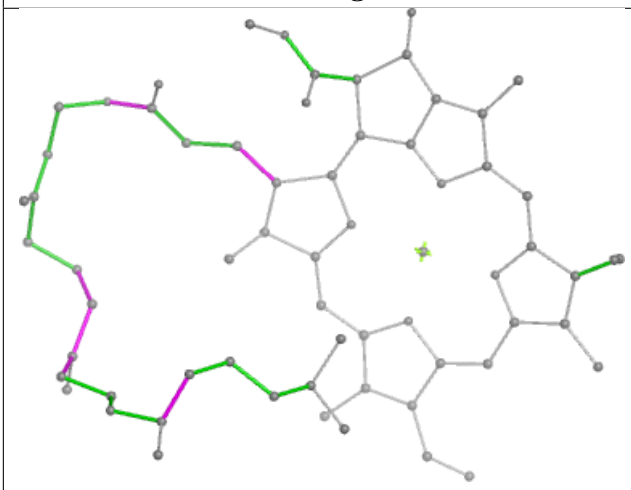


Bond angles



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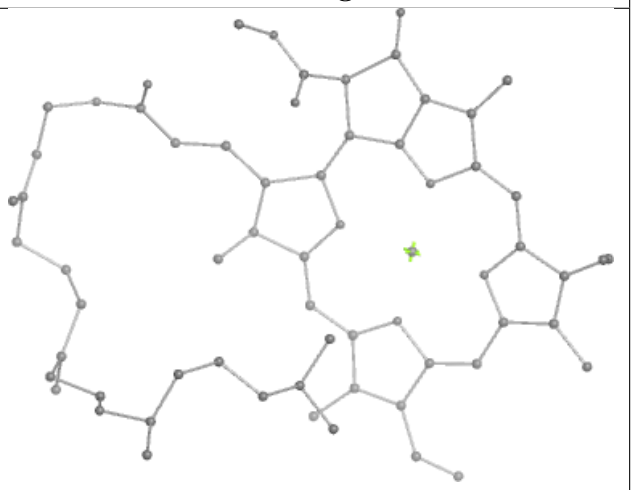

Rings

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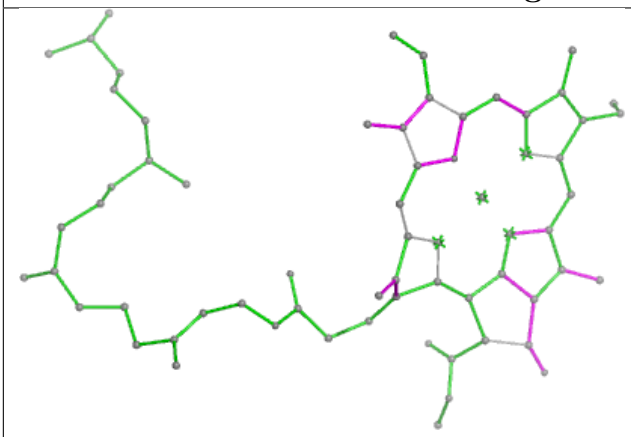

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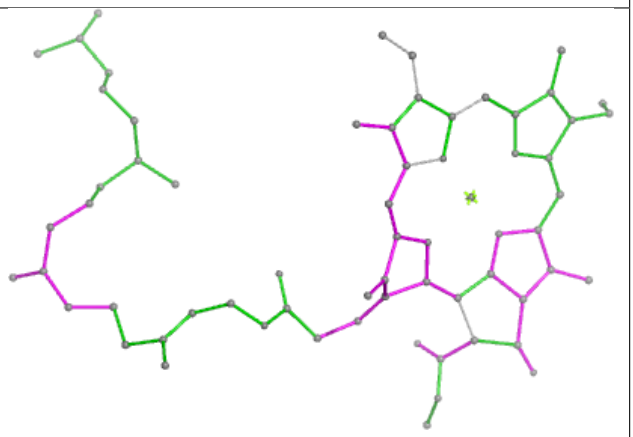
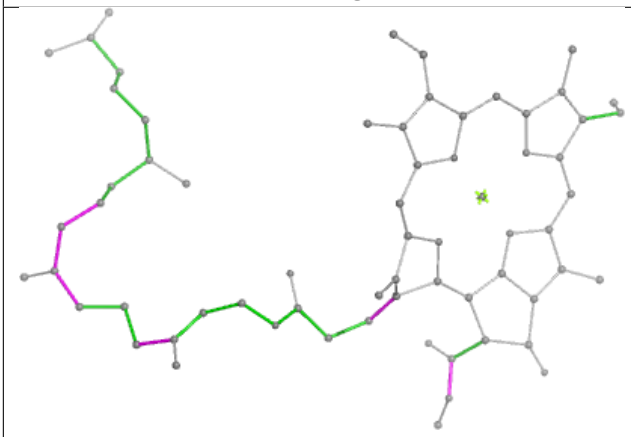


Bond angles



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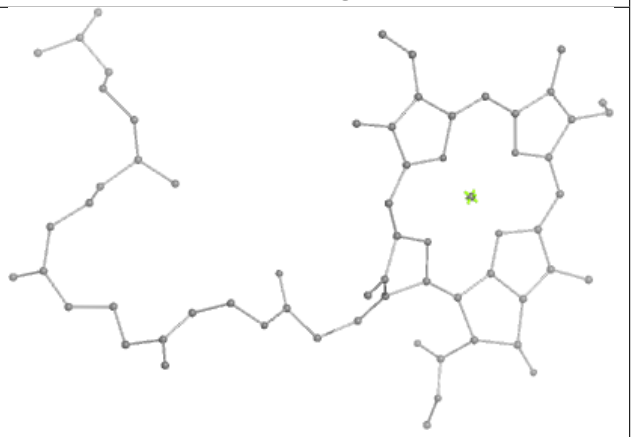
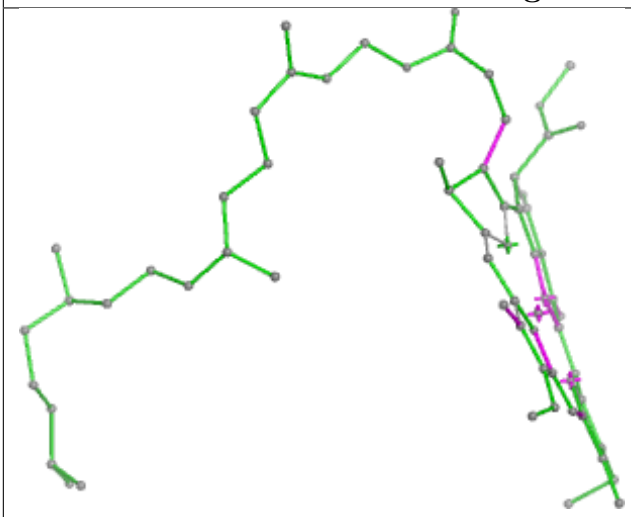
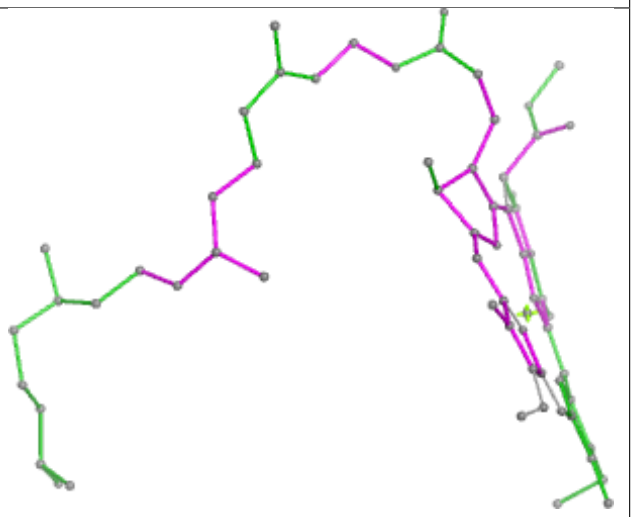


