Full wwPDB EM Validation Report (i)

Feb 26, 2024 – 05:02 AM EST

PDB ID	:	6WJ6
EMDB ID	:	EMD-21690
Title	:	Cryo-EM structure of apo-Photosystem II from Synechocystis sp. PCC 6803
Authors	:	Gisriel, C.J.
Deposited on	:	2020-04-12
Resolution	:	2.58 Å(reported)

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

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

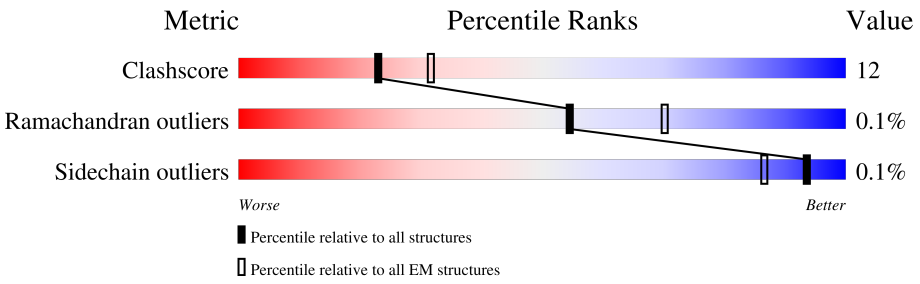
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.58 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	9% 65% 19% 16%
2	B	507	5% 74% 21% 6%
3	C	460	7% 73% 18% 10%
4	D	352	8% 74% 24% .
5	E	81	22% 57% 32% 11%
6	F	44	14% 64% 9% 27%
7	H	64	9% 81% 17% .
8	I	38	18% 76% 16% 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	K	45	51% 49% 29% 22%
10	L	39	13% 59% 21% 21%
11	M	35	23% 71% 11% 17%
12	T	31	32% 71% 23% 6%
13	X	39	26% 62% 28% 10%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	A	402	X	-	-	-
15	CLA	A	403	X	-	-	-
15	CLA	A	405	X	-	-	-
15	CLA	B	601	X	-	-	-
15	CLA	B	602	X	-	-	-
15	CLA	B	603	X	-	-	-
15	CLA	B	604	X	-	-	-
15	CLA	B	605	X	-	-	-
15	CLA	B	606	X	-	-	-
15	CLA	B	607	X	-	-	-
15	CLA	B	608	X	-	-	-
15	CLA	B	609	X	-	-	-
15	CLA	B	610	X	-	-	-
15	CLA	B	611	X	-	-	-
15	CLA	B	612	X	-	-	-
15	CLA	B	613	X	-	-	-
15	CLA	B	614	X	-	-	-
15	CLA	B	615	X	-	-	-
15	CLA	B	616	X	-	-	-
15	CLA	C	502	X	-	-	-
15	CLA	C	503	X	-	-	-
15	CLA	C	504	X	-	-	-
15	CLA	C	505	X	-	-	-
15	CLA	C	506	X	-	-	-
15	CLA	C	507	X	-	-	-
15	CLA	C	508	X	-	-	-
15	CLA	C	509	X	-	-	-
15	CLA	C	510	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	C	511	X	-	-	-
15	CLA	C	512	X	-	-	-
15	CLA	C	513	X	-	-	-
15	CLA	C	514	X	-	-	-
15	CLA	D	402	X	-	-	-
15	CLA	D	405	X	-	-	-
15	CLA	D	406	X	-	-	-

2 Entry composition (i)

There are 28 unique types of molecules in this entry. The entry contains 18884 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 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	302	2357	1552	386	404	15	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	478	3751	2454	628	656	13	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	415	3259	2151	542	553	13	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	18	SER	THR	conflict	UNP P09193

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	342	2734	1812	444	466	12	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	72	603	396	95	111	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	32	255	173	43	38	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	H	63	494	328	79	85	2	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	I	35	276	186	44	46	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	K	35	278	195	39	44	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	L	31	252	169	40	43	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
11	M	29	226	157	33	36	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	T	29	231	157	35	38	1	0	0

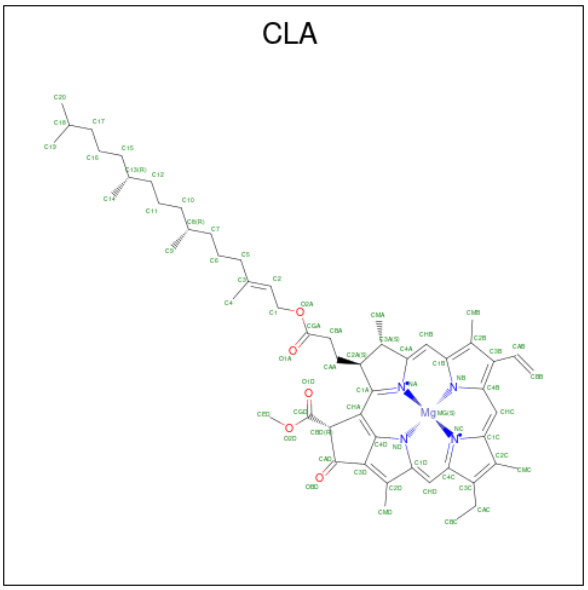
- Molecule 13 is a protein called Photosystem II reaction center X protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	X	35	262	177	40	44	1	0	0

- Molecule 14 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 15 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
15	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
15	A	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
15	A	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
15	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
15	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
15	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
15	B	1	65	55	1	4	5	0

Continued on next page...

Continued from previous page...

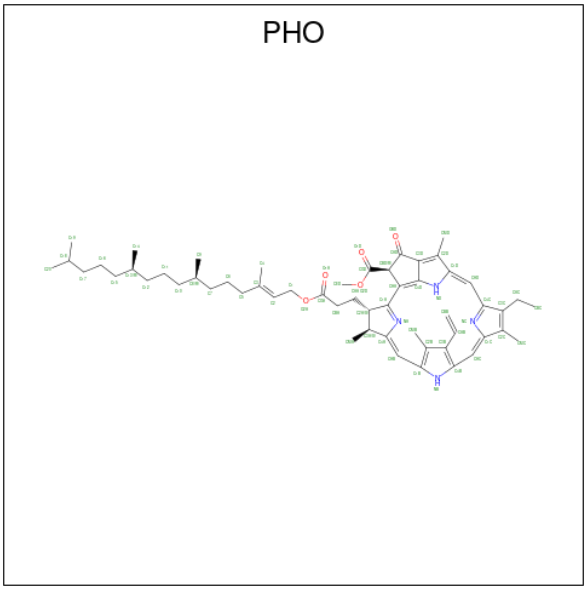
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
15	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
15	B	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
15	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
15	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
15	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
15	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
15	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
15	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
15	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
15	B	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
15	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
15	B	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
15	C	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
15	C	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
15	C	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
15	C	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
15	C	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
15	C	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
15	C	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
15	C	1	65	55	1	4	5	0

Continued on next page...

Continued from previous page...

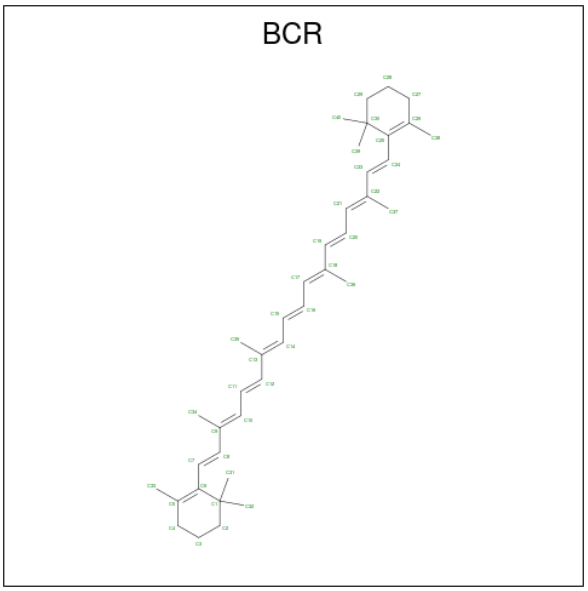
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
15	C	1	65	55	1	4	5	0
15	C	1	45	35	1	4	5	0
15	C	1	65	55	1	4	5	0
15	C	1	65	55	1	4	5	0
15	D	1	65	55	1	4	5	0
15	D	1	65	55	1	4	5	0
15	D	1	65	55	1	4	5	0

- Molecule 16 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



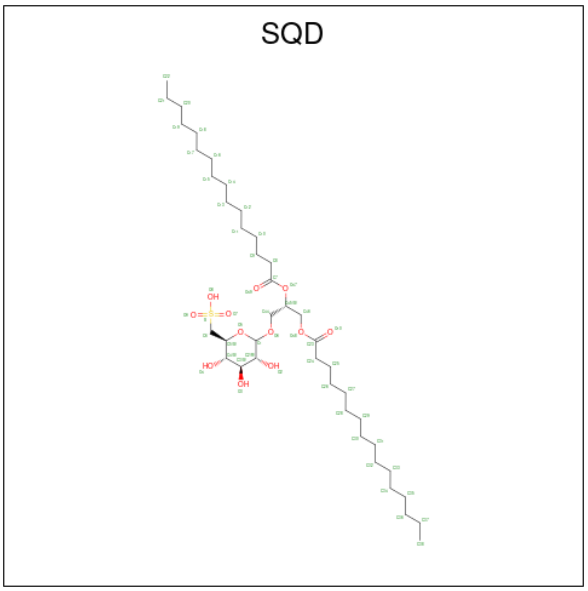
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
16	A	1	64	55	4	5	0
16	D	1	64	55	4	5	0

- Molecule 17 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



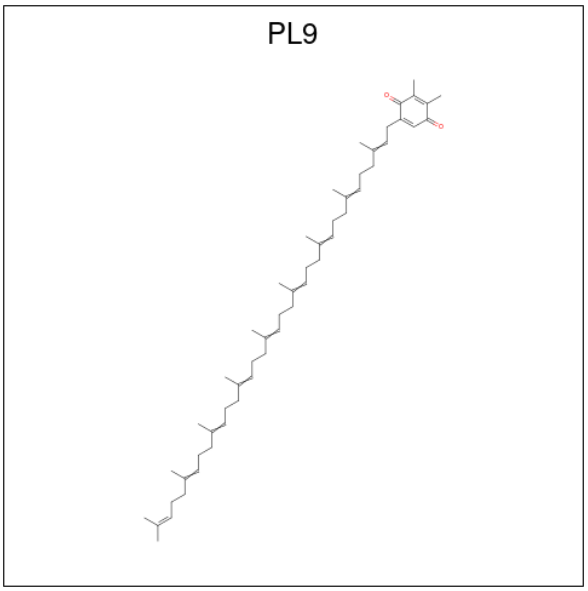
Mol	Chain	Residues	Atoms		AltConf
			Total	C	
17	A	1	40	40	0
17	B	1	40	40	0
17	B	1	40	40	0
17	B	1	40	40	0
17	C	1	40	40	0
17	C	1	40	40	0
17	C	1	40	40	0
17	D	1	40	40	0
17	X	1	40	40	0

- Molecule 18 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



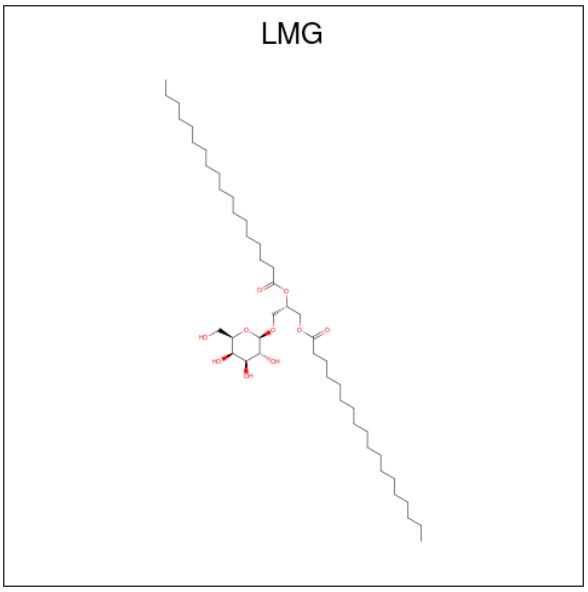
Mol	Chain	Residues	Atoms				AltConf
18	A	1	Total	C	O	S	0
			48	35	12	1	
18	A	1	Total	C	O	S	0
			54	41	12	1	
18	B	1	Total	C	O	S	0
			51	38	12	1	
18	C	1	Total	C	O	S	0
			54	41	12	1	
18	T	1	Total	C	O	S	0
			52	39	12	1	
18	T	1	Total	C	O	S	0
			41	28	12	1	
18	X	1	Total	C	O	S	0
			42	29	12	1	

- Molecule 19 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
			Total	C	O	
19	A	1	15	13	2	0
			Total	C	O	
19	D	1	55	53	2	0

- Molecule 20 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



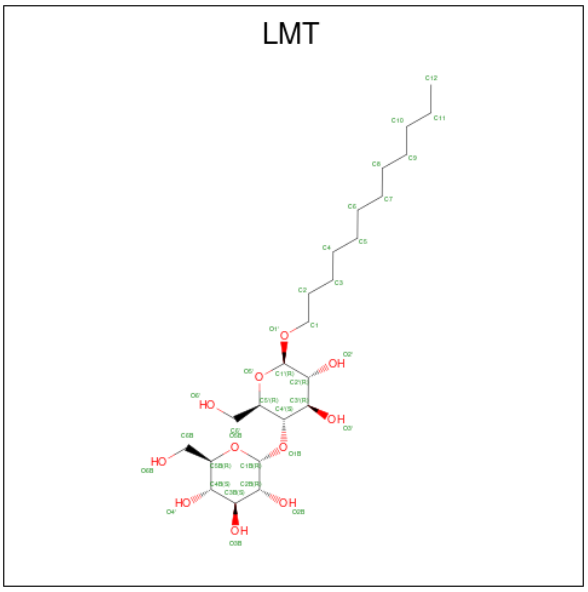
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
20	B	1	51	41	10	0

Continued on next page...

Continued from previous page...

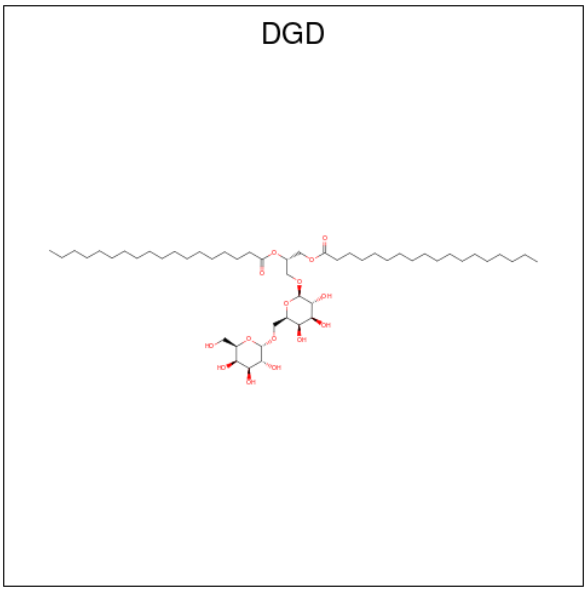
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
20	C	1	51	41	10	0
20	D	1	51	41	10	0

- Molecule 21 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
21	B	1	35	24	11	0
21	B	1	34	23	11	0

- Molecule 22 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).

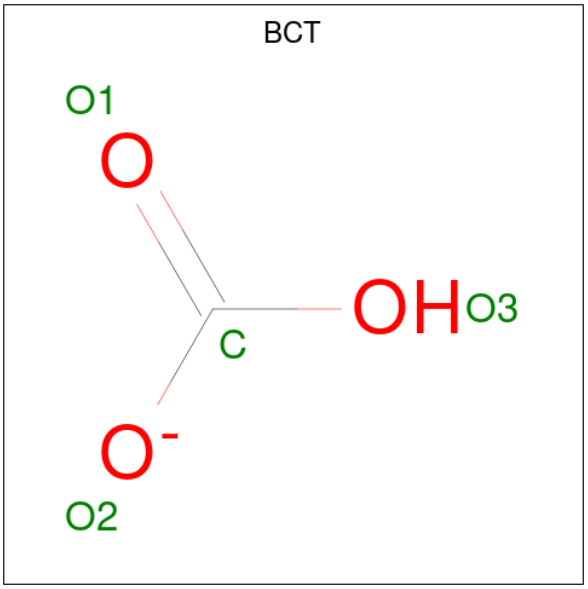


Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
22	C	1	62	47	15	0
			Total	C	O	
22	H	1	62	47	15	0

- Molecule 23 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

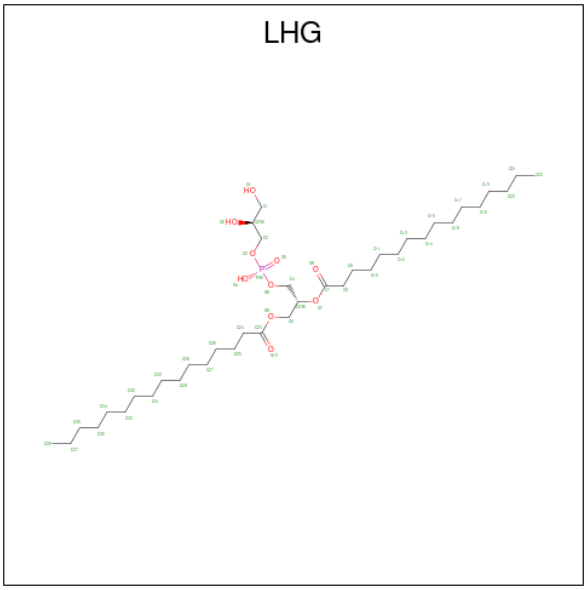
Mol	Chain	Residues	Atoms		AltConf
			Total	Cl	
23	D	1	1	1	0

- Molecule 24 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



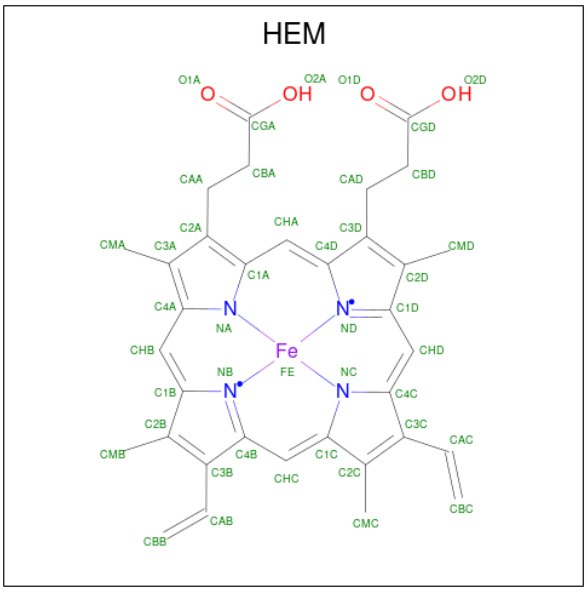
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
24	D	1	4	1	3	0

- Molecule 25 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



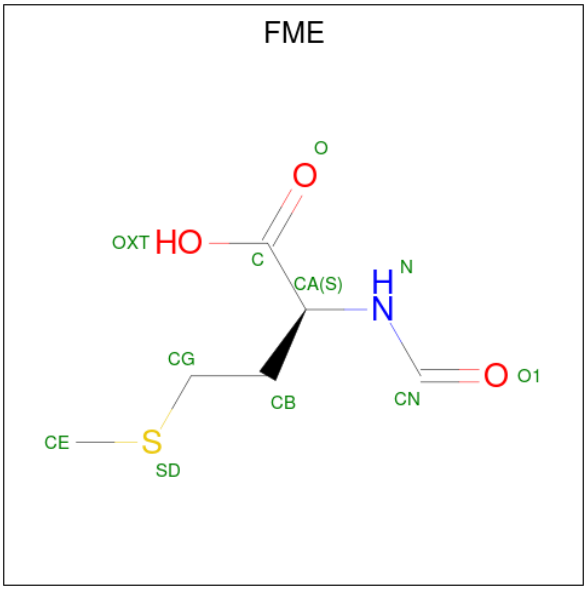
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
25	D	1	49	38	10	1	0
			Total	C	O	P	
25	D	1	49	38	10	1	0
			Total	C	O	P	
25	D	1	46	35	10	1	0
			Total	C	O	P	
25	L	1	49	38	10	1	0

- Molecule 26 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 27 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: $C_6H_{11}NO_3S$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
27	I	1	10	6	1	2	1	0
27	M	1	Total 10	C 6	N 1	O 2	S 1	0
27	T	1	Total 10	C 6	N 1	O 2	S 1	0

- Molecule 28 is water.

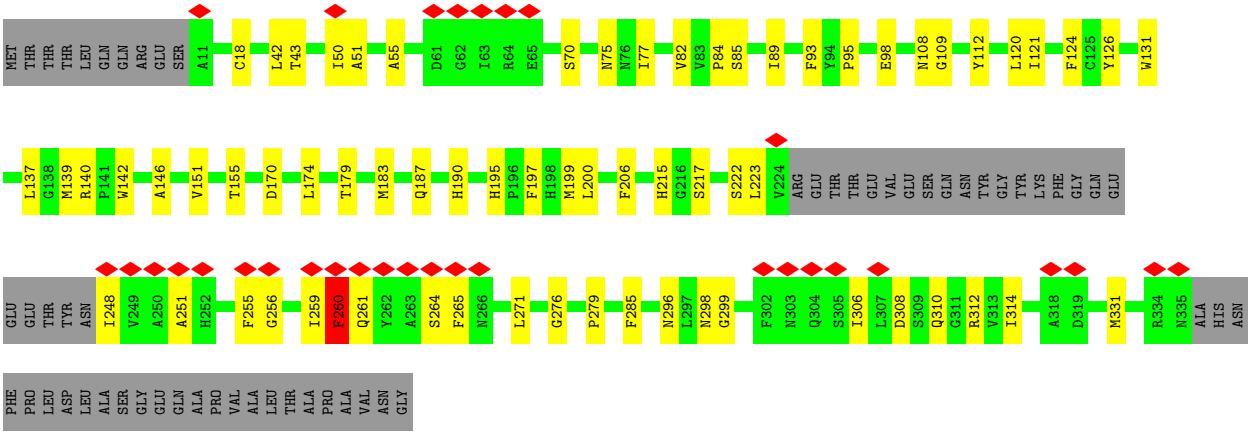
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
28	A	54	54	54	0
28	B	62	62	62	0
28	C	30	30	30	0
28	D	46	46	46	0
28	E	2	2	2	0
28	L	1	1	1	0
28	T	2	2	2	0
28	X	1	1	1	0

3 Residue-property plots (i)

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

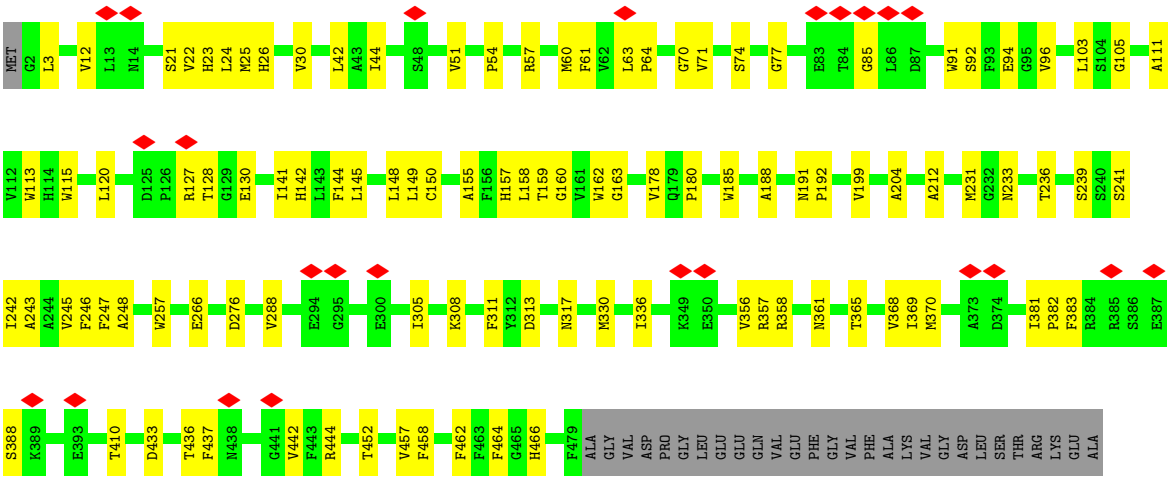
• Molecule 1: Photosystem II protein D1 2

Chain A: 9% 65% 19% 16%



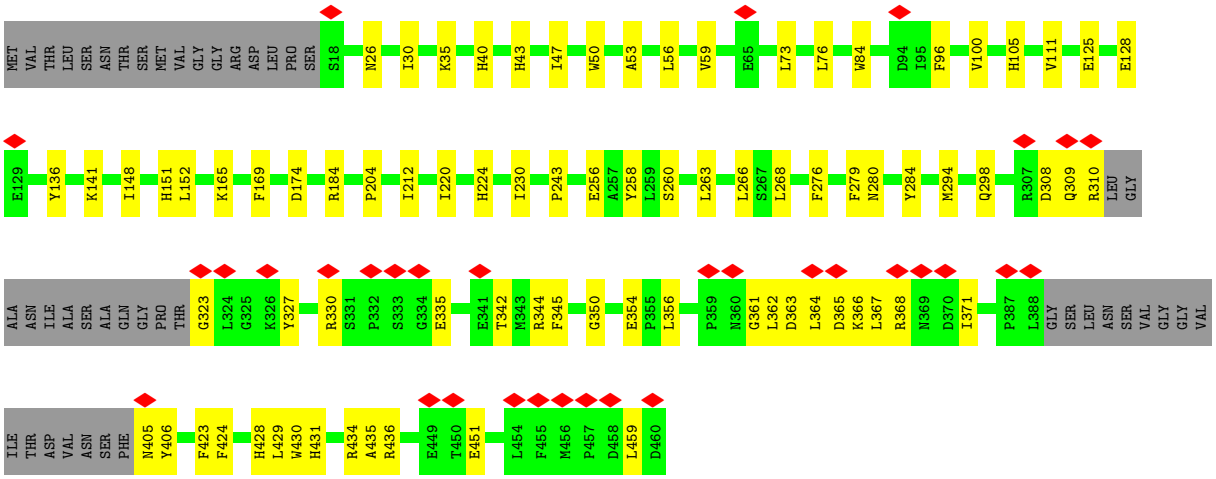
• Molecule 2: Photosystem II CP47 reaction center protein

Chain B: 5% 74% 21% 6%



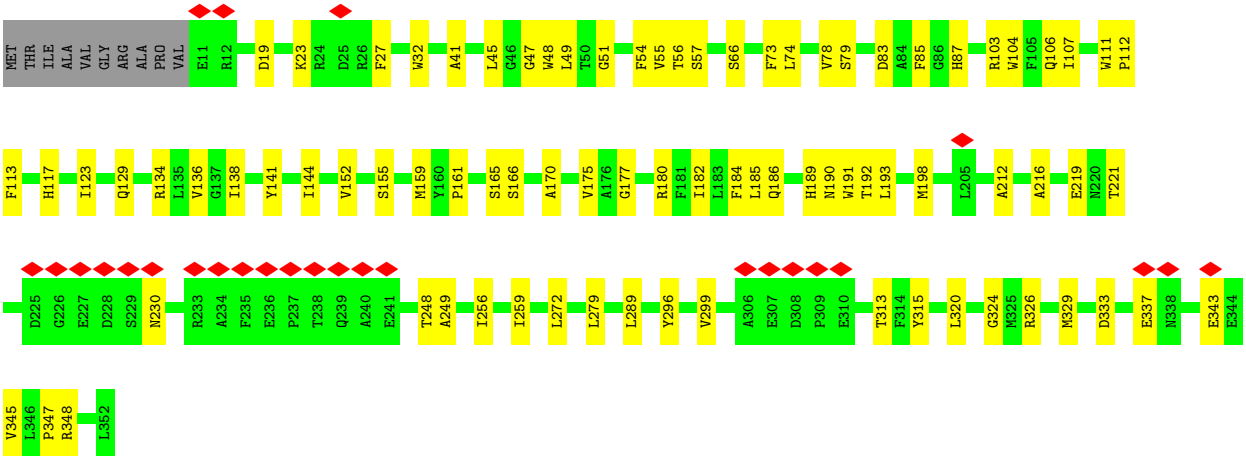
• Molecule 3: Photosystem II CP43 reaction center protein

Chain C:



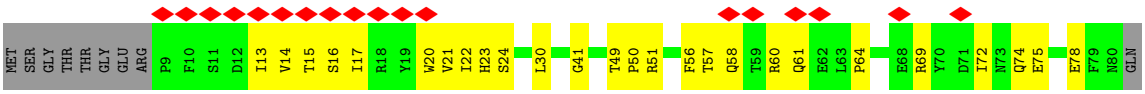
- Molecule 4: Photosystem II D2 protein

Chain D:



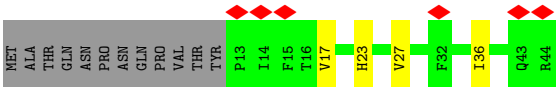
- Molecule 5: Cytochrome b559 subunit alpha

Chain E:



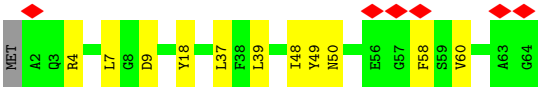
- Molecule 6: Cytochrome b559 subunit beta

Chain F:



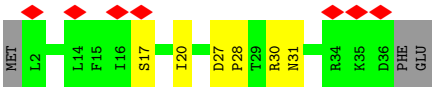
• Molecule 7: Photosystem II reaction center protein H

Chain H:



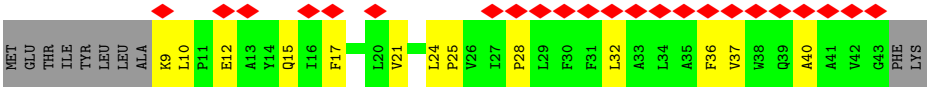
• Molecule 8: Photosystem II reaction center protein I

Chain I:



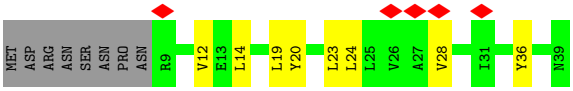
• Molecule 9: Photosystem II reaction center protein K

Chain K:



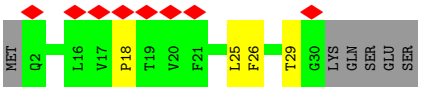
• Molecule 10: Photosystem II reaction center protein L

Chain L:



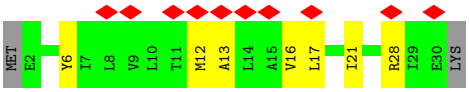
• Molecule 11: Photosystem II reaction center protein M

Chain M:



• Molecule 12: Photosystem II reaction center protein T

Chain T:



• Molecule 13: Photosystem II reaction center X protein

Chain X:

M1
L5
F8
L9
W10
S11
L12
V13
L14
G15
A16
A17
I18
V19
L20
I21
P22
A23
L27
I30
D34
K35
ILE
THR
ARG
SER

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	212640	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	48.07	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.243	Depositor
Minimum map value	-0.114	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.0394	Depositor
Map size (Å)	302.4, 302.4, 302.4	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.18125, 1.18125, 1.18125	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: LMG, SQD, PL9, FME, CLA, BCT, FE2, CL, LMT, DGD, PHO, HEM, LHG, BCR

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	0.29	0/2434	0.42	0/3319
2	B	0.30	0/3881	0.42	0/5285
3	C	0.28	0/3369	0.41	0/4582
4	D	0.30	0/2831	0.42	0/3855
5	E	0.30	0/622	0.44	0/849
6	F	0.27	0/263	0.42	0/357
7	H	0.29	0/506	0.45	0/687
8	I	0.27	0/282	0.45	0/381
9	K	0.28	0/288	0.46	0/397
10	L	0.29	0/257	0.38	0/347
11	M	0.27	0/230	0.37	0/314
12	T	0.27	0/236	0.40	0/321
13	X	0.25	0/267	0.38	0/364
All	All	0.29	0/15466	0.42	0/21058

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	260	PHE	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	2357	0	2284	56	0
2	B	3751	0	3598	84	0
3	C	3259	0	3186	65	0
4	D	2734	0	2623	66	0
5	E	603	0	578	19	0
6	F	255	0	265	4	0
7	H	494	0	508	10	0
8	I	276	0	293	4	0
9	K	278	0	286	10	0
10	L	252	0	262	11	0
11	M	226	0	246	7	0
12	T	231	0	243	4	0
13	X	262	0	289	7	0
14	A	1	0	0	0	0
15	A	170	0	158	10	0
15	B	1010	0	1078	77	0
15	C	815	0	870	65	0
15	D	195	0	216	16	0
16	A	64	0	74	6	0
16	D	64	0	74	4	0
17	A	40	0	49	5	0
17	B	120	0	147	11	0
17	C	120	0	147	13	0
17	D	40	0	49	3	0
17	X	40	0	49	7	0
18	A	102	0	141	8	0
18	B	51	0	69	4	0
18	C	54	0	78	5	0
18	T	93	0	117	6	0
18	X	42	0	48	4	0
19	A	15	0	13	1	0
19	D	55	0	80	0	0
20	B	51	0	72	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	C	51	0	72	8	0
20	D	51	0	72	2	0
21	B	69	0	85	8	0
22	C	62	0	82	2	0
22	H	62	0	82	4	0
23	D	1	0	0	0	0
24	D	4	0	0	0	0
25	D	144	0	213	21	0
25	L	49	0	74	4	0
26	E	43	0	30	5	0
27	I	10	0	10	0	0
27	M	10	0	10	0	0
27	T	10	0	10	0	0
28	A	54	0	0	2	0
28	B	62	0	0	7	0
28	C	30	0	0	1	0
28	D	46	0	0	2	0
28	E	2	0	0	0	0
28	L	1	0	0	0	0
28	T	2	0	0	0	0
28	X	1	0	0	0	0
All	All	18884	0	18930	467	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 12.