Rings

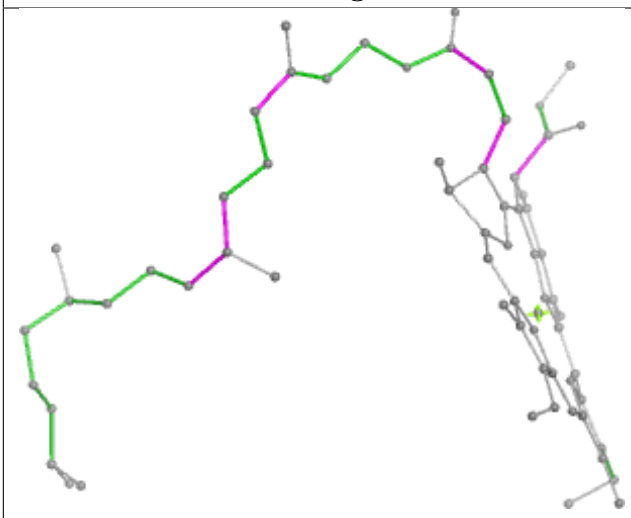
Ligand CLA A 406



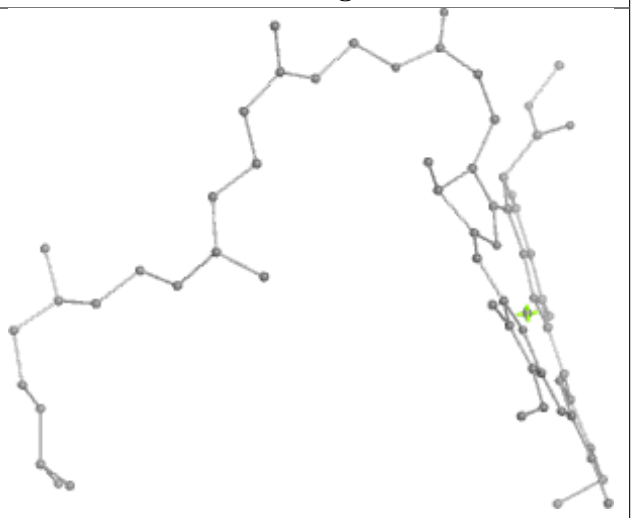
Bond lengths



Bond angles

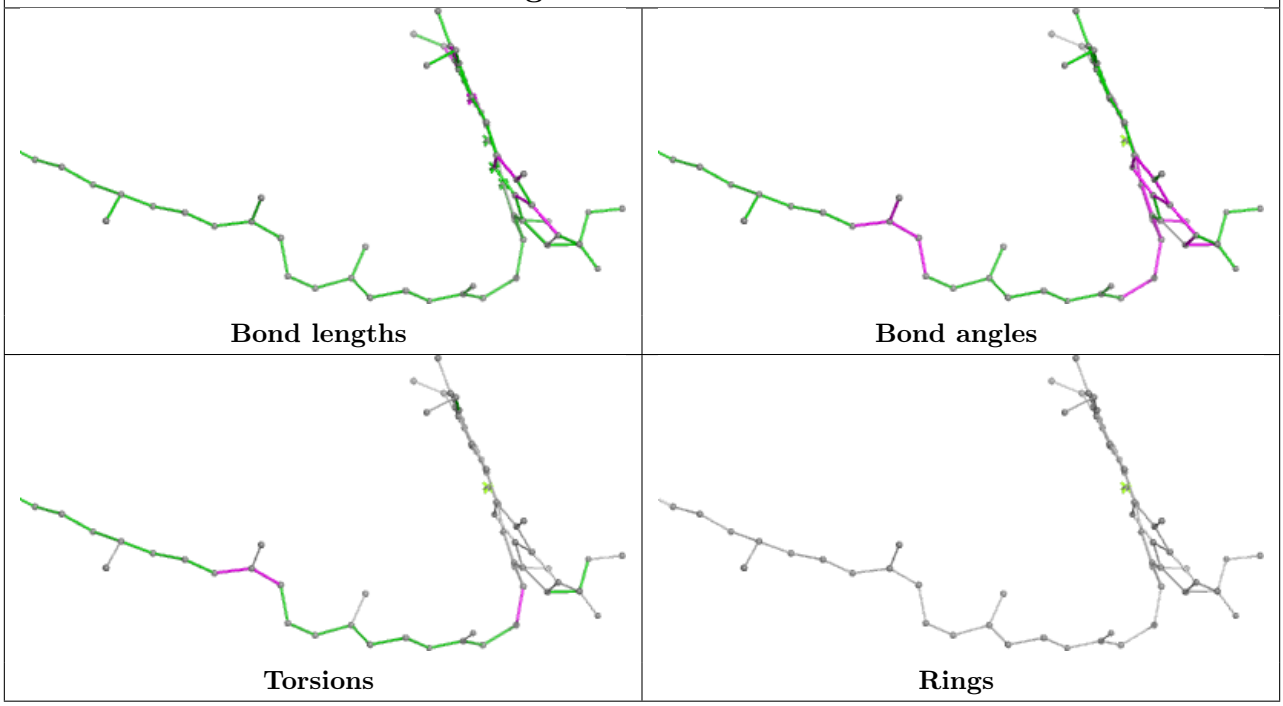


Torsions

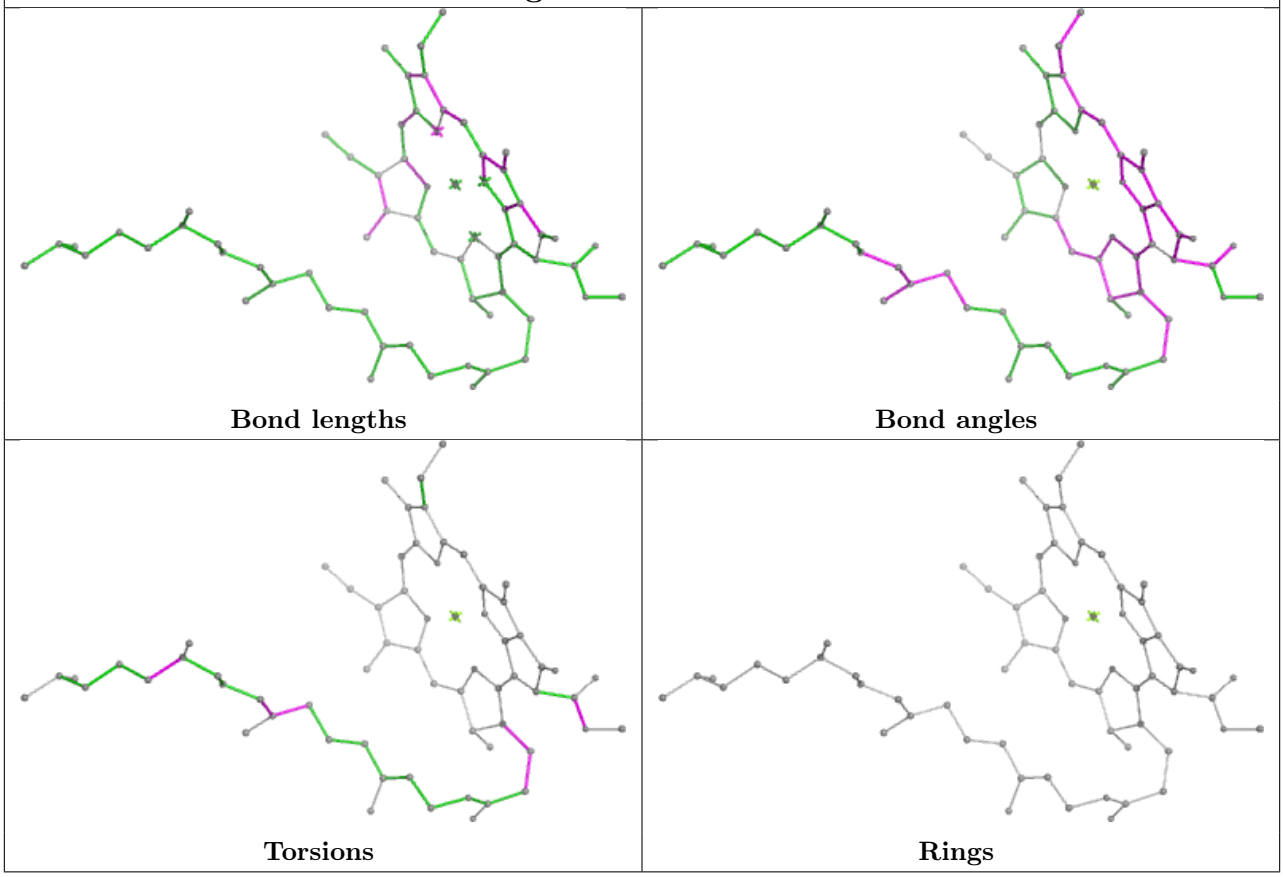


Rings

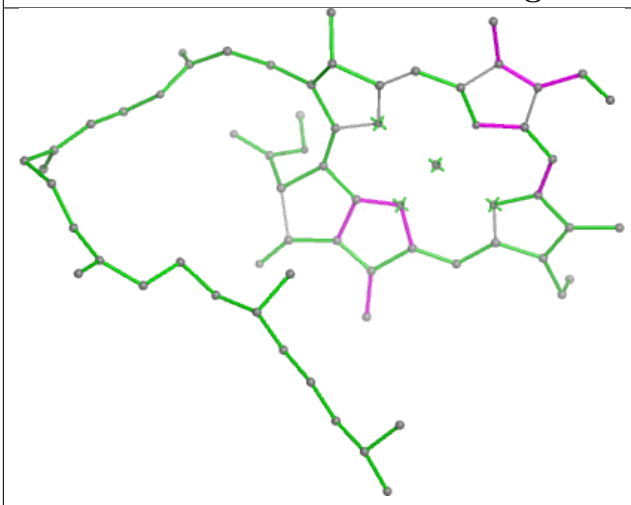
Ligand CLA C 508



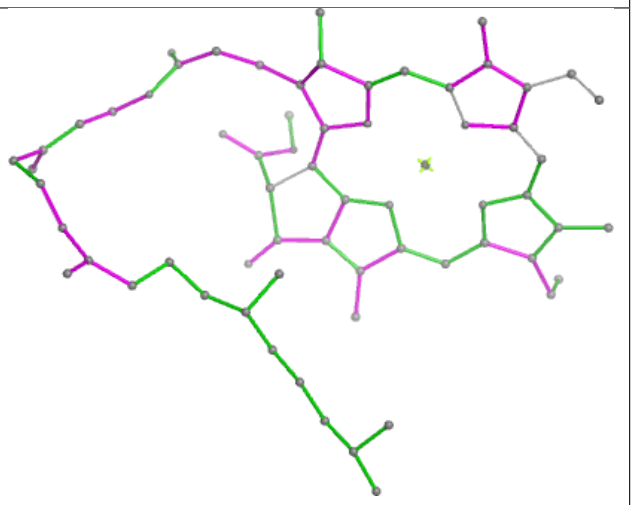
Ligand CLA C 507



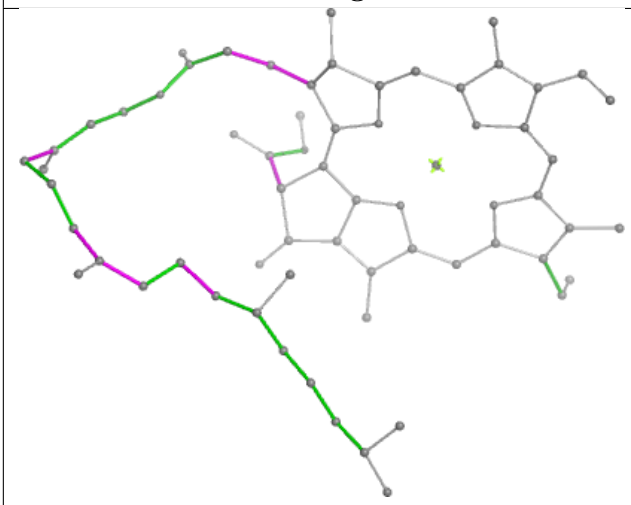
Ligand CLA C 511



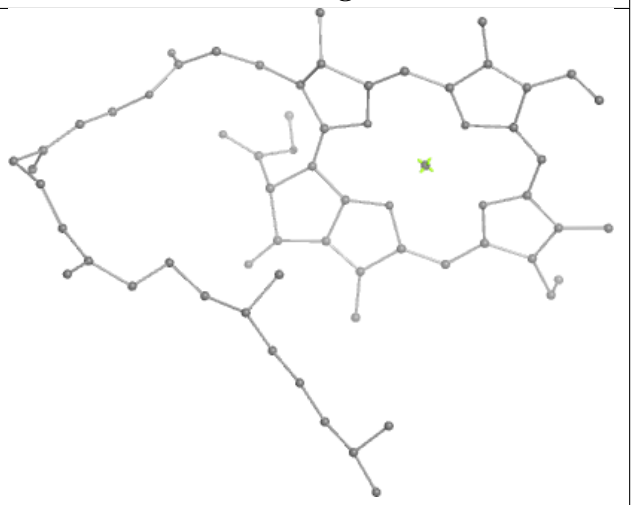
Bond lengths



Bond angles

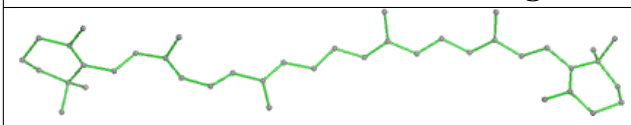


Torsions

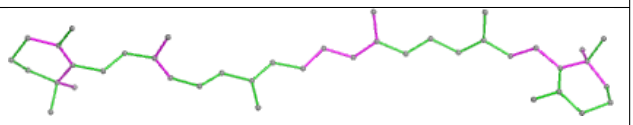


Rings

Ligand BCR F 102



Bond lengths

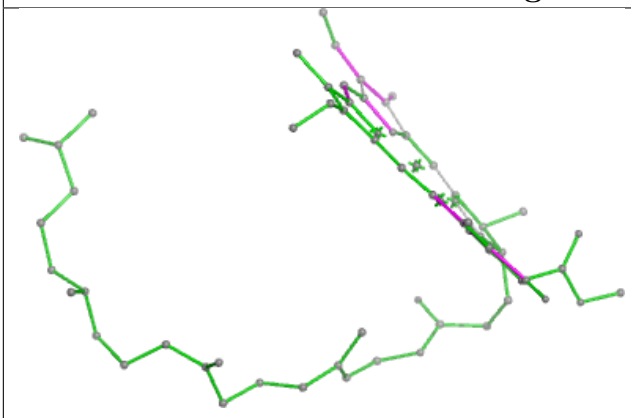


Bond angles

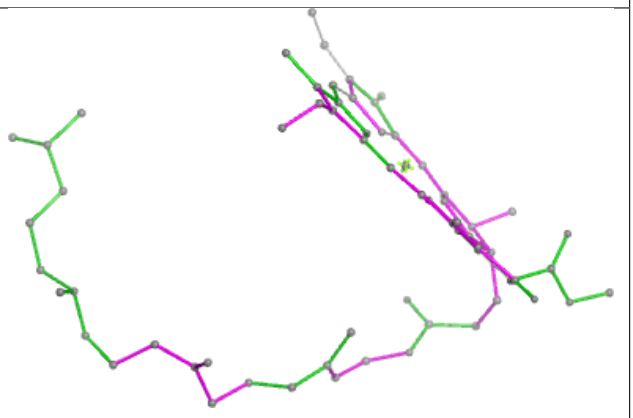
Torsions

Rings

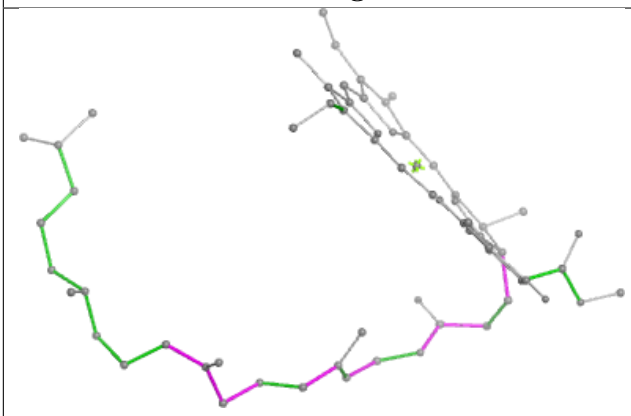
Ligand CLA B 611



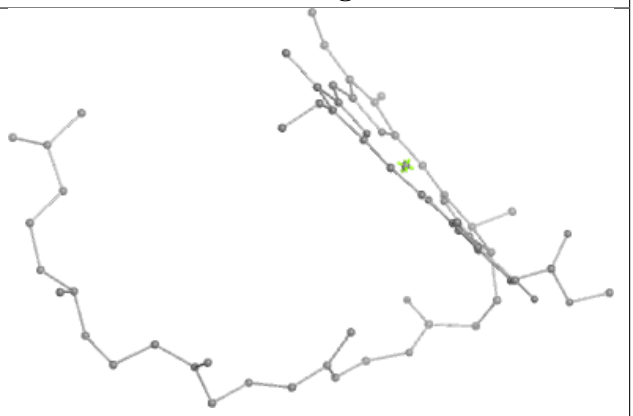
Bond lengths



Bond angles

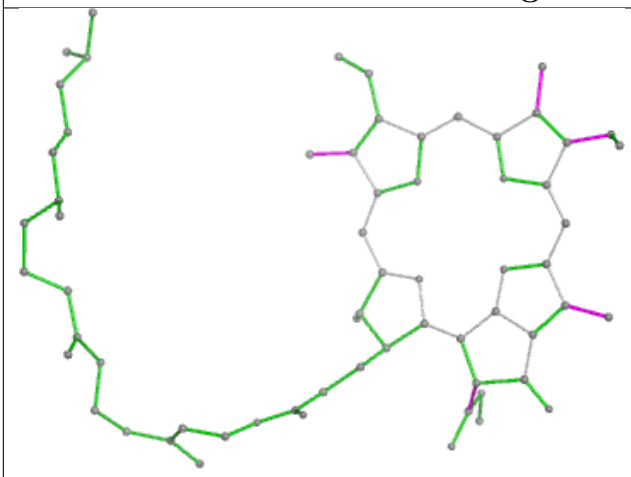


Torsions

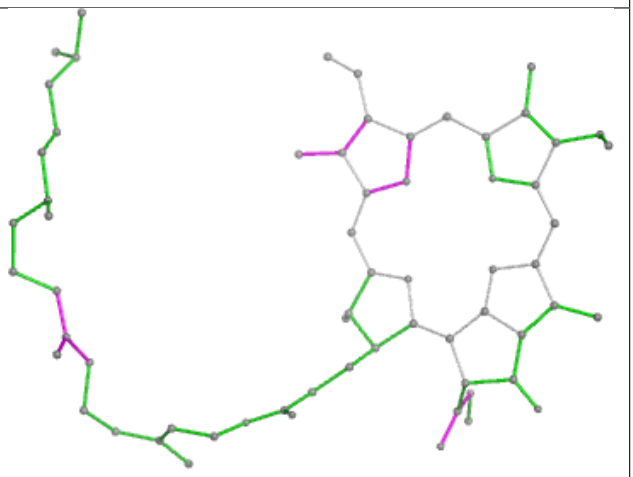


Rings

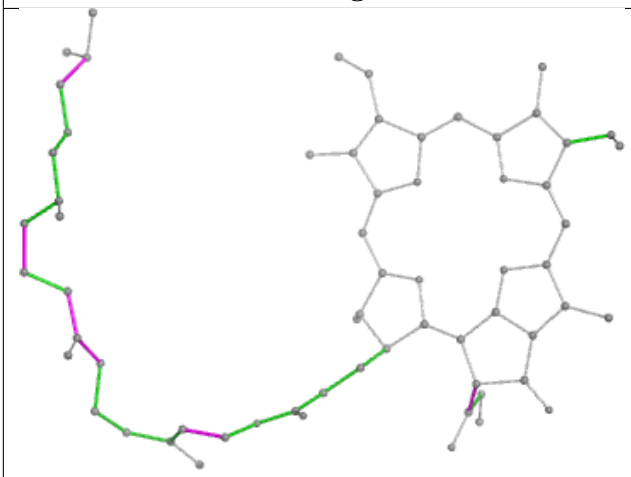
Ligand PHO A 404



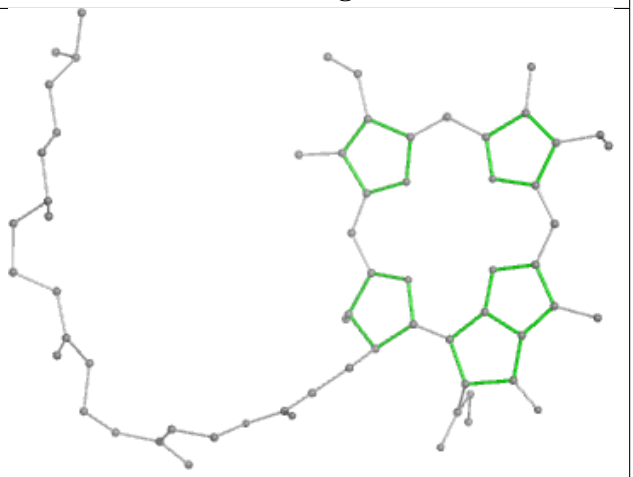
Bond lengths



Bond angles

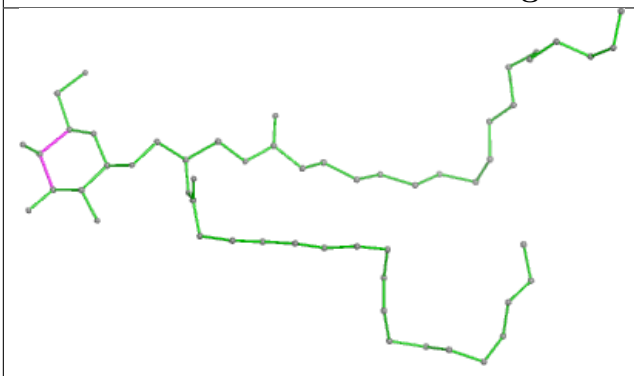


Torsions

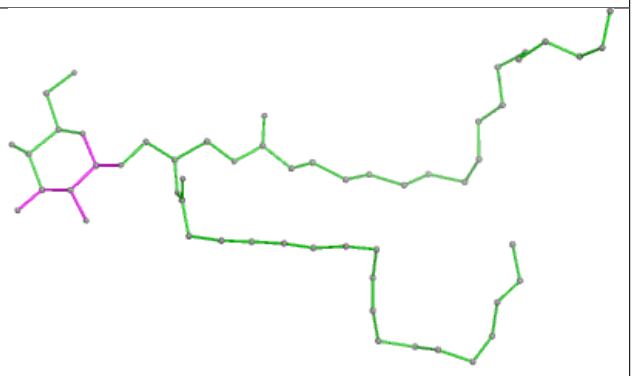


Rings

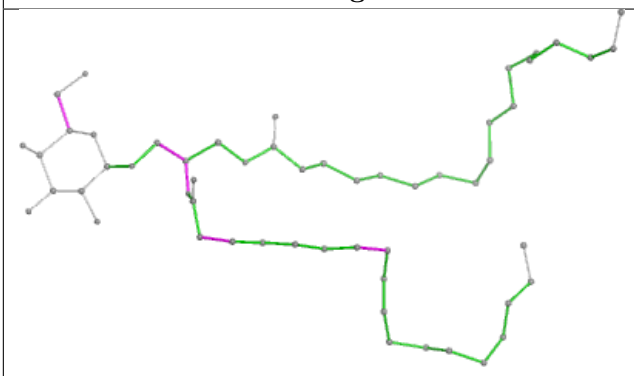
Ligand LMG F 101



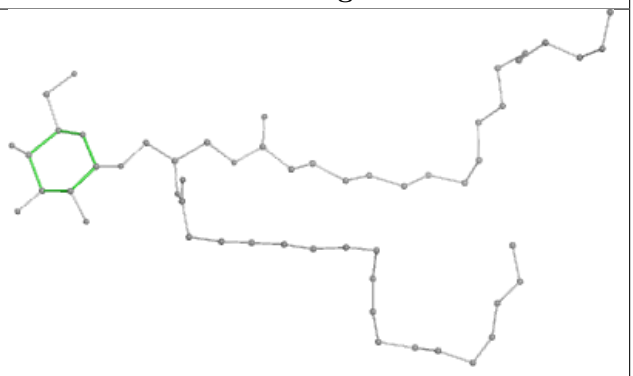
Bond lengths



Bond angles

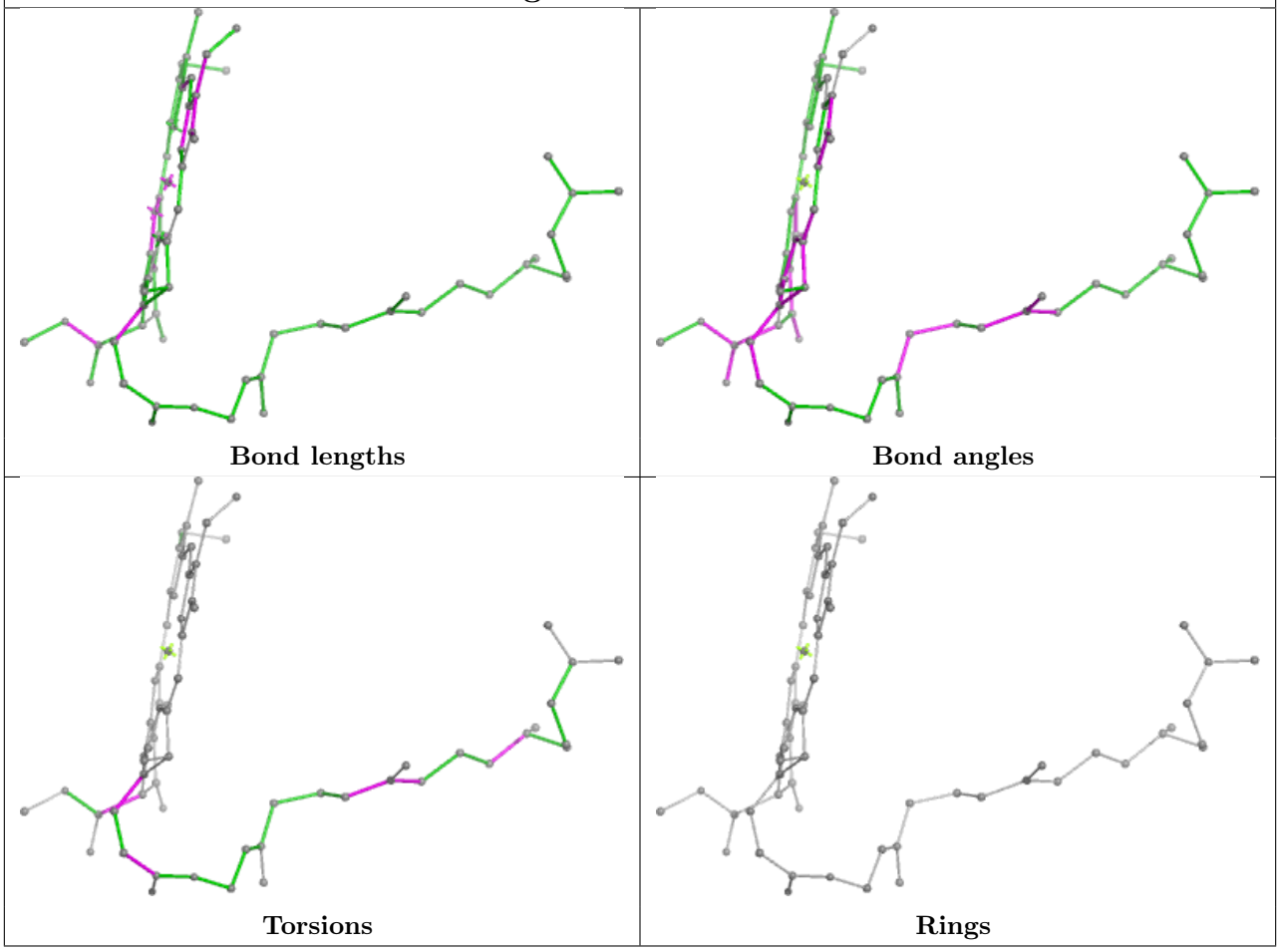


Torsions

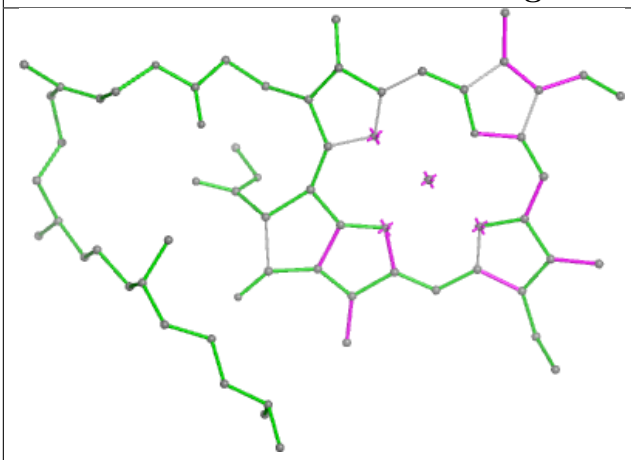


Rings

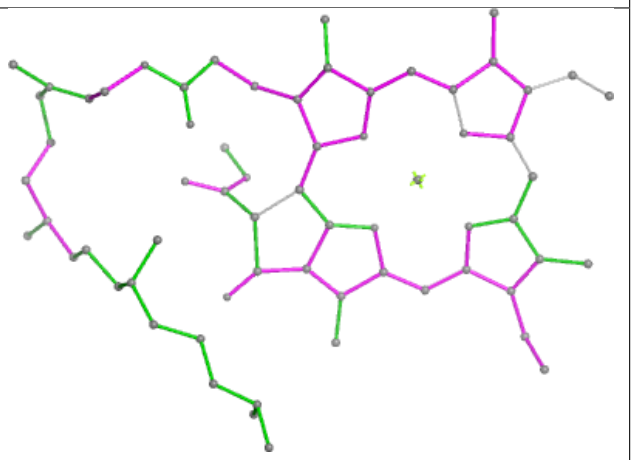