All (467) 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)
4:D:186:GLN:HB2	15:D:405:CLA:HBC1	1.60	0.83
4:D:259:ILE:HD13	25:D:410:LHG:H261	1.61	0.83
3:C:152:LEU:HD21	15:C:507:CLA:HAB	1.60	0.81
4:D:192:THR:HG23	15:D:405:CLA:HBC2	1.64	0.78
1:A:140:ARG:NH2	25:D:411:LHG:O5	2.17	0.77
4:D:313:THR:HG22	4:D:315:TYR:H	1.48	0.77
2:B:25:MET:HG2	17:B:617:BCR:H23C	1.69	0.75
26:E:101:HEM:HBC2	26:E:101:HEM:HHD	1.69	0.75
25:D:410:LHG:H311	12:T:21:ILE:HD11	1.70	0.73
2:B:311:PHE:O	2:B:317:ASN:ND2	2.22	0.72
15:B:610:CLA:HHC	15:B:610:CLA:HBB1	1.71	0.71
3:C:268:LEU:HD12	20:C:501:LMG:H391	1.72	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:D:402:CLA:H121	15:D:402:CLA:HMA1	1.72	0.71
4:D:343:GLU:O	4:D:348:ARG:NH2	2.20	0.70
3:C:298:GLN:OE1	3:C:342:THR:OG1	2.08	0.70
13:X:16:ALA:HA	13:X:19:VAL:HG12	1.73	0.70
5:E:23:HIS:NE2	26:E:101:HEM:ND	2.42	0.68
15:B:605:CLA:HBB1	15:B:605:CLA:HMB1	1.76	0.68
5:E:13:ILE:HG21	26:E:101:HEM:HAD2	1.77	0.67
3:C:363:ASP:HB3	3:C:366:LYS:HB2	1.77	0.66
26:E:101:HEM:NA	6:F:23:HIS:NE2	2.43	0.66
2:B:103:LEU:HD21	15:B:605:CLA:HMC3	1.78	0.66
8:I:28:PRO:O	8:I:31:ASN:ND2	2.29	0.66
1:A:259:ILE:HG22	1:A:260:PHE:H	1.61	0.66
4:D:279:LEU:HD12	16:D:403:PHO:HBC3	1.77	0.65
1:A:82:VAL:HB	1:A:174:LEU:HB2	1.79	0.65
15:B:615:CLA:HBB1	15:B:615:CLA:HMB1	1.80	0.64
2:B:247:PHE:HB2	15:B:608:CLA:HBC1	1.78	0.64
15:C:512:CLA:HBB1	15:C:512:CLA:HMB1	1.78	0.64
15:D:405:CLA:HMB1	15:D:405:CLA:HBB1	1.80	0.64
15:D:402:CLA:HMB1	15:D:402:CLA:HBB1	1.80	0.63
3:C:258:TYR:O	28:C:601:HOH:O	2.14	0.63
15:C:506:CLA:H43	17:C:516:BCR:H331	1.80	0.63
15:D:406:CLA:HBB1	15:D:406:CLA:HMB1	1.80	0.63
5:E:75:GLU:HA	5:E:78:GLU:HG2	1.81	0.63
13:X:1:MET:HA	13:X:5:LEU:HD23	1.79	0.63
2:B:464:PHE:HD2	15:B:611:CLA:HAC2	1.63	0.62
15:B:603:CLA:HBB1	15:B:603:CLA:HMB1	1.81	0.62
15:B:604:CLA:HBB1	15:B:604:CLA:HMB1	1.81	0.62
2:B:243:ALA:HA	2:B:246:PHE:CE1	2.34	0.62
15:B:601:CLA:H12	15:B:601:CLA:H71	1.80	0.62
2:B:127:ARG:HH22	7:H:18:TYR:HB3	1.64	0.62
5:E:57:THR:HG22	5:E:58:GLN:H	1.63	0.62
15:C:504:CLA:H203	15:C:511:CLA:HAB	1.81	0.62
15:C:509:CLA:H62	9:K:36:PHE:HZ	1.65	0.61
3:C:212:ILE:O	3:C:280:ASN:ND2	2.30	0.61
15:C:509:CLA:HBB1	15:C:509:CLA:HMB1	1.82	0.61
15:B:615:CLA:H2	15:B:616:CLA:HBB2	1.82	0.61
3:C:276:PHE:HD2	3:C:284:TYR:HE2	1.48	0.61
15:B:612:CLA:HBB1	15:B:612:CLA:HMB1	1.81	0.61
15:C:502:CLA:HAB	15:C:502:CLA:H71	1.83	0.61
2:B:44:ILE:HD11	15:B:607:CLA:HED1	1.82	0.61
2:B:51:VAL:HG13	2:B:308:LYS:HB2	1.82	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:191:ASN:O	28:B:701:HOH:O	2.16	0.60
15:C:511:CLA:HMB1	15:C:511:CLA:HBB1	1.82	0.60
15:B:615:CLA:H161	7:H:7:LEU:HD21	1.83	0.60
15:C:512:CLA:HBA1	17:C:519:BCR:H282	1.82	0.60
2:B:457:VAL:HG11	20:B:621:LMG:H231	1.83	0.60
15:B:614:CLA:H43	17:B:617:BCR:H383	1.83	0.60
11:M:25:LEU:O	11:M:29:THR:OG1	2.15	0.60
20:C:501:LMG:H382	22:C:517:DGD:HB41	1.83	0.60
4:D:48:TRP:HA	4:D:78:VAL:HG21	1.83	0.60
1:A:140:ARG:NH1	4:D:219:GLU:O	2.34	0.60
15:C:510:CLA:HMB1	15:C:510:CLA:HBB1	1.83	0.60
15:B:608:CLA:HMB1	15:B:608:CLA:HBB1	1.82	0.60
25:D:410:LHG:O3	25:D:410:LHG:O1	2.20	0.60
15:C:507:CLA:HBB1	15:C:507:CLA:HMB1	1.84	0.59
3:C:26:ASN:ND2	15:C:511:CLA:O1A	2.36	0.59
15:B:614:CLA:HBB1	15:B:614:CLA:HMB1	1.84	0.59
2:B:23:HIS:ND1	15:B:615:CLA:OBD	2.29	0.59
1:A:43:THR:HG23	17:A:406:BCR:H362	1.85	0.59
18:A:407:SQD:H121	25:D:411:LHG:H152	1.85	0.58
15:B:611:CLA:HBB1	15:B:611:CLA:HMB1	1.83	0.58
3:C:294:MET:SD	3:C:294:MET:N	2.76	0.58
15:C:504:CLA:H172	15:C:511:CLA:HBB2	1.85	0.58
3:C:30:ILE:HG12	15:C:510:CLA:HMC1	1.85	0.58
3:C:436:ARG:NH2	8:I:27:ASP:OD1	2.36	0.58
4:D:49:LEU:HD22	17:D:407:BCR:H362	1.84	0.58
4:D:324:GLY:HA2	4:D:347:PRO:HG2	1.86	0.58
2:B:120:LEU:HD13	15:B:616:CLA:HMD2	1.86	0.57
2:B:128:THR:HG23	2:B:130:GLU:H	1.69	0.57
1:A:140:ARG:HH22	25:D:411:LHG:HC41	1.69	0.57
4:D:19:ASP:OD2	4:D:32:TRP:NE1	2.25	0.57
4:D:343:GLU:OE1	4:D:348:ARG:NH2	2.38	0.57
1:A:131:TRP:HZ2	3:C:436:ARG:HD2	1.69	0.57
1:A:195:HIS:CE1	1:A:197:PHE:HB2	2.40	0.57
15:A:402:CLA:H201	25:D:410:LHG:H321	1.85	0.57
18:A:409:SQD:H211	18:A:409:SQD:H371	1.84	0.57
2:B:148:LEU:HB3	21:B:623:LMT:H101	1.85	0.57
15:A:405:CLA:HMA2	20:C:501:LMG:H132	1.87	0.56
1:A:89:ILE:HD11	1:A:108:ASN:HB3	1.86	0.56
16:A:404:PHO:HMB3	15:D:402:CLA:H71	1.87	0.56
15:C:503:CLA:HBB1	15:C:503:CLA:HMB1	1.87	0.56
1:A:50:ILE:HG22	17:A:406:BCR:H271	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:D:410:LHG:H171	10:L:24:LEU:HD21	1.86	0.56
25:D:409:LHG:H172	25:L:101:LHG:H302	1.88	0.56
1:A:131:TRP:CD2	15:C:506:CLA:HMA2	2.41	0.56
2:B:248:ALA:HA	15:B:603:CLA:H42	1.88	0.56
3:C:256:GLU:OE2	3:C:431:HIS:ND1	2.31	0.56
1:A:124:PHE:HD1	15:C:506:CLA:HBB2	1.71	0.55
1:A:190:HIS:ND1	1:A:298:ASN:OD1	2.25	0.55
1:A:306:ILE:HG22	1:A:314:ILE:HB	1.88	0.55
4:D:113:PHE:O	4:D:117:HIS:ND1	2.34	0.55
1:A:217:SER:HA	4:D:272:LEU:HD12	1.87	0.55
2:B:30:VAL:HG12	15:B:605:CLA:HHD	1.87	0.55
2:B:365:THR:O	28:B:702:HOH:O	2.18	0.55
15:B:603:CLA:HAB	15:B:605:CLA:H18	1.89	0.55
4:D:141:TYR:OH	25:D:409:LHG:O4	2.18	0.55
4:D:41:ALA:O	4:D:45:LEU:HG	2.07	0.55
15:B:601:CLA:HHD	17:X:102:BCR:H392	1.89	0.55
18:A:407:SQD:O7	4:D:230:ASN:ND2	2.40	0.54
15:B:613:CLA:H192	25:D:409:LHG:H221	1.90	0.54
3:C:335:GLU:HG3	3:C:361:GLY:HA3	1.89	0.54
2:B:160:GLY:HA3	2:B:180:PRO:HB3	1.89	0.54
15:C:507:CLA:H43	17:C:516:BCR:HC31	1.90	0.54
1:A:276:GLY:HA2	4:D:212:ALA:HA	1.90	0.54
15:A:402:CLA:HBB1	15:A:402:CLA:HMB1	1.89	0.54
1:A:308:ASP:OD1	1:A:312:ARG:N	2.41	0.54
2:B:157:HIS:HA	2:B:163:GLY:HA3	1.89	0.54
1:A:296:ASN:ND2	28:A:512:HOH:O	2.41	0.54
5:E:74:GLN:O	5:E:78:GLU:HG2	2.08	0.53
15:A:402:CLA:H102	16:A:404:PHO:HAA1	1.89	0.53
2:B:70:GLY:HA2	2:B:178:VAL:HG11	1.89	0.53
2:B:150:CYS:HB2	15:B:603:CLA:HMC3	1.90	0.53
15:C:508:CLA:H112	17:C:516:BCR:H362	1.89	0.53
16:D:403:PHO:HBB1	16:D:403:PHO:HMB1	1.91	0.53
1:A:248:ILE:N	28:A:511:HOH:O	2.40	0.53
2:B:24:LEU:HD21	15:B:616:CLA:CAB	2.38	0.53
1:A:131:TRP:CH2	15:C:506:CLA:HAA2	2.43	0.53
15:A:405:CLA:HBB1	15:A:405:CLA:HMB1	1.89	0.53
15:B:612:CLA:H171	15:B:613:CLA:HBB2	1.90	0.53
3:C:53:ALA:HB1	9:K:24:LEU:HB3	1.89	0.53
3:C:165:LYS:HA	3:C:169:PHE:HB2	1.90	0.53
15:C:503:CLA:HMB1	15:C:505:CLA:HMC3	1.91	0.53
20:C:501:LMG:H332	15:C:507:CLA:H193	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:PRO:HA	1:A:112:TYR:CG	2.44	0.53
2:B:231:MET:HG2	15:B:610:CLA:HMC1	1.91	0.53
15:B:609:CLA:H42	18:B:620:SQD:H291	1.91	0.53
1:A:255:PHE:CD1	1:A:264:SER:HB3	2.44	0.53
4:D:27:PHE:HE2	6:F:17:VAL:HG13	1.72	0.53
1:A:42:LEU:HD23	17:A:406:BCR:H353	1.91	0.52
1:A:179:THR:O	1:A:183:MET:HG3	2.09	0.52
3:C:424:PHE:CZ	15:C:511:CLA:HMB3	2.45	0.52
13:X:8:PHE:O	13:X:11:SER:OG	2.19	0.52
2:B:383:PHE:CE1	4:D:347:PRO:HB3	2.45	0.52
15:C:502:CLA:HHC	15:C:502:CLA:HBB1	1.92	0.52
10:L:14:LEU:HD22	11:M:25:LEU:HB3	1.89	0.52
2:B:22:VAL:HG22	15:B:614:CLA:HMB3	1.91	0.52
2:B:42:LEU:HD13	2:B:94:GLU:HG3	1.91	0.52
2:B:26:HIS:HB2	15:B:612:CLA:HMB2	1.91	0.52
4:D:74:LEU:HD22	4:D:175:VAL:HG11	1.92	0.52
4:D:85:PHE:HD1	5:E:69:ARG:HG3	1.73	0.52
2:B:233:ASN:O	2:B:236:THR:HG22	2.10	0.52
2:B:357:ARG:NH2	4:D:337:GLU:O	2.34	0.52
3:C:165:LYS:HB2	15:C:503:CLA:H172	1.91	0.52
2:B:74:SER:HA	2:B:92:SER:HB2	1.92	0.51
15:B:608:CLA:H172	15:B:609:CLA:H192	1.90	0.51
3:C:451:GLU:OE2	4:D:248:THR:OG1	2.27	0.51
1:A:146:ALA:HB2	25:D:411:LHG:H261	1.92	0.51
16:A:404:PHO:H51	18:A:409:SQD:H201	1.92	0.51
1:A:18:CYS:SG	8:I:30:ARG:NH2	2.84	0.51
10:L:20:TYR:HE1	18:T:101:SQD:H282	1.76	0.51
4:D:123:ILE:HD11	22:H:101:DGD:HAE1	1.92	0.51
2:B:188:ALA:HA	7:H:58:PHE:CE1	2.45	0.51
25:D:411:LHG:H321	25:D:411:LHG:H142	1.93	0.50
3:C:59:VAL:O	9:K:9:LYS:N	2.45	0.50
3:C:73:LEU:HD13	3:C:76:LEU:HD22	1.94	0.50
4:D:73:PHE:CE2	20:D:412:LMG:H181	2.45	0.50
10:L:28:VAL:HG11	25:L:101:LHG:H201	1.93	0.50
4:D:103:ARG:NH1	4:D:106:GLN:OE1	2.44	0.50
15:C:511:CLA:H203	9:K:32:LEU:HD13	1.94	0.50
3:C:151:HIS:ND1	15:C:508:CLA:OBD	2.40	0.50
4:D:51:GLY:HA3	4:D:78:VAL:HG22	1.93	0.50
4:D:152:VAL:HG21	4:D:279:LEU:HD22	1.92	0.50
2:B:155:ALA:O	2:B:159:THR:OG1	2.29	0.50
3:C:35:LYS:HE2	3:C:125:GLU:HG2	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:17:SER:HA	8:I:20:ILE:HB	1.93	0.50
2:B:462:PHE:CE1	15:B:613:CLA:HMB3	2.46	0.49
3:C:26:ASN:ND2	15:C:509:CLA:O1A	2.44	0.49
3:C:105:HIS:CD2	18:C:518:SQD:H332	2.46	0.49
3:C:294:MET:HG3	3:C:345:PHE:CD1	2.47	0.49
4:D:155:SER:HA	4:D:159:MET:HB2	1.93	0.49
10:L:23:LEU:HD13	18:T:101:SQD:H311	1.93	0.49
4:D:136:VAL:HG23	4:D:138:ILE:HG12	1.93	0.49
15:B:613:CLA:HBB1	15:B:613:CLA:HMB1	1.94	0.49
4:D:198:MET:SD	15:D:402:CLA:HED2	2.52	0.49
2:B:185:TRP:O	28:B:704:HOH:O	2.20	0.49
20:C:501:LMG:H121	15:C:506:CLA:H203	1.95	0.49
1:A:170:ASP:OD2	3:C:344:ARG:NH1	2.39	0.49
5:E:17:ILE:O	5:E:21:VAL:HG23	2.13	0.49
2:B:433:ASP:OD2	2:B:436:THR:OG1	2.29	0.49
20:D:412:LMG:HC91	6:F:36:ILE:HG21	1.93	0.49
5:E:20:TRP:O	5:E:24:SER:OG	2.27	0.49
2:B:158:LEU:HB3	2:B:199:VAL:HG22	1.95	0.49
15:B:601:CLA:HHC	15:B:601:CLA:HBB1	1.95	0.49
28:B:716:HOH:O	4:D:134:ARG:NH1	2.46	0.49
1:A:142:TRP:HZ2	3:C:434:ARG:HB2	1.79	0.48
15:C:507:CLA:HMC2	15:C:508:CLA:H101	1.95	0.48
2:B:127:ARG:NH2	7:H:18:TYR:HB3	2.28	0.48
2:B:266:GLU:OE1	28:B:705:HOH:O	2.20	0.48
15:B:609:CLA:HBB1	15:B:609:CLA:HMB1	1.96	0.48
15:C:502:CLA:H18	15:C:508:CLA:HMB3	1.94	0.48
5:E:22:ILE:HG23	5:E:23:HIS:HD1	1.79	0.48
1:A:195:HIS:HD2	1:A:299:GLY:HA2	1.76	0.48
3:C:308:ASP:OD2	3:C:327:TYR:OH	2.20	0.48
3:C:309:GLN:HB3	3:C:310:ARG:HD2	1.95	0.48
26:E:101:HEM:HMB1	26:E:101:HEM:HBB2	1.96	0.48
3:C:148:ILE:HD13	15:C:507:CLA:HMB3	1.95	0.48
4:D:161:PRO:HB3	4:D:170:ALA:HB2	1.96	0.48
18:X:101:SQD:H242	18:X:101:SQD:H271	1.66	0.48
1:A:85:SER:HA	1:A:109:GLY:HA3	1.96	0.48
1:A:199:MET:SD	15:A:403:CLA:HED2	2.54	0.48
15:B:607:CLA:HMB1	15:B:607:CLA:HBB1	1.95	0.48
15:B:611:CLA:HBB2	15:B:612:CLA:HED2	1.95	0.48
4:D:329:MET:HG2	4:D:333:ASP:HB2	1.96	0.48
17:B:619:BCR:H351	17:B:619:BCR:H15C	1.64	0.48
3:C:204:PRO:O	22:C:517:DGD:HG2	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:276:PHE:CD2	3:C:284:TYR:HE2	2.30	0.48
2:B:149:LEU:HD21	15:B:604:CLA:H8	1.96	0.47
2:B:276:ASP:OD1	2:B:361:ASN:ND2	2.39	0.47
15:B:613:CLA:H43	25:D:409:LHG:H382	1.96	0.47
1:A:120:LEU:HD22	1:A:155:THR:HG22	1.95	0.47
2:B:60:MET:O	28:B:703:HOH:O	2.20	0.47
3:C:260:SER:O	3:C:428:HIS:ND1	2.42	0.47
20:C:501:LMG:H202	20:C:501:LMG:H172	1.63	0.47
3:C:256:GLU:HG2	3:C:435:ALA:HB2	1.97	0.47
2:B:54:PRO:HD2	2:B:57:ARG:HG3	1.97	0.47
15:B:606:CLA:HBC1	21:B:623:LMT:H31	1.96	0.47
15:D:402:CLA:H111	15:D:402:CLA:H152	1.71	0.47
2:B:410:THR:OG1	28:B:706:HOH:O	2.20	0.47
3:C:212:ILE:HG13	3:C:276:PHE:HD1	1.80	0.47
3:C:356:LEU:HD12	3:C:362:LEU:HD22	1.95	0.47
1:A:215:HIS:HA	19:A:408:PL9:O1	2.15	0.47
4:D:47:GLY:HA2	17:D:407:BCR:H332	1.97	0.47
15:A:403:CLA:HMB3	16:D:403:PHO:H152	1.97	0.47
2:B:313:ASP:OD1	2:B:358:ARG:NH2	2.37	0.47
15:B:605:CLA:HMA1	15:B:606:CLA:H3A	1.97	0.47
15:B:609:CLA:H92	15:B:609:CLA:H62	1.72	0.47
17:C:519:BCR:H371	17:C:519:BCR:H24C	1.68	0.47
9:K:37:VAL:HA	9:K:40:ALA:HB3	1.97	0.47
1:A:77:ILE:HD11	12:T:6:TYR:HB3	1.97	0.46
4:D:87:HIS:HB2	22:H:101:DGD:HG11	1.97	0.46
16:A:404:PHO:H61	16:A:404:PHO:H2	1.67	0.46
2:B:204:ALA:CB	15:B:602:CLA:HAB	2.45	0.46
2:B:462:PHE:CZ	15:B:613:CLA:HMB3	2.50	0.46
25:D:411:LHG:H131	25:D:411:LHG:H102	1.66	0.46
1:A:121:ILE:HD11	20:C:501:LMG:H161	1.97	0.46
1:A:124:PHE:CD2	20:C:501:LMG:H221	2.50	0.46
1:A:124:PHE:CD1	15:C:506:CLA:HBB2	2.51	0.46
15:B:611:CLA:H161	15:B:611:CLA:H121	1.63	0.46
4:D:111:TRP:HB3	4:D:112:PRO:HD3	1.96	0.46
9:K:12:GLU:HA	9:K:15:GLN:HG3	1.97	0.46
12:T:13:ALA:O	12:T:17:LEU:HG	2.15	0.46
5:E:41:GLY:O	5:E:51:ARG:NH2	2.48	0.46
3:C:111:VAL:HB	17:C:515:BCR:H362	1.97	0.46
4:D:221:THR:HG21	4:D:249:ALA:HB2	1.97	0.46
4:D:279:LEU:HD21	15:D:405:CLA:HBA1	1.98	0.46
5:E:16:SER:O	5:E:20:TRP:HD1	1.99	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:19:LEU:HD21	18:T:101:SQD:H281	1.98	0.46
3:C:430:TRP:HZ2	25:D:411:LHG:HC31	1.80	0.46
15:C:504:CLA:H62	15:C:504:CLA:H101	1.62	0.46
15:C:506:CLA:HAA1	15:C:506:CLA:HBD	1.97	0.46
5:E:75:GLU:HA	5:E:78:GLU:CG	2.44	0.46
13:X:18:ILE:HD11	18:X:101:SQD:H302	1.95	0.46
1:A:310:GLN:HB2	1:A:312:ARG:HH11	1.81	0.46
3:C:96:PHE:O	3:C:100:VAL:HG23	2.16	0.46
3:C:141:LYS:HB3	3:C:243:PRO:HG2	1.96	0.46
3:C:174:ASP:OD1	3:C:184:ARG:NH2	2.37	0.46
15:C:510:CLA:HMB3	15:C:511:CLA:HAA1	1.98	0.46
1:A:93:PHE:HZ	15:A:405:CLA:HAA1	1.81	0.46
1:A:187:GLN:HB2	15:A:402:CLA:HAC2	1.97	0.46
2:B:12:VAL:HG23	15:B:612:CLA:HMC2	1.98	0.46
1:A:70:SER:O	1:A:75:ASN:HB2	2.16	0.45
18:A:407:SQD:H201	18:A:407:SQD:H171	1.67	0.45
2:B:192:PRO:HG3	7:H:49:TYR:CD1	2.50	0.45
2:B:442:VAL:HG21	4:D:299:VAL:HG11	1.98	0.45
3:C:220:ILE:O	3:C:224:HIS:ND1	2.32	0.45
15:C:506:CLA:HBB1	15:C:506:CLA:HMB1	1.98	0.45
2:B:3:LEU:HD23	2:B:3:LEU:HA	1.86	0.45
15:B:607:CLA:H91	15:B:607:CLA:H112	1.75	0.45
1:A:310:GLN:OE1	1:A:312:ARG:NH1	2.49	0.45
2:B:71:VAL:HG21	2:B:96:VAL:HG21	1.98	0.45
2:B:115:TRP:CH2	15:B:614:CLA:HMA2	2.51	0.45
1:A:265:PHE:HD2	1:A:271:LEU:HA	1.81	0.45
1:A:151:VAL:O	1:A:155:THR:HG23	2.16	0.45
2:B:162:TRP:CG	21:B:623:LMT:H5'	2.51	0.45
3:C:84:TRP:CE2	18:C:518:SQD:H241	2.52	0.45
4:D:54:PHE:O	5:E:49:THR:OG1	2.31	0.45
1:A:222:SER:HB2	1:A:251:ALA:HB2	1.98	0.45
4:D:55:VAL:O	4:D:66:SER:HB3	2.17	0.45
7:H:4:ARG:NH1	7:H:9:ASP:OD2	2.50	0.45
7:H:50:ASN:ND2	22:H:101:DGD:O1G	2.50	0.45
2:B:30:VAL:HG22	15:B:613:CLA:C3C	2.47	0.45
15:B:601:CLA:HMD2	17:X:102:BCR:H393	1.98	0.45
1:A:95:PRO:HG2	1:A:98:GLU:HB2	1.99	0.45
15:B:608:CLA:H91	15:B:608:CLA:H111	1.73	0.45
1:A:206:PHE:CZ	15:D:405:CLA:HBA2	2.52	0.45
15:B:604:CLA:H142	15:B:615:CLA:HMA1	1.98	0.45
15:C:510:CLA:H161	15:C:510:CLA:H192	1.66	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:B:610:CLA:H151	15:B:615:CLA:HBD	1.98	0.45
3:C:43:HIS:HE1	3:C:47:ILE:HD11	1.81	0.45
15:C:511:CLA:H202	15:C:511:CLA:H161	1.67	0.44
17:A:406:BCR:H24C	17:A:406:BCR:H371	1.71	0.44
3:C:128:GLU:OE2	3:C:136:TYR:N	2.51	0.44
15:C:507:CLA:H192	15:C:507:CLA:H141	1.98	0.44
15:B:602:CLA:H61	15:B:602:CLA:H41	1.71	0.44
3:C:50:TRP:HB2	15:C:511:CLA:HAC2	1.99	0.44
15:C:513:CLA:H91	15:C:513:CLA:H112	1.66	0.44
2:B:113:TRP:HA	17:B:619:BCR:H402	1.98	0.44
15:B:603:CLA:H191	7:H:39:LEU:HB2	1.99	0.44
15:B:607:CLA:HBC1	17:B:617:BCR:C10	2.47	0.44
2:B:336:ILE:HB	2:B:433:ASP:HB3	2.00	0.44
17:B:617:BCR:H322	20:B:621:LMG:H112	2.00	0.44
5:E:14:VAL:HG23	5:E:15:THR:HG23	2.00	0.44
5:E:56:PHE:CD1	5:E:61:GLN:HA	2.53	0.44
15:B:606:CLA:NC	21:B:622:LMT:H61	2.32	0.44
15:C:504:CLA:H193	15:C:504:CLA:H161	1.80	0.44
15:C:506:CLA:H62	15:C:506:CLA:H2	1.56	0.44
2:B:239:SER:O	2:B:466:HIS:ND1	2.50	0.44
2:B:242:ILE:HA	2:B:245:VAL:HG22	2.00	0.44
15:B:606:CLA:H142	15:B:606:CLA:H111	1.77	0.44
3:C:405:ASN:OD1	3:C:406:TYR:N	2.49	0.44
4:D:83:ASP:OD2	4:D:166:SER:OG	2.30	0.44
15:B:601:CLA:HHD	17:X:102:BCR:C39	2.48	0.43
3:C:212:ILE:HG21	3:C:279:PHE:HB2	2.00	0.43
25:D:409:LHG:H111	25:L:101:LHG:HC91	2.00	0.43
18:T:101:SQD:H302	18:T:101:SQD:H332	1.59	0.43
3:C:263:LEU:HD21	15:C:509:CLA:HAB	1.99	0.43
15:C:511:CLA:H111	15:C:511:CLA:H91	1.85	0.43
17:C:519:BCR:H351	17:C:519:BCR:H15C	1.73	0.43
15:B:601:CLA:HAC1	17:X:102:BCR:H392	2.00	0.43
15:B:606:CLA:H61	15:B:606:CLA:H101	1.61	0.43
15:B:612:CLA:H102	15:B:612:CLA:H61	1.86	0.43
17:B:618:BCR:H351	17:B:618:BCR:H15C	1.68	0.43
4:D:185:LEU:HG	4:D:189:HIS:CD2	2.53	0.43
15:D:402:CLA:O1A	25:L:101:LHG:H221	2.18	0.43
15:B:604:CLA:CMB	15:B:607:CLA:HAB	2.48	0.43
15:C:512:CLA:HBA1	17:C:519:BCR:C28	2.48	0.43
18:C:518:SQD:H91	18:C:518:SQD:H122	1.71	0.43
5:E:30:LEU:HD21	6:F:27:VAL:HA	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:ALA:HA	1:A:55:ALA:HB2	2.01	0.43
4:D:104:TRP:HZ2	15:D:406:CLA:HED2	1.83	0.43
4:D:19:ASP:O	4:D:23:LYS:HG3	2.19	0.43
2:B:458:PHE:HB3	15:B:604:CLA:HBC2	2.01	0.43
3:C:309:GLN:HE22	3:C:368:ARG:HD3	1.83	0.43
17:C:515:BCR:H15C	17:C:515:BCR:H351	1.69	0.43
1:A:120:LEU:O	1:A:124:PHE:HD2	2.02	0.43
1:A:126:TYR:CE2	16:A:404:PHO:HBA1	2.54	0.43
4:D:190:ASN:HB2	4:D:296:TYR:CD1	2.53	0.43
11:M:25:LEU:HD12	11:M:25:LEU:HA	1.82	0.43
17:X:102:BCR:H371	17:X:102:BCR:H24C	1.73	0.43
2:B:212:ALA:HB2	15:B:609:CLA:HMC3	2.01	0.42
2:B:288:VAL:HG23	2:B:305:ILE:HD11	2.01	0.42
2:B:368:VAL:HG21	2:B:381:ILE:HD12	2.00	0.42
15:C:506:CLA:H3A	15:C:506:CLA:HBA2	1.79	0.42
4:D:165:SER:O	28:D:502:HOH:O	2.22	0.42
5:E:60:ARG:HH22	5:E:64:PRO:HD3	1.83	0.42
18:A:409:SQD:H291	18:T:103:SQD:H101	2.01	0.42
2:B:63:LEU:N	2:B:64:PRO:HD2	2.34	0.42
15:B:611:CLA:H142	15:B:611:CLA:H111	1.81	0.42
3:C:40:HIS:CG	15:C:513:CLA:HMD1	2.54	0.42
15:C:502:CLA:C1D	15:C:504:CLA:H52	2.49	0.42
10:L:14:LEU:HD23	11:M:26:PHE:HB2	2.01	0.42
18:A:409:SQD:H281	18:T:103:SQD:H81	2.01	0.42
2:B:157:HIS:HD2	2:B:158:LEU:HD23	1.84	0.42
21:B:623:LMT:H61	21:B:623:LMT:H91	1.67	0.42
15:C:507:CLA:H62	15:C:507:CLA:H41	1.69	0.42
18:C:518:SQD:H322	18:C:518:SQD:H351	1.77	0.42
2:B:142:HIS:HB3	15:B:610:CLA:H101	2.01	0.42
2:B:142:HIS:ND1	15:B:610:CLA:OBD	2.27	0.42
2:B:243:ALA:HB2	2:B:466:HIS:CE1	2.54	0.42
10:L:14:LEU:H	11:M:29:THR:HG21	1.85	0.42
1:A:256:GLY:O	1:A:261:GLN:HA	2.19	0.42
2:B:77:GLY:O	2:B:85:GLY:N	2.48	0.42
2:B:141:ILE:O	2:B:145:LEU:HG	2.19	0.42
2:B:144:PHE:CE2	2:B:148:LEU:HD11	2.54	0.42
15:B:603:CLA:H2	15:B:605:CLA:H91	2.02	0.42
1:A:223:LEU:HD23	1:A:223:LEU:HA	1.83	0.42
15:C:512:CLA:CHA	15:C:512:CLA:HBA2	2.49	0.42
15:B:608:CLA:HMD1	15:B:610:CLA:CAB	2.50	0.42
17:B:618:BCR:HC31	20:B:621:LMG:H142	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:10:LEU:HD11	9:K:21:VAL:HG21	2.02	0.42
2:B:382:PRO:HG3	2:B:388:SER:HB3	2.00	0.42
15:B:613:CLA:OBD	15:B:614:CLA:HAB	2.18	0.42
15:B:615:CLA:HBA1	15:B:615:CLA:H3A	1.80	0.42
3:C:429:LEU:HD21	15:C:506:CLA:C2B	2.49	0.42
4:D:57:SER:HB3	4:D:79:SER:OG	2.19	0.42
15:D:406:CLA:H2	18:X:101:SQD:H282	2.01	0.42
7:H:37:LEU:HB3	17:X:102:BCR:H14C	2.01	0.42
2:B:61:PHE:CE1	15:B:607:CLA:HMB3	2.54	0.42
2:B:162:TRP:CD2	21:B:623:LMT:H5'	2.55	0.42
1:A:137:LEU:HD12	1:A:139:MET:HE1	2.02	0.42
15:A:402:CLA:H193	15:A:402:CLA:H161	1.70	0.42
3:C:459:LEU:HD23	3:C:459:LEU:HA	1.92	0.42
4:D:107:ILE:HG21	5:E:72:ILE:HD12	2.00	0.42
4:D:161:PRO:HG3	4:D:170:ALA:HB2	2.02	0.42
13:X:18:ILE:HD11	18:X:101:SQD:H262	2.02	0.42
18:B:620:SQD:H152	18:B:620:SQD:H182	1.70	0.41
3:C:56:LEU:HA	3:C:59:VAL:HG12	2.02	0.41
3:C:230:ILE:HG22	15:C:507:CLA:HMC1	2.01	0.41
15:D:406:CLA:H61	15:D:406:CLA:H41	1.45	0.41
25:D:411:LHG:H141	25:D:411:LHG:H171	1.76	0.41
10:L:12:VAL:HG11	11:M:25:LEU:HD11	2.02	0.41
3:C:276:PHE:CZ	15:C:502:CLA:HMA2	2.55	0.41
4:D:141:TYR:HA	4:D:144:ILE:HG12	2.02	0.41
17:X:102:BCR:H351	17:X:102:BCR:H15C	1.76	0.41
16:A:404:PHO:H13	16:A:404:PHO:H102	1.86	0.41
2:B:21:SER:OG	2:B:111:ALA:O	2.30	0.41
2:B:91:TRP:HE1	21:B:622:LMT:H12	1.85	0.41
3:C:169:PHE:CE1	18:C:518:SQD:H131	2.55	0.41
3:C:323:GLY:HA3	3:C:330:ARG:NE	2.34	0.41
3:C:350:GLY:O	3:C:354:GLU:HG2	2.20	0.41
18:A:407:SQD:H182	18:A:407:SQD:H151	1.60	0.41
15:C:514:CLA:H141	15:C:514:CLA:H161	1.69	0.41
2:B:365:THR:HB	4:D:326:ARG:HH21	1.86	0.41
17:B:618:BCR:H24C	17:B:618:BCR:H371	1.80	0.41
18:B:620:SQD:H112	18:B:620:SQD:H82	1.92	0.41
15:C:513:CLA:H61	15:C:513:CLA:H101	1.73	0.41
15:B:602:CLA:H91	15:B:602:CLA:H112	1.64	0.41
3:C:266:LEU:HD12	15:C:510:CLA:HED3	2.02	0.41
25:D:410:LHG:H241	10:L:20:TYR:HB3	2.02	0.41
17:A:406:BCR:H351	17:A:406:BCR:H15C	1.75	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:356:VAL:HG22	2:B:370:MET:HG2	2.03	0.41
3:C:423:PHE:O	15:C:509:CLA:HMC1	2.20	0.41
15:C:514:CLA:H161	15:C:514:CLA:H203	1.82	0.41
13:X:9:LEU:O	13:X:13:VAL:HG23	2.21	0.41
15:B:602:CLA:H193	22:H:101:DGD:HA72	2.02	0.41
17:C:516:BCR:H15C	17:C:516:BCR:H351	1.75	0.41
17:C:519:BCR:HC22	9:K:17:PHE:CD2	2.56	0.41
4:D:177:GLY:O	28:D:501:HOH:O	2.21	0.41
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.55	0.41
13:X:21:ILE:HA	13:X:22:PRO:HA	1.83	0.41
2:B:369:ILE:HD11	4:D:345:VAL:HG21	2.02	0.41
15:B:613:CLA:H3A	15:B:613:CLA:HBA1	1.88	0.41
3:C:367:LEU:HA	3:C:371:ILE:HD11	2.03	0.41
15:C:502:CLA:H151	15:C:508:CLA:HMA1	2.03	0.41
15:C:504:CLA:H111	15:C:504:CLA:H142	1.81	0.41
17:C:519:BCR:HC22	9:K:17:PHE:HD2	1.85	0.41
4:D:56:THR:HG21	5:E:50:PRO:HD3	2.02	0.41
12:T:12:MET:O	12:T:16:VAL:HG23	2.20	0.41
1:A:200:LEU:HD13	1:A:285:PHE:CD1	2.56	0.41
17:B:617:BCR:H15C	17:B:617:BCR:H351	1.80	0.41
15:C:513:CLA:HBA1	15:C:513:CLA:H3A	1.49	0.41
4:D:129:GLN:NE2	16:D:403:PHO:OBD	2.54	0.41
4:D:184:PHE:HD1	4:D:185:LEU:HD12	1.86	0.41
17:D:407:BCR:H371	17:D:407:BCR:H24C	1.77	0.41
25:D:409:LHG:H201	11:M:18:PRO:HG3	2.03	0.41
18:B:620:SQD:H132	18:B:620:SQD:H161	1.47	0.40
15:C:504:CLA:H112	15:C:504:CLA:H93	1.73	0.40
4:D:193:LEU:O	10:L:36:TYR:OH	2.18	0.40
7:H:48:ILE:O	7:H:60:VAL:HG21	2.21	0.40
9:K:25:PRO:O	9:K:28:PRO:HD2	2.20	0.40
2:B:336:ILE:HD11	2:B:437:PHE:CE2	2.56	0.40
21:B:622:LMT:H82	21:B:622:LMT:H112	1.69	0.40
2:B:105:GLY:HA2	17:B:618:BCR:H383	2.03	0.40
2:B:330:MET:HA	2:B:444:ARG:HB2	2.02	0.40
3:C:364:LEU:O	3:C:368:ARG:HG2	2.21	0.40
3:C:365:ASP:HA	3:C:368:ARG:HB2	2.04	0.40
17:C:516:BCR:H24C	17:C:516:BCR:H371	1.79	0.40
4:D:256:ILE:HD13	4:D:256:ILE:HA	1.97	0.40
1:A:331:MET:HE2	4:D:320:LEU:HB3	2.02	0.40
2:B:257:TRP:HB2	2:B:452:THR:HG21	2.04	0.40
1:A:279:PRO:HG2	4:D:212:ALA:HB2	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:241:SER:O	2:B:245:VAL:HG13	2.21	0.40
15:C:502:CLA:H161	15:C:502:CLA:H121	1.84	0.40
4:D:182:ILE:HG23	15:D:405:CLA:CHD	2.51	0.40
4:D:216:ALA:HA	25:D:411:LHG:H252	2.03	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	298/360 (83%)	293 (98%)	4 (1%)	1 (0%)	41	62
2	B	476/507 (94%)	469 (98%)	7 (2%)	0	100	100
3	C	409/460 (89%)	399 (98%)	10 (2%)	0	100	100
4	D	340/352 (97%)	333 (98%)	7 (2%)	0	100	100
5	E	70/81 (86%)	67 (96%)	3 (4%)	0	100	100
6	F	30/44 (68%)	30 (100%)	0	0	100	100
7	H	61/64 (95%)	58 (95%)	3 (5%)	0	100	100
8	I	33/38 (87%)	33 (100%)	0	0	100	100
9	K	33/45 (73%)	33 (100%)	0	0	100	100
10	L	29/39 (74%)	29 (100%)	0	0	100	100
11	M	27/35 (77%)	25 (93%)	2 (7%)	0	100	100
12	T	27/31 (87%)	26 (96%)	1 (4%)	0	100	100
13	X	33/39 (85%)	30 (91%)	3 (9%)	0	100	100
All	All	1866/2095 (89%)	1825 (98%)	40 (2%)	1 (0%)	54	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	260	PHE

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	245/293 (84%)	245 (100%)	0	100	100
2	B	382/404 (95%)	382 (100%)	0	100	100
3	C	326/361 (90%)	326 (100%)	0	100	100
4	D	278/285 (98%)	277 (100%)	1 (0%)	91	97
5	E	66/73 (90%)	66 (100%)	0	100	100
6	F	26/37 (70%)	26 (100%)	0	100	100
7	H	53/54 (98%)	53 (100%)	0	100	100
8	I	31/34 (91%)	31 (100%)	0	100	100
9	K	29/38 (76%)	29 (100%)	0	100	100
10	L	28/36 (78%)	28 (100%)	0	100	100
11	M	26/32 (81%)	26 (100%)	0	100	100
12	T	24/26 (92%)	23 (96%)	1 (4%)	30	53
13	X	29/33 (88%)	29 (100%)	0	100	100
All	All	1543/1706 (90%)	1541 (100%)	2 (0%)	93	98

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	180	ARG
12	T	28	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	195	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	252	HIS
1	A	332	HIS
2	B	157	HIS
2	B	216	HIS
2	B	281	GLN
2	B	291	GLN
2	B	331	ASN
2	B	343	HIS
3	C	309	GLN
3	C	372	GLN
3	C	385	HIS
4	D	142	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 73 ligands modelled in this entry, 2 are monoatomic - leaving 71 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
16	PHO	D	403	-	51,69,69	0.98	3 (5%)	47,99,99	1.22	5 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
20	LMG	D	412	-	51,51,55	1.33	8 (15%)	59,59,63	1.06	3 (5%)
15	CLA	C	512	3	45,53,73	2.58	18 (40%)	52,89,113	2.93	19 (36%)
25	LHG	D	410	-	48,48,48	0.92	2 (4%)	51,54,54	1.08	4 (7%)
17	BCR	B	619	-	41,41,41	2.81	6 (14%)	56,56,56	6.47	20 (35%)
15	CLA	C	502	-	65,73,73	2.25	20 (30%)	76,113,113	2.51	24 (31%)
15	CLA	B	607	28	65,73,73	2.23	19 (29%)	76,113,113	2.52	25 (32%)
17	BCR	C	516	-	41,41,41	2.85	6 (14%)	56,56,56	6.48	21 (37%)
25	LHG	D	411	-	45,45,48	0.96	2 (4%)	48,51,54	1.02	2 (4%)
17	BCR	A	406	-	41,41,41	2.83	7 (17%)	56,56,56	6.45	20 (35%)
15	CLA	A	403	-	55,63,73	2.45	20 (36%)	64,101,113	2.75	24 (37%)
15	CLA	B	605	-	65,73,73	2.24	19 (29%)	76,113,113	2.57	23 (30%)
15	CLA	B	601	28	65,73,73	2.23	19 (29%)	76,113,113	2.67	23 (30%)
15	CLA	B	610	28	65,73,73	2.23	20 (30%)	76,113,113	2.58	23 (30%)
15	CLA	C	513	-	65,73,73	2.24	19 (29%)	76,113,113	2.54	22 (28%)
15	CLA	C	508	28	65,73,73	2.21	19 (29%)	76,113,113	2.65	26 (34%)
15	CLA	D	402	28	65,73,73	2.26	20 (30%)	76,113,113	2.57	27 (35%)
15	CLA	C	506	-	65,73,73	2.25	20 (30%)	76,113,113	2.56	23 (30%)
18	SQD	T	101	-	51,52,54	0.97	5 (9%)	60,63,65	1.55	10 (16%)
27	FME	M	101	-	8,9,10	0.94	0	7,9,11	0.95	0
21	LMT	B	622	-	36,36,36	1.19	6 (16%)	47,47,47	1.10	2 (4%)
20	LMG	B	621	-	51,51,55	1.33	8 (15%)	59,59,63	1.16	4 (6%)
18	SQD	B	620	-	50,51,54	0.98	5 (10%)	59,62,65	1.52	9 (15%)
18	SQD	T	103	-	40,41,54	1.08	3 (7%)	49,52,65	1.73	11 (22%)
27	FME	T	102	-	8,9,10	0.94	0	7,9,11	1.03	1 (14%)
15	CLA	B	602	-	65,73,73	2.25	20 (30%)	76,113,113	2.59	24 (31%)
15	CLA	B	616	-	50,58,73	2.51	19 (38%)	58,95,113	2.87	23 (39%)
25	LHG	D	409	-	48,48,48	0.93	2 (4%)	51,54,54	1.03	2 (3%)
15	CLA	C	503	-	65,73,73	2.25	19 (29%)	76,113,113	2.54	21 (27%)
15	CLA	B	606	-	60,68,73	2.34	20 (33%)	70,107,113	2.58	25 (35%)
18	SQD	X	101	-	41,42,54	1.11	5 (12%)	50,53,65	1.82	12 (24%)
15	CLA	D	406	-	65,73,73	2.25	19 (29%)	76,113,113	2.64	23 (30%)
15	CLA	D	405	-	65,73,73	2.23	19 (29%)	76,113,113	2.59	22 (28%)
15	CLA	A	405	-	50,58,73	2.58	20 (40%)	58,95,113	2.98	24 (41%)
27	FME	I	101	-	8,9,10	0.94	0	7,9,11	1.03	0
15	CLA	A	402	-	65,73,73	2.22	19 (29%)	76,113,113	2.57	25 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
17	BCR	B	618	-	41,41,41	2.85	6 (14%)	56,56,56	6.44	20 (35%)
15	CLA	C	514	-	65,73,73	2.26	20 (30%)	76,113,113	2.53	24 (31%)
15	CLA	B	609	-	65,73,73	2.23	19 (29%)	76,113,113	2.57	21 (27%)
18	SQD	A	409	-	53,54,54	0.97	5 (9%)	62,65,65	1.49	9 (14%)
15	CLA	B	604	-	65,73,73	2.25	20 (30%)	76,113,113	2.57	24 (31%)
15	CLA	C	511	-	65,73,73	2.25	19 (29%)	76,113,113	2.63	24 (31%)
21	LMT	B	623	-	35,35,36	1.20	6 (17%)	46,46,47	1.08	3 (6%)
15	CLA	B	613	-	65,73,73	2.24	19 (29%)	76,113,113	2.60	22 (28%)
17	BCR	X	102	-	41,41,41	2.84	6 (14%)	56,56,56	6.55	21 (37%)
17	BCR	D	407	-	41,41,41	2.82	6 (14%)	56,56,56	6.66	21 (37%)
15	CLA	B	611	-	65,73,73	2.23	19 (29%)	76,113,113	2.51	22 (28%)
15	CLA	C	509	-	55,63,73	2.43	20 (36%)	64,101,113	2.79	25 (39%)
17	BCR	C	515	-	41,41,41	2.82	7 (17%)	56,56,56	6.37	22 (39%)
15	CLA	B	614	-	55,63,73	2.42	20 (36%)	64,101,113	2.76	24 (37%)
20	LMG	C	501	-	51,51,55	1.35	8 (15%)	59,59,63	1.09	3 (5%)
18	SQD	A	407	-	47,48,54	1.00	4 (8%)	56,59,65	1.76	11 (19%)
26	HEM	E	101	6,5	41,50,50	1.53	4 (9%)	45,82,82	1.32	6 (13%)
16	PHO	A	404	-	51,69,69	1.01	4 (7%)	47,99,99	1.20	5 (10%)
19	PL9	A	408	-	15,15,55	1.47	4 (26%)	20,21,69	1.79	4 (20%)
17	BCR	B	617	-	41,41,41	2.83	6 (14%)	56,56,56	6.47	21 (37%)
22	DGD	C	517	-	63,63,67	1.23	7 (11%)	77,77,81	0.96	3 (3%)
15	CLA	B	612	-	65,73,73	2.22	18 (27%)	76,113,113	2.51	21 (27%)
15	CLA	B	615	-	65,73,73	2.25	20 (30%)	76,113,113	2.55	24 (31%)
15	CLA	C	505	28	65,73,73	2.24	20 (30%)	76,113,113	2.61	26 (34%)
15	CLA	C	510	-	65,73,73	2.23	19 (29%)	76,113,113	2.52	22 (28%)
17	BCR	C	519	-	41,41,41	2.85	6 (14%)	56,56,56	6.42	21 (37%)
24	BCT	D	404	14	2,3,3	1.30	0	2,3,3	2.57	1 (50%)
25	LHG	L	101	-	48,48,48	0.92	2 (4%)	51,54,54	1.05	3 (5%)
22	DGD	H	101	-	63,63,67	1.23	8 (12%)	77,77,81	0.99	2 (2%)
15	CLA	C	507	-	65,73,73	2.24	20 (30%)	76,113,113	2.58	25 (32%)
19	PL9	D	408	-	55,55,55	1.26	5 (9%)	68,69,69	1.51	12 (17%)
15	CLA	B	603	-	65,73,73	2.25	19 (29%)	76,113,113	2.57	25 (32%)
18	SQD	C	518	-	53,54,54	0.97	4 (7%)	62,65,65	1.54	9 (14%)
15	CLA	C	504	-	65,73,73	2.24	19 (29%)	76,113,113	2.61	24 (31%)
15	CLA	B	608	-	65,73,73	2.23	19 (29%)	76,113,113	2.52	22 (28%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	PHO	D	403	-	-	8/37/103/103	0/5/6/6
20	LMG	D	412	-	-	16/46/66/70	0/1/1/1
15	CLA	C	512	3	1/1/11/20	6/13/91/115	-
25	LHG	D	410	-	-	25/53/53/53	-
17	BCR	B	619	-	-	9/29/63/63	0/2/2/2
15	CLA	C	502	-	1/1/15/20	10/37/115/115	-
15	CLA	B	607	28	1/1/15/20	16/37/115/115	-
17	BCR	C	516	-	-	2/29/63/63	0/2/2/2
25	LHG	D	411	-	-	29/50/50/53	-
17	BCR	A	406	-	-	7/29/63/63	0/2/2/2
15	CLA	A	403	-	1/1/13/20	10/25/103/115	-
15	CLA	B	605	-	1/1/15/20	14/37/115/115	-
15	CLA	B	601	28	1/1/15/20	18/37/115/115	-
15	CLA	B	610	28	1/1/15/20	5/37/115/115	-
15	CLA	C	513	-	1/1/15/20	18/37/115/115	-
15	CLA	C	508	28	1/1/15/20	15/37/115/115	-
15	CLA	D	402	28	1/1/15/20	9/37/115/115	-
15	CLA	C	506	-	1/1/15/20	11/37/115/115	-
18	SQD	T	101	-	-	25/47/67/69	0/1/1/1
27	FME	M	101	-	-	3/7/9/11	-
21	LMT	B	622	-	-	7/21/61/61	0/2/2/2
20	LMG	B	621	-	-	9/46/66/70	0/1/1/1
18	SQD	B	620	-	-	21/46/66/69	0/1/1/1
18	SQD	T	103	-	-	14/36/56/69	0/1/1/1
27	FME	T	102	-	-	4/7/9/11	-
15	CLA	B	602	-	1/1/15/20	22/37/115/115	-
15	CLA	B	616	-	1/1/12/20	9/19/97/115	-
25	LHG	D	409	-	-	27/53/53/53	-
15	CLA	C	503	-	1/1/15/20	14/37/115/115	-
15	CLA	B	606	-	1/1/14/20	12/31/109/115	-
18	SQD	X	101	-	-	20/37/57/69	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	D	406	-	1/1/15/20	11/37/115/115	-
15	CLA	D	405	-	1/1/15/20	15/37/115/115	-
15	CLA	A	405	-	1/1/12/20	6/19/97/115	-
27	FME	I	101	-	-	2/7/9/11	-
15	CLA	A	402	-	1/1/15/20	9/37/115/115	-
17	BCR	B	618	-	-	9/29/63/63	0/2/2/2
15	CLA	C	514	-	1/1/15/20	17/37/115/115	-
15	CLA	B	609	-	1/1/15/20	19/37/115/115	-
18	SQD	A	409	-	-	22/49/69/69	0/1/1/1
15	CLA	B	604	-	1/1/15/20	17/37/115/115	-
15	CLA	C	511	-	1/1/15/20	11/37/115/115	-
21	LMT	B	623	-	-	9/20/60/61	0/2/2/2
15	CLA	B	613	-	1/1/15/20	15/37/115/115	-
17	BCR	X	102	-	-	10/29/63/63	0/2/2/2
17	BCR	D	407	-	-	11/29/63/63	0/2/2/2
15	CLA	B	611	-	1/1/15/20	16/37/115/115	-
15	CLA	C	509	-	1/1/13/20	14/25/103/115	-
17	BCR	C	515	-	-	13/29/63/63	0/2/2/2
15	CLA	B	614	-	1/1/13/20	10/25/103/115	-
20	LMG	C	501	-	-	15/46/66/70	0/1/1/1
18	SQD	A	407	-	-	15/43/63/69	0/1/1/1
26	HEM	E	101	6,5	-	2/12/54/54	-
16	PHO	A	404	-	-	12/37/103/103	0/5/6/6
19	PL9	A	408	-	-	1/5/25/73	0/1/1/1
17	BCR	B	617	-	-	10/29/63/63	0/2/2/2
22	DGD	C	517	-	-	9/51/91/95	0/2/2/2
15	CLA	B	612	-	1/1/15/20	16/37/115/115	-
15	CLA	B	615	-	1/1/15/20	8/37/115/115	-
15	CLA	C	505	28	1/1/15/20	13/37/115/115	-
15	CLA	C	510	-	1/1/15/20	19/37/115/115	-
17	BCR	C	519	-	-	9/29/63/63	0/2/2/2
25	LHG	L	101	-	-	29/53/53/53	-
22	DGD	H	101	-	-	9/51/91/95	0/2/2/2
15	CLA	C	507	-	1/1/15/20	22/37/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	PL9	D	408	-	-	13/53/73/73	0/1/1/1
15	CLA	B	603	-	1/1/15/20	18/37/115/115	-
18	SQD	C	518	-	-	15/49/69/69	0/1/1/1
15	CLA	C	504	-	1/1/15/20	16/37/115/115	-
15	CLA	B	608	-	1/1/15/20	21/37/115/115	-