Ligand CLA C 506



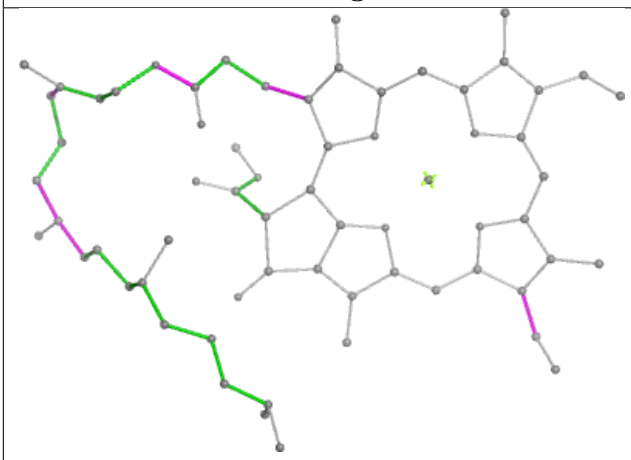
Ligand CLA B 610



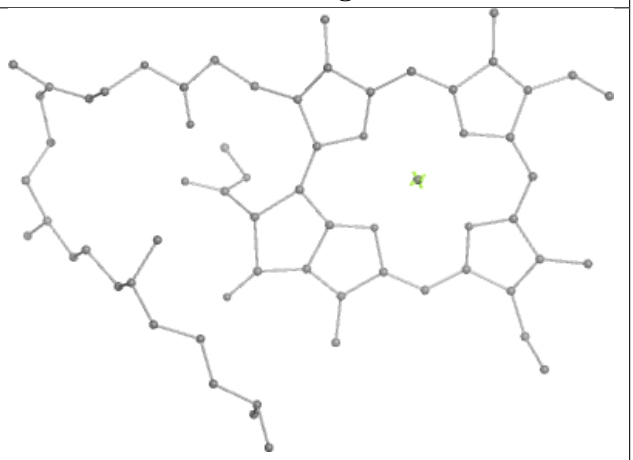
Bond lengths



Bond angles

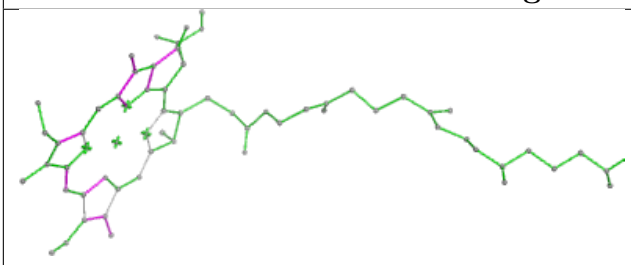


Torsions

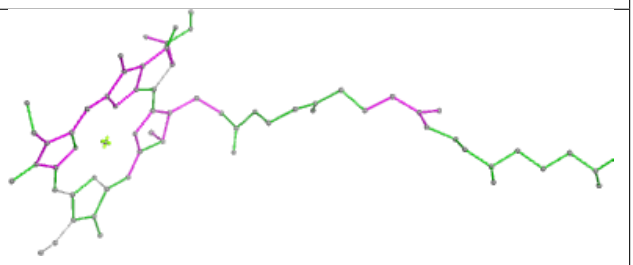


Rings

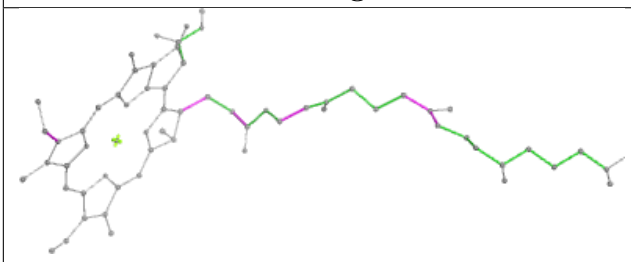
Ligand CLA D 407



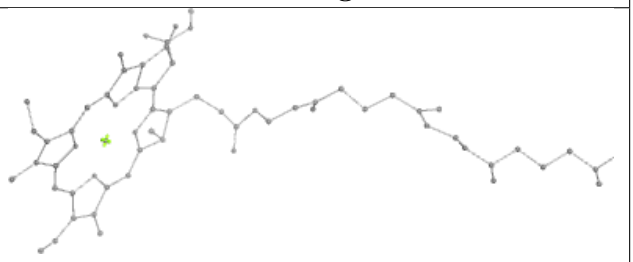
Bond lengths



Bond angles

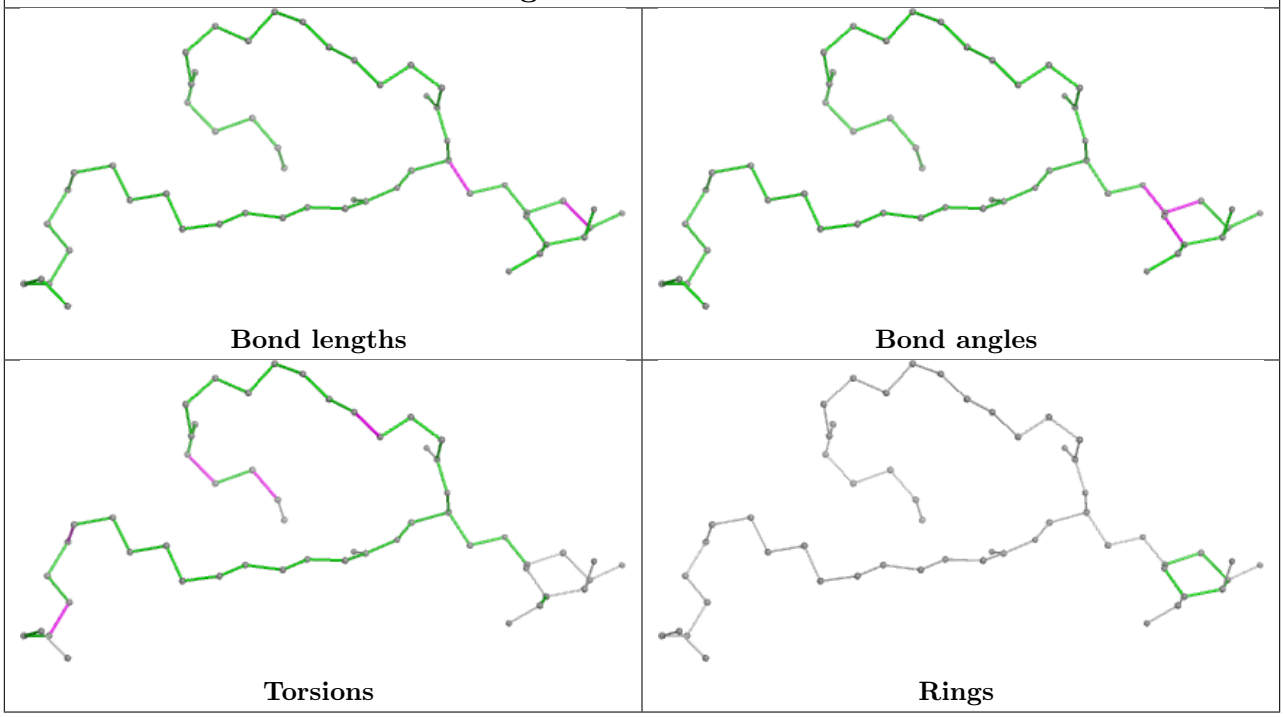


Torsions

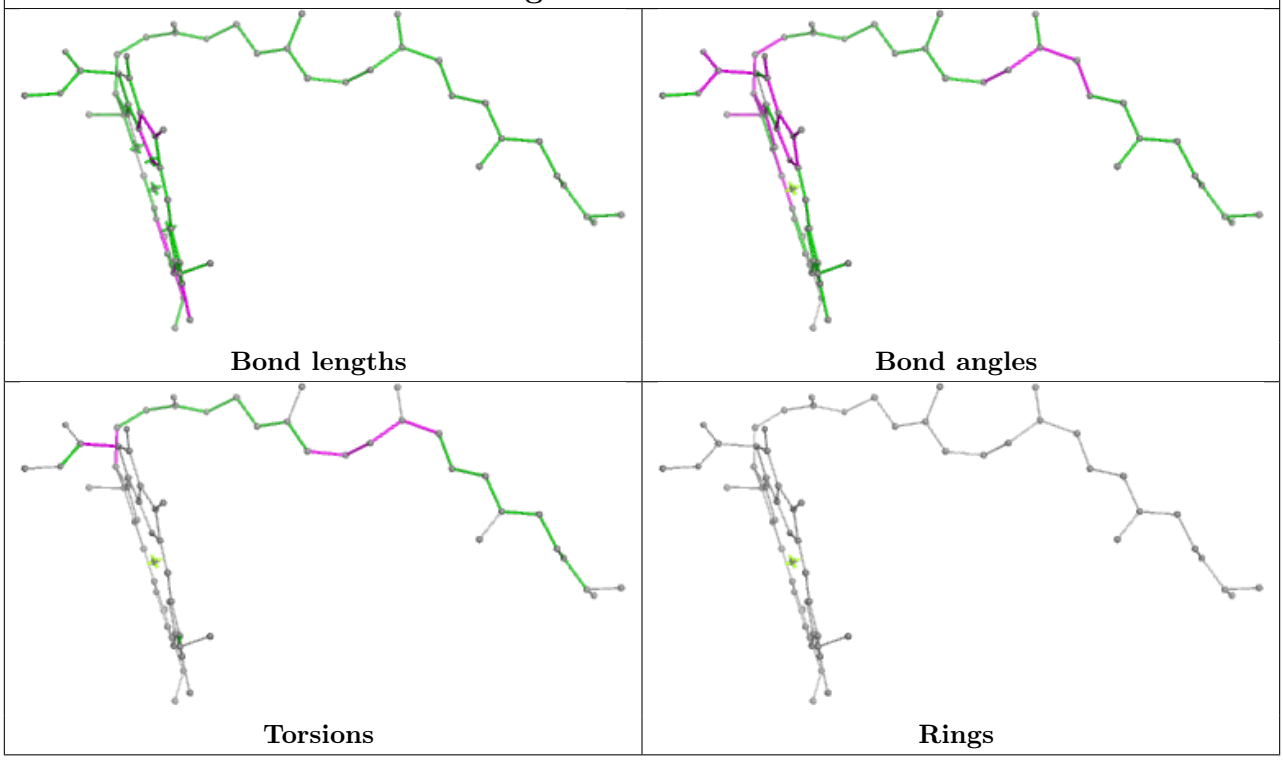


Rings

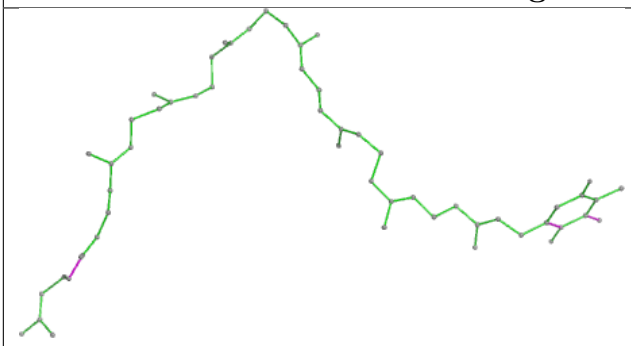
Ligand LMG D 403



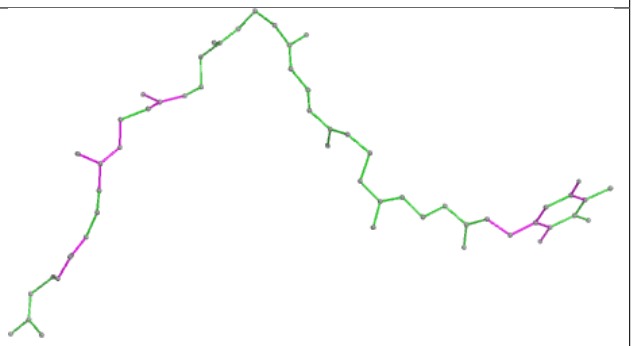
Ligand CLA B 605



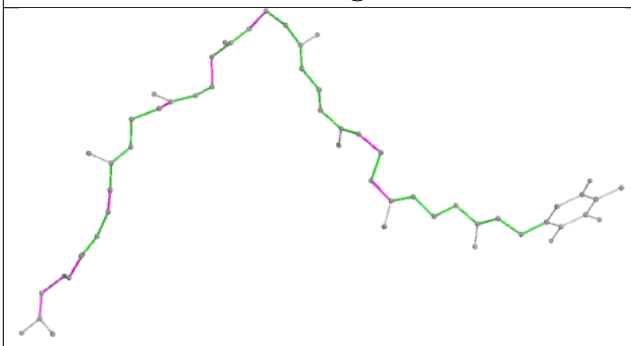
Ligand PL9 D 405



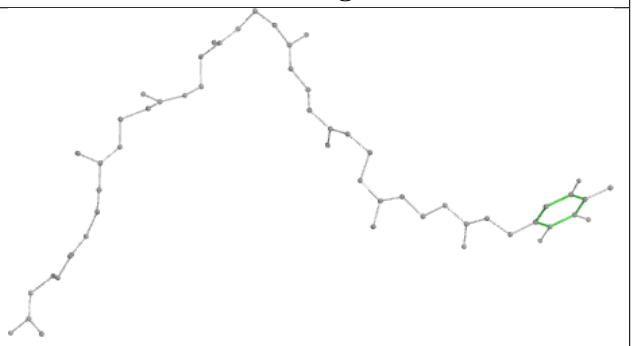