All (844) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	C	515	BCR	C8-C9	-8.42	1.27	1.45
17	B	617	BCR	C8-C9	-8.38	1.27	1.45
17	B	618	BCR	C8-C9	-8.35	1.28	1.45
17	C	519	BCR	C11-C10	-8.32	1.17	1.43
17	C	516	BCR	C8-C9	-8.31	1.28	1.45
17	C	519	BCR	C8-C9	-8.27	1.28	1.45
17	B	619	BCR	C8-C9	-8.27	1.28	1.45
17	X	102	BCR	C11-C10	-8.23	1.17	1.43
17	A	406	BCR	C8-C9	-8.23	1.28	1.45
17	B	618	BCR	C11-C10	-8.18	1.18	1.43
17	D	407	BCR	C8-C9	-8.17	1.28	1.45
17	B	617	BCR	C11-C10	-8.12	1.18	1.43
17	C	516	BCR	C11-C10	-8.09	1.18	1.43
17	D	407	BCR	C11-C10	-8.05	1.18	1.43
17	A	406	BCR	C11-C10	-8.03	1.18	1.43
17	B	619	BCR	C11-C10	-8.02	1.18	1.43
17	X	102	BCR	C8-C9	-8.01	1.28	1.45
17	C	515	BCR	C11-C10	-7.98	1.18	1.43
17	X	102	BCR	C10-C9	-7.71	1.25	1.35
17	C	519	BCR	C10-C9	-7.65	1.25	1.35
15	B	604	CLA	MG-NA	7.63	2.24	2.06
17	D	407	BCR	C10-C9	-7.59	1.25	1.35
17	C	516	BCR	C10-C9	-7.58	1.25	1.35
17	B	618	BCR	C10-C9	-7.57	1.25	1.35
17	X	102	BCR	C20-C21	-7.55	1.20	1.43
15	B	615	CLA	MG-NA	7.53	2.24	2.06
17	A	406	BCR	C20-C21	-7.51	1.20	1.43
17	C	519	BCR	C20-C21	-7.51	1.20	1.43
15	C	513	CLA	MG-NA	7.49	2.24	2.06
15	C	502	CLA	MG-NA	7.49	2.24	2.06
17	B	619	BCR	C10-C9	-7.48	1.25	1.35
15	C	512	CLA	MG-NA	7.48	2.24	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	610	CLA	MG-NA	7.48	2.24	2.06
17	C	516	BCR	C20-C21	-7.45	1.20	1.43
15	A	403	CLA	MG-NA	7.45	2.24	2.06
17	B	618	BCR	C20-C21	-7.45	1.20	1.43
15	C	507	CLA	MG-NA	7.44	2.23	2.06
15	C	503	CLA	MG-NA	7.44	2.23	2.06
15	C	508	CLA	MG-NA	7.43	2.23	2.06
15	B	613	CLA	MG-NA	7.43	2.23	2.06
15	B	601	CLA	MG-NA	7.43	2.23	2.06
17	A	406	BCR	C10-C9	-7.42	1.25	1.35
15	B	603	CLA	MG-NA	7.41	2.23	2.06
15	C	514	CLA	MG-NA	7.40	2.23	2.06
15	A	405	CLA	MG-NA	7.40	2.23	2.06
17	B	618	BCR	C16-C17	-7.39	1.20	1.43
17	B	617	BCR	C10-C9	-7.39	1.26	1.35
15	C	511	CLA	MG-NA	7.39	2.23	2.06
17	A	406	BCR	C16-C17	-7.38	1.20	1.43
15	C	506	CLA	MG-NA	7.38	2.23	2.06
17	C	515	BCR	C20-C21	-7.37	1.20	1.43
17	C	516	BCR	C16-C17	-7.37	1.20	1.43
17	C	515	BCR	C16-C17	-7.36	1.20	1.43
15	B	611	CLA	MG-NA	7.35	2.23	2.06
17	D	407	BCR	C20-C21	-7.34	1.20	1.43
17	C	515	BCR	C10-C9	-7.34	1.26	1.35
15	C	504	CLA	MG-NA	7.34	2.23	2.06
17	B	619	BCR	C20-C21	-7.33	1.20	1.43
17	D	407	BCR	C16-C17	-7.32	1.20	1.43
17	B	617	BCR	C20-C21	-7.32	1.20	1.43
15	D	402	CLA	MG-NA	7.32	2.23	2.06
15	B	608	CLA	MG-NA	7.31	2.23	2.06
15	A	402	CLA	MG-NA	7.30	2.23	2.06
17	X	102	BCR	C16-C17	-7.30	1.20	1.43
15	B	602	CLA	MG-NA	7.28	2.23	2.06
15	C	505	CLA	MG-NA	7.28	2.23	2.06
15	B	607	CLA	MG-NA	7.28	2.23	2.06
17	C	519	BCR	C16-C17	-7.28	1.20	1.43
15	C	510	CLA	MG-NA	7.27	2.23	2.06
17	B	617	BCR	C16-C17	-7.26	1.21	1.43
17	B	619	BCR	C16-C17	-7.26	1.21	1.43
15	B	605	CLA	MG-NA	7.26	2.23	2.06
15	C	509	CLA	MG-NA	7.25	2.23	2.06
15	B	614	CLA	MG-NA	7.25	2.23	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	606	CLA	MG-NA	7.23	2.23	2.06
15	D	406	CLA	MG-NA	7.19	2.23	2.06
15	B	612	CLA	MG-NA	7.16	2.23	2.06
15	D	405	CLA	MG-NA	7.16	2.23	2.06
15	B	616	CLA	MG-NA	7.15	2.23	2.06
15	B	609	CLA	MG-NA	7.14	2.23	2.06
15	B	615	CLA	O2A-C1	5.25	1.60	1.46
15	C	508	CLA	O2A-C1	5.25	1.60	1.46
15	B	606	CLA	O2A-C1	5.23	1.60	1.46
15	D	402	CLA	O2A-C1	5.18	1.60	1.46
15	C	504	CLA	O2A-C1	5.18	1.60	1.46
15	C	513	CLA	O2A-C1	5.17	1.60	1.46
15	C	505	CLA	O2A-C1	5.16	1.60	1.46
15	C	514	CLA	O2D-CGD	5.14	1.45	1.33
15	B	616	CLA	O2A-C1	5.13	1.60	1.46
15	C	507	CLA	O2A-C1	5.13	1.60	1.46
15	C	502	CLA	O2D-CGD	5.12	1.45	1.33
15	D	406	CLA	O2A-C1	5.12	1.60	1.46
15	A	402	CLA	O2D-CGD	5.12	1.45	1.33
15	B	609	CLA	O2D-CGD	5.12	1.45	1.33
15	A	403	CLA	CHC-C1C	5.11	1.48	1.35
15	C	503	CLA	O2A-C1	5.10	1.60	1.46
15	D	405	CLA	C3B-C2B	5.10	1.47	1.40
15	A	402	CLA	O2A-C1	5.10	1.60	1.46
15	B	614	CLA	O2A-C1	5.09	1.60	1.46
15	C	514	CLA	CHC-C1C	5.09	1.48	1.35
15	C	503	CLA	O2D-CGD	5.09	1.45	1.33
15	C	514	CLA	O2A-C1	5.09	1.60	1.46
15	B	601	CLA	O2D-CGD	5.08	1.45	1.33
15	A	405	CLA	O2D-CGD	5.08	1.45	1.33
15	B	603	CLA	O2A-C1	5.08	1.60	1.46
15	B	609	CLA	O2A-C1	5.08	1.60	1.46
15	C	509	CLA	O2A-C1	5.07	1.60	1.46
15	B	602	CLA	O2A-C1	5.07	1.60	1.46
15	C	511	CLA	CHC-C1C	5.07	1.48	1.35
15	B	605	CLA	O2D-CGD	5.06	1.45	1.33
15	A	405	CLA	O2A-C1	5.06	1.60	1.46
15	C	511	CLA	O2D-CGD	5.06	1.45	1.33
15	B	613	CLA	O2D-CGD	5.06	1.45	1.33
15	B	606	CLA	O2D-CGD	5.05	1.45	1.33
15	C	513	CLA	CHC-C1C	5.05	1.47	1.35
15	B	607	CLA	O2A-C1	5.05	1.60	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	C	510	CLA	CHC-C1C	5.04	1.47	1.35
15	B	601	CLA	O2A-C1	5.04	1.60	1.46
15	C	510	CLA	O2A-C1	5.04	1.60	1.46
15	C	505	CLA	CHC-C1C	5.04	1.47	1.35
15	B	610	CLA	O2A-C1	5.03	1.60	1.46
15	C	507	CLA	O2D-CGD	5.03	1.45	1.33
15	B	614	CLA	O2D-CGD	5.03	1.45	1.33
15	B	612	CLA	O2A-C1	5.03	1.60	1.46
15	C	502	CLA	O2A-C1	5.03	1.60	1.46
15	B	611	CLA	O2D-CGD	5.03	1.45	1.33
15	B	608	CLA	O2A-C1	5.03	1.60	1.46
15	C	513	CLA	O2D-CGD	5.02	1.45	1.33
15	C	505	CLA	O2D-CGD	5.02	1.45	1.33
15	C	510	CLA	O2D-CGD	5.02	1.45	1.33
15	A	403	CLA	O2A-C1	5.02	1.60	1.46
15	C	504	CLA	CHC-C1C	5.02	1.47	1.35
15	D	405	CLA	CHC-C1C	5.01	1.47	1.35
15	C	511	CLA	O2A-C1	5.01	1.60	1.46
15	B	602	CLA	O2D-CGD	5.01	1.45	1.33
15	A	402	CLA	CHC-C1C	5.01	1.47	1.35
15	A	403	CLA	O2D-CGD	5.01	1.45	1.33
15	B	602	CLA	CHC-C1C	5.01	1.47	1.35
15	D	402	CLA	O2D-CGD	5.01	1.45	1.33
15	B	615	CLA	O2D-CGD	5.00	1.45	1.33
15	C	512	CLA	O2D-CGD	5.00	1.45	1.33
15	B	605	CLA	O2A-C1	5.00	1.60	1.46
15	B	605	CLA	CHC-C1C	5.00	1.47	1.35
15	C	508	CLA	O2D-CGD	4.98	1.45	1.33
15	B	613	CLA	O2A-C1	4.98	1.60	1.46
15	D	406	CLA	O2D-CGD	4.98	1.45	1.33
15	D	402	CLA	CHC-C1C	4.98	1.47	1.35
15	B	615	CLA	CHC-C1C	4.97	1.47	1.35
15	C	509	CLA	O2D-CGD	4.97	1.45	1.33
15	B	612	CLA	CHC-C1C	4.97	1.47	1.35
15	B	609	CLA	CHC-C1C	4.97	1.47	1.35
15	B	616	CLA	O2D-CGD	4.97	1.45	1.33
15	C	502	CLA	CHC-C1C	4.96	1.47	1.35
15	B	610	CLA	O2D-CGD	4.96	1.45	1.33
15	B	611	CLA	O2A-C1	4.96	1.60	1.46
15	B	612	CLA	O2D-CGD	4.96	1.45	1.33
15	B	606	CLA	CHC-C1C	4.96	1.47	1.35
15	B	608	CLA	CHC-C1C	4.95	1.47	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	601	CLA	CHC-C1C	4.95	1.47	1.35
15	D	406	CLA	CHC-C1C	4.95	1.47	1.35
15	B	607	CLA	CHC-C1C	4.94	1.47	1.35
15	B	608	CLA	O2D-CGD	4.93	1.45	1.33
15	D	405	CLA	O2D-CGD	4.93	1.45	1.33
15	B	603	CLA	CHC-C1C	4.93	1.47	1.35
15	B	613	CLA	CHC-C1C	4.92	1.47	1.35
15	A	405	CLA	CHC-C1C	4.92	1.47	1.35
15	D	406	CLA	C3B-C2B	4.91	1.47	1.40
15	C	506	CLA	O2D-CGD	4.91	1.45	1.33
15	C	503	CLA	CHC-C1C	4.91	1.47	1.35
15	B	607	CLA	O2D-CGD	4.91	1.45	1.33
15	B	604	CLA	O2A-C1	4.90	1.60	1.46
15	C	512	CLA	CHC-C1C	4.90	1.47	1.35
15	C	504	CLA	O2D-CGD	4.90	1.45	1.33
15	D	405	CLA	O2A-C1	4.90	1.59	1.46
26	E	101	HEM	C3C-C2C	-4.89	1.33	1.40
15	C	506	CLA	O2A-C1	4.89	1.59	1.46
15	B	604	CLA	O2D-CGD	4.89	1.45	1.33
15	B	610	CLA	CHC-C1C	4.89	1.47	1.35
15	B	605	CLA	C3B-C2B	4.88	1.47	1.40
15	B	603	CLA	O2D-CGD	4.88	1.45	1.33
15	C	510	CLA	C3B-C2B	4.88	1.47	1.40
15	C	506	CLA	CHC-C1C	4.88	1.47	1.35
15	C	511	CLA	C3B-C2B	4.87	1.47	1.40
15	C	505	CLA	C3B-C2B	4.87	1.47	1.40
15	A	402	CLA	C3B-C2B	4.86	1.47	1.40
15	A	405	CLA	C3B-C2B	4.86	1.47	1.40
15	C	509	CLA	CHC-C1C	4.85	1.47	1.35
15	B	604	CLA	CHC-C1C	4.85	1.47	1.35
15	C	504	CLA	C3B-C2B	4.85	1.47	1.40
15	C	512	CLA	C3B-C2B	4.84	1.47	1.40
15	B	612	CLA	C3B-C2B	4.84	1.47	1.40
15	C	503	CLA	C3B-C2B	4.83	1.47	1.40
15	B	616	CLA	CHC-C1C	4.83	1.47	1.35
15	B	615	CLA	C3B-C2B	4.83	1.47	1.40
15	D	402	CLA	C3B-C2B	4.82	1.47	1.40
15	B	614	CLA	CHC-C1C	4.82	1.47	1.35
15	C	506	CLA	C3B-C2B	4.81	1.47	1.40
15	B	609	CLA	C3B-C2B	4.80	1.47	1.40
15	B	611	CLA	CHC-C1C	4.78	1.47	1.35
15	B	613	CLA	C3B-C2B	4.76	1.47	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	D	402	CLA	CHD-C1D	4.76	1.47	1.38
15	C	507	CLA	CHC-C1C	4.75	1.47	1.35
15	A	403	CLA	CHD-C1D	4.73	1.47	1.38
15	B	616	CLA	C3B-C2B	4.73	1.46	1.40
15	C	514	CLA	C3B-C2B	4.71	1.46	1.40
15	C	508	CLA	CHC-C1C	4.70	1.47	1.35
15	B	608	CLA	C3B-C2B	4.70	1.46	1.40
15	B	603	CLA	C3B-C2B	4.70	1.46	1.40
15	B	607	CLA	C3B-C2B	4.69	1.46	1.40
15	C	502	CLA	CHD-C1D	4.68	1.47	1.38
15	D	402	CLA	C3C-C2C	4.68	1.46	1.36
15	B	606	CLA	C3B-C2B	4.68	1.46	1.40
15	B	604	CLA	C3B-C2B	4.67	1.46	1.40
15	B	606	CLA	CHD-C1D	4.65	1.47	1.38
15	D	405	CLA	C3C-C2C	4.65	1.46	1.36
15	C	507	CLA	CHD-C1D	4.64	1.47	1.38
15	B	614	CLA	C3B-C2B	4.63	1.46	1.40
15	D	406	CLA	CHD-C1D	4.63	1.47	1.38
15	B	613	CLA	CHD-C1D	4.61	1.47	1.38
15	A	403	CLA	C3B-C2B	4.60	1.46	1.40
15	B	602	CLA	C3B-C2B	4.60	1.46	1.40
15	A	403	CLA	C3C-C2C	4.60	1.46	1.36
15	B	603	CLA	C3D-C4D	-4.58	1.33	1.44
15	A	405	CLA	CHD-C1D	4.58	1.47	1.38
15	C	506	CLA	C3D-C4D	-4.56	1.33	1.44
15	C	514	CLA	CHD-C1D	4.56	1.47	1.38
15	C	511	CLA	C3C-C2C	4.56	1.46	1.36
15	C	506	CLA	CHD-C1D	4.55	1.47	1.38
15	B	604	CLA	C3C-C2C	4.54	1.46	1.36
15	B	602	CLA	CHD-C1D	4.54	1.47	1.38
15	B	615	CLA	C3D-C4D	-4.53	1.33	1.44
15	C	514	CLA	C3C-C2C	4.53	1.46	1.36
15	B	601	CLA	C3C-C2C	4.53	1.46	1.36
15	C	511	CLA	CHD-C1D	4.53	1.47	1.38
15	B	611	CLA	C3D-C4D	-4.52	1.34	1.44
15	B	614	CLA	CHD-C1D	4.52	1.47	1.38
15	D	406	CLA	C3C-C2C	4.52	1.46	1.36
15	C	508	CLA	CHD-C1D	4.51	1.47	1.38
15	C	509	CLA	C3D-C4D	-4.51	1.34	1.44
15	B	601	CLA	CHD-C1D	4.51	1.47	1.38
15	B	610	CLA	C3B-C2B	4.51	1.46	1.40
15	B	610	CLA	CHD-C1D	4.51	1.47	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	C	513	CLA	C3C-C2C	4.51	1.46	1.36
15	C	509	CLA	CHD-C1D	4.50	1.47	1.38
15	B	603	CLA	C3C-C2C	4.50	1.46	1.36
15	B	603	CLA	CHD-C1D	4.50	1.47	1.38
15	A	403	CLA	C3D-C4D	-4.50	1.34	1.44
15	B	610	CLA	C3D-C4D	-4.50	1.34	1.44
15	A	405	CLA	C3C-C2C	4.50	1.46	1.36
15	B	612	CLA	C3D-C4D	-4.49	1.34	1.44
15	C	507	CLA	C3C-C2C	4.49	1.46	1.36
15	B	601	CLA	C3D-C4D	-4.49	1.34	1.44
15	B	606	CLA	C3D-C4D	-4.49	1.34	1.44
15	B	611	CLA	C3B-C2B	4.49	1.46	1.40
15	C	503	CLA	CHD-C1D	4.49	1.47	1.38
15	C	504	CLA	C3D-C4D	-4.48	1.34	1.44
15	B	602	CLA	C3D-C4D	-4.48	1.34	1.44
15	D	406	CLA	C3D-C4D	-4.48	1.34	1.44
15	C	512	CLA	C3C-C2C	4.48	1.46	1.36
15	B	605	CLA	C3D-C4D	-4.48	1.34	1.44
15	C	508	CLA	C3D-C4D	-4.48	1.34	1.44
15	B	613	CLA	C3D-C4D	-4.48	1.34	1.44
15	C	509	CLA	C3C-C2C	4.47	1.46	1.36
15	B	604	CLA	CHD-C1D	4.47	1.47	1.38
15	B	608	CLA	C3C-C2C	4.47	1.46	1.36
15	B	607	CLA	CHD-C1D	4.47	1.47	1.38
15	D	402	CLA	C3D-C4D	-4.46	1.34	1.44
15	C	509	CLA	C3B-C2B	4.46	1.46	1.40
15	B	602	CLA	C3C-C2C	4.46	1.46	1.36
15	C	513	CLA	CHD-C1D	4.45	1.47	1.38
15	C	507	CLA	C3D-C4D	-4.45	1.34	1.44
15	D	405	CLA	C3D-C4D	-4.45	1.34	1.44
15	C	504	CLA	C3C-C2C	4.45	1.46	1.36
15	B	605	CLA	CHD-C1D	4.44	1.47	1.38
15	B	609	CLA	CHD-C1D	4.44	1.47	1.38
15	A	405	CLA	C3D-C4D	-4.44	1.34	1.44
15	B	616	CLA	C3D-C4D	-4.44	1.34	1.44
15	C	513	CLA	C3B-C2B	4.44	1.46	1.40
15	B	615	CLA	CHD-C1D	4.44	1.47	1.38
15	C	510	CLA	C3D-C4D	-4.43	1.34	1.44
15	B	611	CLA	CHD-C1D	4.43	1.47	1.38
15	C	505	CLA	CHD-C1D	4.43	1.47	1.38
15	B	607	CLA	C3C-C2C	4.43	1.46	1.36
15	B	610	CLA	C3C-C2C	4.42	1.46	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	C	510	CLA	C3C-C2C	4.42	1.46	1.36
15	B	608	CLA	C3D-C4D	-4.42	1.34	1.44
15	C	505	CLA	C3C-C2C	4.42	1.46	1.36
15	A	402	CLA	C3D-C4D	-4.42	1.34	1.44
15	C	504	CLA	CHD-C1D	4.41	1.47	1.38
15	C	512	CLA	C3D-C4D	-4.41	1.34	1.44
15	B	609	CLA	C3C-C2C	4.40	1.46	1.36
15	B	604	CLA	C3D-C4D	-4.40	1.34	1.44
15	B	614	CLA	C3D-C4D	-4.40	1.34	1.44
15	C	512	CLA	CHD-C1D	4.40	1.46	1.38
15	C	503	CLA	C3C-C2C	4.40	1.46	1.36
15	B	605	CLA	C3C-C2C	4.40	1.46	1.36
15	C	506	CLA	C3C-C2C	4.39	1.46	1.36
15	B	612	CLA	C3C-C2C	4.37	1.46	1.36
15	B	609	CLA	C3D-C4D	-4.37	1.34	1.44
15	C	505	CLA	C3D-C4D	-4.37	1.34	1.44
15	B	606	CLA	C3C-C2C	4.37	1.46	1.36
15	B	611	CLA	C3C-C2C	4.36	1.46	1.36
15	B	614	CLA	C3C-C2C	4.36	1.46	1.36
15	C	510	CLA	CHD-C1D	4.36	1.46	1.38
15	C	503	CLA	C3D-C4D	-4.36	1.34	1.44
15	C	502	CLA	C3C-C2C	4.36	1.46	1.36
15	B	615	CLA	C3C-C2C	4.36	1.46	1.36
15	C	514	CLA	C3D-C4D	-4.35	1.34	1.44
19	D	408	PL9	C7-C3	-4.34	1.46	1.51
15	B	613	CLA	C3C-C2C	4.34	1.45	1.36
15	B	607	CLA	C3D-C4D	-4.33	1.34	1.44
15	A	402	CLA	CHD-C1D	4.33	1.46	1.38
15	B	608	CLA	CHD-C1D	4.33	1.46	1.38
15	B	601	CLA	C3B-C2B	4.32	1.46	1.40
15	B	616	CLA	CHD-C1D	4.32	1.46	1.38
15	C	502	CLA	C3B-C2B	4.31	1.46	1.40
15	C	502	CLA	C3D-C4D	-4.31	1.34	1.44
15	B	616	CLA	C3C-C2C	4.31	1.45	1.36
15	C	508	CLA	C3C-C2C	4.30	1.45	1.36
15	C	511	CLA	C3D-C4D	-4.28	1.34	1.44
25	D	409	LHG	O8-C23	4.28	1.45	1.33
15	B	612	CLA	CHD-C1D	4.27	1.46	1.38
22	C	517	DGD	O1G-C1A	4.25	1.45	1.33
15	C	507	CLA	C3B-C2B	4.25	1.46	1.40
22	H	101	DGD	O1G-C1A	4.24	1.45	1.33
20	C	501	LMG	O8-C28	4.23	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	D	412	LMG	O8-C28	4.20	1.45	1.33
25	D	410	LHG	O8-C23	4.18	1.45	1.33
20	B	621	LMG	O8-C28	4.18	1.45	1.33
25	D	411	LHG	O8-C23	4.18	1.45	1.33
15	C	508	CLA	C3B-C2B	4.17	1.46	1.40
25	L	101	LHG	O8-C23	4.16	1.45	1.33
15	D	402	CLA	CHD-C4C	4.13	1.48	1.39
15	A	402	CLA	C3C-C2C	4.13	1.45	1.36
15	D	405	CLA	CHD-C1D	4.12	1.46	1.38
15	C	513	CLA	C3D-C4D	-4.11	1.34	1.44
25	D	411	LHG	O7-C7	4.07	1.45	1.34
15	B	613	CLA	CHD-C4C	4.06	1.48	1.39
15	A	403	CLA	CHD-C4C	4.06	1.48	1.39
22	C	517	DGD	O2G-C1B	4.04	1.45	1.34
15	C	502	CLA	CHD-C4C	4.04	1.48	1.39
20	C	501	LMG	O7-C10	4.03	1.45	1.34
15	B	606	CLA	CHD-C4C	4.03	1.48	1.39
15	B	602	CLA	CHD-C4C	3.99	1.48	1.39
15	D	406	CLA	CHD-C4C	3.97	1.48	1.39
25	D	410	LHG	O7-C7	3.95	1.45	1.34
15	B	603	CLA	CHD-C4C	3.95	1.48	1.39
20	B	621	LMG	O7-C10	3.94	1.45	1.34
25	L	101	LHG	O7-C7	3.94	1.45	1.34
19	D	408	PL9	C3-C4	-3.94	1.43	1.49
20	D	412	LMG	O7-C10	3.94	1.45	1.34
25	D	409	LHG	O7-C7	3.93	1.45	1.34
15	C	510	CLA	CHD-C4C	3.91	1.48	1.39
15	C	507	CLA	CHD-C4C	3.91	1.48	1.39
15	C	509	CLA	CHD-C4C	3.91	1.48	1.39
15	A	405	CLA	CHD-C4C	3.91	1.48	1.39
15	C	506	CLA	CHD-C4C	3.91	1.48	1.39
15	B	615	CLA	CHD-C4C	3.90	1.48	1.39
22	H	101	DGD	O2G-C1B	3.90	1.45	1.34
15	C	514	CLA	CHD-C4C	3.90	1.48	1.39
15	C	511	CLA	CHD-C4C	3.89	1.48	1.39
15	C	504	CLA	CHD-C4C	3.86	1.48	1.39
15	D	405	CLA	CHD-C4C	3.86	1.48	1.39
15	B	609	CLA	CHD-C4C	3.85	1.48	1.39
15	C	505	CLA	CHD-C4C	3.84	1.48	1.39
15	B	614	CLA	CHD-C4C	3.84	1.48	1.39
15	B	605	CLA	CHD-C4C	3.83	1.48	1.39
15	B	604	CLA	CHD-C4C	3.83	1.48	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	D	405	CLA	C1D-ND	-3.83	1.33	1.37
15	B	607	CLA	CHD-C4C	3.81	1.47	1.39
15	C	508	CLA	CHD-C4C	3.81	1.47	1.39
15	C	513	CLA	CHD-C4C	3.80	1.47	1.39
15	B	610	CLA	CHD-C4C	3.79	1.47	1.39
15	C	503	CLA	CHD-C4C	3.78	1.47	1.39
15	B	612	CLA	CHD-C4C	3.77	1.47	1.39
15	B	601	CLA	CHD-C4C	3.77	1.47	1.39
15	C	512	CLA	CHD-C4C	3.76	1.47	1.39
15	B	612	CLA	C1D-ND	-3.74	1.33	1.37
15	B	608	CLA	CHD-C4C	3.74	1.47	1.39
15	B	611	CLA	CHD-C4C	3.72	1.47	1.39
15	C	511	CLA	OBD-CAD	3.72	1.28	1.22
15	C	505	CLA	OBD-CAD	3.71	1.28	1.22
15	B	608	CLA	C1D-ND	-3.69	1.33	1.37
15	B	616	CLA	CHD-C4C	3.68	1.47	1.39
15	A	402	CLA	CHD-C4C	3.66	1.47	1.39
15	C	506	CLA	OBD-CAD	3.65	1.28	1.22
15	C	514	CLA	OBD-CAD	3.65	1.28	1.22
15	B	602	CLA	OBD-CAD	3.65	1.28	1.22
15	C	503	CLA	OBD-CAD	3.64	1.28	1.22
26	E	101	HEM	C3C-CAC	3.64	1.55	1.47
15	B	603	CLA	C1D-ND	-3.64	1.33	1.37
15	B	601	CLA	OBD-CAD	3.63	1.28	1.22
15	C	513	CLA	OBD-CAD	3.62	1.28	1.22
15	B	607	CLA	OBD-CAD	3.62	1.28	1.22
15	C	502	CLA	OBD-CAD	3.61	1.28	1.22
15	A	405	CLA	OBD-CAD	3.60	1.28	1.22
15	C	512	CLA	OBD-CAD	3.59	1.28	1.22
15	B	610	CLA	OBD-CAD	3.58	1.28	1.22
15	D	406	CLA	OBD-CAD	3.58	1.28	1.22
15	C	510	CLA	OBD-CAD	3.58	1.28	1.22
15	B	604	CLA	OBD-CAD	3.58	1.28	1.22
15	B	609	CLA	C1D-ND	-3.56	1.33	1.37
15	D	402	CLA	OBD-CAD	3.56	1.28	1.22
15	B	608	CLA	OBD-CAD	3.55	1.28	1.22
15	B	612	CLA	OBD-CAD	3.55	1.28	1.22
15	C	506	CLA	C1D-ND	-3.55	1.33	1.37
15	B	614	CLA	OBD-CAD	3.54	1.28	1.22
15	B	615	CLA	OBD-CAD	3.54	1.28	1.22
15	B	613	CLA	OBD-CAD	3.53	1.28	1.22
15	A	403	CLA	OBD-CAD	3.52	1.28	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	609	CLA	OBD-CAD	3.51	1.28	1.22
15	B	611	CLA	C1D-ND	-3.51	1.33	1.37
15	C	504	CLA	OBD-CAD	3.51	1.28	1.22
15	C	509	CLA	OBD-CAD	3.51	1.28	1.22
15	B	605	CLA	C1D-ND	-3.50	1.33	1.37
15	B	603	CLA	OBD-CAD	3.50	1.28	1.22
15	D	405	CLA	OBD-CAD	3.50	1.28	1.22
15	B	606	CLA	OBD-CAD	3.48	1.28	1.22
15	C	508	CLA	OBD-CAD	3.48	1.28	1.22
15	C	507	CLA	OBD-CAD	3.47	1.28	1.22
15	A	402	CLA	OBD-CAD	3.45	1.28	1.22
15	B	605	CLA	OBD-CAD	3.45	1.28	1.22
15	B	607	CLA	C1D-ND	-3.45	1.33	1.37
15	B	611	CLA	OBD-CAD	3.44	1.28	1.22
15	C	509	CLA	C1D-ND	-3.44	1.33	1.37
17	C	519	BCR	C11-C12	-3.40	1.25	1.34
17	X	102	BCR	C11-C12	-3.39	1.25	1.34
17	B	618	BCR	C11-C12	-3.39	1.25	1.34
17	B	617	BCR	C11-C12	-3.38	1.25	1.34
15	C	512	CLA	C1D-ND	-3.38	1.33	1.37
17	C	516	BCR	C11-C12	-3.38	1.25	1.34
17	C	515	BCR	C11-C12	-3.37	1.25	1.34
15	C	513	CLA	C1D-ND	-3.37	1.33	1.37
15	A	405	CLA	C1D-ND	-3.36	1.33	1.37
15	B	616	CLA	C1C-NC	-3.35	1.32	1.37
17	D	407	BCR	C11-C12	-3.34	1.26	1.34
15	A	402	CLA	C1D-ND	-3.34	1.33	1.37
22	H	101	DGD	CAB-C9B	-3.33	1.32	1.51
17	A	406	BCR	C11-C12	-3.32	1.26	1.34
15	B	604	CLA	C1D-ND	-3.32	1.33	1.37
15	C	503	CLA	C1D-ND	-3.31	1.33	1.37
15	B	615	CLA	C1D-ND	-3.31	1.33	1.37
17	B	619	BCR	C11-C12	-3.29	1.26	1.34
22	H	101	DGD	CAA-C9A	-3.27	1.33	1.51
15	B	614	CLA	C1D-ND	-3.26	1.33	1.37
22	C	517	DGD	CDB-CCB	-3.26	1.33	1.51
22	C	517	DGD	CAB-C9B	-3.26	1.33	1.51
15	C	510	CLA	C1D-ND	-3.25	1.33	1.37
20	C	501	LMG	C19-C18	-3.25	1.33	1.51
22	H	101	DGD	CDA-CCA	-3.25	1.33	1.51
22	H	101	DGD	CDB-CCB	-3.25	1.33	1.51
20	B	621	LMG	C22-C21	-3.24	1.33	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	C	501	LMG	C22-C21	-3.24	1.33	1.51
20	D	412	LMG	C37-C36	-3.24	1.33	1.51
20	C	501	LMG	C40-C39	-3.24	1.33	1.51
15	B	611	CLA	MG-ND	-3.23	1.99	2.05
20	B	621	LMG	C19-C18	-3.23	1.33	1.51
15	B	602	CLA	C1D-ND	-3.23	1.33	1.37
22	C	517	DGD	CDA-CCA	-3.23	1.33	1.51
18	A	409	SQD	O48-C23	3.23	1.42	1.33
22	C	517	DGD	CAA-C9A	-3.23	1.33	1.51
15	B	606	CLA	C1D-ND	-3.23	1.33	1.37
20	B	621	LMG	C37-C36	-3.22	1.33	1.51
20	B	621	LMG	C40-C39	-3.22	1.33	1.51
15	C	507	CLA	C1D-ND	-3.21	1.33	1.37
20	C	501	LMG	C37-C36	-3.21	1.33	1.51
20	D	412	LMG	C40-C39	-3.21	1.33	1.51
15	B	610	CLA	C1D-ND	-3.20	1.33	1.37
15	B	616	CLA	OBD-CAD	3.20	1.28	1.22
20	D	412	LMG	C19-C18	-3.20	1.33	1.51
20	D	412	LMG	C22-C21	-3.20	1.33	1.51
15	C	514	CLA	C1D-ND	-3.20	1.33	1.37
18	T	103	SQD	O48-C23	3.19	1.42	1.33
18	T	101	SQD	O48-C23	3.16	1.42	1.33
15	D	406	CLA	C1D-ND	-3.16	1.33	1.37
18	C	518	SQD	O48-C23	3.16	1.42	1.33
15	C	511	CLA	C1D-ND	-3.13	1.33	1.37
15	C	508	CLA	C1D-ND	-3.12	1.33	1.37
15	C	512	CLA	MG-NC	3.12	2.13	2.06
15	B	611	CLA	C3D-C2D	3.12	1.47	1.39
15	C	506	CLA	MG-ND	-3.11	1.99	2.05
15	C	506	CLA	MG-NC	3.10	2.13	2.06
15	C	505	CLA	C1D-ND	-3.10	1.34	1.37
15	B	604	CLA	MG-NC	3.09	2.13	2.06
18	B	620	SQD	O48-C23	3.08	1.42	1.33
15	C	504	CLA	C1D-ND	-3.08	1.34	1.37
15	C	513	CLA	MG-NC	3.07	2.13	2.06
15	A	403	CLA	C1D-ND	-3.07	1.34	1.37
18	A	407	SQD	O48-C23	3.06	1.42	1.33
15	C	513	CLA	C3D-C2D	3.06	1.47	1.39
18	X	101	SQD	O48-C23	3.05	1.42	1.33
15	B	603	CLA	MG-ND	-3.05	1.99	2.05
15	B	613	CLA	C1D-ND	-3.05	1.34	1.37
15	D	402	CLA	C1D-ND	-3.04	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	E	101	HEM	CAB-C3B	3.04	1.55	1.47
15	C	502	CLA	MG-NC	3.04	2.13	2.06
15	C	503	CLA	C3D-C2D	3.03	1.47	1.39
15	B	606	CLA	C3D-C2D	3.02	1.47	1.39
15	B	605	CLA	C3D-C2D	3.02	1.47	1.39
15	B	601	CLA	C1D-ND	-3.02	1.34	1.37
15	C	502	CLA	C1D-ND	-3.02	1.34	1.37
15	B	616	CLA	C1D-ND	-3.02	1.34	1.37
15	D	402	CLA	C3D-C2D	3.01	1.47	1.39
18	X	101	SQD	O47-C7	3.01	1.42	1.34
15	C	507	CLA	C3D-C2D	3.00	1.47	1.39
15	C	502	CLA	C3D-C2D	3.00	1.47	1.39
15	C	508	CLA	MG-ND	-2.99	1.99	2.05
15	B	614	CLA	MG-NC	2.98	2.13	2.06
15	B	609	CLA	C3D-C2D	2.98	1.47	1.39
15	B	602	CLA	C3D-C2D	2.98	1.47	1.39
15	C	514	CLA	C3D-C2D	2.97	1.47	1.39
15	B	613	CLA	MG-NC	2.97	2.13	2.06
15	A	405	CLA	C3D-C2D	2.97	1.47	1.39
15	C	507	CLA	MG-ND	-2.97	1.99	2.05
15	C	509	CLA	C3D-C2D	2.96	1.47	1.39
15	C	509	CLA	C1C-NC	-2.96	1.33	1.37
15	B	614	CLA	C3D-C2D	2.96	1.47	1.39
15	C	505	CLA	C3D-C2D	2.95	1.47	1.39
15	A	403	CLA	MG-NC	2.95	2.13	2.06
15	A	405	CLA	MG-NC	2.95	2.13	2.06
15	C	514	CLA	MG-NC	2.95	2.13	2.06
15	B	607	CLA	C3D-C2D	2.94	1.47	1.39
15	C	512	CLA	C3D-C2D	2.94	1.47	1.39
18	T	101	SQD	O47-C7	2.94	1.42	1.34
15	B	604	CLA	MG-ND	-2.93	2.00	2.05
15	B	602	CLA	MG-NC	2.93	2.13	2.06
15	B	612	CLA	MG-ND	-2.93	2.00	2.05
15	B	614	CLA	MG-ND	-2.92	2.00	2.05
15	C	504	CLA	MG-NC	2.92	2.13	2.06
15	C	507	CLA	MG-NC	2.92	2.13	2.06
15	C	503	CLA	MG-NC	2.92	2.13	2.06
15	D	406	CLA	MG-NC	2.92	2.13	2.06
15	C	510	CLA	C3D-C2D	2.92	1.47	1.39
15	B	607	CLA	MG-NC	2.92	2.13	2.06
15	B	610	CLA	MG-NC	2.92	2.13	2.06
15	B	616	CLA	C3D-C2D	2.91	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	C	511	CLA	C3D-C2D	2.91	1.47	1.39
15	A	403	CLA	C3D-C2D	2.91	1.47	1.39
15	C	511	CLA	MG-NC	2.90	2.13	2.06
15	C	508	CLA	MG-NC	2.90	2.13	2.06
15	B	615	CLA	C3D-C2D	2.90	1.47	1.39
18	C	518	SQD	O47-C7	2.90	1.42	1.34
15	B	605	CLA	MG-ND	-2.90	2.00	2.05
15	C	505	CLA	MG-NC	2.90	2.13	2.06
15	B	608	CLA	MG-ND	-2.90	2.00	2.05
15	B	615	CLA	MG-NC	2.90	2.13	2.06
15	D	402	CLA	MG-NC	2.90	2.13	2.06
15	B	611	CLA	C1C-NC	-2.89	1.33	1.37
18	T	103	SQD	O47-C7	2.89	1.42	1.34
15	D	406	CLA	C3D-C2D	2.89	1.47	1.39
15	B	608	CLA	C3D-C2D	2.89	1.47	1.39
15	B	603	CLA	MG-NC	2.88	2.13	2.06
19	D	408	PL9	C6-C1	-2.87	1.43	1.48
15	C	508	CLA	C3D-C2D	2.87	1.47	1.39
15	C	504	CLA	C3D-C2D	2.87	1.47	1.39
15	B	605	CLA	MG-NC	2.87	2.13	2.06
15	B	606	CLA	MG-NC	2.87	2.13	2.06
15	B	610	CLA	C3D-C2D	2.87	1.47	1.39
15	B	612	CLA	C3D-C2D	2.87	1.46	1.39
15	B	613	CLA	C3D-C2D	2.87	1.46	1.39
15	B	604	CLA	C3D-C2D	2.86	1.46	1.39
18	B	620	SQD	O47-C7	2.85	1.42	1.34
15	B	601	CLA	MG-NC	2.84	2.13	2.06
15	B	612	CLA	C1C-NC	-2.84	1.33	1.37
15	C	502	CLA	C4D-CHA	2.83	1.48	1.38
15	B	603	CLA	C3D-C2D	2.83	1.46	1.39
15	A	402	CLA	MG-NC	2.83	2.13	2.06
15	C	510	CLA	C1C-NC	-2.83	1.33	1.37
15	B	607	CLA	MG-ND	-2.82	2.00	2.05
15	B	609	CLA	MG-NC	2.82	2.13	2.06
15	B	608	CLA	MG-NC	2.82	2.13	2.06
15	C	509	CLA	MG-ND	-2.82	2.00	2.05
18	A	409	SQD	O47-C7	2.81	1.42	1.34
15	B	610	CLA	C1C-NC	-2.81	1.33	1.37
19	A	408	PL9	C7-C3	-2.80	1.48	1.51
16	A	404	PHO	CAC-C3C	-2.80	1.47	1.52
15	C	512	CLA	MG-ND	-2.80	2.00	2.05
15	B	616	CLA	MG-ND	-2.80	2.00	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	C	503	CLA	C1C-NC	-2.79	1.33	1.37
15	A	402	CLA	MG-ND	-2.79	2.00	2.05
15	D	405	CLA	C3D-C2D	2.79	1.46	1.39
15	D	405	CLA	MG-NC	2.78	2.12	2.06
15	C	510	CLA	MG-NC	2.78	2.12	2.06
15	B	614	CLA	C1C-NC	-2.78	1.33	1.37
15	B	604	CLA	C4D-CHA	2.78	1.48	1.38
15	B	607	CLA	C1C-NC	-2.78	1.33	1.37
19	A	408	PL9	C3-C4	-2.77	1.45	1.49
15	B	611	CLA	MG-NC	2.77	2.12	2.06
15	C	504	CLA	C1C-NC	-2.77	1.33	1.37
15	C	508	CLA	C1C-NC	-2.77	1.33	1.37
15	D	405	CLA	MG-ND	-2.76	2.00	2.05
15	C	504	CLA	MG-ND	-2.76	2.00	2.05
15	A	402	CLA	C3D-C2D	2.76	1.46	1.39
15	B	606	CLA	MG-ND	-2.75	2.00	2.05
15	B	612	CLA	MG-NC	2.75	2.12	2.06
15	C	503	CLA	MG-ND	-2.75	2.00	2.05
15	C	514	CLA	MG-ND	-2.74	2.00	2.05
15	B	603	CLA	C1C-NC	-2.74	1.33	1.37
15	B	607	CLA	C4D-CHA	2.74	1.48	1.38
15	B	614	CLA	C4D-CHA	2.74	1.48	1.38
15	C	511	CLA	C4D-CHA	2.73	1.48	1.38
15	B	602	CLA	MG-ND	-2.73	2.00	2.05
15	B	613	CLA	C4D-CHA	2.73	1.48	1.38
15	C	513	CLA	C4D-CHA	2.72	1.48	1.38
15	C	509	CLA	MG-NC	2.72	2.12	2.06
15	A	405	CLA	C1C-NC	-2.72	1.33	1.37
15	B	616	CLA	C4D-CHA	2.72	1.48	1.38
15	C	508	CLA	C4D-CHA	2.72	1.48	1.38
15	B	604	CLA	C1C-NC	-2.71	1.33	1.37
18	A	407	SQD	O47-C7	2.71	1.42	1.34
15	C	503	CLA	C4D-CHA	2.71	1.48	1.38
15	B	609	CLA	MG-ND	-2.71	2.00	2.05
15	D	406	CLA	MG-ND	-2.71	2.00	2.05
15	B	608	CLA	C1C-NC	-2.71	1.33	1.37
15	B	615	CLA	C1C-NC	-2.71	1.33	1.37
15	A	402	CLA	C4D-CHA	2.71	1.48	1.38
15	C	507	CLA	C1C-NC	-2.69	1.33	1.37
15	B	610	CLA	MG-ND	-2.69	2.00	2.05
15	B	605	CLA	C4D-CHA	2.69	1.48	1.38
15	C	504	CLA	C4D-CHA	2.68	1.47	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	C	507	CLA	C4D-CHA	2.68	1.47	1.38
15	B	615	CLA	C4D-CHA	2.68	1.47	1.38
21	B	622	LMT	O2'-C2'	-2.67	1.36	1.43
15	C	505	CLA	C4D-CHA	2.67	1.47	1.38
15	B	602	CLA	C1C-NC	-2.67	1.33	1.37
15	B	610	CLA	C4D-CHA	2.67	1.47	1.38
15	A	405	CLA	MG-ND	-2.67	2.00	2.05
15	B	602	CLA	C4D-CHA	2.66	1.47	1.38
15	B	606	CLA	C4D-CHA	2.66	1.47	1.38
15	B	601	CLA	C4D-CHA	2.66	1.47	1.38
15	B	601	CLA	C3D-C2D	2.66	1.46	1.39
15	B	605	CLA	C1C-NC	-2.66	1.33	1.37
15	A	405	CLA	C4D-CHA	2.66	1.47	1.38
15	A	402	CLA	C1C-NC	-2.65	1.33	1.37
15	C	510	CLA	MG-ND	-2.65	2.00	2.05
15	D	406	CLA	C1C-NC	-2.65	1.33	1.37
15	C	506	CLA	C4D-CHA	2.65	1.47	1.38
15	C	510	CLA	C4D-CHA	2.65	1.47	1.38
15	B	611	CLA	C4D-CHA	2.64	1.47	1.38
15	C	512	CLA	C4D-CHA	2.64	1.47	1.38
15	B	608	CLA	C4D-CHA	2.64	1.47	1.38
15	C	514	CLA	C4D-CHA	2.64	1.47	1.38
15	B	609	CLA	C4D-CHA	2.64	1.47	1.38
15	D	402	CLA	C4D-CHA	2.64	1.47	1.38
15	B	613	CLA	MG-ND	-2.63	2.00	2.05
15	C	506	CLA	C3D-C2D	2.63	1.46	1.39
15	B	609	CLA	C1C-NC	-2.63	1.33	1.37
15	A	403	CLA	C4D-CHA	2.62	1.47	1.38
21	B	623	LMT	O3'-C3'	-2.62	1.36	1.43
15	B	601	CLA	C1C-NC	-2.61	1.33	1.37
15	C	513	CLA	MG-ND	-2.61	2.00	2.05
15	D	406	CLA	C4D-CHA	2.61	1.47	1.38
15	B	616	CLA	MG-NC	2.60	2.12	2.06
15	B	612	CLA	C4D-CHA	2.60	1.47	1.38
15	C	513	CLA	C4B-CHC	2.60	1.48	1.41
15	C	505	CLA	MG-ND	-2.60	2.00	2.05
15	D	402	CLA	C1C-NC	-2.59	1.33	1.37
15	B	603	CLA	C4D-CHA	2.59	1.47	1.38
15	C	509	CLA	C4D-CHA	2.59	1.47	1.38
15	C	502	CLA	MG-ND	-2.58	2.00	2.05
15	D	405	CLA	C1C-NC	-2.58	1.34	1.37
15	C	506	CLA	C1C-NC	-2.58	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	403	CLA	C1D-C2D	2.58	1.50	1.45
15	C	514	CLA	C1C-NC	-2.57	1.34	1.37
15	A	402	CLA	C4B-CHC	2.57	1.48	1.41
15	C	502	CLA	C1C-NC	-2.56	1.34	1.37
15	B	606	CLA	C1C-NC	-2.56	1.34	1.37
15	C	502	CLA	C4B-CHC	2.56	1.48	1.41
21	B	622	LMT	O3'-C3'	-2.56	1.36	1.43
15	B	615	CLA	MG-ND	-2.56	2.00	2.05
15	B	601	CLA	MG-ND	-2.55	2.00	2.05
15	C	505	CLA	C1C-NC	-2.55	1.34	1.37
15	C	512	CLA	C1B-CHB	2.54	1.48	1.41
15	C	511	CLA	MG-ND	-2.54	2.00	2.05
15	D	402	CLA	MG-ND	-2.54	2.00	2.05
15	D	405	CLA	C4B-CHC	2.53	1.48	1.41
16	D	403	PHO	CAC-C3C	-2.53	1.47	1.52
15	C	502	CLA	C1D-C2D	2.53	1.50	1.45
15	B	601	CLA	C1D-C2D	2.53	1.50	1.45
15	D	402	CLA	C1D-C2D	2.52	1.50	1.45
15	B	610	CLA	C4B-CHC	2.52	1.48	1.41
15	C	511	CLA	C1C-NC	-2.52	1.34	1.37
15	A	403	CLA	C4B-CHC	2.51	1.48	1.41
15	A	403	CLA	MG-ND	-2.51	2.00	2.05
15	B	601	CLA	C4B-CHC	2.51	1.48	1.41
15	B	604	CLA	C1B-CHB	2.50	1.48	1.41
15	C	513	CLA	C1B-CHB	2.50	1.47	1.41
15	C	511	CLA	C1D-C2D	2.50	1.50	1.45
15	C	514	CLA	C4B-CHC	2.49	1.47	1.41
15	B	605	CLA	C4B-CHC	2.49	1.47	1.41
21	B	623	LMT	O2'-C2'	-2.48	1.37	1.43
19	A	408	PL9	C6-C1	-2.48	1.44	1.48
15	C	513	CLA	C1C-NC	-2.48	1.34	1.37
15	C	511	CLA	C4B-CHC	2.48	1.47	1.41
15	B	606	CLA	C1D-C2D	2.47	1.50	1.45
15	D	405	CLA	C4D-CHA	2.47	1.47	1.38
15	C	503	CLA	C1B-CHB	2.47	1.47	1.41
15	B	613	CLA	C1C-NC	-2.47	1.34	1.37
15	A	403	CLA	C1C-NC	-2.46	1.34	1.37
15	B	602	CLA	C1D-C2D	2.46	1.50	1.45
15	C	512	CLA	C1C-NC	-2.46	1.34	1.37
15	A	402	CLA	C1B-CHB	2.46	1.47	1.41
15	C	504	CLA	C4B-CHC	2.45	1.47	1.41
15	C	510	CLA	C1B-CHB	2.45	1.47	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	C	505	CLA	C4B-CHC	2.45	1.47	1.41
15	C	511	CLA	C1B-CHB	2.45	1.47	1.41
15	D	406	CLA	C4B-CHC	2.44	1.47	1.41
15	B	609	CLA	C4B-CHC	2.43	1.47	1.41
15	A	405	CLA	C1D-C2D	2.43	1.50	1.45
15	C	512	CLA	C4B-CHC	2.43	1.47	1.41
15	A	405	CLA	C4B-CHC	2.42	1.47	1.41
15	C	504	CLA	C1D-C2D	2.42	1.50	1.45
15	B	613	CLA	C1B-CHB	2.42	1.47	1.41
15	C	504	CLA	C1B-CHB	2.42	1.47	1.41
21	B	623	LMT	O3B-C3B	-2.42	1.37	1.43
15	D	402	CLA	C4B-CHC	2.41	1.47	1.41
15	B	606	CLA	C4B-CHC	2.41	1.47	1.41
15	D	406	CLA	C1B-CHB	2.41	1.47	1.41
15	B	613	CLA	C4B-CHC	2.40	1.47	1.41
15	C	509	CLA	C1D-C2D	2.40	1.50	1.45
15	B	615	CLA	C4B-CHC	2.40	1.47	1.41
15	C	503	CLA	C4B-CHC	2.40	1.47	1.41
15	B	612	CLA	C4B-CHC	2.39	1.47	1.41
15	D	405	CLA	C1B-CHB	2.39	1.47	1.41
15	C	514	CLA	C1B-CHB	2.39	1.47	1.41
15	C	506	CLA	C4B-CHC	2.38	1.47	1.41
15	B	602	CLA	C4B-CHC	2.38	1.47	1.41
15	C	505	CLA	C1B-CHB	2.38	1.47	1.41
15	C	507	CLA	C1B-CHB	2.38	1.47	1.41
15	B	613	CLA	C1D-C2D	2.38	1.50	1.45
15	C	514	CLA	C1D-C2D	2.38	1.50	1.45
15	B	608	CLA	C4B-CHC	2.38	1.47	1.41
15	A	405	CLA	C1B-CHB	2.37	1.47	1.41
15	B	616	CLA	C1B-CHB	2.37	1.47	1.41
15	B	601	CLA	C1B-CHB	2.37	1.47	1.41
15	B	609	CLA	C1B-CHB	2.37	1.47	1.41
15	D	402	CLA	C1B-CHB	2.37	1.47	1.41
15	A	403	CLA	C1B-CHB	2.36	1.47	1.41
15	D	406	CLA	C1D-C2D	2.36	1.50	1.45
15	C	510	CLA	C4B-CHC	2.35	1.47	1.41
15	C	502	CLA	C1B-CHB	2.35	1.47	1.41
21	B	622	LMT	O2B-C2B	-2.35	1.37	1.43
15	B	603	CLA	C4B-CHC	2.35	1.47	1.41
15	B	615	CLA	C1B-CHB	2.34	1.47	1.41
15	B	607	CLA	C4B-CHC	2.34	1.47	1.41
15	C	508	CLA	C4B-CHC	2.34	1.47	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	610	CLA	C1B-CHB	2.34	1.47	1.41
21	B	623	LMT	O2B-C2B	-2.34	1.37	1.43
15	B	607	CLA	C1B-CHB	2.33	1.47	1.41
15	B	604	CLA	C4B-CHC	2.33	1.47	1.41
16	D	403	PHO	CMC-C2C	-2.32	1.46	1.51
15	C	506	CLA	C1B-CHB	2.32	1.47	1.41
15	C	507	CLA	C1D-C2D	2.32	1.49	1.45
15	B	602	CLA	C1B-CHB	2.31	1.47	1.41
15	C	505	CLA	C1D-C2D	2.31	1.49	1.45
15	B	608	CLA	C1B-CHB	2.31	1.47	1.41
15	B	610	CLA	C1D-C2D	2.31	1.49	1.45
18	A	407	SQD	O2-C2	-2.30	1.37	1.43
15	B	614	CLA	C1B-CHB	2.30	1.47	1.41
15	C	509	CLA	C4B-CHC	2.30	1.47	1.41
15	A	403	CLA	C4C-C3C	2.29	1.49	1.45
15	B	611	CLA	C4B-CHC	2.29	1.47	1.41
15	C	509	CLA	C1B-CHB	2.28	1.47	1.41
15	B	605	CLA	C1B-CHB	2.28	1.47	1.41
19	D	408	PL9	C53-C6	-2.28	1.46	1.50
15	C	510	CLA	C1D-C2D	2.28	1.49	1.45
15	B	607	CLA	C1D-C2D	2.27	1.49	1.45
15	C	507	CLA	C4C-C3C	2.26	1.48	1.45
15	B	614	CLA	C4B-CHC	2.26	1.47	1.41
15	B	611	CLA	C1B-CHB	2.26	1.47	1.41
15	C	508	CLA	C1B-CHB	2.26	1.47	1.41
15	B	615	CLA	C1D-C2D	2.24	1.49	1.45
15	B	603	CLA	C1B-CHB	2.24	1.47	1.41
15	B	606	CLA	C1B-CHB	2.24	1.47	1.41
15	D	402	CLA	C4C-C3C	2.23	1.48	1.45
15	B	612	CLA	C1B-CHB	2.22	1.47	1.41
15	B	616	CLA	C4B-CHC	2.21	1.47	1.41
15	C	512	CLA	C1D-C2D	2.21	1.49	1.45
15	D	405	CLA	C1D-C2D	2.19	1.49	1.45
21	B	623	LMT	O4'-C4B	-2.19	1.37	1.43
21	B	622	LMT	O4'-C4B	-2.19	1.37	1.43
15	C	502	CLA	C4C-C3C	2.18	1.48	1.45
15	C	507	CLA	C4B-CHC	2.18	1.47	1.41
16	A	404	PHO	CMC-C2C	-2.18	1.46	1.51
15	B	609	CLA	C1D-C2D	2.17	1.49	1.45
15	C	513	CLA	C1D-C2D	2.17	1.49	1.45
18	A	409	SQD	O2-C2	-2.16	1.37	1.43
16	D	403	PHO	CMD-C2D	-2.16	1.46	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	C	518	SQD	O2-C2	-2.16	1.37	1.43
18	T	101	SQD	O2-C2	-2.15	1.37	1.43
15	C	503	CLA	C1D-C2D	2.14	1.49	1.45
15	B	610	CLA	C4C-C3C	2.14	1.48	1.45
15	C	514	CLA	C4C-C3C	2.14	1.48	1.45
15	A	405	CLA	C4C-C3C	2.14	1.48	1.45
18	B	620	SQD	O2-C2	-2.14	1.37	1.43
15	B	605	CLA	C1D-C2D	2.13	1.49	1.45
16	A	404	PHO	CMD-C2D	-2.12	1.46	1.51
18	T	103	SQD	O2-C2	-2.12	1.38	1.43
21	B	622	LMT	O3B-C3B	-2.12	1.38	1.43
15	B	604	CLA	C1D-C2D	2.12	1.49	1.45
15	B	614	CLA	C4C-C3C	2.11	1.48	1.45
17	A	406	BCR	C30-C25	-2.11	1.50	1.53
15	C	506	CLA	C4C-C3C	2.11	1.48	1.45
15	C	508	CLA	C1D-C2D	2.10	1.49	1.45
15	B	614	CLA	C1D-C2D	2.09	1.49	1.45
15	B	616	CLA	C1D-C2D	2.09	1.49	1.45
18	X	101	SQD	O3-C3	-2.09	1.38	1.43
15	B	604	CLA	C4C-C3C	2.09	1.48	1.45
18	B	620	SQD	O3-C3	-2.09	1.38	1.43
18	A	409	SQD	O4-C4	-2.09	1.38	1.43
18	C	518	SQD	O4-C4	-2.08	1.38	1.43
19	D	408	PL9	C52-C5	-2.08	1.46	1.50
15	C	506	CLA	C1D-C2D	2.08	1.49	1.45
18	X	101	SQD	O2-C2	-2.07	1.38	1.43
15	C	505	CLA	C4C-C3C	2.07	1.48	1.45
18	B	620	SQD	O4-C4	-2.07	1.38	1.43
15	B	603	CLA	C1D-C2D	2.07	1.49	1.45
16	A	404	PHO	CMB-C2B	-2.06	1.46	1.51
19	A	408	PL9	C53-C6	-2.06	1.46	1.50
15	B	602	CLA	C4C-C3C	2.06	1.48	1.45
18	A	409	SQD	O3-C3	-2.06	1.38	1.43
18	A	407	SQD	O3-C3	-2.06	1.38	1.43
18	T	101	SQD	O3-C3	-2.05	1.38	1.43
15	B	606	CLA	C4C-C3C	2.05	1.48	1.45
18	T	101	SQD	O4-C4	-2.05	1.38	1.43
15	B	611	CLA	C1D-C2D	2.03	1.49	1.45
18	X	101	SQD	O4-C4	-2.03	1.38	1.43
21	B	623	LMT	O1'-C1'	-2.03	1.36	1.40
15	A	402	CLA	C1D-C2D	2.03	1.49	1.45
15	C	509	CLA	C4C-C3C	2.03	1.48	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	517	DGD	CGA-CFA	-2.02	1.33	1.49
20	C	501	LMG	C25-C24	-2.02	1.33	1.49
15	B	608	CLA	C1D-C2D	2.02	1.49	1.45
22	H	101	DGD	CGB-CFB	-2.02	1.33	1.49
20	D	412	LMG	C43-C42	-2.01	1.33	1.49
20	B	621	LMG	C25-C24	-2.01	1.33	1.49
15	B	615	CLA	C4C-C3C	2.01	1.48	1.45
22	H	101	DGD	CGA-CFA	-2.01	1.33	1.49
20	C	501	LMG	C43-C42	-2.01	1.33	1.49
21	B	622	LMT	O1'-C1'	-2.00	1.36	1.40
20	B	621	LMG	C43-C42	-2.00	1.33	1.49
26	E	101	HEM	CMB-C2B	2.00	1.55	1.50
20	D	412	LMG	C25-C24	-2.00	1.33	1.49
17	C	515	BCR	C30-C25	-2.00	1.51	1.53

All (1144) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	D	407	BCR	C20-C21-C22	23.19	160.40	127.31
17	C	516	BCR	C20-C21-C22	21.49	157.99	127.31
17	B	617	BCR	C20-C21-C22	21.21	157.57	127.31
17	D	407	BCR	C15-C16-C17	20.88	166.25	123.47
17	C	515	BCR	C20-C21-C22	20.85	157.07	127.31
17	B	617	BCR	C15-C16-C17	20.83	166.14	123.47
17	X	102	BCR	C15-C16-C17	20.80	166.07	123.47
17	B	618	BCR	C20-C21-C22	20.76	156.93	127.31
17	A	406	BCR	C15-C16-C17	20.73	165.95	123.47
17	C	516	BCR	C15-C16-C17	20.67	165.81	123.47
17	B	619	BCR	C20-C21-C22	20.60	156.71	127.31
17	B	618	BCR	C15-C16-C17	20.59	165.65	123.47
17	X	102	BCR	C20-C21-C22	20.55	156.64	127.31
17	A	406	BCR	C20-C21-C22	20.55	156.63	127.31
17	C	519	BCR	C20-C21-C22	20.46	156.51	127.31
17	C	519	BCR	C15-C16-C17	20.35	165.16	123.47
17	D	407	BCR	C16-C17-C18	20.31	156.30	127.31
17	B	619	BCR	C15-C16-C17	20.22	164.90	123.47
17	C	515	BCR	C15-C16-C17	20.20	164.85	123.47
17	C	519	BCR	C16-C17-C18	19.82	155.59	127.31
17	C	516	BCR	C16-C17-C18	19.49	155.13	127.31
17	B	618	BCR	C16-C17-C18	19.40	155.00	127.31
17	A	406	BCR	C16-C17-C18	19.07	154.53	127.31
17	C	515	BCR	C16-C17-C18	19.00	154.42	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	X	102	BCR	C16-C17-C18	18.93	154.33	127.31
17	B	619	BCR	C16-C17-C18	18.68	153.97	127.31
17	B	617	BCR	C16-C17-C18	18.66	153.94	127.31
17	X	102	BCR	C10-C11-C12	18.18	179.94	123.22
17	D	407	BCR	C10-C11-C12	17.51	177.86	123.22
17	B	618	BCR	C10-C11-C12	17.43	177.61	123.22
17	B	619	BCR	C10-C11-C12	17.34	177.34	123.22
17	C	516	BCR	C10-C11-C12	17.31	177.23	123.22
17	B	617	BCR	C10-C11-C12	17.14	176.71	123.22
17	C	519	BCR	C10-C11-C12	16.91	175.99	123.22
17	A	406	BCR	C10-C11-C12	16.77	175.56	123.22
17	C	515	BCR	C10-C11-C12	16.41	174.42	123.22
17	A	406	BCR	C11-C10-C9	13.72	146.89	127.31
17	B	617	BCR	C11-C10-C9	13.48	146.54	127.31
17	B	619	BCR	C11-C10-C9	13.29	146.27	127.31
17	A	406	BCR	C21-C20-C19	13.15	164.25	123.22
17	C	515	BCR	C21-C20-C19	13.12	164.15	123.22
17	B	619	BCR	C16-C15-C14	13.05	150.20	123.47
17	X	102	BCR	C21-C20-C19	13.01	163.82	123.22
17	X	102	BCR	C11-C10-C9	13.00	145.87	127.31
17	C	519	BCR	C21-C20-C19	13.00	163.78	123.22
17	B	618	BCR	C21-C20-C19	12.96	163.67	123.22
17	B	619	BCR	C21-C20-C19	12.96	163.65	123.22
17	B	617	BCR	C21-C20-C19	12.79	163.12	123.22
17	C	515	BCR	C16-C15-C14	12.73	149.55	123.47
17	B	618	BCR	C16-C15-C14	12.54	149.16	123.47
17	B	618	BCR	C11-C10-C9	12.53	145.19	127.31
17	D	407	BCR	C11-C10-C9	12.45	145.08	127.31
17	X	102	BCR	C16-C15-C14	12.44	148.96	123.47
17	C	516	BCR	C21-C20-C19	12.42	161.99	123.22
17	D	407	BCR	C16-C15-C14	12.42	148.93	123.47
17	C	516	BCR	C11-C10-C9	12.30	144.87	127.31
17	C	519	BCR	C16-C15-C14	12.25	148.57	123.47
17	C	519	BCR	C11-C10-C9	12.09	144.57	127.31
17	B	617	BCR	C16-C15-C14	12.07	148.21	123.47
17	C	516	BCR	C16-C15-C14	12.07	148.20	123.47
17	D	407	BCR	C21-C20-C19	11.93	160.45	123.22
17	A	406	BCR	C16-C15-C14	11.86	147.76	123.47
17	C	515	BCR	C11-C10-C9	11.79	144.13	127.31
17	A	406	BCR	C11-C12-C13	11.44	158.56	126.42
17	C	516	BCR	C11-C12-C13	11.09	157.56	126.42
17	B	617	BCR	C11-C12-C13	10.87	156.96	126.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	X	102	BCR	C11-C12-C13	10.73	156.56	126.42
17	B	619	BCR	C11-C12-C13	10.60	156.20	126.42
17	D	407	BCR	C11-C12-C13	10.60	156.18	126.42
17	C	519	BCR	C11-C12-C13	10.50	155.91	126.42
17	B	618	BCR	C11-C12-C13	10.32	155.40	126.42
17	C	515	BCR	C11-C12-C13	10.01	154.53	126.42
15	B	601	CLA	CMD-C2D-C1D	9.20	140.93	124.71
15	C	506	CLA	CMD-C2D-C1D	8.52	139.74	124.71
15	C	504	CLA	CMD-C2D-C1D	8.32	139.38	124.71
15	B	613	CLA	CMD-C2D-C1D	8.32	139.37	124.71
17	D	407	BCR	C20-C19-C18	8.26	149.62	126.42
15	B	606	CLA	CMD-C2D-C1D	8.23	139.22	124.71
15	A	403	CLA	CMD-C2D-C1D	8.19	139.14	124.71
15	B	602	CLA	CMD-C2D-C1D	8.12	139.03	124.71
15	D	406	CLA	CMD-C2D-C1D	8.10	138.99	124.71
15	C	511	CLA	CMD-C2D-C1D	8.06	138.92	124.71
15	C	502	CLA	CMD-C2D-C1D	8.06	138.91	124.71
15	A	405	CLA	CMD-C2D-C1D	8.04	138.88	124.71
15	C	505	CLA	CMD-C2D-C1D	8.04	138.88	124.71
15	D	405	CLA	CMD-C2D-C1D	8.03	138.86	124.71
15	C	514	CLA	CMD-C2D-C1D	8.00	138.81	124.71
15	B	610	CLA	CMD-C2D-C1D	7.97	138.77	124.71
15	D	402	CLA	CMD-C2D-C1D	7.97	138.76	124.71
15	A	402	CLA	CMD-C2D-C1D	7.96	138.74	124.71
15	B	604	CLA	CMD-C2D-C1D	7.95	138.73	124.71
15	C	510	CLA	CMD-C2D-C1D	7.95	138.72	124.71
15	C	508	CLA	CMD-C2D-C1D	7.94	138.72	124.71
15	C	509	CLA	CMD-C2D-C1D	7.94	138.71	124.71
15	B	615	CLA	CMD-C2D-C1D	7.90	138.63	124.71
15	B	607	CLA	CMD-C2D-C1D	7.89	138.61	124.71
15	C	512	CLA	CMD-C2D-C1D	7.87	138.57	124.71
15	B	603	CLA	CMD-C2D-C1D	7.86	138.57	124.71
15	C	507	CLA	CMD-C2D-C1D	7.82	138.49	124.71
15	B	614	CLA	CMD-C2D-C1D	7.79	138.44	124.71
15	B	609	CLA	CMD-C2D-C1D	7.66	138.21	124.71
15	B	605	CLA	CMD-C2D-C1D	7.63	138.17	124.71
15	B	616	CLA	CMD-C2D-C1D	7.62	138.15	124.71
17	B	617	BCR	C20-C19-C18	7.57	147.67	126.42
15	B	612	CLA	CMD-C2D-C1D	7.49	137.92	124.71
15	C	503	CLA	CMD-C2D-C1D	7.44	137.82	124.71
15	B	611	CLA	CMD-C2D-C1D	7.39	137.74	124.71
17	C	516	BCR	C20-C19-C18	7.38	147.15	126.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	B	608	CLA	CMD-C2D-C1D	7.28	137.55	124.71
15	D	405	CLA	C2D-C1D-ND	7.22	115.42	110.10
15	C	507	CLA	C2C-C1C-NC	7.16	116.68	109.97
15	C	513	CLA	CMD-C2D-C1D	7.08	137.20	124.71
15	C	513	CLA	C2D-C1D-ND	7.08	115.32	110.10
15	C	508	CLA	C2C-C1C-NC	7.06	116.58	109.97
15	B	604	CLA	C2C-C1C-NC	6.86	116.40	109.97
15	B	609	CLA	C2D-C1D-ND	6.84	115.15	110.10
15	B	613	CLA	C2C-C1C-NC	6.83	116.37	109.97
15	C	505	CLA	C2D-C1D-ND	6.82	115.13	110.10
15	A	405	CLA	C2C-C1C-NC	6.82	116.36	109.97
15	A	402	CLA	C2D-C1D-ND	6.80	115.11	110.10
15	B	616	CLA	C2D-C1D-ND	6.80	115.11	110.10
15	B	614	CLA	C2C-C1C-NC	6.78	116.32	109.97
17	C	519	BCR	C20-C19-C18	6.76	145.40	126.42
15	C	506	CLA	C2C-C1C-NC	6.74	116.28	109.97
17	X	102	BCR	C20-C19-C18	6.72	145.29	126.42
17	B	619	BCR	C20-C19-C18	6.71	145.26	126.42
15	D	402	CLA	C2C-C1C-NC	6.70	116.25	109.97
15	B	615	CLA	C2D-C1D-ND	6.69	115.03	110.10
15	C	512	CLA	C2D-C1D-ND	6.69	115.03	110.10
15	C	510	CLA	C2D-C1D-ND	6.68	115.03	110.10
15	B	610	CLA	C2C-C1C-NC	6.68	116.23	109.97
15	C	511	CLA	C2D-C1D-ND	6.66	115.01	110.10
15	C	512	CLA	C2C-C1C-NC	6.65	116.20	109.97
15	C	503	CLA	C2D-C1D-ND	6.65	115.00	110.10
15	B	605	CLA	C2D-C1D-ND	6.64	115.00	110.10
17	B	618	BCR	C20-C19-C18	6.60	144.96	126.42
15	B	608	CLA	C2D-C1D-ND	6.59	114.96	110.10
15	B	607	CLA	C2D-C1D-ND	6.58	114.95	110.10
15	B	615	CLA	C2C-C1C-NC	6.58	116.13	109.97
15	C	502	CLA	C2C-C1C-NC	6.57	116.12	109.97
15	C	506	CLA	O2D-CGD-CBD	6.54	122.90	111.27
15	C	503	CLA	C2C-C1C-NC	6.54	116.10	109.97
15	C	504	CLA	C2D-C1D-ND	6.54	114.92	110.10
15	B	603	CLA	C2C-C1C-NC	6.53	116.09	109.97
15	C	513	CLA	C2C-C1C-NC	6.50	116.06	109.97
17	C	515	BCR	C20-C19-C18	6.50	144.68	126.42
15	B	601	CLA	C2D-C1D-ND	6.50	114.89	110.10
15	C	510	CLA	C2C-C1C-NC	6.50	116.06	109.97
15	B	610	CLA	C2D-C1D-ND	6.48	114.88	110.10
15	C	511	CLA	C2C-C1C-NC	6.48	116.04	109.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	D	406	CLA	C2C-C1C-NC	6.47	116.03	109.97
15	B	601	CLA	C2C-C1C-NC	6.45	116.01	109.97
15	B	602	CLA	C2C-C1C-NC	6.45	116.01	109.97
15	B	608	CLA	C2C-C1C-NC	6.44	116.01	109.97
15	C	514	CLA	C2D-C1D-ND	6.43	114.84	110.10
15	B	613	CLA	C2D-C1D-ND	6.42	114.83	110.10
15	C	504	CLA	C2C-C1C-NC	6.39	115.96	109.97
15	A	405	CLA	C2D-C1D-ND	6.38	114.80	110.10
15	D	406	CLA	C2D-C1D-ND	6.37	114.80	110.10
15	B	602	CLA	C2D-C1D-ND	6.37	114.80	110.10
15	C	509	CLA	C2D-C1D-ND	6.36	114.79	110.10
15	C	508	CLA	C2D-C1D-ND	6.35	114.78	110.10
15	B	611	CLA	C2D-C1D-ND	6.34	114.77	110.10
15	A	403	CLA	C2D-C1D-ND	6.34	114.77	110.10
15	B	612	CLA	C2D-C1D-ND	6.34	114.77	110.10
17	A	406	BCR	C20-C19-C18	6.34	144.21	126.42
15	C	505	CLA	C2C-C1C-NC	6.32	115.89	109.97
15	B	607	CLA	C2C-C1C-NC	6.31	115.89	109.97
15	B	612	CLA	C2C-C1C-NC	6.31	115.88	109.97
15	B	609	CLA	C2C-C1C-NC	6.31	115.88	109.97
15	D	402	CLA	C2D-C1D-ND	6.31	114.75	110.10
15	B	614	CLA	C2D-C1D-ND	6.30	114.75	110.10
15	B	611	CLA	C2C-C1C-NC	6.29	115.87	109.97
15	A	403	CLA	C2C-C1C-NC	6.29	115.87	109.97
15	C	509	CLA	C2C-C1C-NC	6.29	115.86	109.97
15	C	502	CLA	C2D-C1D-ND	6.29	114.74	110.10
15	B	606	CLA	C2C-C1C-NC	6.26	115.83	109.97
15	B	605	CLA	C2C-C1C-NC	6.23	115.81	109.97
15	C	514	CLA	C2C-C1C-NC	6.21	115.79	109.97
15	D	405	CLA	C2C-C1C-NC	6.20	115.78	109.97
15	B	604	CLA	C2D-C1D-ND	6.18	114.66	110.10
15	B	616	CLA	O2D-CGD-CBD	6.11	122.12	111.27
15	C	507	CLA	C2D-C1D-ND	6.10	114.60	110.10
15	B	616	CLA	C2C-C1C-NC	6.09	115.68	109.97
15	A	402	CLA	C2C-C1C-NC	6.05	115.64	109.97
15	B	603	CLA	C2D-C1D-ND	6.03	114.55	110.10
15	B	614	CLA	C4A-NA-C1A	5.99	109.40	106.71
15	B	601	CLA	CHD-C1D-ND	-5.94	118.99	124.45
15	B	606	CLA	C2D-C1D-ND	5.93	114.47	110.10
15	B	605	CLA	O2D-CGD-CBD	5.93	121.81	111.27
15	C	509	CLA	O2A-C1-C2	5.91	124.17	108.64
15	C	508	CLA	C1C-C2C-C3C	-5.88	100.77	106.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	D	405	CLA	CHD-C1D-ND	-5.86	119.07	124.45
15	C	511	CLA	O2D-CGD-CBD	5.86	121.67	111.27
15	C	508	CLA	O2D-CGD-CBD	5.83	121.63	111.27
15	D	406	CLA	O2D-CGD-CBD	5.83	121.63	111.27
17	C	515	BCR	C24-C23-C22	-5.79	117.49	126.23
15	B	603	CLA	O2D-CGD-CBD	5.76	121.50	111.27
15	D	406	CLA	O2A-C1-C2	5.74	123.72	108.64
15	A	405	CLA	O2D-CGD-CBD	5.72	121.43	111.27
15	C	513	CLA	O2D-CGD-CBD	5.71	121.42	111.27
15	B	604	CLA	O2D-CGD-CBD	5.71	121.42	111.27
15	C	508	CLA	O2A-C1-C2	5.71	123.64	108.64
15	B	606	CLA	CHD-C1D-ND	-5.68	119.23	124.45
15	B	612	CLA	O2D-CGD-CBD	5.68	121.36	111.27
15	C	505	CLA	O2D-CGD-CBD	5.68	121.36	111.27
17	B	619	BCR	C24-C23-C22	-5.68	117.66	126.23
15	C	509	CLA	CHD-C1D-ND	-5.67	119.25	124.45
15	C	505	CLA	O2A-C1-C2	5.67	123.53	108.64
15	B	613	CLA	C1C-C2C-C3C	-5.65	101.02	106.96
15	C	507	CLA	O2A-C1-C2	5.59	123.32	108.64
15	D	402	CLA	C1C-C2C-C3C	-5.55	101.12	106.96
15	C	511	CLA	C1C-C2C-C3C	-5.52	101.15	106.96
15	C	504	CLA	O2A-C1-C2	5.52	123.14	108.64
15	D	402	CLA	CHD-C1D-ND	-5.51	119.39	124.45
15	D	406	CLA	CHD-C1D-ND	-5.50	119.39	124.45
15	B	601	CLA	O2A-C1-C2	5.49	123.08	108.64
15	C	502	CLA	C1C-C2C-C3C	-5.49	101.18	106.96
15	A	405	CLA	C1C-C2C-C3C	-5.49	101.18	106.96
15	D	405	CLA	C1C-C2C-C3C	-5.49	101.19	106.96
15	C	507	CLA	C1C-C2C-C3C	-5.48	101.19	106.96
15	C	507	CLA	O2D-CGD-CBD	5.48	121.00	111.27
15	B	602	CLA	O2A-C1-C2	5.48	123.03	108.64
15	A	403	CLA	CHD-C1D-ND	-5.47	119.43	124.45
15	B	610	CLA	O2D-CGD-CBD	5.47	120.98	111.27
15	D	406	CLA	C1C-C2C-C3C	-5.47	101.21	106.96
15	C	503	CLA	O2D-CGD-CBD	5.46	120.97	111.27
17	X	102	BCR	C7-C8-C9	-5.46	117.99	126.23
15	B	609	CLA	C1C-C2C-C3C	-5.45	101.22	106.96
19	A	408	PL9	C7-C3-C4	5.45	121.31	116.88
15	B	602	CLA	CHD-C1D-ND	-5.44	119.45	124.45
15	B	606	CLA	O2D-CGD-CBD	5.44	120.94	111.27
15	A	402	CLA	O2A-C1-C2	5.43	122.91	108.64
15	C	513	CLA	C1C-C2C-C3C	-5.43	101.25	106.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	C	512	CLA	C1C-C2C-C3C	-5.42	101.26	106.96
15	B	608	CLA	C1C-C2C-C3C	-5.42	101.26	106.96
17	C	519	BCR	C24-C23-C22	-5.41	118.06	126.23
15	C	502	CLA	CHD-C1D-ND	-5.39	119.50	124.45
15	C	504	CLA	CHD-C1D-ND	-5.39	119.50	124.45
15	B	615	CLA	C1C-C2C-C3C	-5.37	101.31	106.96
15	B	603	CLA	O2A-CGA-O1A	-5.36	110.06	123.59
15	B	604	CLA	C1C-C2C-C3C	-5.35	101.33	106.96
15	C	502	CLA	O2D-CGD-CBD	5.35	120.78	111.27
15	A	405	CLA	CHD-C1D-ND	-5.35	119.54	124.45
15	B	611	CLA	O2A-CGA-O1A	-5.34	110.12	123.59
15	C	506	CLA	C1C-C2C-C3C	-5.33	101.35	106.96
15	B	605	CLA	C1C-C2C-C3C	-5.33	101.36	106.96
15	B	609	CLA	O2A-CGA-O1A	-5.32	110.15	123.59
15	B	616	CLA	C3D-C2D-C1D	-5.32	98.57	105.83
15	C	503	CLA	O2A-C1-C2	5.32	122.61	108.64
15	B	601	CLA	C1C-C2C-C3C	-5.32	101.37	106.96
15	B	603	CLA	C1C-C2C-C3C	-5.31	101.37	106.96
15	B	605	CLA	CHD-C1D-ND	-5.30	119.58	124.45
15	C	510	CLA	CHD-C1D-ND	-5.30	119.58	124.45
15	B	603	CLA	CHD-C1D-ND	-5.30	119.58	124.45
15	B	612	CLA	C1C-C2C-C3C	-5.30	101.39	106.96
15	C	504	CLA	C3D-C2D-C1D	-5.30	98.60	105.83
15	B	602	CLA	O2D-CGD-CBD	5.29	120.67	111.27
15	C	505	CLA	CHD-C1D-ND	-5.29	119.59	124.45
15	B	609	CLA	CHD-C1D-ND	-5.29	119.59	124.45
15	B	610	CLA	C1C-C2C-C3C	-5.29	101.40	106.96
15	C	514	CLA	CHD-C1D-ND	-5.29	119.60	124.45
15	C	508	CLA	C3D-C2D-C1D	-5.28	98.63	105.83
15	B	602	CLA	C1C-C2C-C3C	-5.28	101.41	106.96
15	C	512	CLA	C4A-NA-C1A	5.26	109.07	106.71
15	B	614	CLA	C1C-C2C-C3C	-5.26	101.43	106.96
15	D	405	CLA	C3D-C2D-C1D	-5.26	98.66	105.83
15	B	615	CLA	CHD-C1D-ND	-5.25	119.63	124.45
15	C	506	CLA	C2D-C1D-ND	5.25	113.97	110.10
15	C	511	CLA	O2A-C1-C2	5.25	122.44	108.64
15	C	510	CLA	O2A-CGA-O1A	-5.25	110.34	123.59
15	C	505	CLA	C3D-C2D-C1D	-5.25	98.67	105.83
15	C	510	CLA	C1C-C2C-C3C	-5.25	101.44	106.96
15	B	616	CLA	C4A-NA-C1A	5.25	109.07	106.71
15	C	505	CLA	C1C-C2C-C3C	-5.25	101.44	106.96
15	C	510	CLA	C3D-C2D-C1D	-5.25	98.67	105.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	C	504	CLA	O2D-CGD-CBD	5.25	120.59	111.27
15	B	613	CLA	CHD-C1D-ND	-5.24	119.63	124.45
17	B	618	BCR	C7-C8-C9	-5.23	118.33	126.23
15	B	609	CLA	O2D-CGD-CBD	5.23	120.56	111.27
15	B	613	CLA	C3D-C2D-C1D	-5.22	98.70	105.83
15	B	611	CLA	CHD-C1D-ND	-5.21	119.67	124.45
15	C	512	CLA	C3D-C2D-C1D	-5.21	98.73	105.83
15	B	607	CLA	CHD-C1D-ND	-5.20	119.67	124.45
15	B	613	CLA	O2A-C1-C2	5.20	122.31	108.64
15	B	601	CLA	C3D-C2D-C1D	-5.20	98.73	105.83
15	C	511	CLA	CHD-C1D-ND	-5.20	119.68	124.45
15	A	403	CLA	C1C-C2C-C3C	-5.20	101.49	106.96
15	C	504	CLA	C1C-C2C-C3C	-5.19	101.50	106.96
15	B	615	CLA	O2D-CGD-CBD	5.18	120.48	111.27
15	B	615	CLA	O2A-C1-C2	5.18	122.25	108.64
15	B	611	CLA	O2A-C1-C2	5.18	122.25	108.64
15	B	610	CLA	O2A-CGA-O1A	-5.17	110.53	123.59
15	B	611	CLA	O2D-CGD-CBD	5.17	120.45	111.27
15	C	512	CLA	O2D-CGD-CBD	5.16	120.44	111.27
15	C	510	CLA	C4A-NA-C1A	5.16	109.03	106.71
17	X	102	BCR	C24-C23-C22	-5.16	118.44	126.23
15	B	607	CLA	O2D-CGD-CBD	5.16	120.44	111.27
15	D	405	CLA	C1D-ND-C4D	-5.16	102.67	106.33
15	B	615	CLA	C3D-C2D-C1D	-5.15	98.80	105.83
15	B	602	CLA	C3D-C2D-C1D	-5.15	98.80	105.83
15	C	511	CLA	C3D-C2D-C1D	-5.15	98.81	105.83
15	C	514	CLA	O2A-CGA-O1A	-5.15	110.61	123.59
15	B	606	CLA	C1C-C2C-C3C	-5.14	101.56	106.96
15	B	601	CLA	O2A-CGA-O1A	-5.13	110.64	123.59
15	B	607	CLA	C3D-C2D-C1D	-5.13	98.83	105.83
15	A	402	CLA	C3D-C2D-C1D	-5.12	98.84	105.83
15	C	503	CLA	C1C-C2C-C3C	-5.12	101.57	106.96
15	C	514	CLA	C1C-C2C-C3C	-5.11	101.58	106.96
15	B	607	CLA	C1C-C2C-C3C	-5.11	101.58	106.96
17	B	619	BCR	C7-C8-C9	-5.11	118.51	126.23
15	B	605	CLA	C3D-C2D-C1D	-5.11	98.86	105.83
15	A	402	CLA	C4A-NA-C1A	5.11	109.00	106.71
15	C	507	CLA	CHD-C1D-ND	-5.11	119.76	124.45
15	C	503	CLA	C3D-C2D-C1D	-5.11	98.86	105.83
15	C	509	CLA	C3D-C2D-C1D	-5.10	98.87	105.83
15	B	604	CLA	C4A-NA-C1A	5.10	109.00	106.71
15	A	403	CLA	C3D-C2D-C1D	-5.09	98.88	105.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	B	610	CLA	C3D-C2D-C1D	-5.09	98.88	105.83
15	B	609	CLA	C3D-C2D-C1D	-5.09	98.88	105.83
15	D	402	CLA	C3D-C2D-C1D	-5.09	98.89	105.83
15	A	405	CLA	C3D-C2D-C1D	-5.08	98.90	105.83
15	B	610	CLA	CHD-C1D-ND	-5.06	119.80	124.45
15	B	612	CLA	CHD-C1D-ND	-5.06	119.80	124.45
15	C	512	CLA	CHD-C1D-ND	-5.06	119.80	124.45
18	A	407	SQD	O5-C5-C4	5.06	118.88	109.69
15	B	609	CLA	C4A-NA-C1A	5.05	108.98	106.71
15	C	514	CLA	O2D-CGD-CBD	5.05	120.23	111.27
17	A	406	BCR	C24-C23-C22	-5.04	118.62	126.23
15	B	609	CLA	O2A-C1-C2	5.03	121.87	108.64
15	A	403	CLA	O2A-CGA-O1A	-5.03	110.89	123.59
15	C	507	CLA	C3D-C2D-C1D	-5.03	98.96	105.83
15	A	405	CLA	O2A-C1-C2	5.03	121.85	108.64
15	A	402	CLA	C1C-C2C-C3C	-5.03	101.67	106.96
15	C	514	CLA	C3D-C2D-C1D	-5.03	98.97	105.83
15	D	406	CLA	C3D-C2D-C1D	-5.02	98.98	105.83
15	C	511	CLA	O2A-CGA-O1A	-5.00	110.96	123.59
15	B	601	CLA	O2D-CGD-CBD	5.00	120.15	111.27
15	C	502	CLA	C3D-C2D-C1D	-4.99	99.02	105.83
15	B	602	CLA	O2A-CGA-O1A	-4.99	111.00	123.59
15	C	513	CLA	O2A-CGA-O1A	-4.98	111.03	123.59
15	B	616	CLA	O2A-CGA-O1A	-4.97	111.05	123.59
15	D	406	CLA	O2A-CGA-O1A	-4.97	111.05	123.59
15	C	513	CLA	C3D-C2D-C1D	-4.97	99.05	105.83
17	C	515	BCR	C7-C8-C9	-4.97	118.73	126.23
15	B	604	CLA	C3D-C2D-C1D	-4.96	99.06	105.83
15	B	614	CLA	C3D-C2D-C1D	-4.96	99.06	105.83
15	C	504	CLA	O2A-CGA-O1A	-4.96	111.08	123.59
15	C	513	CLA	C1D-ND-C4D	-4.96	102.81	106.33
15	B	613	CLA	O2A-CGA-O1A	-4.96	111.08	123.59
15	A	402	CLA	O2A-CGA-O1A	-4.96	111.09	123.59
15	B	613	CLA	O2D-CGD-CBD	4.95	120.07	111.27
15	B	606	CLA	C3D-C2D-C1D	-4.94	99.08	105.83
15	B	614	CLA	CHD-C1D-ND	-4.94	119.91	124.45
15	A	405	CLA	C4A-NA-C1A	4.94	108.93	106.71
15	B	611	CLA	C1C-C2C-C3C	-4.94	101.76	106.96
17	B	618	BCR	C24-C23-C22	-4.93	118.78	126.23
15	B	616	CLA	O2A-C1-C2	4.93	121.59	108.64
15	C	509	CLA	O2D-CGD-CBD	4.93	120.02	111.27
19	D	408	PL9	C7-C3-C4	4.92	120.88	116.88