Bond lengths



Bond angles

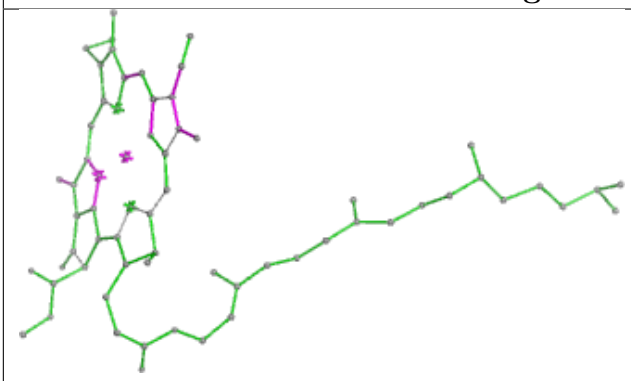


Torsions

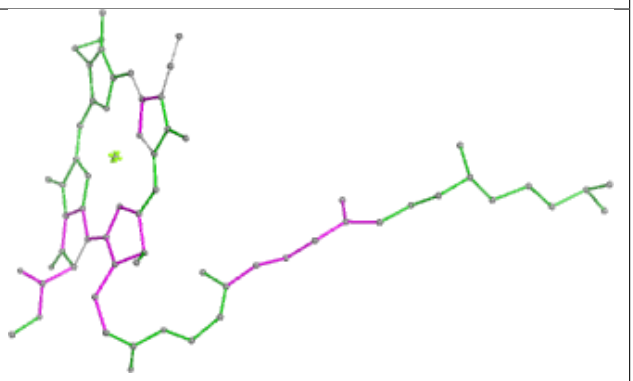


Rings

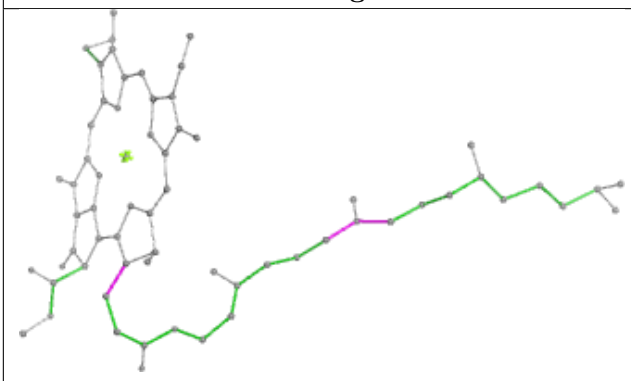
Ligand CLA D 408



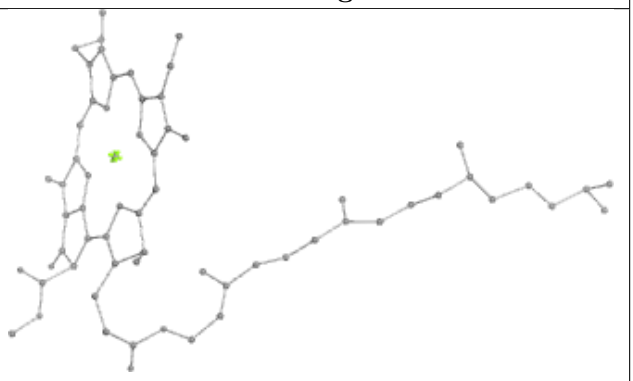
Bond lengths



Bond angles

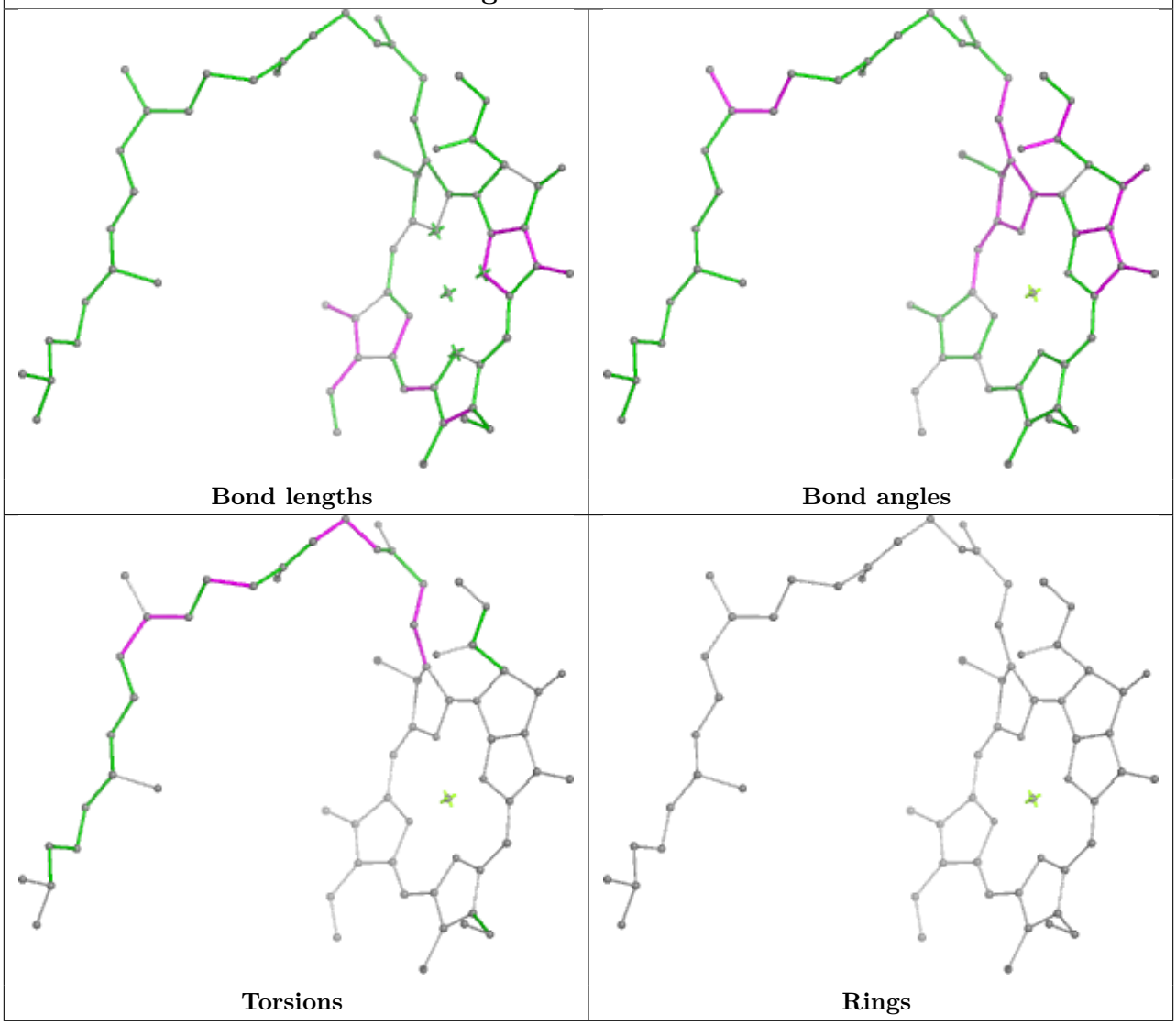


Torsions



Rings

Ligand CLA C 509



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.

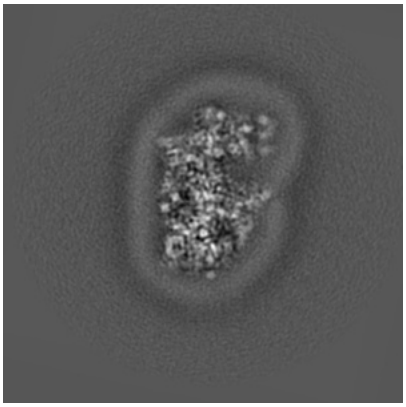
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-12337. These allow visual inspection of the internal detail of the map and identification of artifacts.

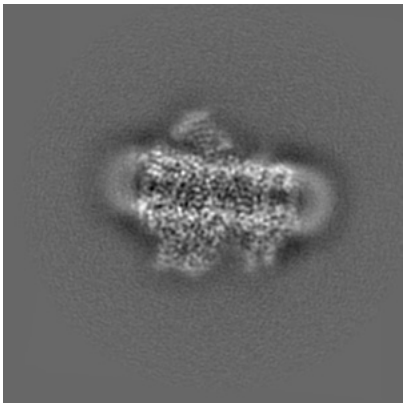
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

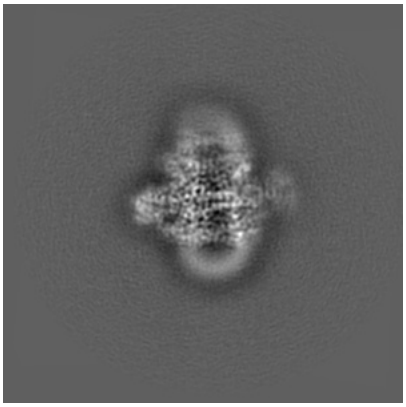