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	C	502	CLA	O2A-CGA-O1A	-4.92	111.18	123.59
15	C	508	CLA	CHD-C1D-ND	-4.91	119.94	124.45
15	A	405	CLA	O2A-CGA-O1A	-4.91	111.19	123.59
15	B	608	CLA	O2D-CGD-CBD	4.91	120.00	111.27
15	C	503	CLA	CHD-C1D-ND	-4.91	119.94	124.45
15	C	513	CLA	CHD-C1D-ND	-4.89	119.96	124.45
15	B	611	CLA	C3D-C2D-C1D	-4.89	99.16	105.83
15	C	513	CLA	O2A-C1-C2	4.89	121.48	108.64
15	B	601	CLA	C1D-ND-C4D	-4.89	102.86	106.33
15	B	613	CLA	C4A-NA-C1A	4.89	108.90	106.71
15	B	608	CLA	O2A-CGA-O1A	-4.88	111.27	123.59
15	B	614	CLA	O2A-CGA-O1A	-4.88	111.27	123.59
15	C	503	CLA	O2A-CGA-O1A	-4.87	111.29	123.59
15	B	608	CLA	O2A-C1-C2	4.85	121.39	108.64
15	B	608	CLA	C3D-C2D-C1D	-4.85	99.21	105.83
15	C	505	CLA	O2A-CGA-O1A	-4.84	111.37	123.59
15	C	509	CLA	C1C-C2C-C3C	-4.84	101.87	106.96
18	B	620	SQD	O7-S-C6	4.84	112.69	106.94
15	C	506	CLA	C4A-NA-C1A	4.82	108.87	106.71
15	C	508	CLA	C4A-NA-C1A	4.82	108.87	106.71
15	C	509	CLA	O2A-CGA-O1A	-4.82	111.44	123.59
15	B	615	CLA	O2A-CGA-O1A	-4.81	111.45	123.59
15	A	403	CLA	O2D-CGD-CBD	4.81	119.81	111.27
15	B	607	CLA	C4A-NA-C1A	4.81	108.87	106.71
15	B	605	CLA	O2A-CGA-O1A	-4.80	111.47	123.59
15	B	606	CLA	O2A-CGA-O1A	-4.80	111.48	123.59
15	B	612	CLA	O2A-CGA-O1A	-4.79	111.49	123.59
20	B	621	LMG	O7-C10-C11	4.79	121.81	111.50
15	B	604	CLA	O2A-CGA-O1A	-4.78	111.52	123.59
15	B	615	CLA	C1D-ND-C4D	-4.78	102.94	106.33
15	C	505	CLA	C4A-NA-C1A	4.77	108.85	106.71
15	C	505	CLA	C1D-ND-C4D	-4.77	102.95	106.33
15	B	603	CLA	O2A-C1-C2	4.77	121.17	108.64
15	C	512	CLA	O2A-CGA-O1A	-4.77	111.42	123.30
15	A	402	CLA	CHD-C1D-ND	-4.77	120.08	124.45
15	A	403	CLA	C1D-ND-C4D	-4.76	102.95	106.33
15	C	511	CLA	C1D-ND-C4D	-4.76	102.96	106.33
15	D	405	CLA	O2A-C1-C2	4.73	121.07	108.64
15	A	402	CLA	C1D-ND-C4D	-4.73	102.97	106.33
15	D	406	CLA	C1D-ND-C4D	-4.73	102.97	106.33
15	C	506	CLA	O2A-CGA-O1A	-4.73	111.67	123.59
15	D	402	CLA	O2A-C1-C2	4.72	121.05	108.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	B	603	CLA	C3D-C2D-C1D	-4.72	99.39	105.83
15	B	612	CLA	C3D-C2D-C1D	-4.72	99.39	105.83
15	B	608	CLA	CHD-C1D-ND	-4.72	120.12	124.45
15	C	514	CLA	O2A-C1-C2	4.71	121.03	108.64
15	D	405	CLA	O2D-CGD-CBD	4.71	119.64	111.27
15	D	405	CLA	O2A-CGA-O1A	-4.71	111.71	123.59
15	B	605	CLA	O2A-C1-C2	4.70	120.98	108.64
15	B	610	CLA	C1D-ND-C4D	-4.70	103.00	106.33
15	B	614	CLA	O2D-CGD-CBD	4.70	119.61	111.27
15	B	608	CLA	C1D-ND-C4D	-4.69	103.01	106.33
15	D	402	CLA	C1D-ND-C4D	-4.68	103.01	106.33
15	A	403	CLA	O2A-C1-C2	4.67	120.92	108.64
15	C	507	CLA	O2A-CGA-O1A	-4.67	111.80	123.59
17	X	102	BCR	C38-C26-C25	-4.67	119.29	124.53
15	B	610	CLA	O2A-C1-C2	4.66	120.89	108.64
15	B	609	CLA	C1D-ND-C4D	-4.66	103.02	106.33
15	C	506	CLA	CHD-C1D-ND	-4.66	120.17	124.45
15	C	509	CLA	C4A-NA-C1A	4.65	108.80	106.71
15	B	601	CLA	C4A-NA-C1A	4.65	108.80	106.71
15	C	511	CLA	C4A-NA-C1A	4.65	108.80	106.71
15	B	608	CLA	C4A-NA-C1A	4.64	108.79	106.71
15	B	612	CLA	C4A-NA-C1A	4.64	108.79	106.71
15	C	507	CLA	C4A-NA-C1A	4.63	108.79	106.71
15	C	508	CLA	O2A-CGA-O1A	-4.62	111.92	123.59
15	B	604	CLA	CHD-C1D-ND	-4.61	120.22	124.45
15	C	504	CLA	C1D-ND-C4D	-4.60	103.06	106.33
15	D	402	CLA	C4A-NA-C1A	4.60	108.77	106.71
17	B	617	BCR	C38-C26-C25	-4.59	119.37	124.53
15	C	510	CLA	C1D-ND-C4D	-4.59	103.08	106.33
15	B	616	CLA	C1D-ND-C4D	-4.58	103.08	106.33
15	B	612	CLA	O2A-C1-C2	4.58	120.67	108.64
15	C	504	CLA	C4A-NA-C1A	4.58	108.77	106.71
15	C	510	CLA	O2D-CGD-CBD	4.57	119.39	111.27
17	C	516	BCR	C24-C23-C22	-4.55	119.36	126.23
15	D	406	CLA	C4A-NA-C1A	4.54	108.75	106.71
15	B	614	CLA	O2A-C1-C2	4.53	120.55	108.64
15	C	514	CLA	C1D-ND-C4D	-4.52	103.12	106.33
15	D	402	CLA	O2A-CGA-O1A	-4.50	112.23	123.59
15	C	509	CLA	C1D-ND-C4D	-4.49	103.15	106.33
17	D	407	BCR	C24-C23-C22	-4.49	119.45	126.23
15	D	405	CLA	C4A-NA-C1A	4.48	108.72	106.71
15	B	616	CLA	CHD-C1D-ND	-4.48	120.33	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	B	602	CLA	C1D-ND-C4D	-4.48	103.15	106.33
15	C	513	CLA	C4A-NA-C1A	4.48	108.72	106.71
15	C	502	CLA	C1D-ND-C4D	-4.48	103.15	106.33
17	D	407	BCR	C38-C26-C25	-4.48	119.50	124.53
15	B	605	CLA	C4A-NA-C1A	4.48	108.72	106.71
15	C	512	CLA	C1D-ND-C4D	-4.47	103.16	106.33
15	A	402	CLA	O2D-CGD-CBD	4.47	119.20	111.27
15	A	405	CLA	C1D-ND-C4D	-4.47	103.16	106.33
15	B	603	CLA	C4A-NA-C1A	4.46	108.71	106.71
15	C	503	CLA	C4A-NA-C1A	4.46	108.71	106.71
15	C	503	CLA	C1D-ND-C4D	-4.44	103.18	106.33
15	B	612	CLA	C1D-ND-C4D	-4.43	103.19	106.33
15	B	607	CLA	O2A-CGA-O1A	-4.42	112.44	123.59
15	B	605	CLA	C1D-ND-C4D	-4.41	103.20	106.33
17	C	516	BCR	C38-C26-C25	-4.41	119.57	124.53
15	B	609	CLA	O2A-CGA-CBA	4.41	125.75	111.91
15	B	613	CLA	C1D-ND-C4D	-4.39	103.22	106.33
15	B	603	CLA	O2A-CGA-CBA	4.38	125.66	111.91
15	C	506	CLA	C3D-C2D-C1D	-4.36	99.88	105.83
17	A	406	BCR	C38-C26-C25	-4.36	119.64	124.53
17	B	618	BCR	C33-C5-C6	-4.34	119.66	124.53
15	C	506	CLA	O2A-C1-C2	4.34	120.03	108.64
15	B	602	CLA	C4A-NA-C1A	4.33	108.65	106.71
15	A	402	CLA	O2A-CGA-CBA	4.33	125.48	111.91
15	B	611	CLA	C4A-NA-C1A	4.32	108.65	106.71
15	B	603	CLA	C1D-ND-C4D	-4.31	103.27	106.33
15	C	513	CLA	O2A-CGA-CBA	4.30	125.41	111.91
15	B	611	CLA	C1D-ND-C4D	-4.29	103.28	106.33
15	D	402	CLA	O2D-CGD-CBD	4.27	118.86	111.27
15	C	502	CLA	C4A-NA-C1A	4.27	108.63	106.71
15	B	607	CLA	C1D-ND-C4D	-4.26	103.31	106.33
17	C	519	BCR	C33-C5-C6	-4.25	119.75	124.53
17	C	519	BCR	C7-C8-C9	-4.21	119.88	126.23
18	X	101	SQD	O47-C7-C8	4.20	120.55	111.50
15	A	403	CLA	C4A-NA-C1A	4.18	108.58	106.71
18	X	101	SQD	C4-C3-C2	4.17	118.10	110.82
15	B	610	CLA	O2A-CGA-CBA	4.17	124.98	111.91
15	B	602	CLA	C1-C2-C3	-4.17	118.84	126.04
15	A	405	CLA	C1-C2-C3	-4.15	120.04	126.75
15	B	601	CLA	O2A-CGA-CBA	4.15	124.92	111.91
15	C	511	CLA	O2A-CGA-CBA	4.14	124.89	111.91
15	B	614	CLA	C1D-ND-C4D	-4.13	103.40	106.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	D	402	CLA	C1-C2-C3	-4.12	118.91	126.04
18	A	407	SQD	O7-S-C6	4.12	111.83	106.94
15	B	616	CLA	C1C-C2C-C3C	-4.12	102.63	106.96
15	B	611	CLA	O2A-CGA-CBA	4.11	124.81	111.91
15	B	615	CLA	C4A-NA-C1A	4.11	108.55	106.71
17	A	406	BCR	C33-C5-C6	-4.09	119.93	124.53
20	C	501	LMG	O7-C10-C11	4.09	120.32	111.50
15	B	606	CLA	C1D-ND-C4D	-4.09	103.43	106.33
15	D	406	CLA	O2A-CGA-CBA	4.08	124.72	111.91
15	B	616	CLA	O2A-CGA-CBA	4.08	124.70	111.91
15	C	514	CLA	O2A-CGA-CBA	4.06	124.66	111.91
15	C	511	CLA	C1-C2-C3	-4.05	119.03	126.04
15	C	507	CLA	C1D-ND-C4D	-4.04	103.47	106.33
18	A	407	SQD	C1-O5-C5	4.03	121.59	113.69
18	A	407	SQD	O9-S-C6	4.02	111.72	106.94
18	X	101	SQD	O7-S-C6	4.02	111.72	106.94
15	C	514	CLA	C4A-NA-C1A	4.02	108.51	106.71
15	B	613	CLA	C1-C2-C3	-4.01	119.10	126.04
25	D	410	LHG	O7-C7-C8	4.01	120.15	111.50
17	X	102	BCR	C33-C5-C6	-4.01	120.03	124.53
15	B	604	CLA	O2A-C1-C2	4.01	119.17	108.64
18	C	518	SQD	O9-S-C6	4.00	111.70	106.94
15	B	614	CLA	O2A-CGA-CBA	3.99	124.43	111.91
15	C	510	CLA	O2A-CGA-CBA	3.99	124.42	111.91
15	B	610	CLA	C4A-NA-C1A	3.99	108.50	106.71
15	C	508	CLA	C1D-ND-C4D	-3.99	103.50	106.33
15	B	604	CLA	C1D-ND-C4D	-3.98	103.51	106.33
15	C	510	CLA	O2A-C1-C2	3.97	119.06	108.64
15	A	403	CLA	O2A-CGA-CBA	3.96	124.33	111.91
18	T	101	SQD	O7-S-C6	3.95	111.63	106.94
17	C	515	BCR	C38-C26-C25	-3.95	120.10	124.53
22	H	101	DGD	O2G-C1B-C2B	3.92	119.96	111.50
15	C	503	CLA	C1-C2-C3	-3.92	119.26	126.04
15	B	612	CLA	CMB-C2B-C3B	3.92	132.01	124.68
15	B	612	CLA	O2A-CGA-CBA	3.90	124.15	111.91
17	B	617	BCR	C33-C5-C6	-3.90	120.15	124.53
15	B	613	CLA	O2A-CGA-CBA	3.90	124.14	111.91
15	B	602	CLA	O2A-CGA-CBA	3.89	124.11	111.91
15	A	405	CLA	O2A-CGA-CBA	3.88	124.10	111.91
17	B	617	BCR	C24-C23-C22	-3.88	120.37	126.23
15	B	607	CLA	O2A-C1-C2	3.88	118.83	108.64
15	C	504	CLA	O2A-CGA-CBA	3.88	124.09	111.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B	619	BCR	C33-C5-C6	-3.87	120.18	124.53
15	B	606	CLA	CMB-C2B-C3B	3.87	131.93	124.68
15	C	508	CLA	O2A-CGA-CBA	3.87	124.06	111.91
18	T	103	SQD	O9-S-C6	3.86	111.53	106.94
25	D	411	LHG	O7-C7-C8	3.85	119.81	111.50
15	C	507	CLA	O2A-CGA-CBA	3.85	124.00	111.91
15	C	505	CLA	O2A-CGA-CBA	3.84	123.97	111.91
20	D	412	LMG	O7-C10-C11	3.84	119.78	111.50
15	C	506	CLA	C1D-ND-C4D	-3.84	103.61	106.33
17	B	617	BCR	C36-C18-C17	-3.83	117.56	122.92
15	C	509	CLA	O2A-CGA-CBA	3.83	123.93	111.91
18	C	518	SQD	O9-S-O7	-3.83	100.70	113.95
17	X	102	BCR	C15-C14-C13	-3.82	121.86	127.31
18	B	620	SQD	O9-S-O7	-3.82	100.73	113.95
25	D	409	LHG	O7-C7-C8	3.82	119.72	111.50
18	T	103	SQD	O7-S-C6	3.80	111.46	106.94
15	B	606	CLA	C4A-NA-C1A	3.80	108.42	106.71
15	D	406	CLA	C1-C2-C3	-3.79	119.48	126.04
15	B	603	CLA	CMB-C2B-C3B	3.79	131.76	124.68
17	D	407	BCR	C7-C8-C9	-3.78	120.52	126.23
18	A	409	SQD	O8-S-C6	3.78	111.76	105.74
15	C	503	CLA	O2A-CGA-CBA	3.76	123.71	111.91
18	A	409	SQD	O9-S-C6	3.75	111.39	106.94
15	B	605	CLA	CMB-C2B-C3B	3.74	131.67	124.68
18	A	409	SQD	O9-S-O7	-3.73	101.03	113.95
18	T	101	SQD	O9-S-O7	-3.72	101.06	113.95
15	B	604	CLA	O2A-CGA-CBA	3.72	123.59	111.91
15	D	402	CLA	O2A-CGA-CBA	3.72	123.58	111.91
15	B	604	CLA	CMA-C3A-C4A	3.71	121.75	111.77
15	B	611	CLA	C1-C2-C3	-3.71	119.63	126.04
15	D	405	CLA	O2A-CGA-CBA	3.71	123.54	111.91
25	L	101	LHG	O7-C7-C8	3.70	119.47	111.50
18	T	103	SQD	O9-S-O7	-3.69	101.16	113.95
17	C	516	BCR	C33-C5-C6	-3.69	120.38	124.53
15	B	608	CLA	CMB-C2B-C3B	3.68	131.56	124.68
15	D	406	CLA	CMB-C2B-C3B	3.67	131.54	124.68
18	X	101	SQD	O9-S-C6	3.66	111.29	106.94
18	A	407	SQD	O9-S-O7	-3.65	101.32	113.95
15	B	605	CLA	C1-C2-C3	-3.65	119.73	126.04
15	B	605	CLA	O2A-CGA-CBA	3.65	123.35	111.91
15	C	507	CLA	C1-C2-C3	-3.64	119.74	126.04
15	B	608	CLA	O2A-CGA-CBA	3.64	123.32	111.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	406	BCR	C7-C8-C9	-3.63	120.75	126.23
21	B	622	LMT	O5'-C5'-C4'	3.63	117.40	109.75
18	T	101	SQD	O47-C7-C8	3.61	119.29	111.50
17	B	619	BCR	C36-C18-C17	-3.58	117.90	122.92
17	C	516	BCR	C7-C8-C9	-3.58	120.82	126.23
15	B	608	CLA	C1-C2-C3	-3.58	119.85	126.04
18	C	518	SQD	O47-C7-C8	3.58	119.22	111.50
15	A	405	CLA	CMB-C2B-C3B	3.58	131.37	124.68
18	X	101	SQD	O9-S-O7	-3.58	101.57	113.95
17	C	515	BCR	C36-C18-C17	-3.57	117.92	122.92
18	B	620	SQD	O47-C7-C8	3.56	119.18	111.50
15	B	615	CLA	O2A-CGA-CBA	3.56	123.07	111.91
15	B	606	CLA	O2A-CGA-CBA	3.55	123.06	111.91
15	C	502	CLA	O2A-CGA-CBA	3.55	123.06	111.91
15	C	506	CLA	O2A-CGA-CBA	3.55	123.05	111.91
15	C	506	CLA	C1-C2-C3	-3.54	119.91	126.04
17	C	515	BCR	C19-C18-C17	3.54	124.37	118.94
15	C	509	CLA	CMB-C2B-C3B	3.54	131.30	124.68
18	T	101	SQD	O9-S-C6	3.54	111.14	106.94
15	D	402	CLA	CMB-C2B-C3B	3.53	131.28	124.68
15	B	606	CLA	O2A-C1-C2	3.52	117.90	108.64
15	D	405	CLA	CMB-C2B-C3B	3.52	131.27	124.68
15	B	611	CLA	CMB-C2B-C3B	3.50	131.23	124.68
18	T	103	SQD	O5-C5-C4	3.49	116.04	109.69
18	A	409	SQD	C44-O6-C1	3.48	120.55	113.74
17	C	515	BCR	C33-C5-C6	-3.48	120.62	124.53
17	B	619	BCR	C19-C18-C17	3.48	124.28	118.94
15	A	402	CLA	CMC-C2C-C1C	3.47	130.33	125.04
15	B	607	CLA	O2A-CGA-CBA	3.46	122.77	111.91
18	C	518	SQD	O8-S-C6	3.45	111.23	105.74
19	A	408	PL9	C7-C3-C2	-3.43	118.79	123.30
16	D	403	PHO	CMB-C2B-C3B	3.41	131.07	124.68
15	A	402	CLA	CMB-C2B-C3B	3.39	131.02	124.68
18	X	101	SQD	C1-C2-C3	3.37	117.01	110.00
15	B	607	CLA	CMB-C2B-C3B	3.37	130.97	124.68
15	B	615	CLA	CMB-C2B-C3B	3.36	130.96	124.68
15	D	405	CLA	C1-C2-C3	-3.35	120.24	126.04
15	C	512	CLA	CMA-C3A-C4A	3.35	120.78	111.77
15	B	602	CLA	CMB-C2B-C3B	3.34	130.92	124.68
17	C	519	BCR	C28-C27-C26	-3.34	108.12	114.08
15	B	601	CLA	C1-C2-C3	-3.34	120.27	126.04
18	A	407	SQD	O47-C7-C8	3.33	118.69	111.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	C	506	CLA	CMB-C2B-C3B	3.33	130.91	124.68
19	D	408	PL9	C7-C3-C2	-3.33	118.92	123.30
15	C	505	CLA	C1-C2-C3	-3.32	120.30	126.04
15	B	610	CLA	C1-C2-C3	-3.32	120.30	126.04
17	X	102	BCR	C36-C18-C17	-3.31	118.28	122.92
15	B	604	CLA	C4-C3-C5	3.31	120.84	115.27
15	C	512	CLA	CMB-C2B-C3B	3.31	130.86	124.68
18	C	518	SQD	O7-S-C6	3.31	110.87	106.94
15	C	514	CLA	CMB-C2B-C3B	3.29	130.83	124.68
15	C	504	CLA	C1-C2-C3	-3.29	120.36	126.04
17	D	407	BCR	C33-C5-C6	-3.27	120.85	124.53
18	T	103	SQD	C4-C3-C2	3.26	116.52	110.82
25	D	410	LHG	C5-O7-C7	-3.26	109.78	117.79
15	C	503	CLA	CMB-C2B-C3B	3.25	130.77	124.68
15	A	405	CLA	CMA-C3A-C4A	3.25	120.50	111.77
15	C	502	CLA	O2A-C1-C2	3.24	117.14	108.64
18	T	103	SQD	O47-C7-C8	3.23	118.47	111.50
15	C	510	CLA	CMB-C2B-C3B	3.22	130.70	124.68
22	C	517	DGD	O2G-C1B-C2B	3.21	118.43	111.50
15	C	504	CLA	CMB-C2B-C3B	3.21	130.68	124.68
15	B	609	CLA	CMB-C2B-C3B	3.21	130.68	124.68
17	C	519	BCR	C38-C26-C25	-3.20	120.93	124.53
17	D	407	BCR	C3-C4-C5	-3.19	108.38	114.08
15	C	511	CLA	CMB-C2B-C3B	3.19	130.64	124.68
15	B	616	CLA	C1-C2-C3	-3.19	121.60	126.75
15	A	403	CLA	C1-C2-C3	-3.17	120.56	126.04
15	B	601	CLA	CMD-C2D-C3D	-3.16	120.33	127.61
17	D	407	BCR	C36-C18-C17	-3.16	118.49	122.92
15	C	506	CLA	O2D-CGD-O1D	-3.16	117.66	123.84
17	B	618	BCR	C36-C18-C17	-3.16	118.50	122.92
15	D	405	CLA	C4-C3-C5	3.16	120.58	115.27
15	C	504	CLA	CMA-C3A-C4A	3.15	120.24	111.77
15	C	514	CLA	C1-C2-C3	-3.15	120.59	126.04
15	B	616	CLA	CMB-C2B-C3B	3.15	130.57	124.68
15	C	506	CLA	CMD-C2D-C3D	-3.15	120.38	127.61
15	A	403	CLA	CMA-C3A-C4A	3.14	120.21	111.77
15	B	604	CLA	O2D-CGD-O1D	-3.12	117.73	123.84
15	B	614	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
15	C	512	CLA	O2A-CGA-CBA	3.10	123.99	114.03
15	C	508	CLA	C4-C3-C5	3.10	120.48	115.27
15	B	609	CLA	C1-C2-C3	-3.10	120.68	126.04
18	A	407	SQD	O6-C1-C2	3.09	113.12	108.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	409	SQD	O47-C7-C8	3.07	118.11	111.50
24	D	404	BCT	O2-C-O1	-3.07	111.59	119.55
15	D	406	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
15	C	505	CLA	CMB-C2B-C3B	3.05	130.39	124.68
18	C	518	SQD	C4-C3-C2	3.05	116.15	110.82
15	A	403	CLA	CMB-C2B-C3B	3.05	130.38	124.68
15	B	612	CLA	C1-C2-C3	-3.05	120.77	126.04
18	A	407	SQD	C3-C4-C5	3.05	115.67	110.24
18	B	620	SQD	O9-S-C6	3.05	110.56	106.94
17	B	619	BCR	C38-C26-C25	-3.04	121.11	124.53
15	B	607	CLA	C4-C3-C5	3.04	120.39	115.27
17	C	516	BCR	C36-C18-C17	-3.04	118.66	122.92
15	C	508	CLA	CMC-C2C-C1C	3.04	129.67	125.04
15	C	509	CLA	C1-C2-C3	-3.04	120.79	126.04
17	C	519	BCR	C34-C9-C10	-3.03	118.68	122.92
17	A	406	BCR	C19-C18-C17	3.02	123.57	118.94
17	X	102	BCR	C34-C9-C10	-3.01	118.70	122.92
15	C	508	CLA	CMB-C2B-C3B	3.01	130.31	124.68
18	X	101	SQD	O6-C1-C2	3.01	113.00	108.30
17	B	619	BCR	C15-C14-C13	-3.01	123.01	127.31
15	C	509	CLA	CAA-C2A-C3A	-3.01	104.54	112.78
17	B	617	BCR	C19-C18-C17	3.00	123.55	118.94
15	B	615	CLA	CMC-C2C-C1C	3.00	129.60	125.04
15	B	613	CLA	CMB-C2B-C3B	2.99	130.28	124.68
17	C	516	BCR	C33-C5-C4	2.99	119.36	113.62
18	A	409	SQD	O7-S-C6	2.99	110.49	106.94
15	B	612	CLA	CMC-C2C-C1C	2.98	129.58	125.04
15	C	509	CLA	CMA-C3A-C4A	2.98	119.79	111.77
25	L	101	LHG	O8-C23-C24	2.98	121.25	111.91
15	C	502	CLA	CMC-C2C-C1C	2.98	129.57	125.04
18	T	103	SQD	C44-O6-C1	2.97	119.54	113.74
15	C	508	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
17	B	617	BCR	C7-C8-C9	-2.96	121.76	126.23
15	B	605	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
15	B	608	CLA	C4-C3-C5	2.96	120.25	115.27
17	B	619	BCR	C34-C9-C10	-2.96	118.78	122.92
15	D	402	CLA	C3D-C4D-ND	2.95	115.02	110.24
15	C	502	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
15	B	606	CLA	CAA-C2A-C3A	-2.95	104.71	112.78
15	B	605	CLA	CMC-C2C-C1C	2.95	129.53	125.04
15	B	608	CLA	CMA-C3A-C4A	2.94	119.69	111.77
15	B	604	CLA	C1-C2-C3	-2.94	120.96	126.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	C	502	CLA	C4-C3-C5	2.94	120.22	115.27
17	C	516	BCR	C3-C4-C5	-2.93	108.84	114.08
15	B	610	CLA	CMB-C2B-C3B	2.93	130.16	124.68
15	A	405	CLA	O2D-CGD-O1D	-2.93	118.12	123.84
15	B	604	CLA	CMB-C2B-C3B	2.92	130.14	124.68
15	C	506	CLA	C4D-C3D-CAD	2.92	111.53	108.10
15	C	505	CLA	CMC-C2C-C1C	2.92	129.48	125.04
16	A	404	PHO	O1D-CGD-CBD	2.91	129.59	124.74
15	B	612	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
15	C	512	CLA	CMC-C2C-C1C	2.91	129.47	125.04
18	B	620	SQD	O8-S-C6	2.91	110.37	105.74
15	C	514	CLA	CMC-C2C-C1C	2.90	129.46	125.04
17	B	617	BCR	C37-C22-C21	-2.90	118.86	122.92
17	B	618	BCR	C19-C18-C17	2.90	123.39	118.94
15	B	609	CLA	CMC-C2C-C1C	2.89	129.44	125.04
15	B	601	CLA	CMC-C2C-C1C	2.89	129.44	125.04
16	D	403	PHO	O1D-CGD-CBD	2.89	129.54	124.74
15	D	405	CLA	C3D-C4D-ND	2.88	114.90	110.24
18	T	101	SQD	O8-S-C6	2.88	110.33	105.74
15	C	513	CLA	CMC-C2C-C1C	2.88	129.43	125.04
17	X	102	BCR	C33-C5-C4	2.88	119.15	113.62
15	D	402	CLA	CMA-C3A-C4A	2.88	119.51	111.77
15	B	601	CLA	CMA-C3A-C4A	2.88	119.51	111.77
15	B	614	CLA	C4-C3-C5	2.88	120.11	115.27
15	C	509	CLA	C3D-C4D-ND	2.87	114.89	110.24
15	B	611	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
15	C	503	CLA	CMA-C3A-C4A	2.87	119.50	111.77
16	A	404	PHO	O2D-CGD-O1D	-2.87	118.22	123.84
15	C	507	CLA	CMB-C2B-C3B	2.87	130.05	124.68
15	B	607	CLA	CAA-C2A-C3A	-2.87	104.92	112.78
18	X	101	SQD	O48-C23-C24	2.87	120.90	111.91
15	D	406	CLA	C3D-C4D-ND	2.87	114.87	110.24
15	C	513	CLA	C1-C2-C3	-2.87	121.09	126.04
15	B	608	CLA	C3D-C4D-ND	2.86	114.87	110.24
15	B	608	CLA	CMC-C2C-C1C	2.86	129.40	125.04
16	A	404	PHO	CMB-C2B-C3B	2.86	130.03	124.68
17	D	407	BCR	C38-C26-C27	2.86	119.11	113.62
17	X	102	BCR	C38-C26-C27	2.86	119.10	113.62
15	B	611	CLA	CAC-C3C-C4C	2.85	128.51	124.81
15	B	613	CLA	CMC-C2C-C1C	2.85	129.38	125.04
15	C	506	CLA	CMC-C2C-C1C	2.85	129.38	125.04
22	H	101	DGD	O1G-C1A-C2A	2.85	120.84	111.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	A	403	CLA	C3D-C4D-ND	2.84	114.84	110.24
18	T	101	SQD	O6-C1-C2	2.84	112.74	108.30
15	B	610	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
15	B	604	CLA	C3C-C4C-NC	2.84	113.76	110.57
15	B	607	CLA	CMA-C3A-C4A	2.84	119.41	111.77
15	B	612	CLA	C4-C3-C5	2.84	120.05	115.27
15	C	508	CLA	CBC-CAC-C3C	-2.83	104.62	112.43
15	B	614	CLA	CMB-C2B-C3B	2.83	129.98	124.68
15	C	505	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
15	B	610	CLA	C4-C3-C5	2.83	120.03	115.27
15	C	511	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
15	B	601	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
15	D	405	CLA	CMC-C2C-C1C	2.82	129.34	125.04
15	C	513	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
18	T	101	SQD	C4-C3-C2	2.82	115.74	110.82
19	D	408	PL9	C40-C39-C41	2.81	120.00	115.27
15	C	513	CLA	C3D-C4D-ND	2.81	114.78	110.24
15	D	402	CLA	CAA-C2A-C3A	-2.81	105.09	112.78
15	C	513	CLA	C4-C3-C5	2.80	119.99	115.27
15	B	610	CLA	CMA-C3A-C4A	2.80	119.29	111.77
15	B	616	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
17	C	519	BCR	C36-C18-C17	-2.79	119.01	122.92
15	B	606	CLA	C1-O2A-CGA	2.79	123.77	116.44
19	D	408	PL9	C22-C23-C24	-2.79	120.94	127.66
15	B	612	CLA	C3D-C4D-ND	2.79	114.74	110.24
15	B	614	CLA	CMC-C2C-C1C	2.78	129.28	125.04
15	B	603	CLA	C4-C3-C5	2.78	119.95	115.27
15	B	605	CLA	C4-C3-C5	2.78	119.95	115.27
15	A	405	CLA	C3D-C4D-ND	2.78	114.73	110.24
17	X	102	BCR	C19-C18-C17	2.77	123.20	118.94
15	B	602	CLA	C3D-C4D-ND	2.77	114.73	110.24
15	B	602	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
15	B	611	CLA	C3D-C4D-ND	2.77	114.72	110.24
15	C	510	CLA	C4-C3-C5	2.77	119.92	115.27
16	D	403	PHO	O2D-CGD-O1D	-2.77	118.43	123.84
17	A	406	BCR	C36-C18-C17	-2.76	119.06	122.92
15	B	602	CLA	C4-C3-C5	2.76	119.91	115.27
15	B	603	CLA	CMA-C3A-C4A	2.76	119.19	111.77
15	B	603	CLA	C3D-C4D-ND	2.76	114.70	110.24
18	T	103	SQD	O8-S-C6	2.76	110.13	105.74
15	B	610	CLA	C3D-C4D-ND	2.75	114.69	110.24
15	A	402	CLA	CAC-C3C-C4C	2.75	128.38	124.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	C	508	CLA	CMA-C3A-C4A	2.75	119.16	111.77
20	D	412	LMG	C8-O7-C10	-2.74	111.04	117.79
17	B	619	BCR	C37-C22-C21	-2.74	119.08	122.92
15	C	503	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
15	C	511	CLA	CMC-C2C-C1C	2.73	129.20	125.04
15	C	513	CLA	C3C-C4C-NC	2.73	113.64	110.57
15	C	514	CLA	C3D-C4D-ND	2.73	114.65	110.24
15	B	616	CLA	C3C-C4C-NC	2.72	113.63	110.57
20	B	621	LMG	C8-O7-C10	-2.72	111.09	117.79
15	C	506	CLA	C4-C3-C5	2.72	119.84	115.27
15	C	512	CLA	C3C-C4C-NC	2.72	113.62	110.57
15	C	511	CLA	C3D-C4D-ND	2.71	114.63	110.24
15	C	509	CLA	C4-C3-C5	2.71	119.83	115.27
18	T	101	SQD	O5-C5-C4	2.71	114.62	109.69
15	C	507	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
15	A	403	CLA	C4-C3-C5	2.71	119.83	115.27
15	B	609	CLA	C3D-C4D-ND	2.71	114.62	110.24
15	C	508	CLA	C1-O2A-CGA	2.70	123.54	116.44
15	A	403	CLA	CMC-C2C-C1C	2.70	129.16	125.04
15	D	406	CLA	CMC-C2C-C1C	2.70	129.16	125.04
15	B	601	CLA	C3C-C4C-NC	2.70	113.60	110.57
15	C	504	CLA	CMC-C2C-C1C	2.70	129.16	125.04
15	B	615	CLA	C3D-C4D-ND	2.70	114.60	110.24
15	C	502	CLA	C1-O2A-CGA	2.70	123.52	116.44
15	B	602	CLA	CMC-C2C-C1C	2.70	129.15	125.04
15	C	502	CLA	C3D-C4D-ND	2.69	114.60	110.24
15	B	607	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
15	B	613	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
21	B	623	LMT	C1'-O5'-C5'	-2.69	108.42	113.69
15	C	505	CLA	C3D-C4D-ND	2.68	114.58	110.24
15	C	504	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
15	B	606	CLA	C3D-C4D-ND	2.67	114.56	110.24
15	B	606	CLA	CMC-C2C-C1C	2.67	129.11	125.04
15	C	504	CLA	C3D-C4D-ND	2.67	114.56	110.24
15	C	509	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
15	C	510	CLA	C3D-C4D-ND	2.66	114.55	110.24
15	B	615	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
15	C	503	CLA	C3D-C4D-ND	2.66	114.55	110.24
15	B	603	CLA	CMC-C2C-C1C	2.66	129.09	125.04
17	A	406	BCR	C37-C22-C21	-2.66	119.20	122.92
18	A	407	SQD	O8-S-C6	2.65	109.97	105.74
19	D	408	PL9	C27-C28-C29	-2.65	121.27	127.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	D	406	CLA	CMA-C3A-C4A	2.65	118.90	111.77
15	B	606	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
15	B	601	CLA	C4-C3-C5	2.65	119.73	115.27
15	D	406	CLA	CAA-C2A-C3A	-2.65	105.52	112.78
25	D	409	LHG	O8-C23-C24	2.65	120.23	111.91
17	D	407	BCR	C34-C9-C10	-2.65	119.21	122.92
17	B	618	BCR	C38-C26-C25	-2.64	121.56	124.53
15	B	601	CLA	C3D-C4D-ND	2.64	114.51	110.24
20	C	501	LMG	O8-C28-C29	2.63	120.17	111.91
15	B	605	CLA	C3D-C4D-ND	2.63	114.49	110.24
15	C	512	CLA	C3D-C4D-ND	2.63	114.48	110.24
15	C	514	CLA	CMA-C3A-C4A	2.62	118.83	111.77
15	B	608	CLA	C3C-C4C-NC	2.62	113.51	110.57
15	B	610	CLA	CMC-C2C-C1C	2.62	129.02	125.04
15	C	502	CLA	CMB-C2B-C3B	2.62	129.57	124.68
15	A	405	CLA	CMC-C2C-C1C	2.61	129.02	125.04
15	B	610	CLA	C3C-C4C-NC	2.61	113.49	110.57
17	X	102	BCR	C37-C22-C21	-2.60	119.28	122.92
15	B	612	CLA	C3C-C4C-NC	2.59	113.48	110.57
15	B	614	CLA	C3C-C4C-NC	2.59	113.48	110.57
15	C	506	CLA	C3C-C4C-NC	2.59	113.48	110.57
15	B	603	CLA	C1-C2-C3	-2.59	121.56	126.04
15	C	514	CLA	C4-C3-C5	2.59	119.63	115.27
16	A	404	PHO	C1-C2-C3	-2.59	121.57	126.04
26	E	101	HEM	C4D-ND-C1D	2.59	107.74	105.07
15	C	505	CLA	CMA-C3A-C4A	2.59	118.72	111.77
15	B	603	CLA	O2D-CGD-O1D	-2.58	118.78	123.84
17	C	519	BCR	C37-C22-C21	-2.58	119.30	122.92
15	B	614	CLA	C4D-C3D-CAD	2.58	111.14	108.10
17	A	406	BCR	C35-C13-C12	2.58	122.14	118.08
15	C	507	CLA	CMA-C3A-C4A	2.58	118.70	111.77
15	D	405	CLA	C3C-C4C-NC	2.58	113.46	110.57
15	C	514	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
15	C	506	CLA	C3D-C4D-ND	2.57	114.40	110.24
15	B	606	CLA	CMD-C2D-C3D	-2.57	121.70	127.61
18	A	409	SQD	O48-C23-C24	2.57	119.98	111.91
15	C	507	CLA	C3D-C4D-ND	2.57	114.39	110.24
15	B	601	CLA	C4D-C3D-CAD	2.57	111.12	108.10
18	C	518	SQD	O48-C23-C24	2.56	119.96	111.91
15	A	402	CLA	C3D-C4D-ND	2.56	114.38	110.24
17	C	519	BCR	C3-C4-C5	-2.55	109.52	114.08
15	C	510	CLA	C3C-C4C-NC	2.55	113.44	110.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	C	503	CLA	C3C-C4C-NC	2.55	113.43	110.57
18	X	101	SQD	O8-S-C6	2.55	109.81	105.74
15	B	601	CLA	CMB-C2B-C3B	2.55	129.45	124.68
15	B	607	CLA	CMC-C2C-C1C	2.55	128.92	125.04
15	B	611	CLA	C4-C3-C5	2.55	119.56	115.27
18	C	518	SQD	C44-O6-C1	2.55	118.72	113.74
15	B	614	CLA	C1-C2-C3	-2.55	121.64	126.04
15	C	511	CLA	C4-C3-C5	2.55	119.55	115.27
15	B	603	CLA	C3C-C4C-NC	2.55	113.43	110.57
15	C	511	CLA	C3C-C4C-NC	2.55	113.43	110.57
15	A	402	CLA	C3C-C4C-NC	2.54	113.42	110.57
18	B	620	SQD	O6-C1-C2	2.53	112.26	108.30
15	C	502	CLA	CMA-C3A-C4A	2.53	118.58	111.77
17	B	618	BCR	C15-C14-C13	-2.53	123.70	127.31
15	B	602	CLA	CMA-C3A-C4A	2.53	118.57	111.77
17	C	515	BCR	C3-C4-C5	-2.52	109.57	114.08
15	B	607	CLA	C3C-C4C-NC	2.52	113.40	110.57
15	C	510	CLA	CMC-C2C-C1C	2.52	128.88	125.04
25	D	411	LHG	O8-C23-C24	2.52	119.81	111.91
15	B	608	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
15	B	609	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
15	A	403	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
17	C	515	BCR	C34-C9-C10	-2.51	119.41	122.92
15	D	405	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
15	B	616	CLA	C3D-C4D-ND	2.51	114.29	110.24
21	B	623	LMT	O1'-C1'-C2'	2.50	112.21	108.30
15	B	614	CLA	CAC-C3C-C4C	2.50	128.06	124.81
17	C	515	BCR	C15-C14-C13	-2.50	123.74	127.31
15	B	610	CLA	C4D-C3D-CAD	2.50	111.04	108.10
15	C	504	CLA	C3C-C4C-NC	2.50	113.38	110.57
17	A	406	BCR	C38-C26-C27	2.50	118.42	113.62
15	B	615	CLA	C3C-C4C-NC	2.50	113.37	110.57
25	D	410	LHG	O8-C23-C24	2.49	119.74	111.91
15	B	616	CLA	C4C-C3C-C2C	-2.49	103.27	106.90
15	B	609	CLA	C4-C3-C5	2.49	119.46	115.27
15	A	402	CLA	CMA-C3A-C4A	2.49	118.46	111.77
15	C	513	CLA	CMA-C3A-C4A	2.49	118.45	111.77
15	B	607	CLA	C3D-C4D-ND	2.48	114.26	110.24
15	C	508	CLA	C1-C2-C3	-2.48	121.75	126.04
15	A	402	CLA	C4D-C3D-CAD	2.48	111.02	108.10
17	B	619	BCR	C38-C26-C27	2.48	118.38	113.62
15	C	506	CLA	O1D-CGD-CBD	-2.48	119.42	124.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	B	609	CLA	C3C-C4C-NC	2.48	113.35	110.57
15	C	512	CLA	O2D-CGD-O1D	-2.48	119.00	123.84
15	B	613	CLA	CMD-C2D-C3D	-2.47	121.92	127.61
15	D	402	CLA	CED-O2D-CGD	2.47	121.52	115.94
15	B	615	CLA	C1-C2-C3	-2.46	121.78	126.04
17	B	617	BCR	C3-C4-C5	-2.46	109.68	114.08
22	C	517	DGD	O1G-C1A-C2A	2.46	119.62	111.91
20	B	621	LMG	O8-C28-C29	2.46	119.62	111.91
15	C	513	CLA	CMB-C2B-C3B	2.45	129.27	124.68
15	B	613	CLA	C3D-C4D-ND	2.45	114.20	110.24
18	B	620	SQD	C1-O5-C5	2.45	118.50	113.69
15	D	405	CLA	C4D-C3D-CAD	2.45	110.98	108.10
15	A	403	CLA	CMD-C2D-C3D	-2.45	121.98	127.61
18	X	101	SQD	O5-C1-C2	2.45	115.53	110.35
15	D	406	CLA	C4-C3-C5	2.45	119.39	115.27
15	C	514	CLA	C3C-C4C-NC	2.45	113.31	110.57
15	C	505	CLA	C4-C3-C5	2.45	119.39	115.27
15	B	605	CLA	C3C-C4C-NC	2.44	113.31	110.57
15	B	614	CLA	OBD-CAD-C3D	-2.44	122.65	128.52
15	B	616	CLA	O1D-CGD-CBD	-2.44	119.50	124.48
17	B	618	BCR	C37-C22-C21	-2.44	119.51	122.92
15	C	504	CLA	CMD-C2D-C3D	-2.43	122.02	127.61
15	B	610	CLA	CAC-C3C-C4C	2.43	127.97	124.81
15	B	614	CLA	C3D-C4D-ND	2.43	114.17	110.24
19	D	408	PL9	C7-C8-C9	-2.43	122.75	126.79
15	D	406	CLA	CMD-C2D-C3D	-2.43	122.03	127.61
15	C	503	CLA	C4-C3-C5	2.43	119.36	115.27
17	D	407	BCR	C19-C18-C17	2.43	122.67	118.94
15	B	604	CLA	C4D-C3D-CAD	2.42	110.95	108.10
15	B	603	CLA	CMD-C2D-C3D	-2.42	122.05	127.61
18	A	407	SQD	O48-C23-C24	2.42	119.49	111.91
15	C	507	CLA	C4-C3-C5	2.42	119.34	115.27
17	C	519	BCR	C19-C18-C17	2.41	122.65	118.94
19	D	408	PL9	C20-C19-C21	2.41	119.33	115.27
25	L	101	LHG	C5-O7-C7	-2.41	111.86	117.79
15	B	602	CLA	C3C-C4C-NC	2.41	113.27	110.57
15	C	502	CLA	CMD-C2D-C3D	-2.41	122.07	127.61
18	B	620	SQD	O5-C5-C4	2.41	114.06	109.69
18	T	101	SQD	C44-O6-C1	2.41	118.44	113.74
17	A	406	BCR	C23-C24-C25	-2.40	120.45	127.20
15	C	514	CLA	C4D-C3D-CAD	2.40	110.93	108.10
15	B	613	CLA	C4-C3-C5	2.40	119.31	115.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	B	615	CLA	C1-O2A-CGA	2.40	122.73	116.44
17	C	516	BCR	C19-C18-C17	2.40	122.62	118.94
15	C	505	CLA	C4D-C3D-CAD	2.39	110.92	108.10
15	A	402	CLA	O2D-CGD-O1D	-2.39	119.16	123.84
15	C	514	CLA	CAA-C2A-C3A	-2.39	106.23	112.78
15	C	502	CLA	CAA-C2A-C3A	-2.39	106.23	112.78
17	C	515	BCR	C37-C22-C21	-2.39	119.58	122.92
15	A	405	CLA	C3C-C4C-NC	2.38	113.24	110.57
15	C	506	CLA	CAC-C3C-C4C	2.37	127.89	124.81
15	C	507	CLA	C3C-C4C-NC	2.37	113.23	110.57
15	C	505	CLA	C3C-C4C-NC	2.37	113.23	110.57
15	C	503	CLA	CMC-C2C-C1C	2.37	128.65	125.04
15	D	402	CLA	C4-C3-C5	2.37	119.26	115.27
15	B	615	CLA	C4-C3-C5	2.37	119.25	115.27
15	B	615	CLA	CMA-C3A-C4A	2.37	118.13	111.77
15	B	602	CLA	CMD-C2D-C3D	-2.37	122.17	127.61
26	E	101	HEM	CBA-CAA-C2A	-2.36	108.58	112.62
15	C	507	CLA	CAC-C3C-C4C	2.36	127.88	124.81
18	T	103	SQD	C1-O5-C5	2.36	118.33	113.69
26	E	101	HEM	C4B-CHC-C1C	2.36	125.67	122.56
15	B	606	CLA	C4-C3-C5	2.36	119.24	115.27
15	B	604	CLA	CMC-C2C-C1C	2.36	128.63	125.04
26	E	101	HEM	C4C-CHD-C1D	2.35	125.66	122.56
17	C	516	BCR	C8-C7-C6	-2.35	120.61	127.20
15	B	604	CLA	CMD-C2D-C3D	-2.35	122.21	127.61
15	B	602	CLA	C4D-C3D-CAD	2.35	110.86	108.10
15	C	514	CLA	CMD-C2D-C3D	-2.35	122.22	127.61
18	X	101	SQD	C44-O6-C1	2.35	118.32	113.74
15	A	405	CLA	CMD-C2D-C3D	-2.35	122.22	127.61
15	B	606	CLA	CAC-C3C-C4C	2.34	127.85	124.81
15	B	603	CLA	C4D-C3D-CAD	2.34	110.86	108.10
17	C	516	BCR	C37-C22-C21	-2.34	119.64	122.92
15	C	510	CLA	O2D-CGD-O1D	-2.34	119.26	123.84
15	B	604	CLA	C3D-C4D-ND	2.34	114.02	110.24
15	B	603	CLA	O1D-CGD-CBD	-2.34	119.70	124.48
15	C	503	CLA	CAC-C3C-C4C	2.34	127.84	124.81
15	C	508	CLA	C3D-C4D-ND	2.34	114.02	110.24
15	C	514	CLA	CAC-C3C-C4C	2.34	127.84	124.81
15	C	510	CLA	CED-O2D-CGD	2.33	121.21	115.94
26	E	101	HEM	C1B-NB-C4B	2.33	107.48	105.07
15	B	615	CLA	CAC-C3C-C4C	2.33	127.83	124.81
15	A	402	CLA	C4-C3-C5	2.33	119.19	115.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	C	502	CLA	CAC-C3C-C4C	2.33	127.83	124.81
15	C	511	CLA	CMD-C2D-C3D	-2.32	122.27	127.61
15	B	606	CLA	CMA-C3A-C4A	2.32	118.01	111.77
15	C	504	CLA	C1-O2A-CGA	2.32	122.53	116.44
20	D	412	LMG	O8-C28-C29	2.32	119.18	111.91
15	C	508	CLA	C3C-C4C-NC	2.32	113.17	110.57
15	C	504	CLA	C4D-C3D-CAD	2.32	110.83	108.10
15	B	613	CLA	C1-O2A-CGA	2.32	122.52	116.44
15	B	603	CLA	CAA-C2A-C3A	-2.31	106.44	112.78
18	B	620	SQD	O48-C23-C24	2.31	119.17	111.91
15	C	509	CLA	CAC-C3C-C4C	2.31	127.81	124.81
15	B	611	CLA	CMA-C3A-C4A	2.31	117.98	111.77
15	C	509	CLA	C3C-C4C-NC	2.31	113.16	110.57
16	A	404	PHO	CMC-C2C-C3C	2.31	129.30	124.94
16	D	403	PHO	C1-C2-C3	-2.31	122.05	126.04
17	A	406	BCR	C3-C4-C5	-2.31	109.96	114.08
15	B	605	CLA	CAA-C2A-C3A	-2.31	106.47	112.78
17	C	515	BCR	C33-C5-C4	2.30	118.04	113.62
15	B	616	CLA	CAC-C3C-C4C	2.30	127.80	124.81
15	D	406	CLA	C3C-C4C-NC	2.30	113.15	110.57
17	B	618	BCR	C33-C5-C4	2.29	118.02	113.62
17	B	617	BCR	C32-C1-C6	-2.29	106.58	110.30
15	D	402	CLA	CMC-C2C-C1C	2.29	128.53	125.04
22	C	517	DGD	C2G-O2G-C1B	-2.29	112.15	117.79
15	D	402	CLA	CMD-C2D-C3D	-2.29	122.35	127.61
17	D	407	BCR	C33-C5-C4	2.29	118.01	113.62
21	B	623	LMT	O5'-C1'-C2'	-2.29	105.50	110.35
15	B	610	CLA	CMD-C2D-C3D	-2.29	122.35	127.61
17	C	515	BCR	C38-C26-C27	2.28	118.00	113.62
15	C	511	CLA	C4D-C3D-CAD	2.28	110.78	108.10
15	A	402	CLA	CAA-CBA-CGA	-2.28	106.60	113.25
15	D	402	CLA	O2D-CGD-O1D	-2.28	119.39	123.84
15	B	612	CLA	C4D-C3D-CAD	2.28	110.78	108.10
15	C	507	CLA	C1-O2A-CGA	2.27	122.41	116.44
15	A	405	CLA	CAA-C2A-C3A	-2.27	106.56	112.78
15	B	611	CLA	CMC-C2C-C1C	2.27	128.49	125.04
15	A	403	CLA	CAA-C2A-C3A	-2.26	106.58	112.78
15	B	607	CLA	C1-O2A-CGA	2.26	122.38	116.44
15	A	405	CLA	C5-C3-C4	2.26	119.60	114.60
15	B	616	CLA	C5-C3-C4	2.26	119.60	114.60
15	C	505	CLA	CAC-C3C-C4C	2.26	127.74	124.81
17	B	618	BCR	C34-C9-C10	-2.26	119.76	122.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	A	402	CLA	CMD-C2D-C3D	-2.26	122.42	127.61
15	C	509	CLA	CMD-C2D-C3D	-2.26	122.42	127.61
17	B	617	BCR	C8-C7-C6	-2.25	120.88	127.20
17	C	516	BCR	C23-C24-C25	-2.25	120.89	127.20
19	D	408	PL9	O1-C4-C3	-2.24	118.25	120.72
18	T	103	SQD	O48-C23-C24	2.24	118.94	111.91
15	C	505	CLA	CMD-C2D-C3D	-2.24	122.46	127.61
15	A	403	CLA	C3C-C4C-NC	2.24	113.08	110.57
17	B	619	BCR	C30-C25-C26	-2.24	119.46	122.61
15	A	402	CLA	C1-C2-C3	-2.24	122.17	126.04
15	D	402	CLA	C6-C5-C3	-2.24	107.58	113.45
15	B	613	CLA	C3C-C4C-NC	2.24	113.08	110.57
15	B	608	CLA	C1-O2A-CGA	2.23	122.30	116.44
15	D	405	CLA	CMD-C2D-C3D	-2.23	122.48	127.61
15	B	614	CLA	CMD-C2D-C3D	-2.22	122.50	127.61
18	X	101	SQD	C45-O47-C7	2.22	123.26	117.79
17	X	102	BCR	C3-C4-C5	-2.22	110.11	114.08
15	C	512	CLA	C4D-C3D-CAD	2.22	110.71	108.10
15	C	504	CLA	C4-C3-C5	2.21	119.00	115.27
15	C	507	CLA	CHC-C1C-C2C	-2.21	120.60	126.72
15	C	505	CLA	C1-O2A-CGA	2.21	122.25	116.44
15	B	606	CLA	C4D-C3D-CAD	2.21	110.70	108.10
15	C	513	CLA	C4D-C3D-CAD	2.20	110.69	108.10
15	C	507	CLA	CMD-C2D-C3D	-2.20	122.55	127.61
15	B	607	CLA	CMD-C2D-C3D	-2.20	122.56	127.61
15	B	607	CLA	C4D-C3D-CAD	2.20	110.69	108.10
15	B	615	CLA	CMD-C2D-C3D	-2.19	122.57	127.61
15	C	508	CLA	OBD-CAD-C3D	-2.19	123.24	128.52
15	B	607	CLA	CAC-C3C-C4C	2.19	127.65	124.81
15	C	504	CLA	CAC-C3C-C4C	2.19	127.65	124.81
17	C	516	BCR	C35-C13-C12	2.19	121.52	118.08
15	A	403	CLA	CAC-C3C-C4C	2.18	127.64	124.81
15	C	511	CLA	O1D-CGD-CBD	-2.18	120.01	124.48
20	B	621	LMG	O7-C10-O9	-2.18	118.44	123.70
15	C	510	CLA	CMD-C2D-C3D	-2.18	122.60	127.61
15	B	616	CLA	CMA-C3A-C4A	2.18	117.63	111.77
15	B	615	CLA	C4D-C3D-CAD	2.18	110.66	108.10
15	C	505	CLA	CAA-C2A-C3A	-2.17	106.83	112.78
15	B	611	CLA	C3C-C4C-NC	2.17	113.01	110.57
15	C	508	CLA	C4D-C3D-CAD	2.17	110.66	108.10
16	D	403	PHO	CMC-C2C-C3C	2.17	129.04	124.94
18	A	407	SQD	C44-O6-C1	2.17	117.97	113.74

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	C	507	CLA	CMC-C2C-C1C	2.16	128.33	125.04
15	B	613	CLA	C4D-C3D-CAD	2.16	110.64	108.10
15	C	502	CLA	C4D-C3D-CAD	2.16	110.64	108.10
15	D	402	CLA	C4D-C3D-CAD	2.16	110.64	108.10
15	B	616	CLA	CHC-C1C-C2C	-2.16	120.74	126.72
15	C	508	CLA	CMD-C2D-C3D	-2.15	122.66	127.61
18	T	103	SQD	C3-C4-C5	2.15	114.07	110.24
17	B	617	BCR	C38-C26-C27	2.15	117.74	113.62
15	D	406	CLA	C4D-C3D-CAD	2.14	110.62	108.10
15	B	612	CLA	CMD-C2D-C3D	-2.14	122.69	127.61
21	B	622	LMT	C3B-C4B-C5B	-2.14	106.42	110.24
15	C	512	CLA	CMD-C2D-C3D	-2.14	122.70	127.61
15	B	606	CLA	C3C-C4C-NC	2.14	112.97	110.57
15	A	403	CLA	C4D-C3D-CAD	2.14	110.61	108.10
15	B	604	CLA	CAA-C2A-C3A	-2.14	106.93	112.78
18	A	409	SQD	O47-C7-O49	-2.13	118.54	123.70
19	D	408	PL9	C32-C33-C34	-2.13	122.53	127.66
18	T	101	SQD	O47-C7-O49	-2.12	118.57	123.70
15	B	605	CLA	O1D-CGD-CBD	-2.12	120.15	124.48
15	C	511	CLA	CMA-C3A-C4A	2.12	117.47	111.77
15	D	402	CLA	CAC-C3C-C4C	2.12	127.56	124.81
15	A	402	CLA	C6-C5-C3	-2.11	107.91	113.45
19	D	408	PL9	O2-C1-C2	-2.11	116.95	121.78
15	B	614	CLA	CED-O2D-CGD	2.11	120.70	115.94
15	B	604	CLA	CAC-C3C-C4C	2.10	127.54	124.81
15	C	502	CLA	C3C-C4C-NC	2.10	112.93	110.57
15	B	607	CLA	C1-C2-C3	-2.10	122.41	126.04
15	B	601	CLA	CAC-C3C-C4C	2.10	127.54	124.81
17	C	519	BCR	C33-C5-C4	2.10	117.65	113.62
15	B	609	CLA	C4D-C3D-CAD	2.10	110.57	108.10
15	B	603	CLA	CAC-C3C-C4C	2.10	127.53	124.81
15	B	608	CLA	C4D-C3D-CAD	2.09	110.56	108.10
19	D	408	PL9	O2-C1-C6	2.09	124.21	120.59
15	A	405	CLA	C4D-C3D-CAD	2.09	110.56	108.10
19	A	408	PL9	O1-C4-C3	-2.09	118.42	120.72
15	B	602	CLA	CAA-C2A-C3A	-2.09	107.06	112.78
17	C	519	BCR	C38-C26-C27	2.08	117.62	113.62
27	T	102	FME	C-CA-N	2.08	113.48	109.73
15	D	402	CLA	C3C-C4C-NC	2.07	112.89	110.57
15	C	509	CLA	C1-O2A-CGA	2.07	121.88	116.44
17	D	407	BCR	C23-C24-C25	-2.07	121.40	127.20
15	C	509	CLA	CHC-C1C-C2C	-2.07	121.01	126.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	A	405	CLA	CAC-C3C-C4C	2.07	127.49	124.81
15	C	513	CLA	O1D-CGD-CBD	-2.07	120.26	124.48
17	B	617	BCR	C33-C5-C4	2.06	117.57	113.62
15	B	602	CLA	CAC-C3C-C4C	2.05	127.47	124.81
15	B	606	CLA	C6-C5-C3	-2.05	108.07	113.45
19	D	408	PL9	C31-C32-C33	-2.05	105.14	111.88
15	D	405	CLA	CED-O2D-CGD	2.05	120.57	115.94
25	D	410	LHG	O7-C7-O9	-2.05	118.75	123.70
15	B	609	CLA	CMD-C2D-C3D	-2.05	122.91	127.61
20	C	501	LMG	C8-O7-C10	-2.04	112.76	117.79
18	C	518	SQD	C1-C2-C3	2.04	114.25	110.00
17	D	407	BCR	C37-C22-C21	-2.04	120.07	122.92
15	C	510	CLA	CMA-C3A-C4A	2.04	117.25	111.77
15	D	402	CLA	CHC-C1C-C2C	-2.04	121.09	126.72
15	C	510	CLA	C1-C2-C3	-2.03	122.52	126.04
15	C	508	CLA	O1D-CGD-CBD	-2.03	120.32	124.48
19	A	408	PL9	O2-C1-C2	-2.03	117.12	121.78
17	C	515	BCR	C29-C28-C27	2.03	115.92	111.38
18	A	409	SQD	O5-C5-C4	2.03	113.38	109.69
26	E	101	HEM	CMA-C3A-C4A	-2.03	125.35	128.46
15	C	505	CLA	O1D-CGD-CBD	-2.03	120.34	124.48
15	C	509	CLA	CED-O2D-CGD	2.02	120.51	115.94
17	B	618	BCR	C38-C26-C27	2.02	117.50	113.62
15	C	511	CLA	CAA-C2A-C3A	-2.02	107.26	112.78
15	B	605	CLA	CMD-C2D-C3D	-2.02	122.98	127.61
15	C	507	CLA	CAA-C2A-C3A	-2.01	107.26	112.78
15	B	605	CLA	C4D-C3D-CAD	2.01	110.47	108.10
15	B	611	CLA	CHC-C1C-C2C	-2.00	121.19	126.72

All (35) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
15	A	402	CLA	ND
15	A	403	CLA	ND
15	A	405	CLA	ND
15	B	601	CLA	ND
15	B	602	CLA	ND
15	B	603	CLA	ND
15	B	604	CLA	ND
15	B	605	CLA	ND
15	B	606	CLA	ND
15	B	607	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
15	B	608	CLA	ND
15	B	609	CLA	ND
15	B	610	CLA	ND
15	B	611	CLA	ND
15	B	612	CLA	ND
15	B	613	CLA	ND
15	B	614	CLA	ND
15	B	615	CLA	ND
15	B	616	CLA	ND
15	C	502	CLA	ND
15	C	503	CLA	ND
15	C	504	CLA	ND
15	C	505	CLA	ND
15	C	506	CLA	ND
15	C	507	CLA	ND
15	C	508	CLA	ND
15	C	509	CLA	ND
15	C	510	CLA	ND
15	C	511	CLA	ND
15	C	512	CLA	ND
15	C	513	CLA	ND
15	C	514	CLA	ND
15	D	402	CLA	ND
15	D	405	CLA	ND
15	D	406	CLA	ND

All (923) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	A	403	CLA	CHA-CBD-CGD-O1D
15	A	403	CLA	CHA-CBD-CGD-O2D
15	B	601	CLA	CBA-CGA-O2A-C1
15	B	601	CLA	O1A-CGA-O2A-C1
15	B	601	CLA	CAD-CBD-CGD-O1D
15	B	601	CLA	CAD-CBD-CGD-O2D
15	B	601	CLA	C14-C13-C15-C16
15	B	604	CLA	CHA-CBD-CGD-O1D
15	B	604	CLA	CHA-CBD-CGD-O2D
15	B	604	CLA	CAD-CBD-CGD-O1D
15	B	605	CLA	C2-C3-C5-C6
15	B	605	CLA	C4-C3-C5-C6
15	B	606	CLA	CHA-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	B	606	CLA	CHA-CBD-CGD-O2D
15	B	607	CLA	CHA-CBD-CGD-O1D
15	B	607	CLA	CHA-CBD-CGD-O2D
15	B	607	CLA	CAD-CBD-CGD-O1D
15	B	607	CLA	CBD-CGD-O2D-CED
15	B	608	CLA	CHA-CBD-CGD-O1D
15	B	608	CLA	CBD-CGD-O2D-CED
15	B	608	CLA	C2-C3-C5-C6
15	B	608	CLA	C4-C3-C5-C6
15	B	609	CLA	CBD-CGD-O2D-CED
15	B	610	CLA	CBD-CGD-O2D-CED
15	B	611	CLA	C11-C12-C13-C14
15	B	612	CLA	C1A-C2A-CAA-CBA
15	B	612	CLA	C3A-C2A-CAA-CBA
15	B	612	CLA	C2-C1-O2A-CGA
15	B	614	CLA	CAD-CBD-CGD-O1D
15	B	614	CLA	CAD-CBD-CGD-O2D
15	B	616	CLA	CHA-CBD-CGD-O2D
15	C	502	CLA	CBD-CGD-O2D-CED
15	C	503	CLA	CBD-CGD-O2D-CED
15	C	503	CLA	C14-C13-C15-C16
15	C	507	CLA	C1A-C2A-CAA-CBA
15	C	507	CLA	CBD-CGD-O2D-CED
15	C	509	CLA	C1A-C2A-CAA-CBA
15	C	509	CLA	CHA-CBD-CGD-O1D
15	C	509	CLA	CHA-CBD-CGD-O2D
15	C	510	CLA	C2-C1-O2A-CGA
15	C	512	CLA	C1A-C2A-CAA-CBA
15	C	512	CLA	CHA-CBD-CGD-O1D
15	C	512	CLA	CBD-CGD-O2D-CED
15	C	513	CLA	C1A-C2A-CAA-CBA
15	C	513	CLA	C3A-C2A-CAA-CBA
15	C	513	CLA	CBD-CGD-O2D-CED
15	D	402	CLA	C1A-C2A-CAA-CBA
15	D	402	CLA	CHA-CBD-CGD-O1D
15	D	402	CLA	CHA-CBD-CGD-O2D
15	D	405	CLA	C1A-C2A-CAA-CBA
15	D	405	CLA	C3A-C2A-CAA-CBA
16	A	404	PHO	C3A-C2A-CAA-CBA
17	A	406	BCR	C1-C6-C7-C8
17	B	617	BCR	C1-C6-C7-C8
17	B	617	BCR	C11-C10-C9-C34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	B	617	BCR	C36-C18-C19-C20
17	B	617	BCR	C37-C22-C23-C24
17	B	618	BCR	C7-C8-C9-C10
17	B	618	BCR	C7-C8-C9-C34
17	B	618	BCR	C11-C10-C9-C8
17	B	618	BCR	C11-C10-C9-C34
17	B	618	BCR	C10-C11-C12-C13
17	B	619	BCR	C11-C10-C9-C8
17	B	619	BCR	C11-C10-C9-C34
17	B	619	BCR	C23-C24-C25-C30
17	C	515	BCR	C7-C8-C9-C10
17	C	515	BCR	C7-C8-C9-C34
17	C	515	BCR	C11-C10-C9-C8
17	C	515	BCR	C11-C10-C9-C34
17	C	515	BCR	C37-C22-C23-C24
17	C	515	BCR	C23-C24-C25-C30
17	C	519	BCR	C11-C10-C9-C8
17	C	519	BCR	C11-C10-C9-C34
17	C	519	BCR	C10-C11-C12-C13
17	D	407	BCR	C11-C10-C9-C8
17	D	407	BCR	C11-C10-C9-C34
17	D	407	BCR	C10-C11-C12-C13
17	D	407	BCR	C17-C18-C19-C20
17	D	407	BCR	C36-C18-C19-C20
17	X	102	BCR	C7-C8-C9-C10
17	X	102	BCR	C7-C8-C9-C34
17	X	102	BCR	C11-C10-C9-C8
17	X	102	BCR	C11-C10-C9-C34
17	X	102	BCR	C10-C11-C12-C13
18	A	407	SQD	O5-C1-O6-C44
18	A	409	SQD	O5-C1-O6-C44
18	B	620	SQD	C8-C7-O47-C45
18	B	620	SQD	O5-C5-C6-S
18	C	518	SQD	C2-C1-O6-C44
18	C	518	SQD	O5-C1-O6-C44
18	C	518	SQD	O49-C7-O47-C45
18	C	518	SQD	C8-C7-O47-C45
18	C	518	SQD	O10-C23-O48-C46
18	C	518	SQD	C24-C23-O48-C46
18	T	101	SQD	O49-C7-O47-C45
18	T	101	SQD	C8-C7-O47-C45
18	T	101	SQD	C24-C23-O48-C46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	T	103	SQD	C2-C1-O6-C44
18	T	103	SQD	O5-C1-O6-C44
18	T	103	SQD	C46-C45-O47-C7
18	T	103	SQD	C24-C23-O48-C46
18	X	101	SQD	O5-C1-O6-C44
18	X	101	SQD	O49-C7-O47-C45
18	X	101	SQD	C8-C7-O47-C45
19	D	408	PL9	C12-C13-C14-C16
19	D	408	PL9	C18-C19-C21-C22
19	D	408	PL9	C20-C19-C21-C22
20	C	501	LMG	C2-C1-O1-C7
20	C	501	LMG	O6-C1-O1-C7
21	B	623	LMT	C2-C1-O1'-C1'
25	D	409	LHG	O1-C1-C2-C3
25	D	409	LHG	C4-O6-P-O5
25	D	410	LHG	O1-C1-C2-C3
25	D	410	LHG	C4-O6-P-O3
25	D	411	LHG	O1-C1-C2-C3
25	D	411	LHG	C3-O3-P-O4
25	D	411	LHG	C3-O3-P-O5
25	D	411	LHG	C4-O6-P-O3
25	D	411	LHG	C4-O6-P-O4
25	D	411	LHG	C4-O6-P-O5
25	L	101	LHG	C3-O3-P-O5
27	M	101	FME	N-CA-CB-CG
27	M	101	FME	C-CA-CB-CG
27	T	102	FME	N-CA-CB-CG
27	T	102	FME	C-CA-CB-CG
15	A	402	CLA	O1D-CGD-O2D-CED
15	A	402	CLA	CBD-CGD-O2D-CED
15	B	603	CLA	CBD-CGD-O2D-CED
15	B	606	CLA	CBD-CGD-O2D-CED
15	B	611	CLA	CBD-CGD-O2D-CED
15	B	613	CLA	CBD-CGD-O2D-CED
15	C	511	CLA	CBD-CGD-O2D-CED
15	C	514	CLA	CBD-CGD-O2D-CED
15	D	405	CLA	CBD-CGD-O2D-CED
15	D	406	CLA	CBD-CGD-O2D-CED
16	A	404	PHO	CBD-CGD-O2D-CED
15	B	602	CLA	O1A-CGA-O2A-C1
18	T	101	SQD	O10-C23-O48-C46
18	T	103	SQD	O10-C23-O48-C46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	B	608	CLA	O1D-CGD-O2D-CED
15	C	502	CLA	O1D-CGD-O2D-CED
15	C	503	CLA	O1D-CGD-O2D-CED
15	C	507	CLA	O1D-CGD-O2D-CED
15	C	512	CLA	O1D-CGD-O2D-CED
15	C	513	CLA	O1D-CGD-O2D-CED
15	B	602	CLA	CBA-CGA-O2A-C1
15	A	405	CLA	CBD-CGD-O2D-CED
15	B	605	CLA	CBD-CGD-O2D-CED
15	C	504	CLA	CBD-CGD-O2D-CED
15	C	510	CLA	CBD-CGD-O2D-CED
15	A	405	CLA	O1A-CGA-O2A-C1
15	B	614	CLA	O1A-CGA-O2A-C1
18	A	409	SQD	O10-C23-O48-C46
18	B	620	SQD	O10-C23-O48-C46
15	B	607	CLA	O1D-CGD-O2D-CED
15	B	609	CLA	O1D-CGD-O2D-CED
15	B	610	CLA	O1D-CGD-O2D-CED
15	C	509	CLA	CBD-CGD-O2D-CED
18	B	620	SQD	O49-C7-O47-C45
18	T	103	SQD	O49-C7-O47-C45
20	D	412	LMG	O9-C10-O7-C8
15	B	604	CLA	C3-C5-C6-C7
15	B	613	CLA	C3-C5-C6-C7
15	A	405	CLA	CBA-CGA-O2A-C1
15	B	614	CLA	CBA-CGA-O2A-C1
18	A	409	SQD	C8-C7-O47-C45
20	D	412	LMG	C11-C10-O7-C8
15	B	606	CLA	O1D-CGD-O2D-CED
15	B	611	CLA	O1D-CGD-O2D-CED
15	B	613	CLA	O1D-CGD-O2D-CED
15	B	614	CLA	C4-C3-C5-C6
15	B	614	CLA	C2-C3-C5-C6
15	A	402	CLA	C2A-CAA-CBA-CGA
15	B	606	CLA	C2A-CAA-CBA-CGA
15	C	507	CLA	C2A-CAA-CBA-CGA
15	C	508	CLA	C2A-CAA-CBA-CGA
15	C	513	CLA	C2A-CAA-CBA-CGA
20	B	621	LMG	C17-C18-C19-C20
20	C	501	LMG	C17-C18-C19-C20
20	D	412	LMG	C17-C18-C19-C20
20	D	412	LMG	C20-C21-C22-C23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	D	412	LMG	C35-C36-C37-C38
20	D	412	LMG	C38-C39-C40-C41
22	C	517	DGD	C8A-C9A-CAA-CBA
22	H	101	DGD	CBA-CCA-CDA-CEA
22	H	101	DGD	CBB-CCB-CDB-CEB
15	B	612	CLA	CBA-CGA-O2A-C1
15	C	510	CLA	CBA-CGA-O2A-C1
18	B	620	SQD	C24-C23-O48-C46
16	A	404	PHO	O1D-CGD-O2D-CED
15	C	514	CLA	O1D-CGD-O2D-CED
15	C	510	CLA	O1A-CGA-O2A-C1
15	B	602	CLA	CBD-CGD-O2D-CED
15	B	614	CLA	CBD-CGD-O2D-CED
15	B	616	CLA	CBD-CGD-O2D-CED
15	C	505	CLA	CBD-CGD-O2D-CED
15	B	603	CLA	O1D-CGD-O2D-CED
15	D	406	CLA	O1D-CGD-O2D-CED
25	D	411	LHG	O2-C2-C3-O3
15	A	402	CLA	C3-C5-C6-C7
15	B	616	CLA	CBA-CGA-O2A-C1
15	C	511	CLA	CBA-CGA-O2A-C1
15	C	513	CLA	CBA-CGA-O2A-C1
18	A	409	SQD	C24-C23-O48-C46
15	C	513	CLA	O1A-CGA-O2A-C1
15	D	405	CLA	O1D-CGD-O2D-CED
22	C	517	DGD	O6E-C5E-C6E-O5E
27	M	101	FME	CA-CB-CG-SD
15	C	511	CLA	O1D-CGD-O2D-CED
15	B	616	CLA	O1A-CGA-O2A-C1
15	C	511	CLA	O1A-CGA-O2A-C1
15	B	602	CLA	C4-C3-C5-C6
15	C	508	CLA	C4-C3-C5-C6
15	C	509	CLA	C4-C3-C5-C6
15	D	406	CLA	C4-C3-C5-C6
15	B	602	CLA	C2-C3-C5-C6
15	C	508	CLA	C2-C3-C5-C6
15	C	509	CLA	C2-C3-C5-C6
15	D	406	CLA	C2-C3-C5-C6
15	B	616	CLA	C2A-CAA-CBA-CGA
15	B	612	CLA	O1A-CGA-O2A-C1
21	B	622	LMT	C4'-C5'-C6'-O6'
19	D	408	PL9	C9-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	C	505	CLA	CBA-CGA-O2A-C1
15	B	605	CLA	O1D-CGD-O2D-CED
25	D	411	LHG	C1-C2-C3-O3
16	A	404	PHO	C3-C5-C6-C7
15	C	504	CLA	O1D-CGD-O2D-CED
15	B	607	CLA	CBA-CGA-O2A-C1
15	B	609	CLA	CBA-CGA-O2A-C1
15	C	508	CLA	CBD-CGD-O2D-CED
15	B	615	CLA	C10-C11-C12-C13
15	B	602	CLA	C13-C15-C16-C17
15	B	607	CLA	C13-C15-C16-C17
15	B	607	CLA	C15-C16-C17-C18
15	B	613	CLA	C15-C16-C17-C18
15	D	405	CLA	C10-C11-C12-C13
15	D	406	CLA	C8-C10-C11-C12
15	D	402	CLA	C3-C5-C6-C7
15	B	607	CLA	O1A-CGA-O2A-C1
15	B	609	CLA	O1A-CGA-O2A-C1
21	B	623	LMT	C4B-C5B-C6B-O6B
15	B	601	CLA	C11-C10-C8-C9
15	B	602	CLA	C11-C10-C8-C9
15	B	602	CLA	C14-C13-C15-C16
15	B	604	CLA	C6-C7-C8-C9
15	B	609	CLA	C6-C7-C8-C9
15	C	510	CLA	C6-C7-C8-C9
15	C	510	CLA	C14-C13-C15-C16
15	C	513	CLA	C14-C13-C15-C16
15	C	514	CLA	C14-C13-C15-C16
15	D	406	CLA	C6-C7-C8-C9
15	C	505	CLA	C13-C15-C16-C17
15	B	610	CLA	C2A-CAA-CBA-CGA
17	B	619	BCR	C7-C8-C9-C34
17	B	619	BCR	C7-C8-C9-C10
18	T	101	SQD	C7-C8-C9-C10
25	D	411	LHG	C23-C24-C25-C26
15	B	602	CLA	C15-C16-C17-C18
15	C	514	CLA	C8-C10-C11-C12
15	A	405	CLA	O1D-CGD-O2D-CED
27	T	102	FME	CA-CB-CG-SD
15	A	402	CLA	C15-C16-C17-C18
15	B	609	CLA	C5-C6-C7-C8
15	B	615	CLA	C15-C16-C17-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	C	504	CLA	C8-C10-C11-C12
15	C	504	CLA	C15-C16-C17-C18
22	H	101	DGD	O6E-C5E-C6E-O5E
18	A	407	SQD	C7-C8-C9-C10
18	A	409	SQD	C23-C24-C25-C26
15	C	510	CLA	O1D-CGD-O2D-CED
15	B	602	CLA	C5-C6-C7-C8
15	B	603	CLA	C5-C6-C7-C8
15	B	606	CLA	C8-C10-C11-C12
15	C	507	CLA	C13-C15-C16-C17
15	C	513	CLA	C10-C11-C12-C13
18	T	103	SQD	C23-C24-C25-C26
25	D	409	LHG	C23-C24-C25-C26
25	D	411	LHG	C7-C8-C9-C10
18	A	407	SQD	C15-C16-C17-C18
15	B	601	CLA	C13-C15-C16-C17
15	B	602	CLA	C8-C10-C11-C12
15	B	604	CLA	C15-C16-C17-C18
15	B	615	CLA	C5-C6-C7-C8
15	C	505	CLA	C8-C10-C11-C12
15	C	508	CLA	C10-C11-C12-C13
15	C	513	CLA	C15-C16-C17-C18
15	B	605	CLA	CBA-CGA-O2A-C1
15	C	507	CLA	CBA-CGA-O2A-C1
18	C	518	SQD	C9-C10-C11-C12
25	D	411	LHG	C30-C31-C32-C33
15	B	614	CLA	C2-C1-O2A-CGA
15	B	615	CLA	C2-C1-O2A-CGA
15	C	509	CLA	C2-C1-O2A-CGA
15	D	402	CLA	C2-C1-O2A-CGA
15	B	613	CLA	C5-C6-C7-C8
15	C	511	CLA	C15-C16-C17-C18
15	D	405	CLA	C8-C10-C11-C12
20	C	501	LMG	C10-C11-C12-C13
21	B	623	LMT	C4'-C5'-C6'-O6'
18	T	101	SQD	C24-C25-C26-C27
15	C	506	CLA	C8-C10-C11-C12
15	B	601	CLA	C11-C10-C8-C7
15	B	602	CLA	C11-C12-C13-C15
15	B	606	CLA	C6-C7-C8-C10
15	C	502	CLA	C12-C13-C15-C16
15	C	504	CLA	C12-C13-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	C	513	CLA	C6-C7-C8-C10
15	C	514	CLA	C11-C12-C13-C15
16	D	403	PHO	C12-C13-C15-C16
25	D	410	LHG	C23-C24-C25-C26
15	C	514	CLA	CBA-CGA-O2A-C1
15	C	509	CLA	O1D-CGD-O2D-CED
15	B	608	CLA	C15-C16-C17-C18
15	C	506	CLA	C13-C15-C16-C17
15	C	514	CLA	C5-C6-C7-C8
21	B	623	LMT	O5'-C1'-O1'-C1
15	C	503	CLA	C13-C15-C16-C17
15	C	507	CLA	C5-C6-C7-C8
17	A	406	BCR	C10-C11-C12-C13
17	B	619	BCR	C10-C11-C12-C13
17	C	515	BCR	C10-C11-C12-C13
19	A	408	PL9	C7-C8-C9-C11
25	L	101	LHG	O2-C2-C3-O3
15	B	613	CLA	C10-C11-C12-C13
15	D	405	CLA	C13-C15-C16-C17
15	B	604	CLA	CBD-CGD-O2D-CED
15	C	505	CLA	O1A-CGA-O2A-C1
15	C	507	CLA	O1A-CGA-O2A-C1
15	B	608	CLA	C13-C15-C16-C17
15	C	514	CLA	C13-C15-C16-C17
15	B	608	CLA	C8-C10-C11-C12
15	B	609	CLA	C15-C16-C17-C18
25	D	410	LHG	C3-O3-P-O6
25	D	411	LHG	C3-O3-P-O6
25	L	101	LHG	C3-O3-P-O6
21	B	623	LMT	O5'-C5'-C6'-O6'
15	A	403	CLA	C3-C5-C6-C7
15	C	506	CLA	C3-C5-C6-C7
18	B	620	SQD	C13-C14-C15-C16
15	B	613	CLA	CBA-CGA-O2A-C1
15	C	503	CLA	C15-C16-C17-C18
15	C	510	CLA	C15-C16-C17-C18
15	C	511	CLA	C5-C6-C7-C8
25	L	101	LHG	C1-C2-C3-O3
22	C	517	DGD	C4E-C5E-C6E-O5E
15	D	406	CLA	CBA-CGA-O2A-C1
15	B	613	CLA	C8-C10-C11-C12
18	T	103	SQD	C8-C7-O47-C45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	A	406	BCR	C11-C10-C9-C34
18	A	409	SQD	C17-C18-C19-C20
18	T	101	SQD	C15-C16-C17-C18
18	X	101	SQD	C11-C10-C9-C8
25	D	409	LHG	C26-C27-C28-C29
25	D	410	LHG	C29-C30-C31-C32
15	B	605	CLA	O1A-CGA-O2A-C1
18	T	101	SQD	C26-C27-C28-C29
18	X	101	SQD	C9-C10-C11-C12
20	D	412	LMG	C15-C16-C17-C18
20	D	412	LMG	C18-C19-C20-C21
22	H	101	DGD	CCA-CDA-CEA-CFA
18	T	101	SQD	C46-C45-O47-C7
15	B	614	CLA	O1D-CGD-O2D-CED
18	A	409	SQD	C32-C33-C34-C35
18	T	101	SQD	C9-C10-C11-C12
18	T	101	SQD	C10-C11-C12-C13
25	L	101	LHG	C2-C3-O3-P
18	A	407	SQD	C13-C14-C15-C16
21	B	623	LMT	C3-C4-C5-C6
22	C	517	DGD	C4B-C5B-C6B-C7B
18	B	620	SQD	C24-C25-C26-C27
18	T	101	SQD	C17-C18-C19-C20
20	C	501	LMG	C16-C17-C18-C19
15	B	616	CLA	O1D-CGD-O2D-CED
17	A	406	BCR	C11-C10-C9-C8
17	B	617	BCR	C11-C10-C9-C8
15	A	403	CLA	CBA-CGA-O2A-C1
18	B	620	SQD	C31-C32-C33-C34
25	D	410	LHG	C31-C32-C33-C34
25	L	101	LHG	C16-C17-C18-C19
15	C	514	CLA	O1A-CGA-O2A-C1
15	A	403	CLA	C6-C7-C8-C9
15	B	611	CLA	C16-C17-C18-C20
15	B	602	CLA	O1D-CGD-O2D-CED
18	A	409	SQD	C9-C10-C11-C12
25	D	409	LHG	C30-C31-C32-C33
18	A	409	SQD	C14-C15-C16-C17
17	B	617	BCR	C17-C18-C19-C20
15	D	406	CLA	C3-C5-C6-C7
25	D	410	LHG	C11-C12-C13-C14
25	D	410	LHG	C18-C19-C20-C21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	D	410	LHG	C26-C27-C28-C29
18	A	407	SQD	C14-C15-C16-C17
25	D	409	LHG	C13-C14-C15-C16
15	B	612	CLA	C16-C17-C18-C20
18	A	409	SQD	C13-C14-C15-C16
18	B	620	SQD	C27-C28-C29-C30
18	T	101	SQD	C11-C12-C13-C14
18	X	101	SQD	C24-C25-C26-C27
25	L	101	LHG	C34-C35-C36-C37
27	I	101	FME	CA-CB-CG-SD
15	C	505	CLA	O1D-CGD-O2D-CED
18	X	101	SQD	C12-C13-C14-C15
15	C	511	CLA	C8-C10-C11-C12
15	B	613	CLA	O1A-CGA-O2A-C1
18	B	620	SQD	C28-C29-C30-C31
20	C	501	LMG	C18-C19-C20-C21
16	A	404	PHO	CBA-CGA-O2A-C1
20	D	412	LMG	C36-C37-C38-C39
15	C	508	CLA	C3A-C2A-CAA-CBA
15	C	507	CLA	C15-C16-C17-C18
21	B	622	LMT	C2-C1-O1'-C1'
18	C	518	SQD	C17-C18-C19-C20
20	B	621	LMG	C12-C13-C14-C15
15	A	403	CLA	C6-C7-C8-C10
18	A	409	SQD	C12-C13-C14-C15
18	B	620	SQD	C34-C35-C36-C37
15	C	510	CLA	C3-C5-C6-C7
27	T	102	FME	CB-CG-SD-CE
25	L	101	LHG	C23-C24-C25-C26
25	D	410	LHG	O1-C1-C2-O2
25	D	411	LHG	O1-C1-C2-O2
18	X	101	SQD	C11-C12-C13-C14
25	D	411	LHG	C13-C14-C15-C16
15	D	406	CLA	O1A-CGA-O2A-C1
15	C	514	CLA	C10-C11-C12-C13
20	D	412	LMG	O6-C5-C6-O5
21	B	623	LMT	O5B-C5B-C6B-O6B
25	D	409	LHG	C28-C29-C30-C31
15	A	403	CLA	C2-C1-O2A-CGA
15	C	504	CLA	C2-C1-O2A-CGA
15	C	508	CLA	C2-C1-O2A-CGA
15	C	514	CLA	C2-C1-O2A-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	D	408	PL9	C42-C43-C44-C46
15	B	605	CLA	C15-C16-C17-C18
15	A	403	CLA	O1A-CGA-O2A-C1
25	L	101	LHG	C33-C34-C35-C36
17	A	406	BCR	C5-C6-C7-C8
17	A	406	BCR	C23-C24-C25-C30
17	B	617	BCR	C5-C6-C7-C8
17	B	618	BCR	C23-C24-C25-C26
17	B	618	BCR	C23-C24-C25-C30
17	B	619	BCR	C23-C24-C25-C26
17	C	515	BCR	C1-C6-C7-C8
17	C	515	BCR	C5-C6-C7-C8
17	C	515	BCR	C23-C24-C25-C26
17	C	516	BCR	C23-C24-C25-C26
17	C	516	BCR	C23-C24-C25-C30
17	C	519	BCR	C1-C6-C7-C8
17	C	519	BCR	C5-C6-C7-C8
17	D	407	BCR	C1-C6-C7-C8
17	D	407	BCR	C5-C6-C7-C8
17	D	407	BCR	C23-C24-C25-C26
17	D	407	BCR	C23-C24-C25-C30
17	X	102	BCR	C1-C6-C7-C8
17	X	102	BCR	C5-C6-C7-C8
17	X	102	BCR	C23-C24-C25-C26
17	X	102	BCR	C23-C24-C25-C30
25	L	101	LHG	C27-C28-C29-C30
15	B	609	CLA	C13-C15-C16-C17
20	D	412	LMG	C11-C12-C13-C14
16	D	403	PHO	CBD-CGD-O2D-CED
25	D	410	LHG	C16-C17-C18-C19
15	C	507	CLA	C4-C3-C5-C6
15	B	604	CLA	C6-C7-C8-C10
15	B	615	CLA	C11-C10-C8-C7
15	C	510	CLA	C6-C7-C8-C10
16	A	404	PHO	O1A-CGA-O2A-C1
21	B	622	LMT	C7-C8-C9-C10
15	C	504	CLA	C13-C15-C16-C17
25	D	410	LHG	C7-C8-C9-C10
15	C	509	CLA	CBA-CGA-O2A-C1
25	L	101	LHG	C17-C18-C19-C20
18	B	620	SQD	C7-C8-C9-C10
15	B	611	CLA	C15-C16-C17-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	B	621	LMG	C33-C34-C35-C36
15	C	508	CLA	O1D-CGD-O2D-CED
22	H	101	DGD	C6B-C7B-C8B-C9B
15	B	604	CLA	C16-C17-C18-C20
21	B	623	LMT	C1-C2-C3-C4
18	X	101	SQD	C27-C28-C29-C30
25	L	101	LHG	C11-C10-C9-C8
15	C	513	CLA	C8-C10-C11-C12
15	B	611	CLA	C16-C17-C18-C19
15	C	511	CLA	C13-C15-C16-C17
19	D	408	PL9	C30-C29-C31-C32
18	A	407	SQD	C9-C10-C11-C12
15	B	602	CLA	C11-C12-C13-C14
15	B	615	CLA	C11-C10-C8-C9
15	C	504	CLA	C14-C13-C15-C16
15	C	505	CLA	C6-C7-C8-C9
15	C	507	CLA	C14-C13-C15-C16
15	C	514	CLA	C11-C12-C13-C14
16	D	403	PHO	C14-C13-C15-C16
18	T	101	SQD	C25-C26-C27-C28
17	B	617	BCR	C21-C22-C23-C24
15	A	403	CLA	C1A-C2A-CAA-CBA
15	B	603	CLA	C1A-C2A-CAA-CBA
15	B	604	CLA	C1A-C2A-CAA-CBA
15	B	606	CLA	C1A-C2A-CAA-CBA
15	C	502	CLA	C1A-C2A-CAA-CBA
15	C	508	CLA	C1A-C2A-CAA-CBA
15	D	406	CLA	C1A-C2A-CAA-CBA
15	B	604	CLA	C16-C17-C18-C19
18	A	409	SQD	O49-C7-O47-C45
18	T	101	SQD	C32-C33-C34-C35
25	D	411	LHG	C24-C25-C26-C27
15	C	508	CLA	C13-C15-C16-C17
15	B	611	CLA	CBA-CGA-O2A-C1
25	D	409	LHG	O6-C4-C5-C6
19	D	408	PL9	C12-C13-C14-C15
25	D	411	LHG	C11-C10-C9-C8
25	D	411	LHG	C11-C12-C13-C14
15	B	607	CLA	C10-C11-C12-C13
25	D	409	LHG	O2-C2-C3-O3
25	D	409	LHG	C25-C26-C27-C28
25	L	101	LHG	C28-C29-C30-C31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	C	518	SQD	C24-C25-C26-C27
15	B	604	CLA	O1D-CGD-O2D-CED
18	A	407	SQD	C19-C20-C21-C22
18	X	101	SQD	C13-C14-C15-C16
25	D	409	LHG	O1-C1-C2-O2
15	B	601	CLA	C5-C6-C7-C8
25	D	410	LHG	C13-C14-C15-C16
18	T	103	SQD	C9-C10-C11-C12
15	C	507	CLA	C2-C3-C5-C6
16	A	404	PHO	C2A-CAA-CBA-CGA
20	B	621	LMG	O6-C5-C6-O5
18	T	101	SQD	C31-C32-C33-C34
15	A	402	CLA	C13-C15-C16-C17
15	B	605	CLA	C5-C6-C7-C8
20	D	412	LMG	C29-C28-O8-C9
25	D	411	LHG	O6-C4-C5-O7
15	C	509	CLA	O1A-CGA-O2A-C1
18	T	103	SQD	C24-C25-C26-C27
15	C	508	CLA	C5-C6-C7-C8
18	X	101	SQD	C2-C1-O6-C44
18	C	518	SQD	C15-C16-C17-C18
15	B	611	CLA	C8-C10-C11-C12
15	B	602	CLA	C12-C13-C15-C16
15	B	611	CLA	C12-C13-C15-C16
15	B	613	CLA	C6-C7-C8-C10
15	C	506	CLA	C6-C7-C8-C10
15	C	507	CLA	C12-C13-C15-C16
15	C	510	CLA	C12-C13-C15-C16
15	B	603	CLA	C6-C7-C8-C9
15	B	606	CLA	C6-C7-C8-C9
15	C	502	CLA	C11-C10-C8-C9
15	C	502	CLA	C14-C13-C15-C16
15	C	508	CLA	C6-C7-C8-C9
15	C	510	CLA	C11-C12-C13-C14
25	L	101	LHG	C14-C15-C16-C17
15	C	505	CLA	C5-C6-C7-C8
15	C	507	CLA	C8-C10-C11-C12
15	B	611	CLA	O1A-CGA-O2A-C1
17	C	515	BCR	C21-C22-C23-C24
25	D	409	LHG	C1-C2-C3-O3
18	C	518	SQD	C10-C11-C12-C13
15	B	601	CLA	C16-C17-C18-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	D	410	LHG	O6-C4-C5-C6
25	D	409	LHG	C11-C12-C13-C14
25	D	410	LHG	C30-C31-C32-C33
15	A	402	CLA	C16-C17-C18-C20
15	B	608	CLA	C3A-C2A-CAA-CBA
15	C	506	CLA	C3A-C2A-CAA-CBA
18	B	620	SQD	C29-C30-C31-C32
21	B	622	LMT	C6-C7-C8-C9
15	B	608	CLA	C5-C6-C7-C8
15	C	507	CLA	C16-C17-C18-C19
18	A	409	SQD	C44-C45-C46-O48
18	B	620	SQD	O6-C44-C45-C46
25	D	411	LHG	C4-C5-C6-O8
18	C	518	SQD	C11-C12-C13-C14
25	D	409	LHG	C27-C28-C29-C30
18	B	620	SQD	C14-C15-C16-C17
18	T	101	SQD	C27-C28-C29-C30
25	D	411	LHG	C10-C11-C12-C13
25	D	409	LHG	O6-C4-C5-O7
25	D	410	LHG	O6-C4-C5-O7
15	A	402	CLA	C16-C17-C18-C19
25	D	409	LHG	C33-C34-C35-C36
20	D	412	LMG	O10-C28-O8-C9
19	D	408	PL9	C34-C36-C37-C38
25	D	410	LHG	C35-C36-C37-C38
15	B	609	CLA	C2-C1-O2A-CGA
15	C	513	CLA	C6-C7-C8-C9
15	C	514	CLA	C11-C10-C8-C9
16	A	404	PHO	C14-C13-C15-C16
25	D	411	LHG	C31-C32-C33-C34
16	A	404	PHO	C1A-C2A-CAA-CBA
15	B	612	CLA	C16-C17-C18-C19
15	D	405	CLA	C16-C17-C18-C20
17	A	406	BCR	C23-C24-C25-C26
17	C	519	BCR	C23-C24-C25-C26
16	D	403	PHO	O1D-CGD-O2D-CED
18	A	409	SQD	C27-C28-C29-C30
15	A	403	CLA	C5-C6-C7-C8
15	B	608	CLA	C10-C11-C12-C13
25	D	411	LHG	O6-C4-C5-C6
15	B	601	CLA	C12-C13-C15-C16
15	B	603	CLA	C6-C7-C8-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	B	603	CLA	C12-C13-C15-C16
15	B	609	CLA	C11-C10-C8-C7
15	B	611	CLA	C11-C12-C13-C15
15	C	502	CLA	C11-C10-C8-C7
15	C	503	CLA	C12-C13-C15-C16
15	C	508	CLA	C6-C7-C8-C10
15	C	513	CLA	C12-C13-C15-C16
15	C	514	CLA	C11-C10-C8-C7
19	D	408	PL9	C43-C44-C46-C47
18	A	407	SQD	C24-C25-C26-C27
15	C	507	CLA	C16-C17-C18-C20
15	B	613	CLA	C13-C15-C16-C17
15	C	505	CLA	C15-C16-C17-C18
25	L	101	LHG	C8-C7-O7-C5
25	D	410	LHG	C24-C25-C26-C27
15	B	607	CLA	CAD-CBD-CGD-O2D
15	C	504	CLA	CAD-CBD-CGD-O2D
15	C	506	CLA	CAD-CBD-CGD-O2D
16	A	404	PHO	CAD-CBD-CGD-O2D
18	X	101	SQD	C44-C45-O47-C7
15	C	505	CLA	C3-C5-C6-C7
22	C	517	DGD	C5A-C6A-C7A-C8A
15	B	606	CLA	C10-C11-C12-C13
25	D	411	LHG	C2-C3-O3-P
15	B	601	CLA	C8-C10-C11-C12
15	C	508	CLA	C8-C10-C11-C12
22	H	101	DGD	CCB-CDB-CEB-CFB
15	B	601	CLA	C16-C17-C18-C19
15	B	605	CLA	CHA-CBD-CGD-O1D
15	B	605	CLA	CHA-CBD-CGD-O2D
15	B	608	CLA	CHA-CBD-CGD-O2D
15	B	609	CLA	CHA-CBD-CGD-O1D
15	B	609	CLA	CHA-CBD-CGD-O2D
15	B	612	CLA	CHA-CBD-CGD-O1D
15	B	616	CLA	CHA-CBD-CGD-O1D
15	C	503	CLA	CHA-CBD-CGD-O1D
15	C	503	CLA	CHA-CBD-CGD-O2D
15	C	505	CLA	CHA-CBD-CGD-O1D
15	C	505	CLA	CHA-CBD-CGD-O2D
15	C	507	CLA	CHA-CBD-CGD-O1D
15	C	507	CLA	CHA-CBD-CGD-O2D
15	C	512	CLA	CHA-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	A	409	SQD	C2-C1-O6-C44
15	D	402	CLA	C2C-C3C-CAC-CBC
18	B	620	SQD	O6-C44-C45-O47
18	X	101	SQD	O47-C45-C46-O48
15	B	604	CLA	CBA-CGA-O2A-C1
25	L	101	LHG	O1-C1-C2-O2
15	B	611	CLA	C4-C3-C5-C6
19	D	408	PL9	C4-C3-C7-C8
25	L	101	LHG	O9-C7-O7-C5
15	B	609	CLA	C11-C10-C8-C9
18	A	409	SQD	C5-C6-S-O8
17	C	519	BCR	C36-C18-C19-C20
20	D	412	LMG	C37-C38-C39-C40
25	L	101	LHG	O1-C1-C2-C3
20	B	621	LMG	C32-C33-C34-C35
15	B	607	CLA	C1A-C2A-CAA-CBA
15	C	504	CLA	C1A-C2A-CAA-CBA
15	C	510	CLA	C16-C17-C18-C19
18	B	620	SQD	C32-C33-C34-C35
15	C	507	CLA	C2-C1-O2A-CGA
15	B	612	CLA	CBD-CGD-O2D-CED
18	A	409	SQD	C28-C29-C30-C31
18	A	407	SQD	C12-C13-C14-C15
25	D	410	LHG	C34-C35-C36-C37
25	D	410	LHG	C3-O3-P-O5
25	D	410	LHG	C4-O6-P-O4
25	L	101	LHG	C3-O3-P-O4
15	D	405	CLA	C15-C16-C17-C18
15	B	604	CLA	C10-C11-C12-C13
15	B	605	CLA	CAD-CBD-CGD-O1D
15	B	609	CLA	CAD-CBD-CGD-O1D
15	B	612	CLA	CAD-CBD-CGD-O1D
15	C	503	CLA	CAD-CBD-CGD-O1D
15	C	505	CLA	CAD-CBD-CGD-O1D
15	C	507	CLA	CAD-CBD-CGD-O1D
15	C	513	CLA	CAD-CBD-CGD-O1D
18	A	409	SQD	O5-C5-C6-S
18	T	103	SQD	C5-C6-S-O7
21	B	622	LMT	O5'-C5'-C6'-O6'
20	C	501	LMG	C37-C38-C39-C40
18	C	518	SQD	C29-C30-C31-C32
15	B	607	CLA	C16-C17-C18-C19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	B	602	CLA	C6-C7-C8-C10
15	B	607	CLA	C12-C13-C15-C16
15	B	608	CLA	C12-C13-C15-C16
15	B	609	CLA	C6-C7-C8-C10
15	B	611	CLA	C2-C3-C5-C6
15	B	611	CLA	C6-C7-C8-C10
15	C	510	CLA	C11-C10-C8-C7
15	C	510	CLA	C11-C12-C13-C15
15	D	406	CLA	C6-C7-C8-C10
26	E	101	HEM	C2A-CAA-CBA-CGA
15	B	604	CLA	O1A-CGA-O2A-C1
15	C	511	CLA	C16-C17-C18-C20
22	H	101	DGD	C4E-C5E-C6E-O5E
25	D	409	LHG	C7-C8-C9-C10
18	T	101	SQD	O6-C44-C45-O47
25	D	411	LHG	O7-C5-C6-O8
18	B	620	SQD	C12-C13-C14-C15
25	D	409	LHG	C29-C30-C31-C32
15	B	603	CLA	C14-C13-C15-C16
15	B	608	CLA	C3-C5-C6-C7
15	C	510	CLA	C16-C17-C18-C20
15	D	405	CLA	C16-C17-C18-C19
25	D	411	LHG	C16-C17-C18-C19
15	D	402	CLA	C2A-CAA-CBA-CGA
20	C	501	LMG	C13-C14-C15-C16
19	D	408	PL9	C47-C48-C49-C50
27	I	101	FME	CB-CG-SD-CE
20	D	412	LMG	C14-C15-C16-C17
22	H	101	DGD	O2G-C1B-C2B-C3B
25	D	409	LHG	C35-C36-C37-C38
15	B	603	CLA	C2-C1-O2A-CGA
15	B	616	CLA	C2-C1-O2A-CGA
15	D	405	CLA	CAA-CBA-CGA-O2A
15	B	615	CLA	O1A-CGA-O2A-C1
15	B	611	CLA	C13-C15-C16-C17
18	A	407	SQD	C18-C19-C20-C21
17	B	617	BCR	C23-C24-C25-C26
17	B	617	BCR	C23-C24-C25-C30
17	C	519	BCR	C23-C24-C25-C30
22	H	101	DGD	CAB-CBB-CCB-CDB
18	A	407	SQD	C10-C11-C12-C13
16	D	403	PHO	C16-C17-C18-C19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	X	101	SQD	C10-C11-C12-C13
25	D	409	LHG	C4-O6-P-O3
25	L	101	LHG	C4-O6-P-O3
16	D	403	PHO	CHA-CBD-CGD-O2D
15	B	615	CLA	CBA-CGA-O2A-C1
18	X	101	SQD	C44-C45-C46-O48
20	B	621	LMG	C7-C8-C9-O8
18	T	101	SQD	C30-C31-C32-C33
15	C	514	CLA	C12-C13-C15-C16
15	B	602	CLA	C6-C7-C8-C9
15	B	608	CLA	C14-C13-C15-C16
15	B	611	CLA	C6-C7-C8-C9
15	B	613	CLA	C6-C7-C8-C9
15	C	506	CLA	C6-C7-C8-C9
15	B	613	CLA	C16-C17-C18-C20
15	C	503	CLA	C16-C17-C18-C20
15	B	605	CLA	C8-C10-C11-C12
18	T	101	SQD	C11-C10-C9-C8
15	B	612	CLA	C15-C16-C17-C18
17	C	519	BCR	C17-C18-C19-C20
18	X	101	SQD	C28-C29-C30-C31
21	B	623	LMT	C6-C7-C8-C9
15	C	504	CLA	C5-C6-C7-C8
17	C	515	BCR	C9-C10-C11-C12
17	D	407	BCR	C9-C10-C11-C12
17	D	407	BCR	C15-C16-C17-C18
25	D	411	LHG	C32-C33-C34-C35
15	B	612	CLA	O1D-CGD-O2D-CED
18	B	620	SQD	C26-C27-C28-C29
18	A	409	SQD	C7-C8-C9-C10
15	D	405	CLA	C2-C1-O2A-CGA
15	B	608	CLA	C16-C17-C18-C20
20	B	621	LMG	C34-C35-C36-C37
15	B	603	CLA	C2A-CAA-CBA-CGA
15	B	609	CLA	C3A-C2A-CAA-CBA
25	L	101	LHG	C13-C14-C15-C16
25	D	409	LHG	C24-C25-C26-C27
15	B	608	CLA	C11-C12-C13-C14
18	C	518	SQD	C32-C33-C34-C35
15	B	601	CLA	O1D-CGD-O2D-CED
20	C	501	LMG	O9-C10-O7-C8
18	T	103	SQD	C26-C27-C28-C29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	D	410	LHG	C9-C10-C11-C12
25	D	409	LHG	C31-C32-C33-C34
15	B	607	CLA	C16-C17-C18-C20
16	D	403	PHO	C16-C17-C18-C20
15	C	510	CLA	C8-C10-C11-C12
25	D	409	LHG	C34-C35-C36-C37
15	D	402	CLA	C4C-C3C-CAC-CBC
15	A	402	CLA	C1A-C2A-CAA-CBA
15	B	608	CLA	C1A-C2A-CAA-CBA
15	B	601	CLA	C6-C7-C8-C10
15	B	603	CLA	C11-C12-C13-C15
15	C	504	CLA	O1A-CGA-O2A-C1
17	B	618	BCR	C9-C10-C11-C12
25	D	410	LHG	C10-C11-C12-C13
15	C	504	CLA	CBA-CGA-O2A-C1
18	B	620	SQD	C10-C11-C12-C13
22	C	517	DGD	CDB-CEB-CFB-CGB
25	D	411	LHG	C9-C10-C11-C12
25	D	409	LHG	C19-C20-C21-C22
18	A	407	SQD	O47-C45-C46-O48
17	C	515	BCR	C19-C20-C21-C22
17	X	102	BCR	C13-C14-C15-C16
15	B	603	CLA	C8-C10-C11-C12
18	A	409	SQD	C10-C11-C12-C13
15	C	511	CLA	C4-C3-C5-C6
16	A	404	PHO	C2-C1-O2A-CGA
20	C	501	LMG	C14-C15-C16-C17
25	D	409	LHG	C32-C33-C34-C35
25	L	101	LHG	C26-C27-C28-C29
15	C	509	CLA	C2A-CAA-CBA-CGA
17	B	619	BCR	C9-C10-C11-C12
15	B	603	CLA	C4-C3-C5-C6
19	D	408	PL9	C45-C44-C46-C47
15	C	504	CLA	C10-C11-C12-C13
18	X	101	SQD	C25-C26-C27-C28
18	C	518	SQD	C45-C44-O6-C1
18	X	101	SQD	C45-C44-O6-C1
20	D	412	LMG	C8-C7-O1-C1
20	B	621	LMG	C14-C15-C16-C17
18	X	101	SQD	C29-C30-C31-C32
25	L	101	LHG	C10-C11-C12-C13
15	C	503	CLA	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	B	609	CLA	C2-C3-C5-C6
25	L	101	LHG	O7-C5-C6-O8
25	D	410	LHG	O8-C23-C24-C25
15	C	503	CLA	C16-C17-C18-C19
15	C	502	CLA	CAA-CBA-CGA-O2A
15	B	601	CLA	C6-C7-C8-C9
15	B	603	CLA	C11-C12-C13-C14
15	B	606	CLA	C11-C10-C8-C9
15	B	607	CLA	C14-C13-C15-C16
15	C	503	CLA	C11-C12-C13-C14
15	C	510	CLA	C11-C10-C8-C9
18	A	407	SQD	C11-C12-C13-C14
15	C	509	CLA	C5-C6-C7-C8
15	B	603	CLA	O1A-CGA-O2A-C1
20	C	501	LMG	O8-C28-C29-C30
15	B	603	CLA	CAD-CBD-CGD-O2D
15	B	604	CLA	CAD-CBD-CGD-O2D
15	B	610	CLA	CAD-CBD-CGD-O2D
15	C	510	CLA	CAD-CBD-CGD-O2D
15	B	613	CLA	C16-C17-C18-C19
15	C	502	CLA	C2A-CAA-CBA-CGA
15	C	511	CLA	C2A-CAA-CBA-CGA
15	B	604	CLA	C2-C1-O2A-CGA
15	B	602	CLA	CAA-CBA-CGA-O2A
19	D	408	PL9	C28-C29-C31-C32
15	C	504	CLA	CAA-CBA-CGA-O2A
15	C	509	CLA	CAA-CBA-CGA-O2A
16	D	403	PHO	C2C-C3C-CAC-CBC
25	L	101	LHG	O6-C4-C5-O7
22	C	517	DGD	O2G-C1B-C2B-C3B
21	B	622	LMT	C5-C6-C7-C8
21	B	622	LMT	O5B-C1B-O1B-C4'
15	B	608	CLA	C16-C17-C18-C19
15	B	614	CLA	C6-C7-C8-C9
15	B	602	CLA	CHA-CBD-CGD-O1D
15	B	602	CLA	CHA-CBD-CGD-O2D
15	B	612	CLA	CHA-CBD-CGD-O2D
15	C	508	CLA	CHA-CBD-CGD-O1D
15	C	513	CLA	CHA-CBD-CGD-O1D
15	C	507	CLA	CAA-CBA-CGA-O2A
25	D	409	LHG	O8-C23-C24-C25
18	T	103	SQD	O47-C45-C46-O48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	D	405	CLA	CBA-CGA-O2A-C1
15	D	402	CLA	C15-C16-C17-C18
15	B	608	CLA	CAA-CBA-CGA-O2A
15	C	506	CLA	CAA-CBA-CGA-O2A
18	A	409	SQD	O48-C23-C24-C25
15	B	601	CLA	CBD-CGD-O2D-CED
15	B	605	CLA	C11-C12-C13-C14
18	T	103	SQD	C25-C26-C27-C28
25	L	101	LHG	C30-C31-C32-C33
18	T	101	SQD	C4-C5-C6-S
16	A	404	PHO	C10-C11-C12-C13
20	C	501	LMG	C39-C40-C41-C42
15	C	504	CLA	CAA-CBA-CGA-O1A
17	B	619	BCR	C21-C22-C23-C24
15	B	612	CLA	C13-C15-C16-C17
15	B	609	CLA	C1A-C2A-CAA-CBA
15	C	506	CLA	C1A-C2A-CAA-CBA
25	D	409	LHG	O10-C23-C24-C25
18	A	407	SQD	C17-C18-C19-C20
25	D	411	LHG	C25-C26-C27-C28
15	B	603	CLA	CBA-CGA-O2A-C1
15	B	602	CLA	CAA-CBA-CGA-O1A
15	C	509	CLA	CAA-CBA-CGA-O1A
20	C	501	LMG	O10-C28-C29-C30
25	D	410	LHG	O10-C23-C24-C25
18	A	407	SQD	C44-C45-C46-O48
18	T	101	SQD	O6-C44-C45-C46
15	C	502	CLA	CAA-CBA-CGA-O1A
18	A	409	SQD	O10-C23-C24-C25
15	B	608	CLA	CAA-CBA-CGA-O1A
15	D	405	CLA	O1A-CGA-O2A-C1
22	C	517	DGD	C3B-C4B-C5B-C6B
25	L	101	LHG	C4-O6-P-O5
25	L	101	LHG	O7-C7-C8-C9
15	C	507	CLA	CAA-CBA-CGA-O1A
18	T	101	SQD	O49-C7-C8-C9
15	A	405	CLA	CAD-CBD-CGD-O1D
15	B	610	CLA	CAD-CBD-CGD-O1D
18	T	101	SQD	O5-C5-C6-S
18	T	101	SQD	C5-C6-S-O9
26	E	101	HEM	C4D-C3D-CAD-CBD
20	B	621	LMG	C31-C32-C33-C34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	C	506	CLA	C11-C12-C13-C14
15	A	405	CLA	CAA-CBA-CGA-O2A
20	C	501	LMG	O7-C10-C11-C12
15	B	602	CLA	C11-C10-C8-C7
15	B	603	CLA	C2-C3-C5-C6
15	B	605	CLA	C11-C12-C13-C15
15	B	612	CLA	C11-C10-C8-C7
15	B	613	CLA	C11-C10-C8-C7
15	C	513	CLA	C11-C12-C13-C15
15	C	506	CLA	CAA-CBA-CGA-O1A
25	D	411	LHG	C14-C15-C16-C17
22	C	517	DGD	O6D-C5D-C6D-O5D
15	B	601	CLA	CAA-CBA-CGA-O2A
15	C	514	CLA	CAA-CBA-CGA-O2A
15	C	513	CLA	C3-C5-C6-C7
17	B	618	BCR	C11-C12-C13-C14
25	L	101	LHG	O9-C7-C8-C9
15	C	503	CLA	CAA-CBA-CGA-O2A
15	B	616	CLA	CAA-CBA-CGA-O2A
18	B	620	SQD	O48-C23-C24-C25
18	X	101	SQD	O47-C7-C8-C9
15	B	606	CLA	C11-C12-C13-C14
15	C	512	CLA	CAA-CBA-CGA-O2A
15	B	612	CLA	C8-C10-C11-C12
15	C	514	CLA	CAA-CBA-CGA-O1A
20	C	501	LMG	O9-C10-C11-C12
15	B	609	CLA	C4-C3-C5-C6
15	D	405	CLA	C4-C3-C5-C6