6.1.1 Primary map



X



Y

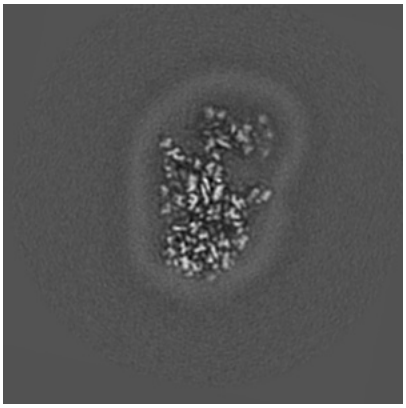


Z

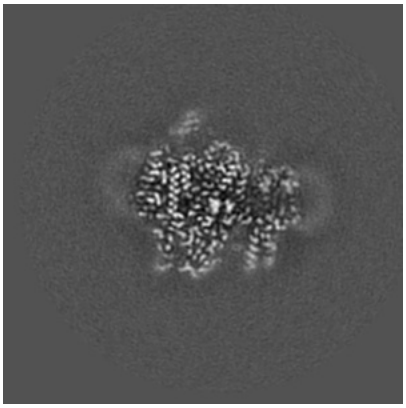
The images above show the map projected in three orthogonal directions.

6.2 Central slices

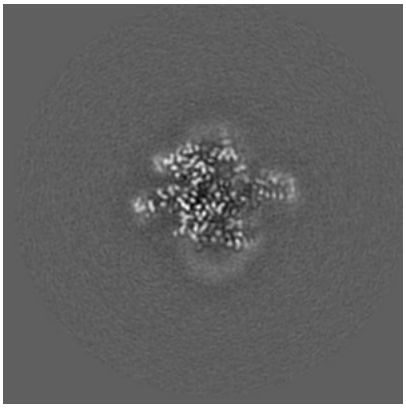
6.2.1 Primary map



X Index: 130



Y Index: 130

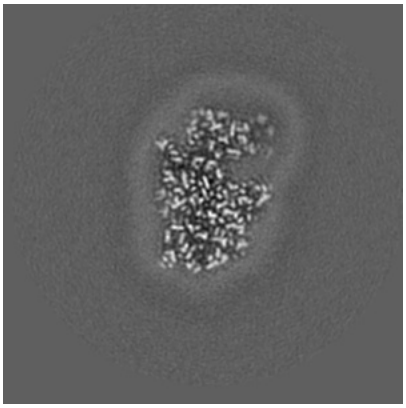


Z Index: 130

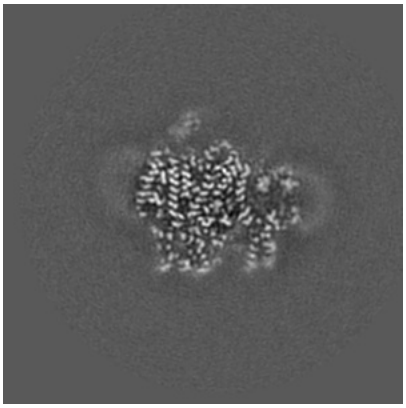
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

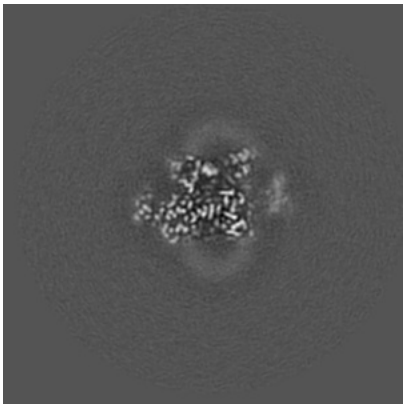
6.3.1 Primary map



X Index: 125



Y Index: 129

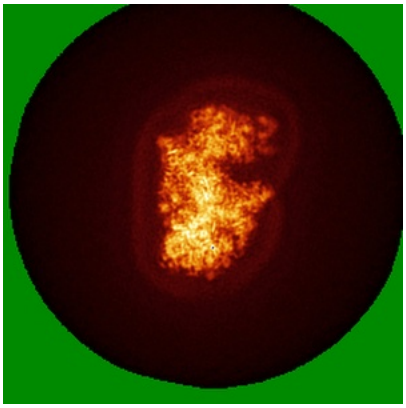


Z Index: 116

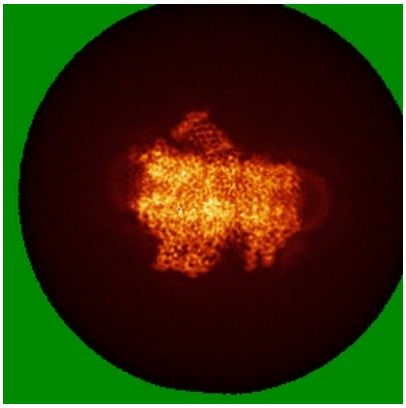
The images above show the largest variance slices of the map in three orthogonal directions.

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

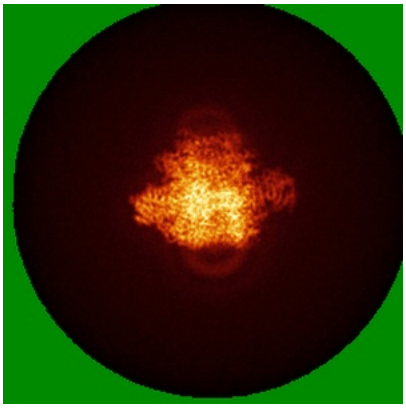
6.4.1 Primary map



X



Y



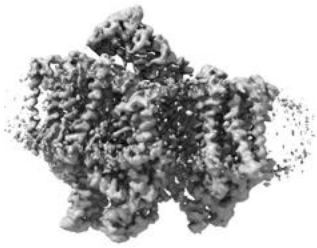
Z

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

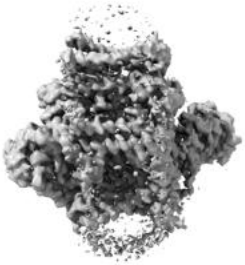
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.006. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

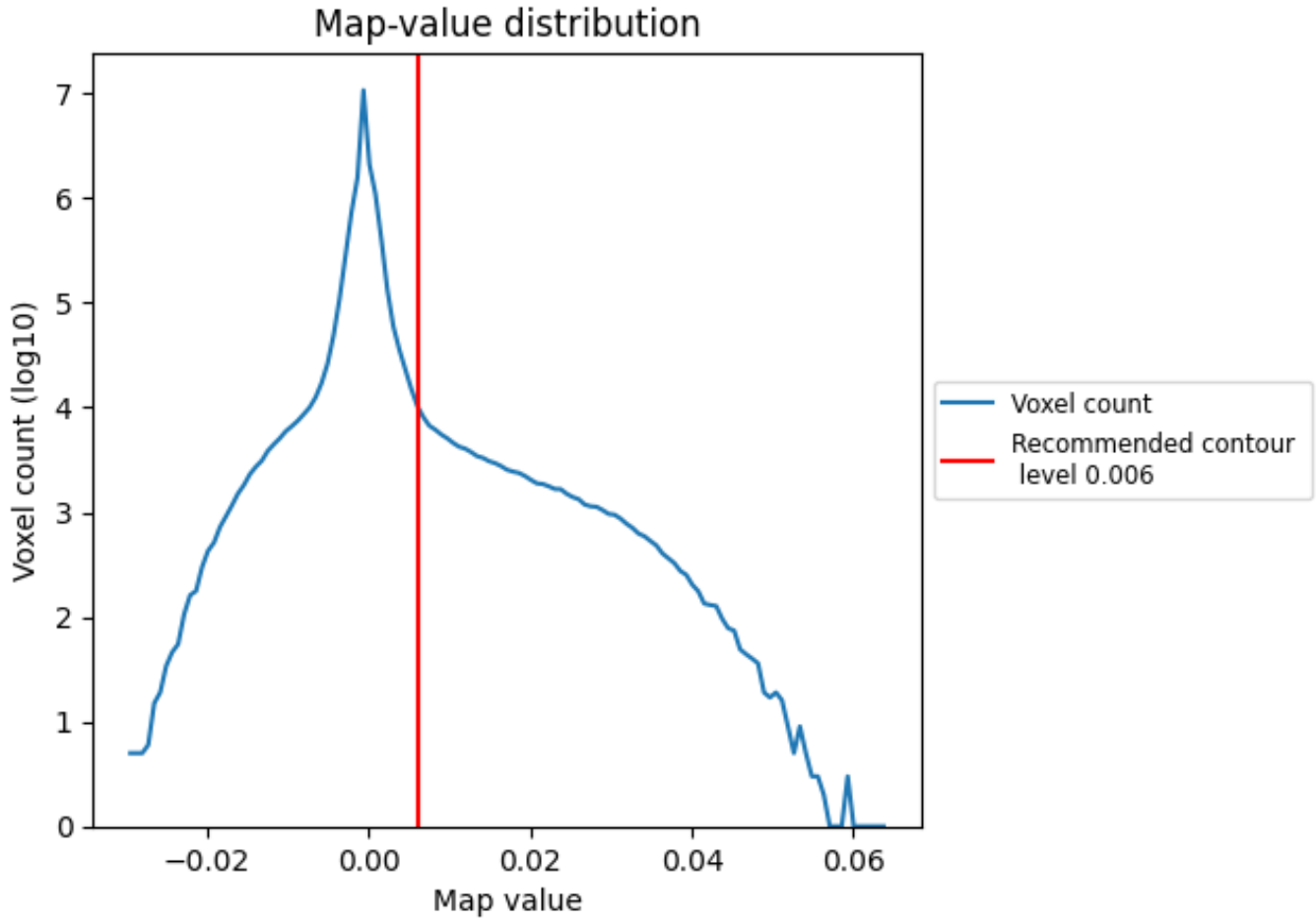
6.6 Mask visualisation (i)

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

7 Map analysis

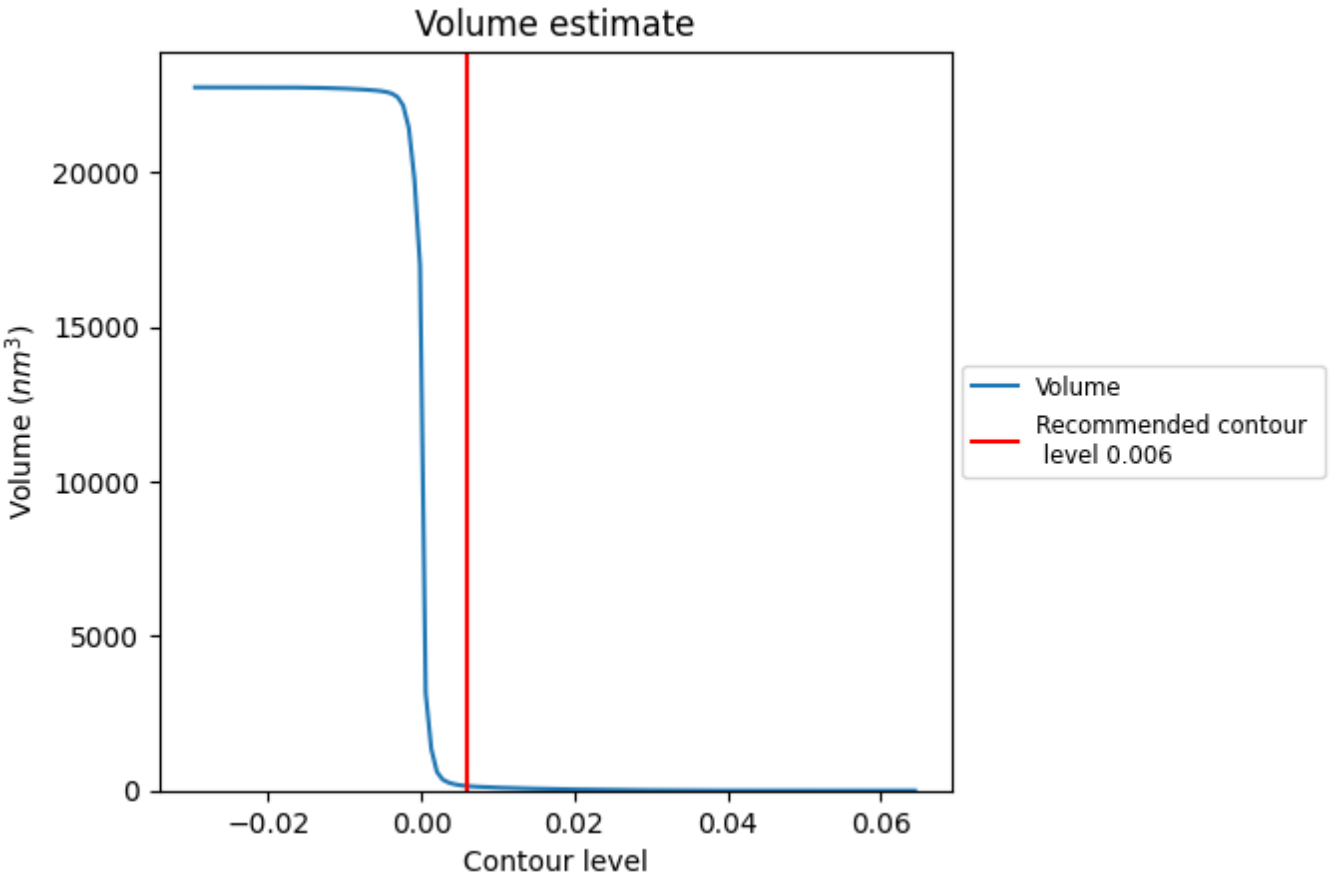
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

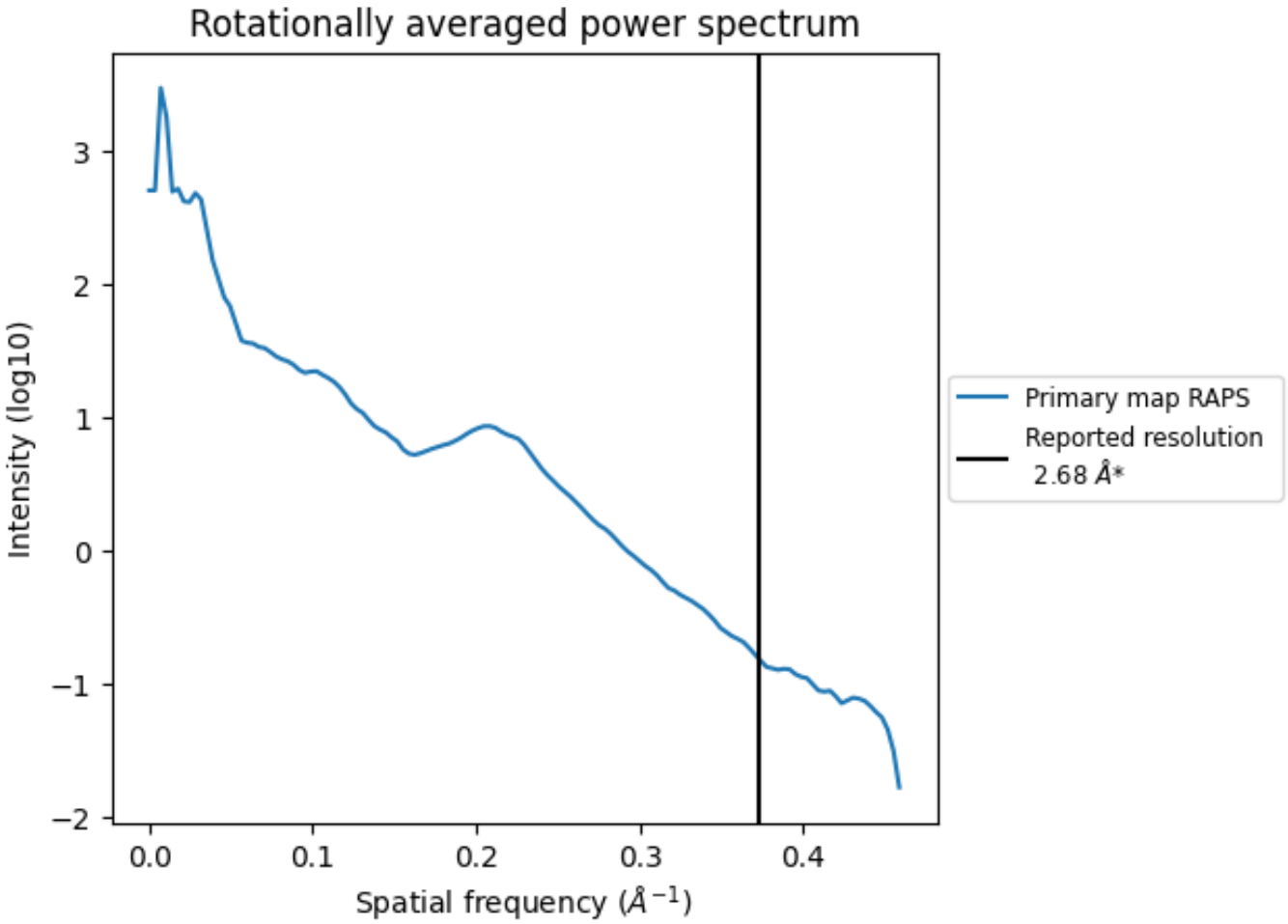
7.2 Volume estimate



The volume at the recommended contour level is 147 nm^3; this corresponds to an approximate mass of 133 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 0.373 $Å^{-1}$