There are no ring outliers.

66 monomers are involved in 267 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	D	403	PHO	4	0
20	D	412	LMG	2	0
15	C	512	CLA	4	0
25	D	410	LHG	6	0
17	B	619	BCR	2	0
15	C	502	CLA	7	0
15	B	607	CLA	6	0
17	C	516	BCR	5	0
25	D	411	LHG	9	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	A	406	BCR	5	0
15	A	403	CLA	2	0
15	B	605	CLA	6	0
15	B	601	CLA	6	0
15	B	610	CLA	6	0
15	C	513	CLA	4	0
15	C	508	CLA	5	0
15	D	402	CLA	6	0
15	C	506	CLA	11	0
18	T	101	SQD	4	0
21	B	622	LMT	3	0
20	B	621	LMG	3	0
18	B	620	SQD	4	0
18	T	103	SQD	2	0
15	B	602	CLA	4	0
15	B	616	CLA	3	0
25	D	409	LHG	6	0
15	C	503	CLA	3	0
15	B	606	CLA	5	0
18	X	101	SQD	4	0
15	D	406	CLA	4	0
15	D	405	CLA	6	0
15	A	405	CLA	3	0
15	A	402	CLA	5	0
17	B	618	BCR	4	0
15	C	514	CLA	2	0
15	B	609	CLA	5	0
18	A	409	SQD	4	0
15	B	604	CLA	5	0
15	C	511	CLA	10	0
21	B	623	LMT	5	0
15	B	613	CLA	9	0
17	X	102	BCR	7	0
17	D	407	BCR	3	0
15	B	611	CLA	5	0
15	C	509	CLA	5	0
17	C	515	BCR	2	0
15	B	614	CLA	5	0
20	C	501	LMG	8	0
18	A	407	SQD	4	0
26	E	101	HEM	5	0
16	A	404	PHO	6	0

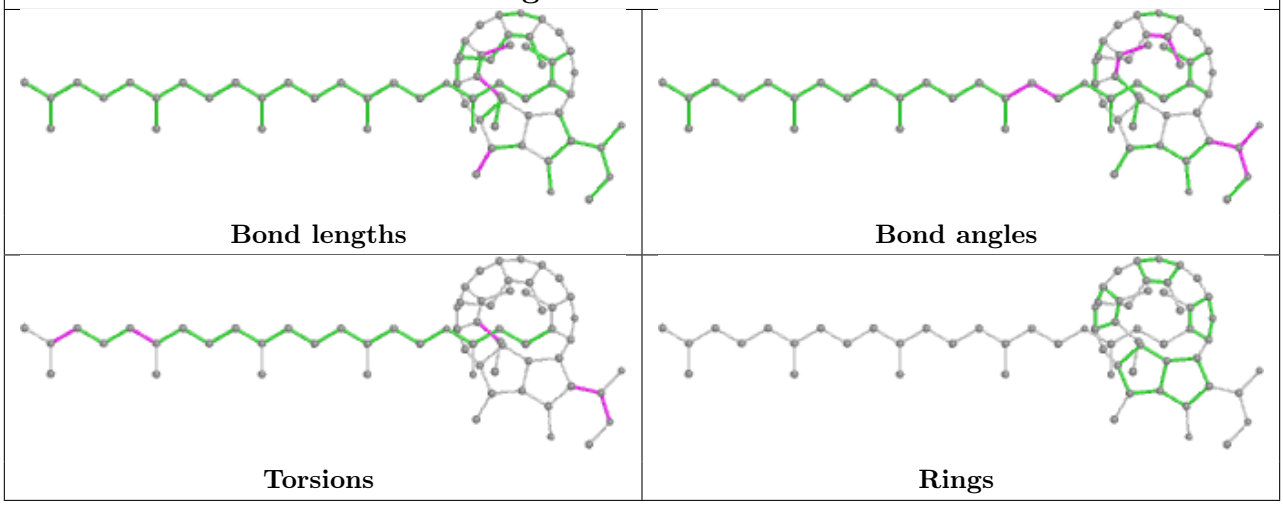
Continued on next page...

Continued from previous page...

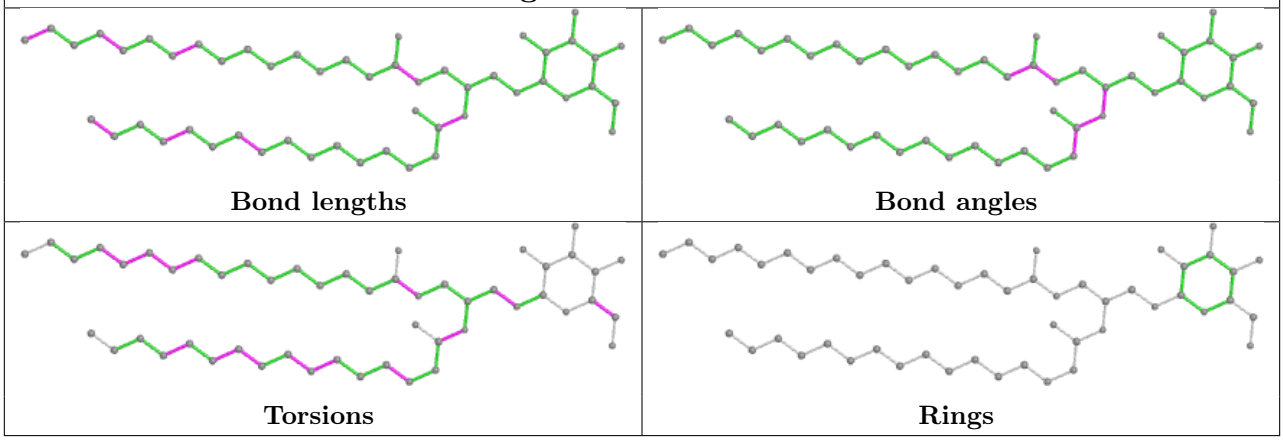
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	408	PL9	1	0
17	B	617	BCR	5	0
22	C	517	DGD	2	0
15	B	612	CLA	6	0
15	B	615	CLA	7	0
15	C	505	CLA	1	0
15	C	510	CLA	5	0
17	C	519	BCR	6	0
25	L	101	LHG	4	0
22	H	101	DGD	4	0
15	C	507	CLA	9	0
15	B	603	CLA	6	0
18	C	518	SQD	5	0
15	C	504	CLA	7	0
15	B	608	CLA	5	0

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.

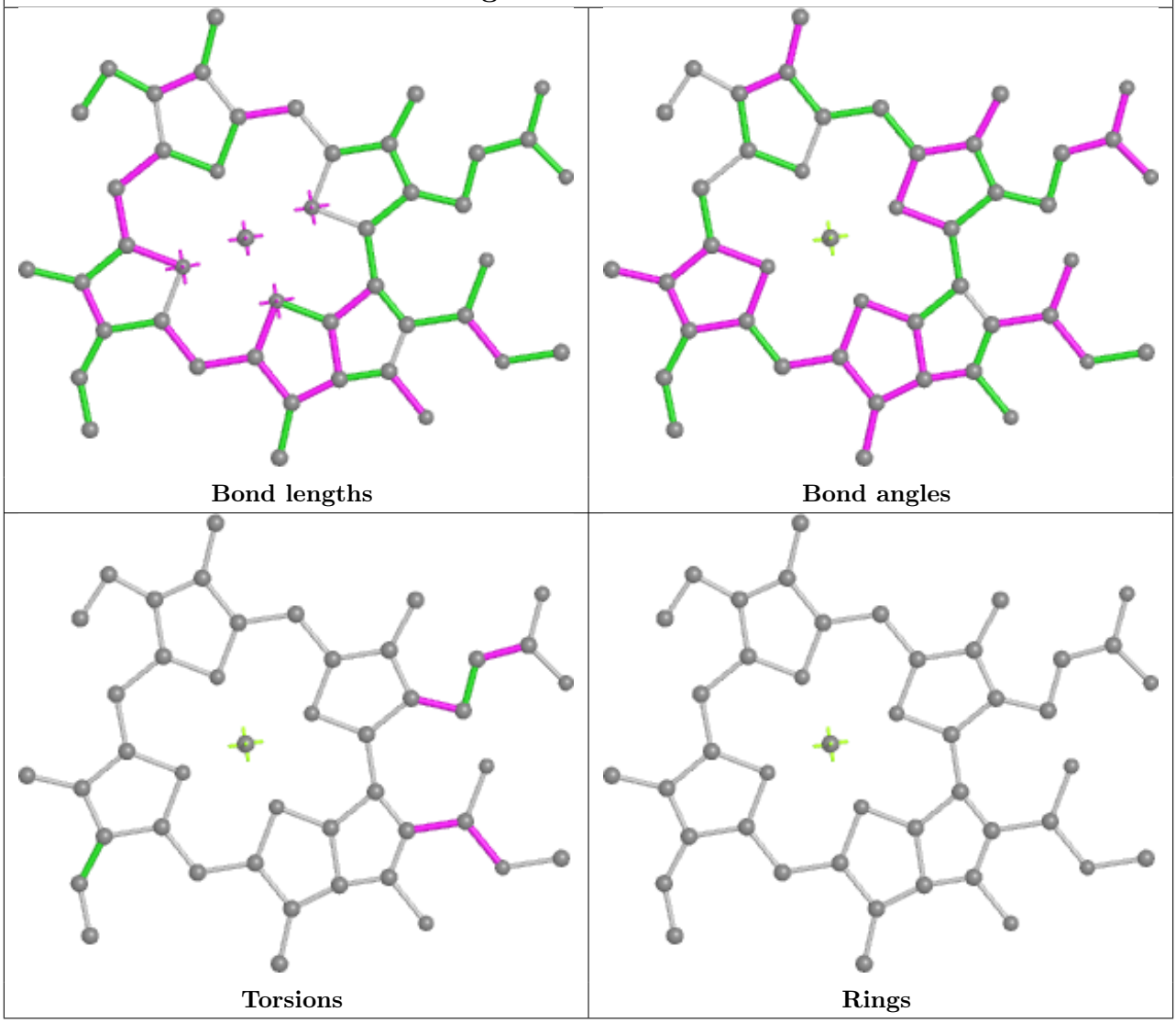
Ligand PHO D 403



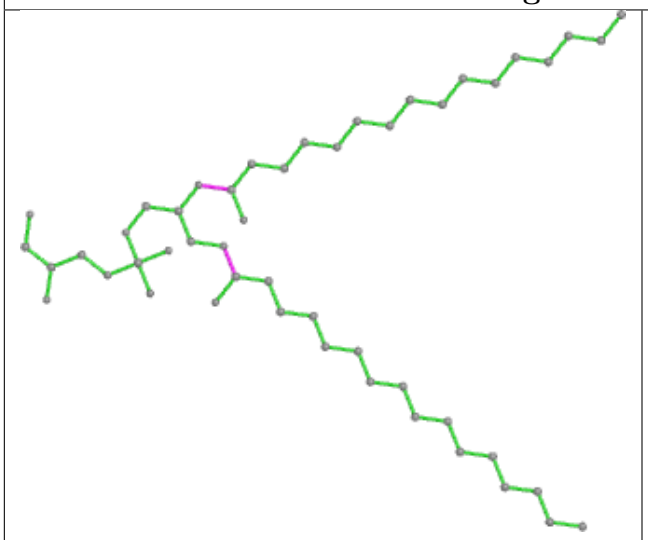
Ligand LMG D 412



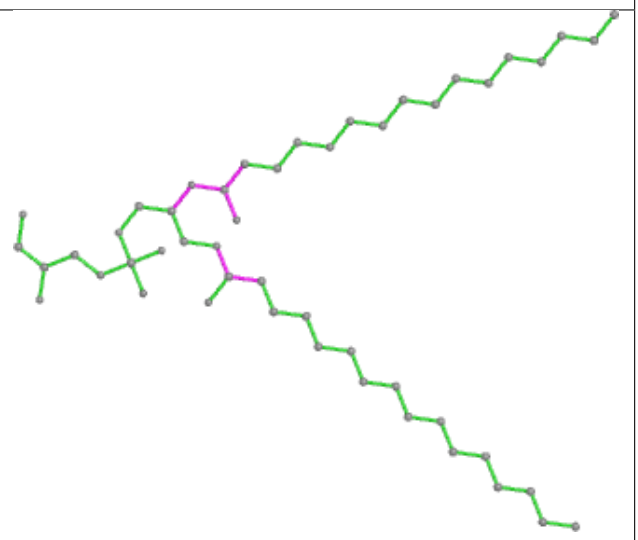
Ligand CLA C 512



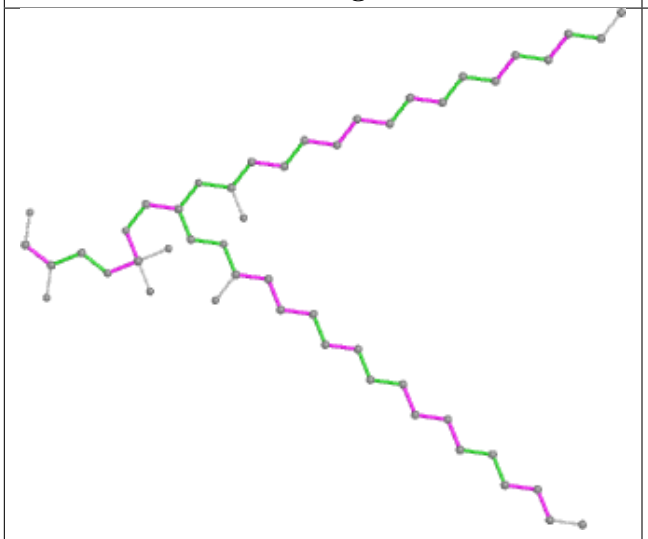
Ligand LHG D 410



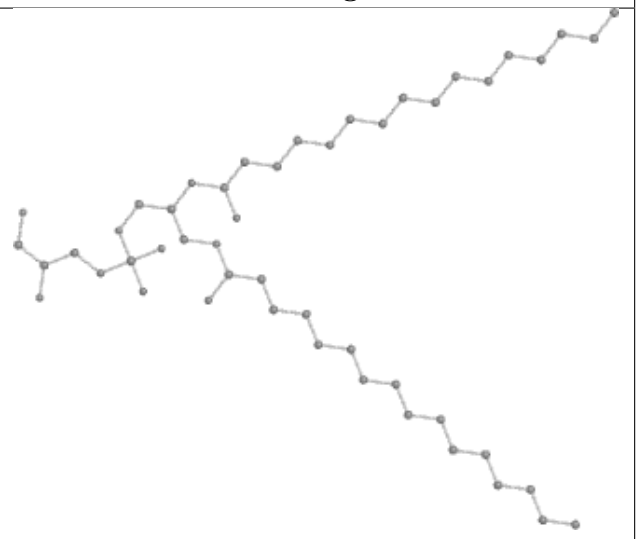
Bond lengths



Bond angles

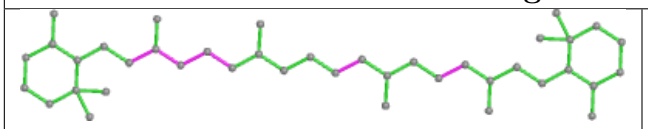


Torsions

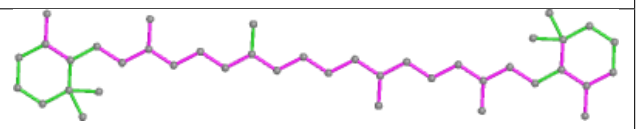


Rings

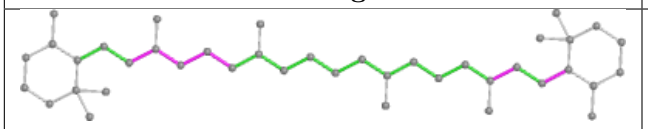
Ligand BCR B 619



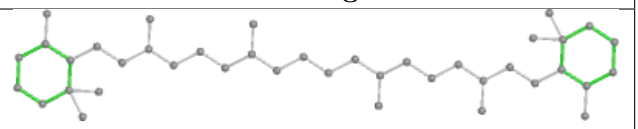
Bond lengths



Bond angles

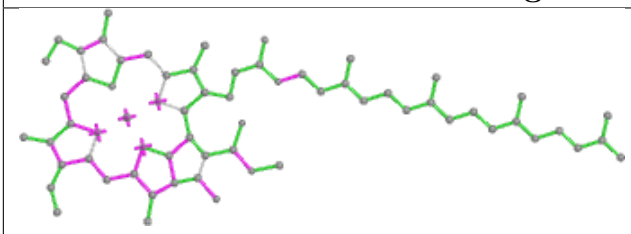


Torsions

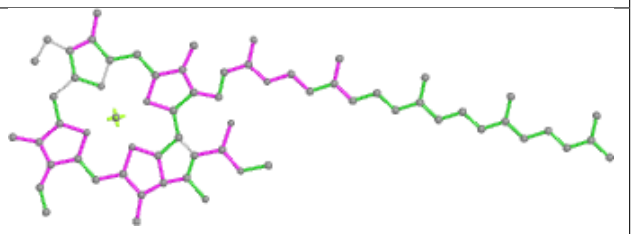


Rings

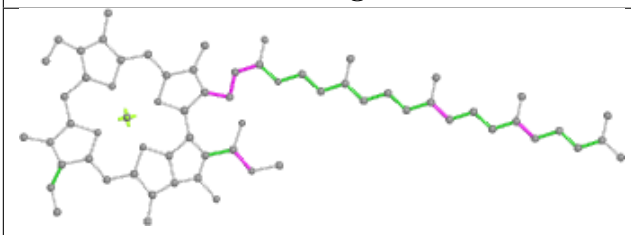
Ligand CLA C 502



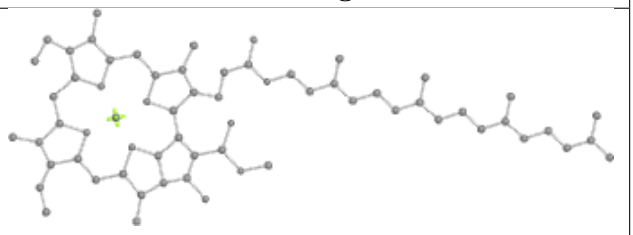
Bond lengths



Bond angles

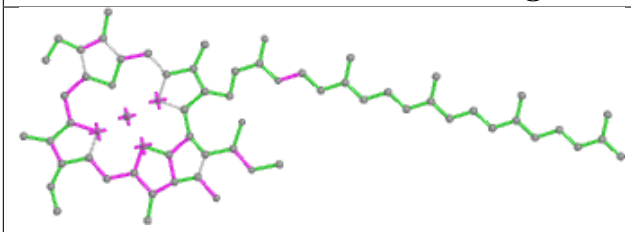


Torsions

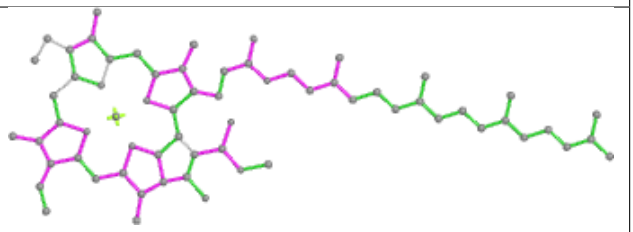


Rings

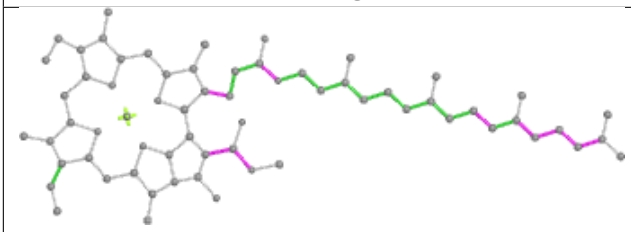
Ligand CLA B 607



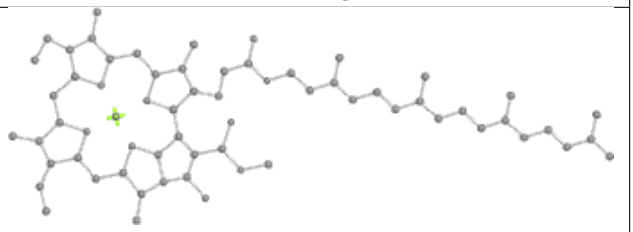
Bond lengths



Bond angles

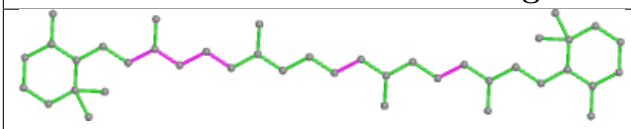


Torsions

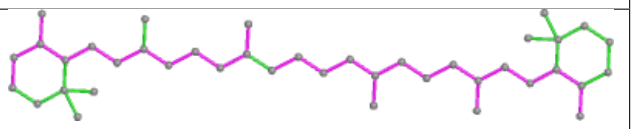


Rings

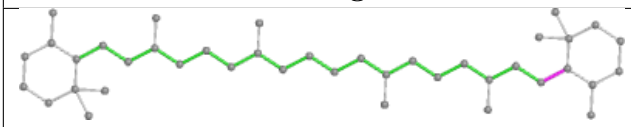
Ligand BCR C 516



Bond lengths



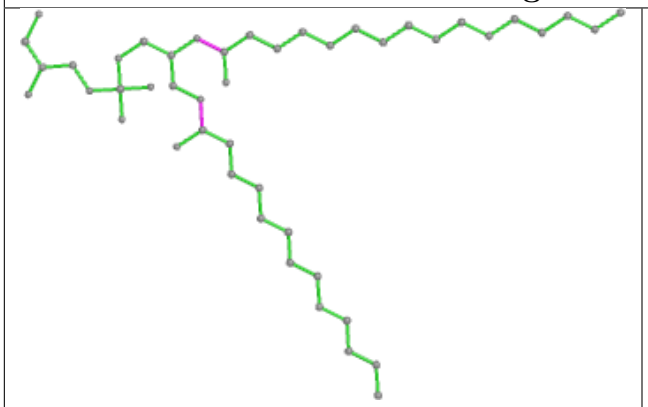
Bond angles



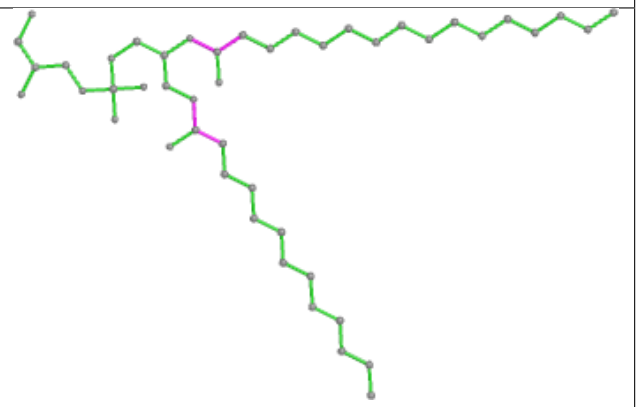
Torsions

Rings

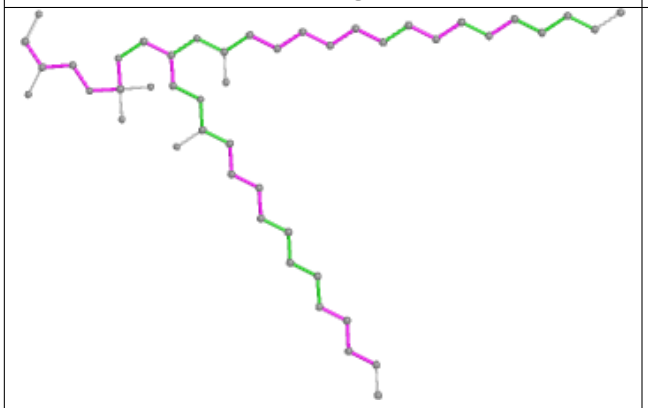
Ligand LHG D 411



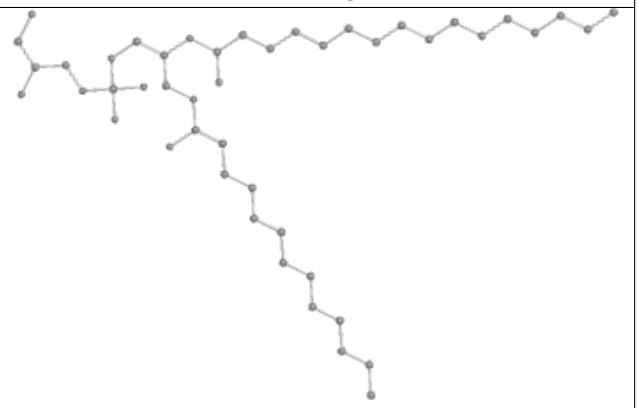
Bond lengths



Bond angles

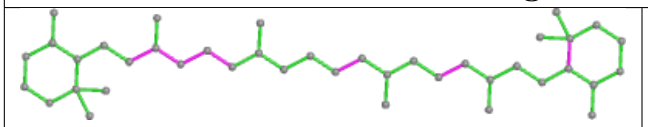


Torsions

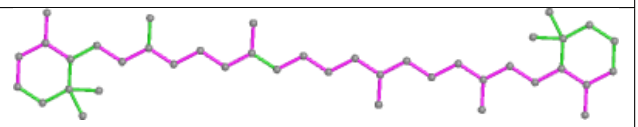


Rings

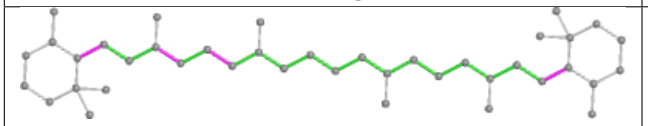
Ligand BCR A 406



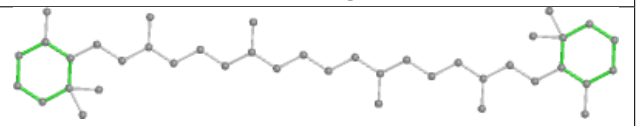
Bond lengths



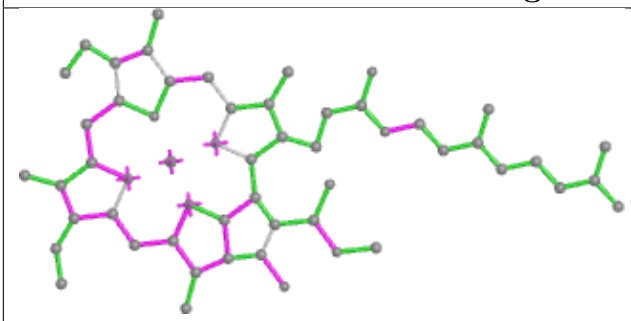
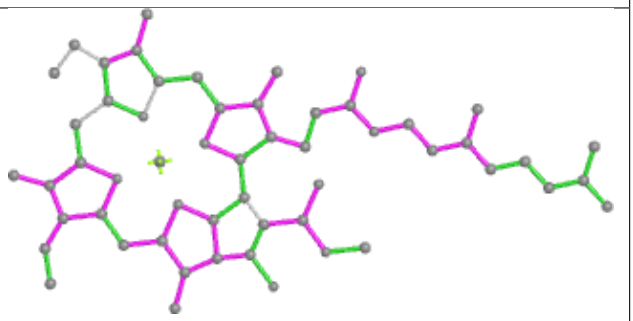
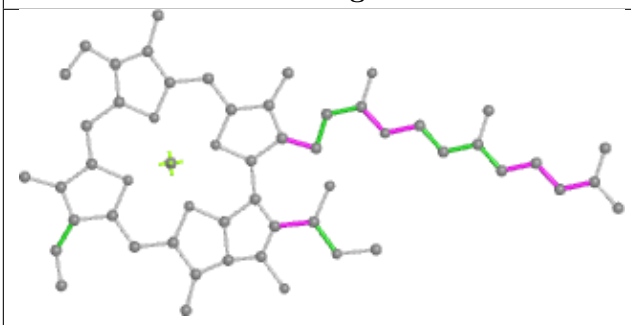
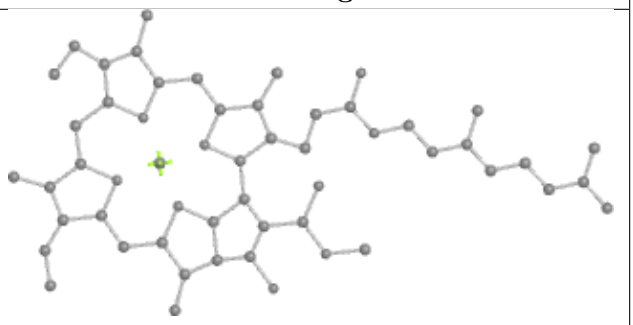
Bond angles

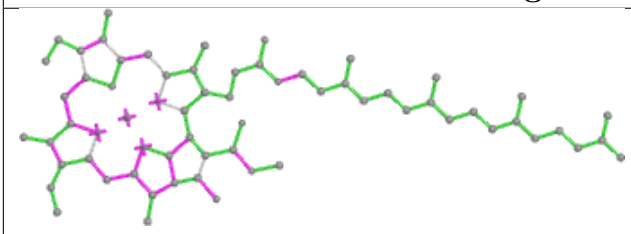
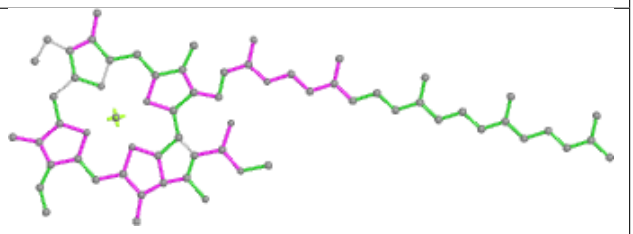
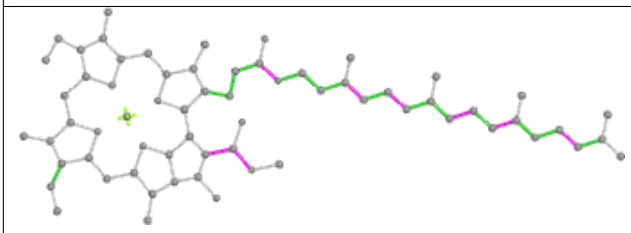
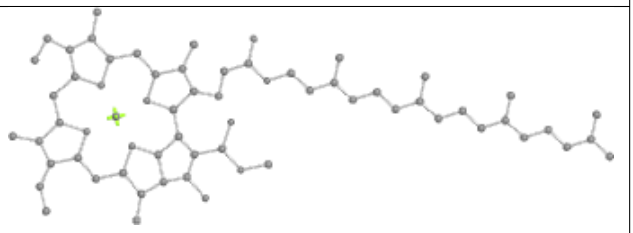


Torsions

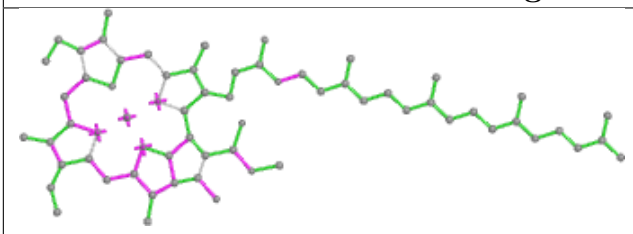


Rings

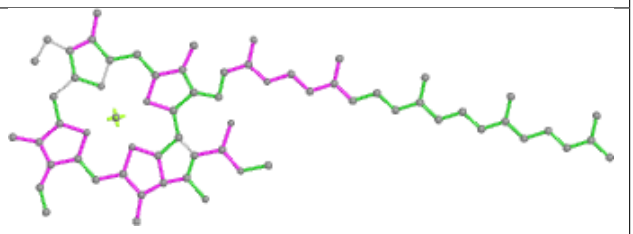
Ligand CLA A 403	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 605	
 Bond lengths	 Bond angles
 Torsions	 Rings