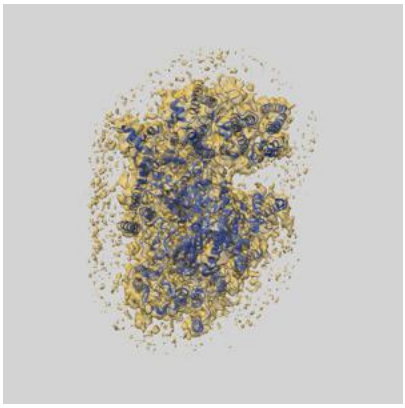
8 Fourier-Shell correlation (i)

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

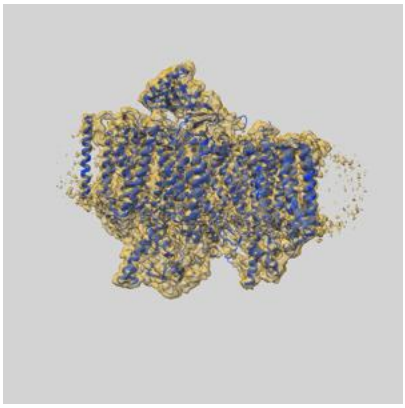
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-12337 and PDB model 7NHQ. Per-residue inclusion information can be found in section 3 on page 14.

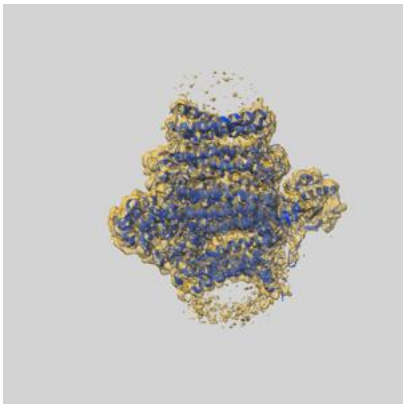
9.1 Map-model overlay



X



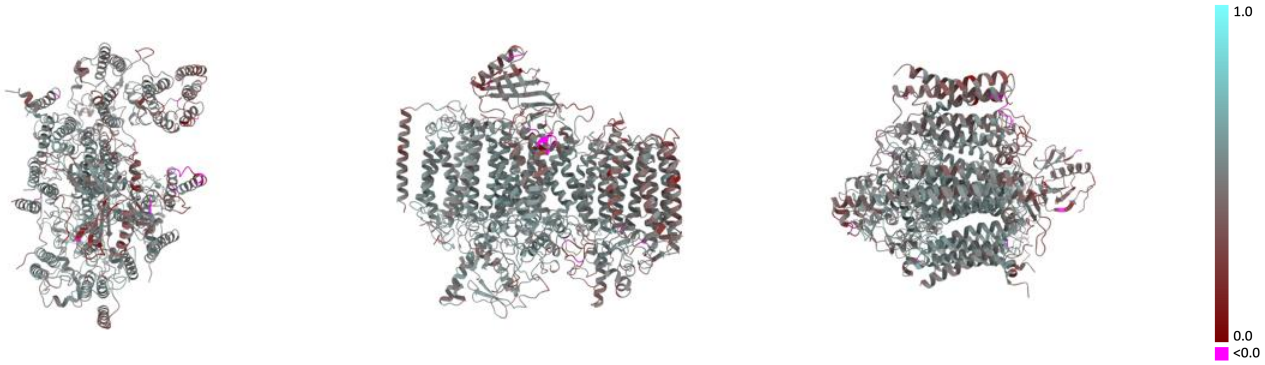
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.006 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.

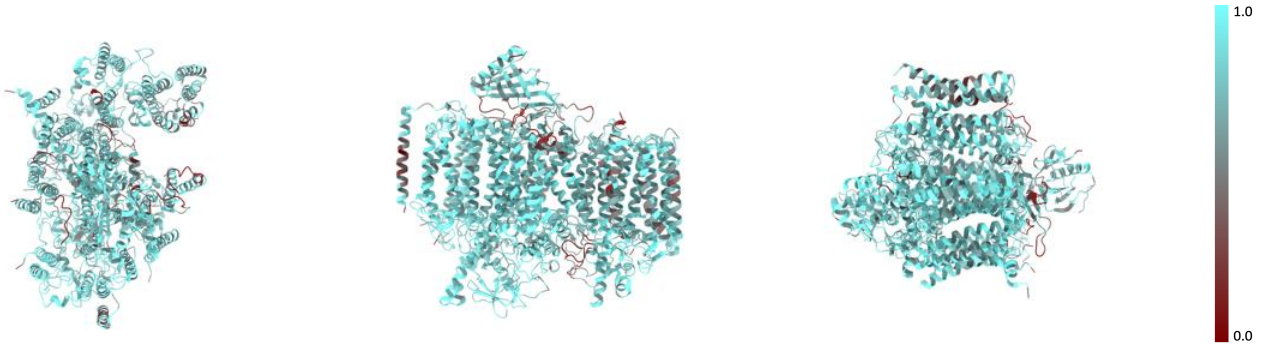
9.2 Q-score mapped to coordinate model (i)



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.

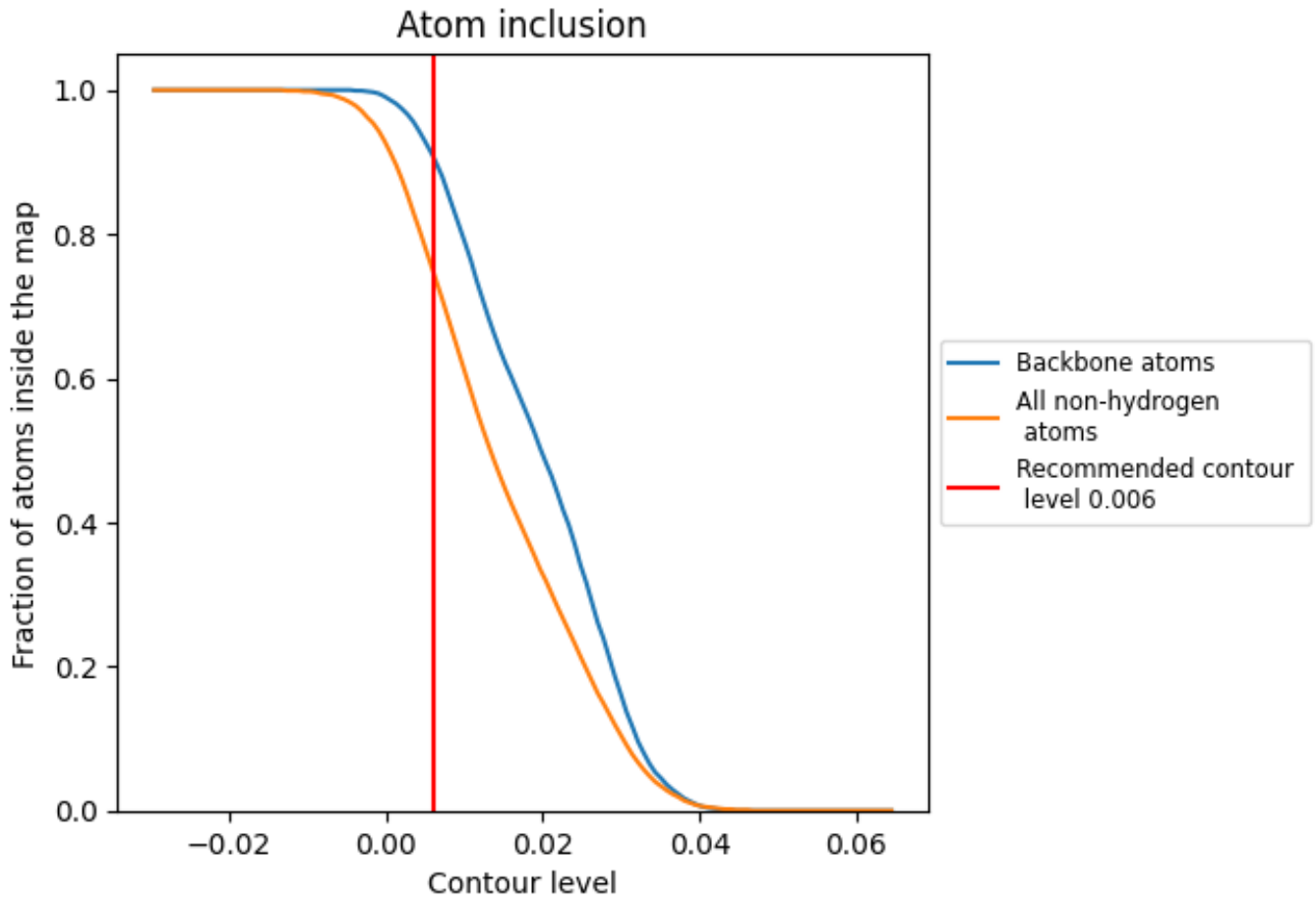
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.006).

9.4 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 75% 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 (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7510	0.4650
2	0.7490	0.3980
3	0.4990	0.4070
A	0.7660	0.4900
B	0.8120	0.4970
C	0.7050	0.4280
D	0.8150	0.5250
E	0.7010	0.3620
F	0.5680	0.3920
H	0.8410	0.4930
I	0.6230	0.3870
K	0.5780	0.3990
L	0.8020	0.5130
M	0.6800	0.4440
T	0.7420	0.4800
X	0.7790	0.4710
Z	0.6720	0.3760
y	0.5240	0.3410