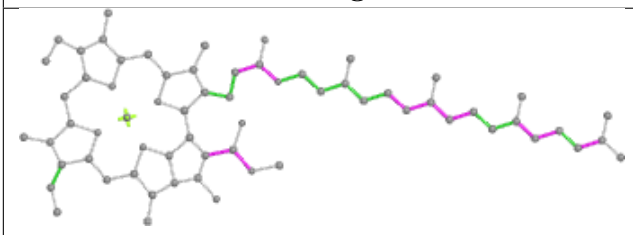
Ligand CLA B 601



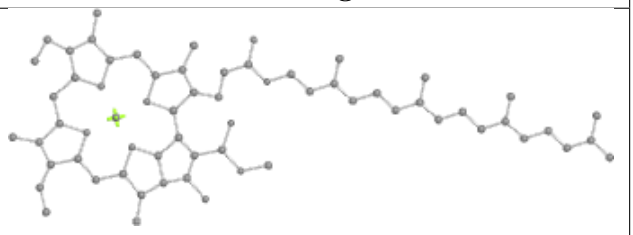
Bond lengths



Bond angles

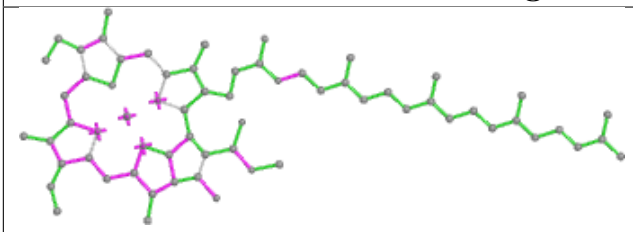


Torsions

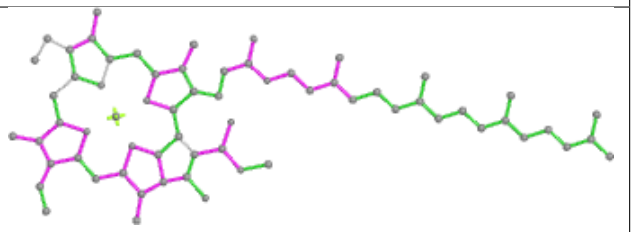


Rings

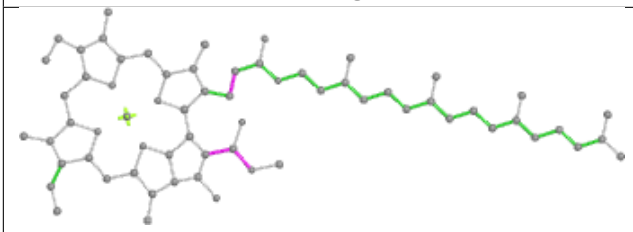
Ligand CLA B 610



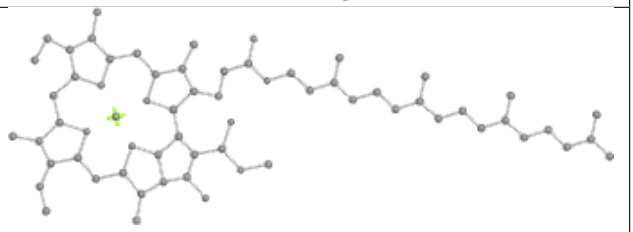
Bond lengths



Bond angles

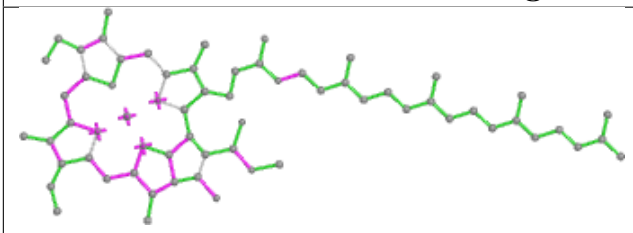


Torsions

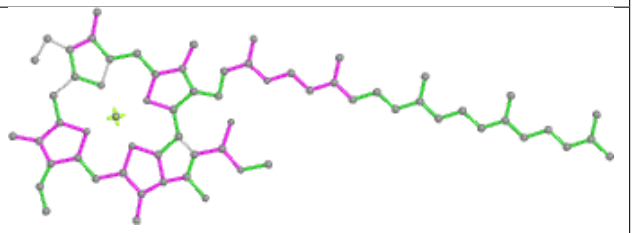


Rings

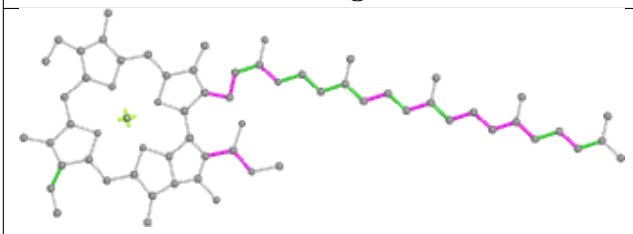
Ligand CLA C 513



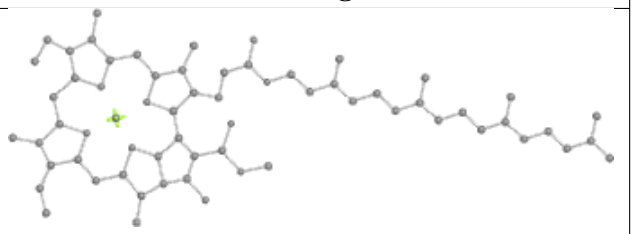
Bond lengths



Bond angles

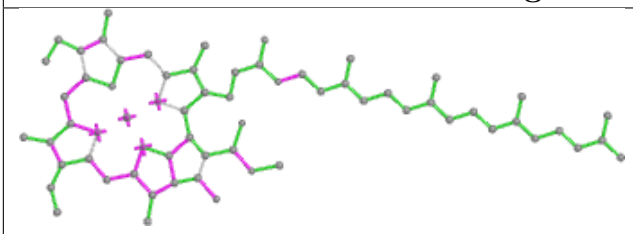


Torsions

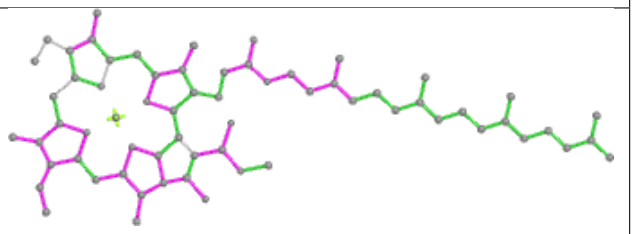


Rings

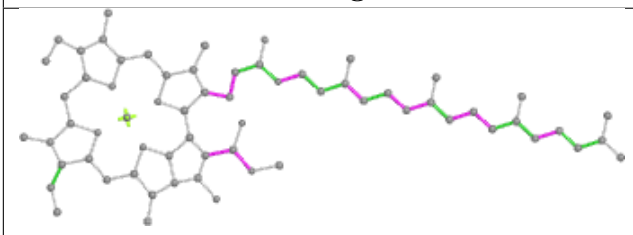
Ligand CLA C 508



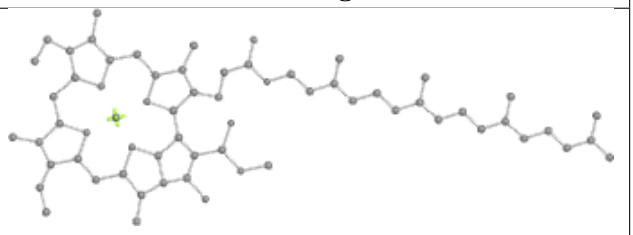
Bond lengths



Bond angles

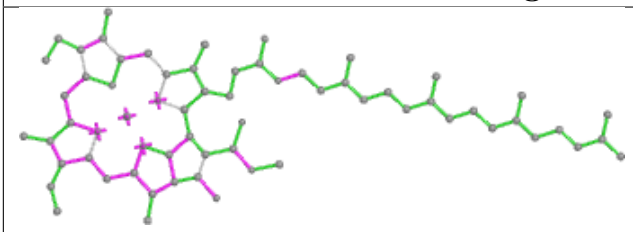


Torsions

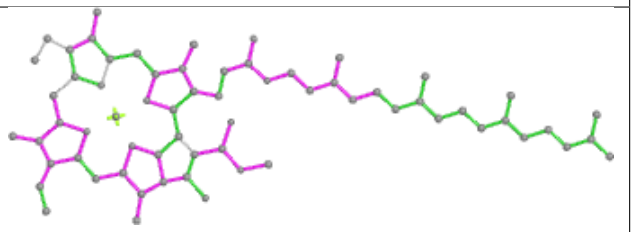


Rings

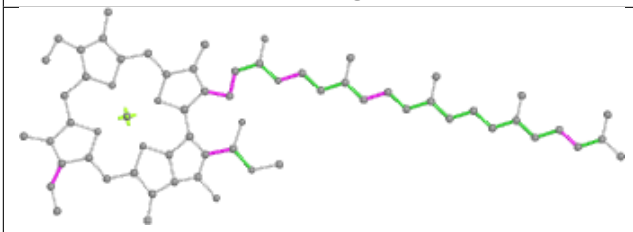
Ligand CLA D 402



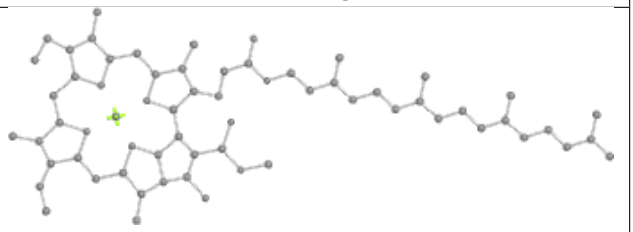
Bond lengths



Bond angles

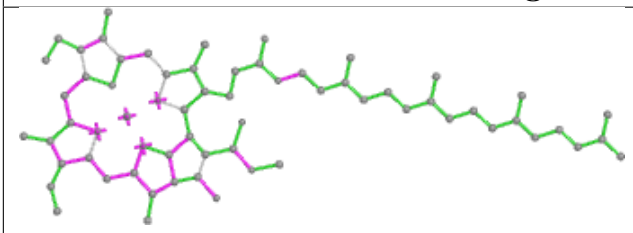


Torsions

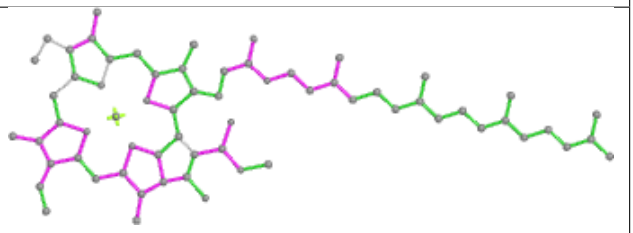


Rings

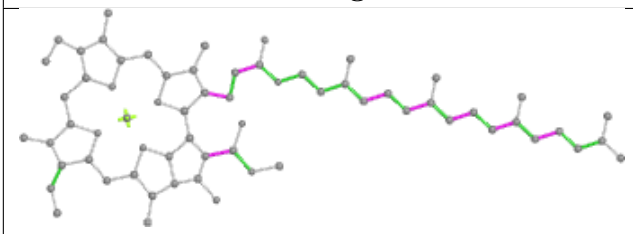
Ligand CLA C 506



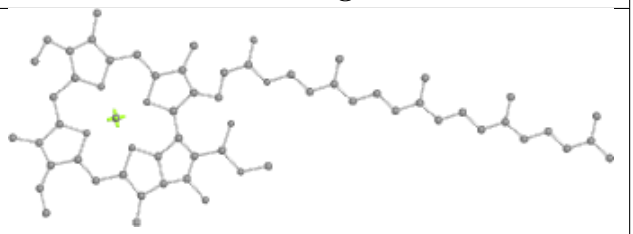
Bond lengths



Bond angles

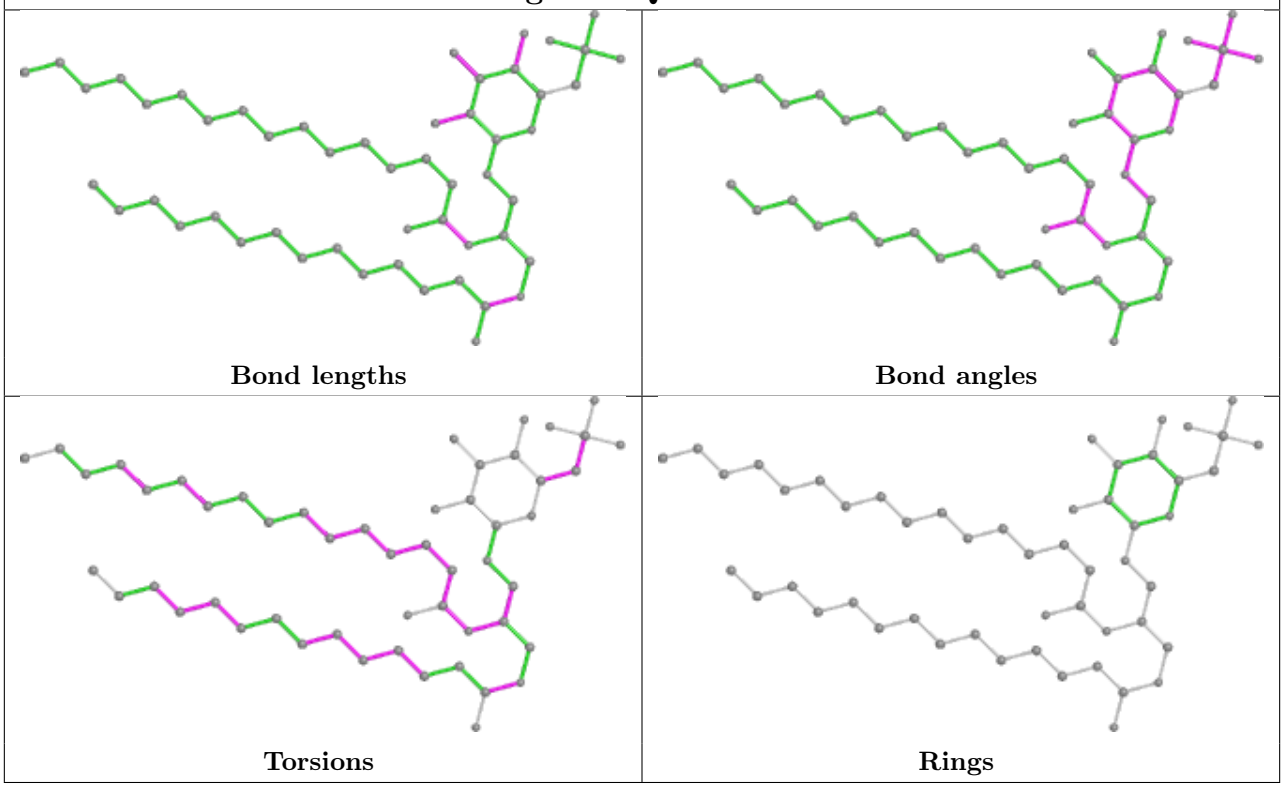


Torsions

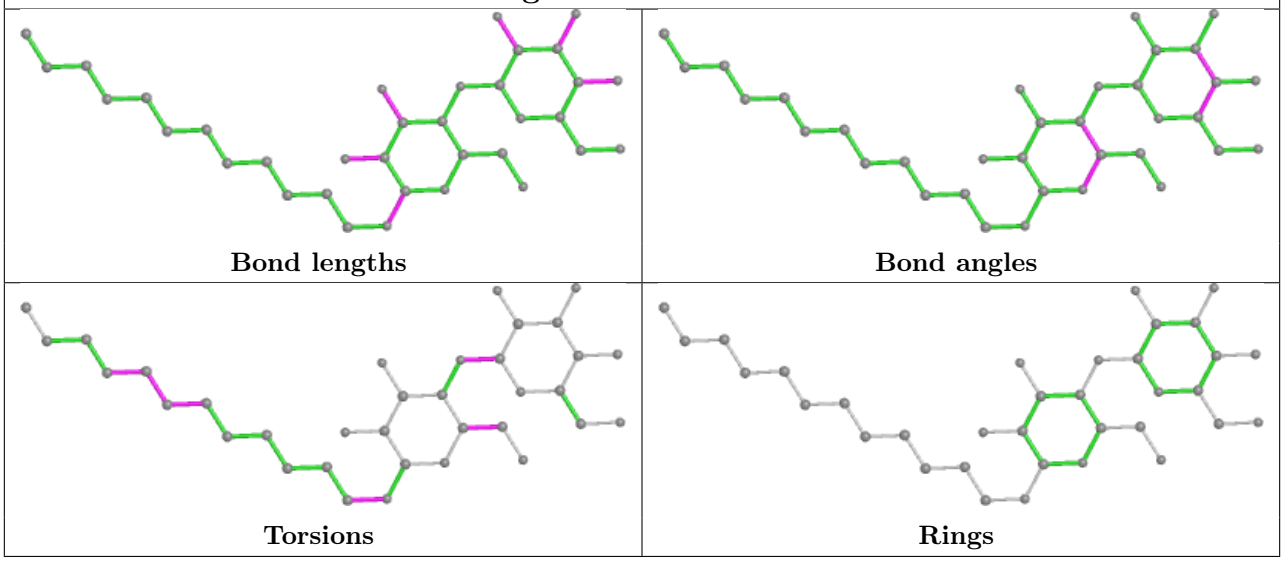


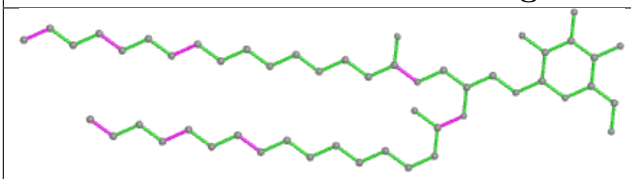
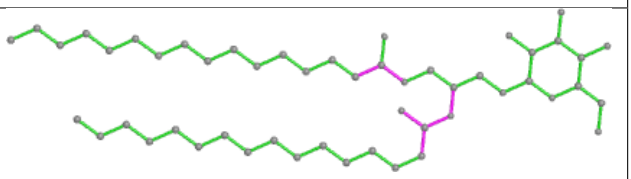
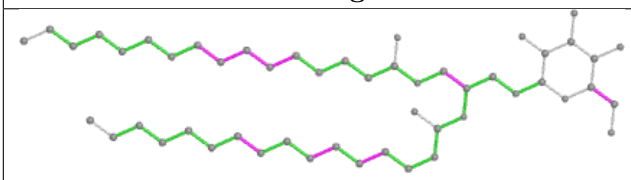
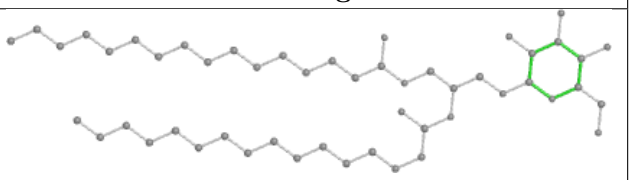
Rings

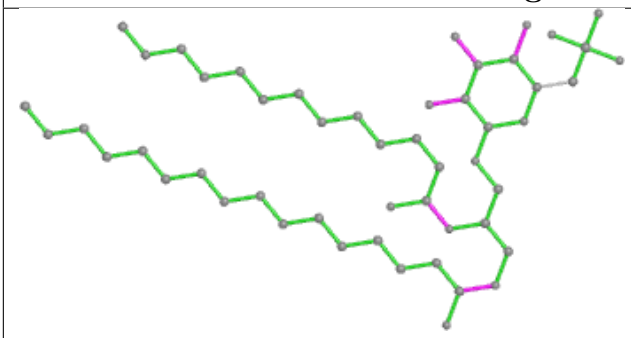
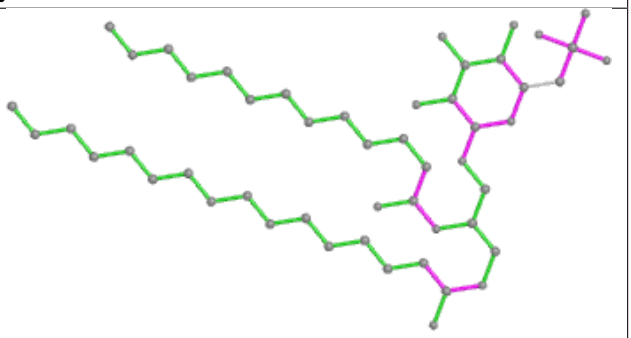
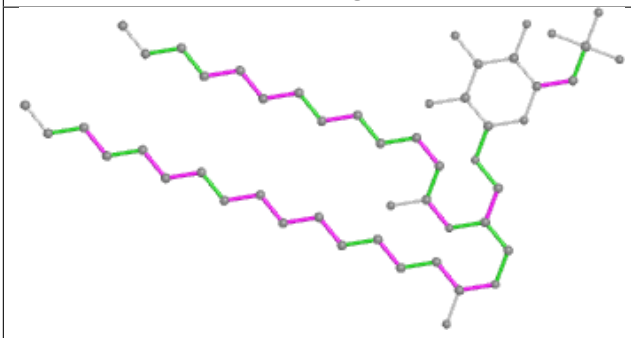
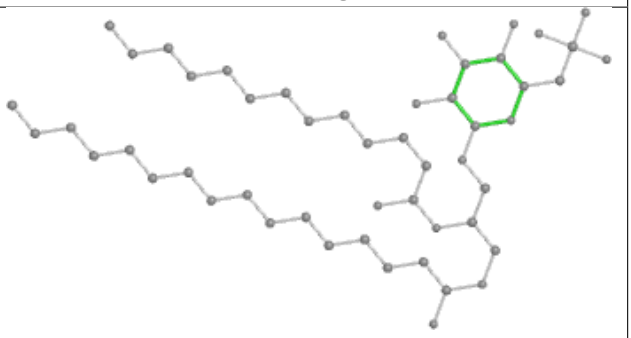
Ligand SQD T 101



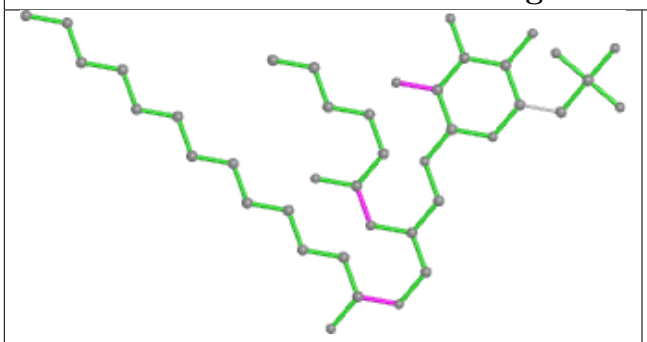
Ligand LMT B 622



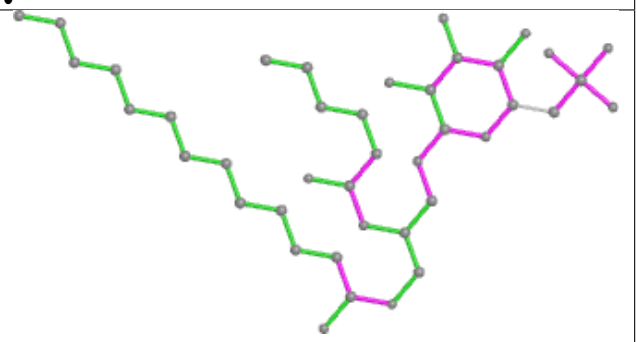
Ligand LMG B 621	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SQD B 620	
 Bond lengths	 Bond angles
 Torsions	 Rings

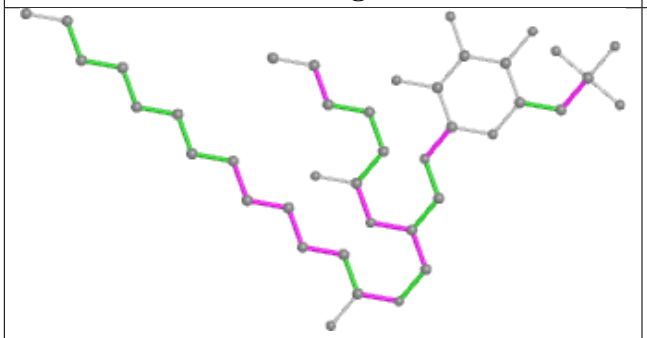
Ligand SQD T 103



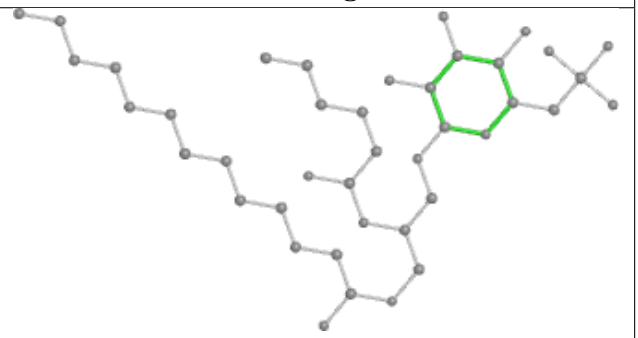
Bond lengths



Bond angles

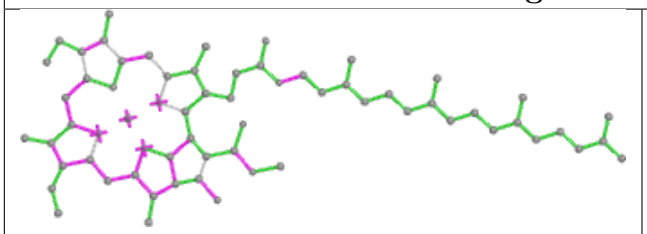


Torsions

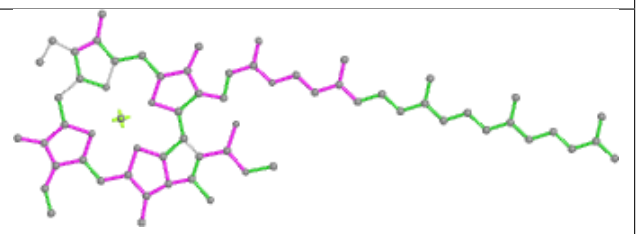


Rings

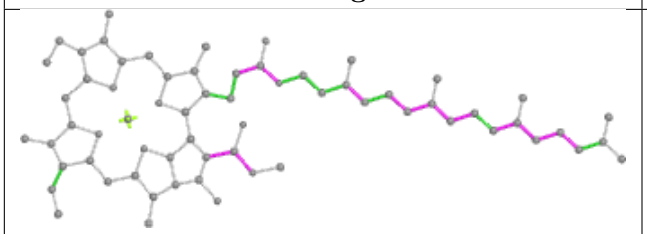
Ligand CLA B 602



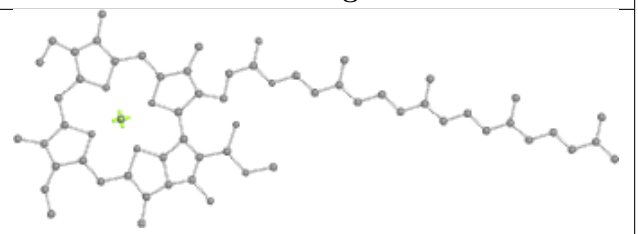
Bond lengths



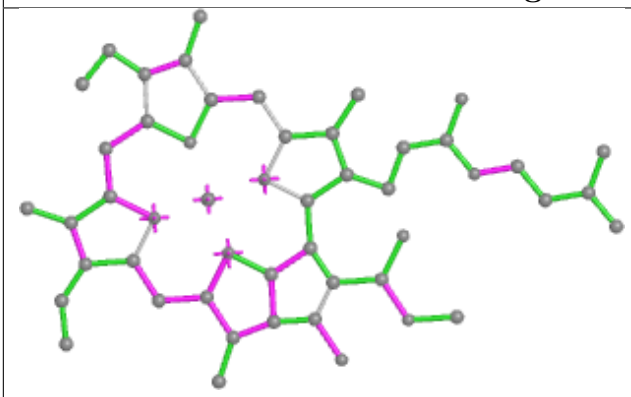
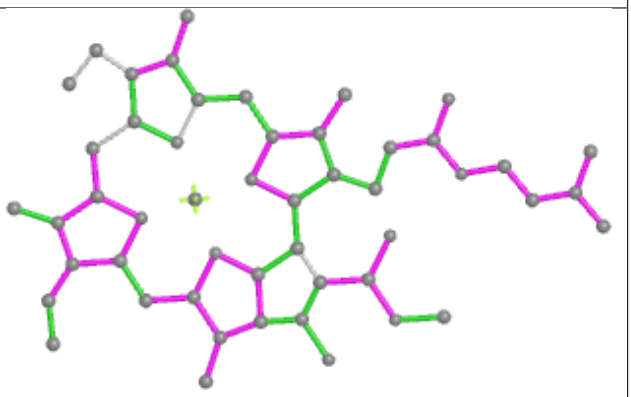
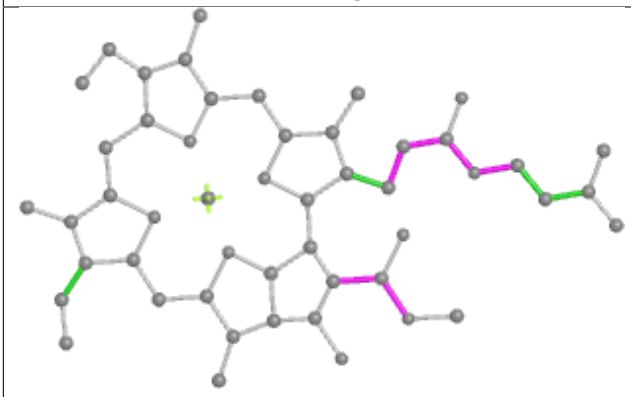
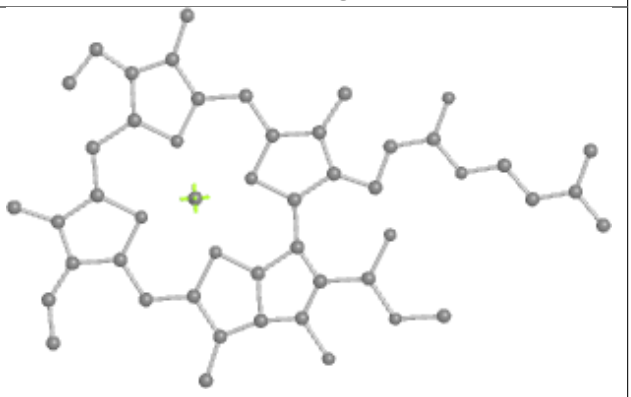
Bond angles



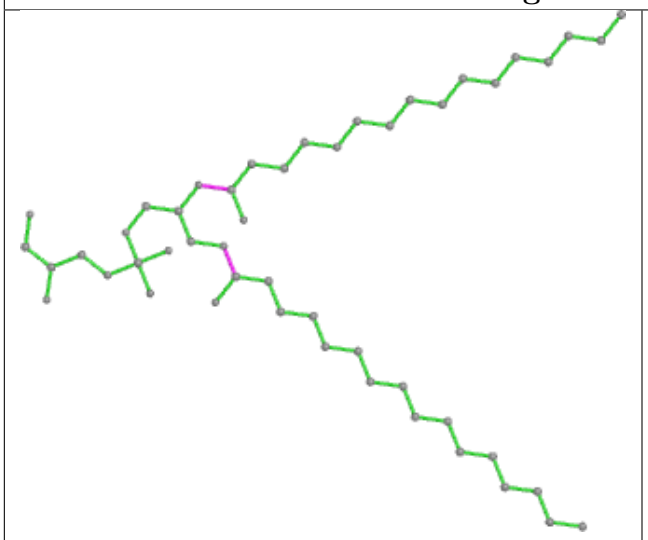
Torsions



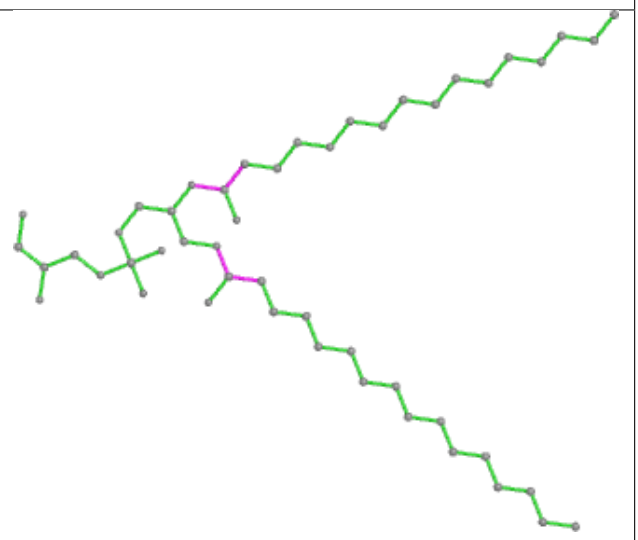
Rings

Ligand CLA B 616	
 Bond lengths	 Bond angles
 Torsions	 Rings

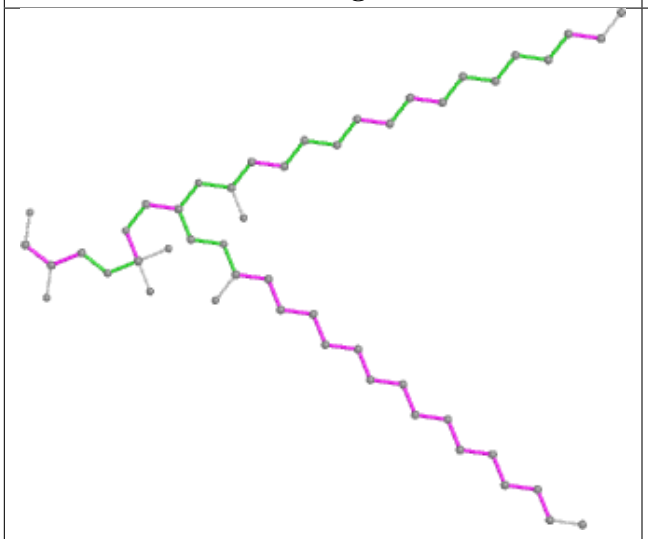
Ligand LHG D 409



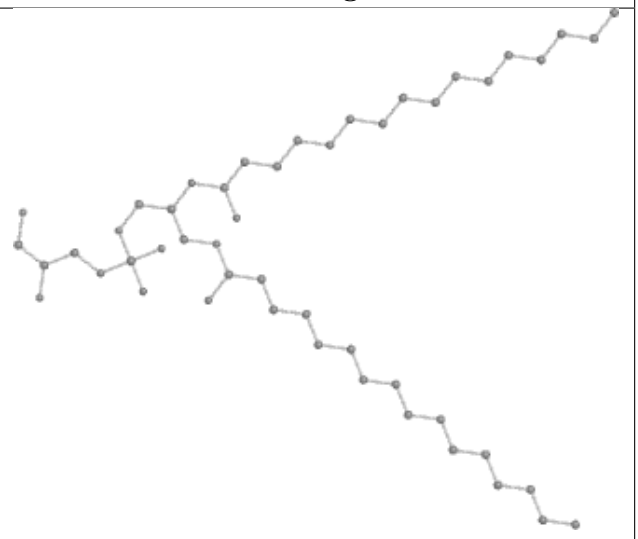
Bond lengths



Bond angles

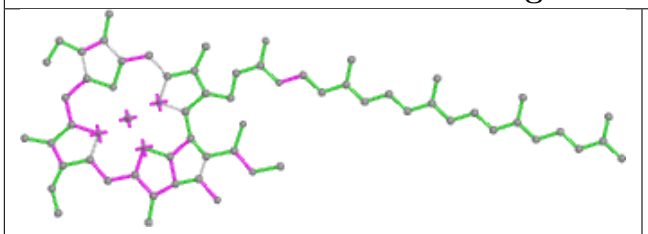


Torsions

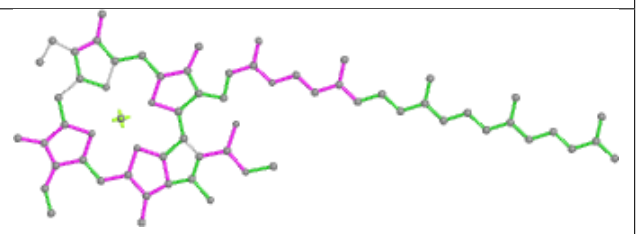


Rings

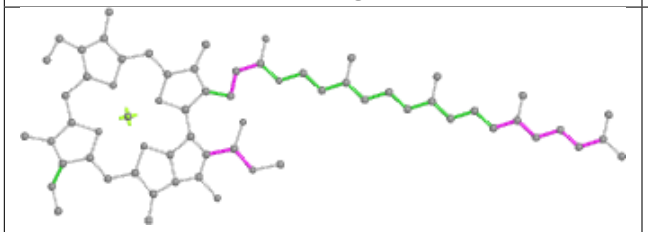
Ligand CLA C 503



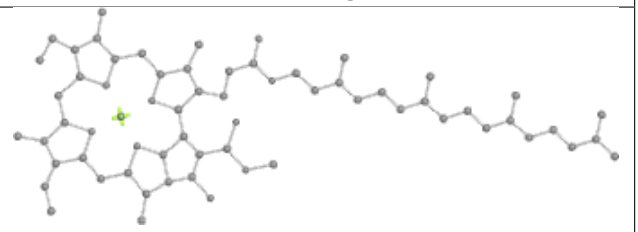
Bond lengths



Bond angles

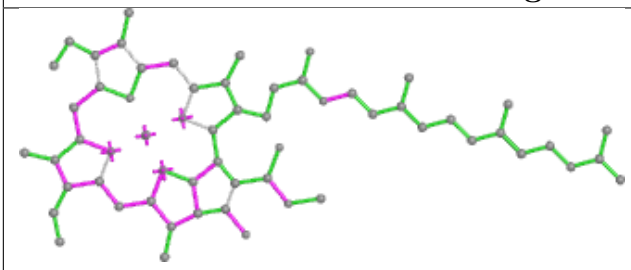


Torsions

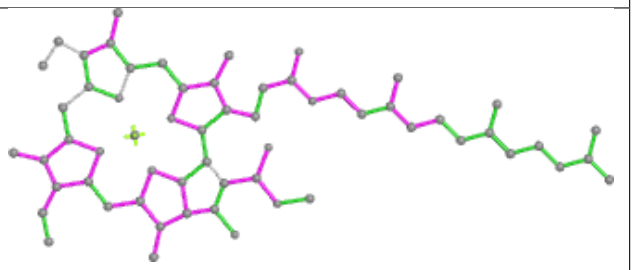


Rings

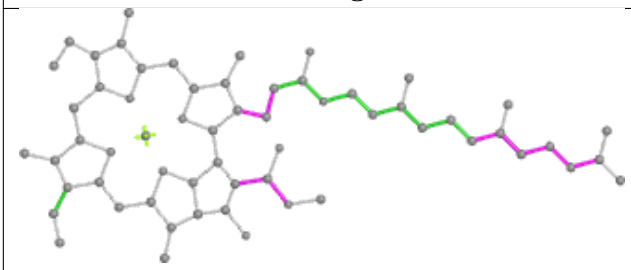
Ligand CLA B 606



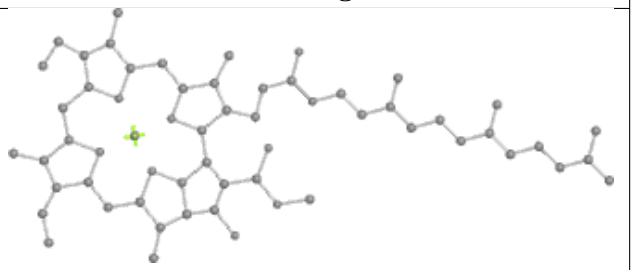
Bond lengths



Bond angles

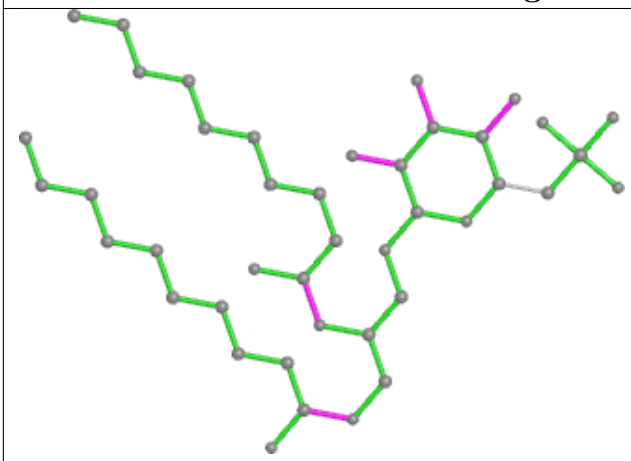


Torsions

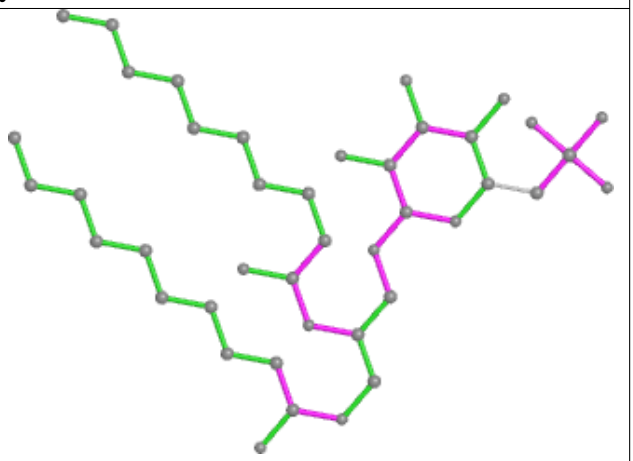


Rings

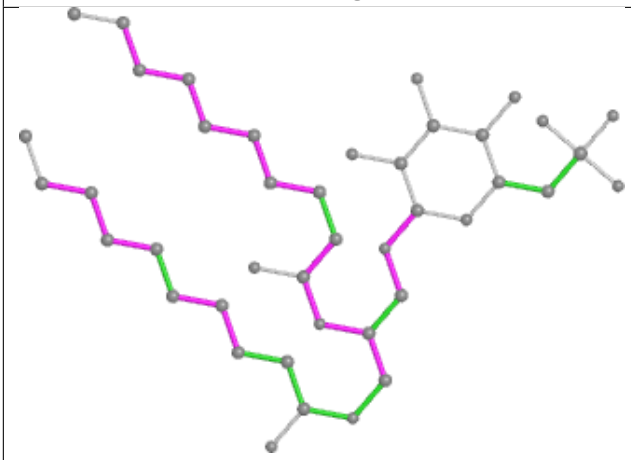
Ligand SQD X 101



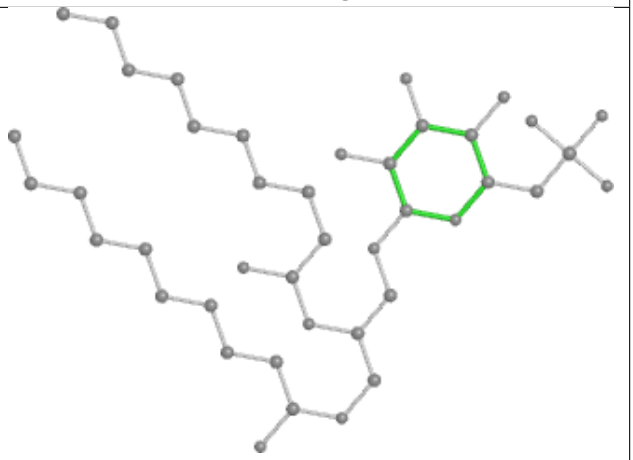
Bond lengths



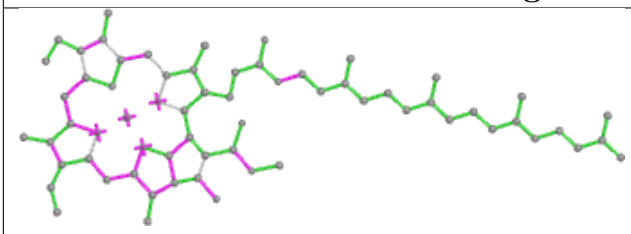
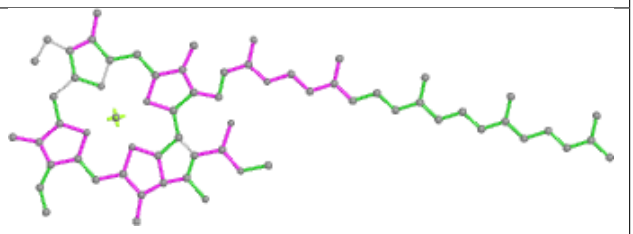
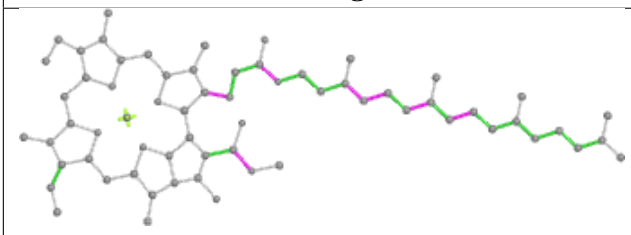
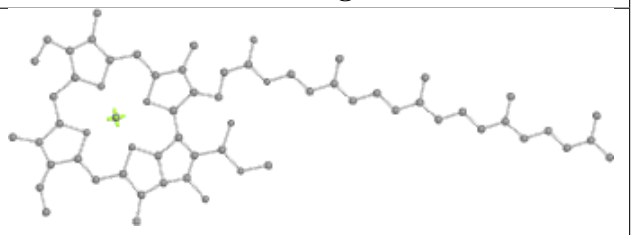
Bond angles

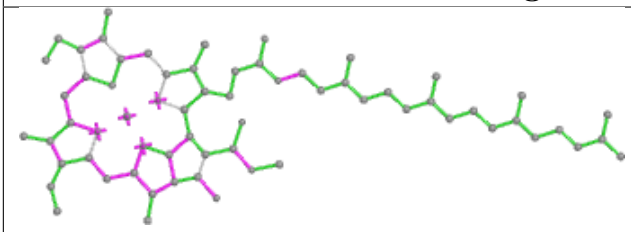
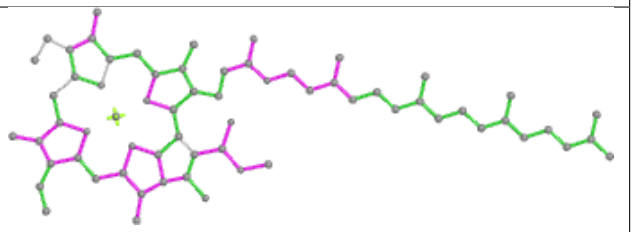
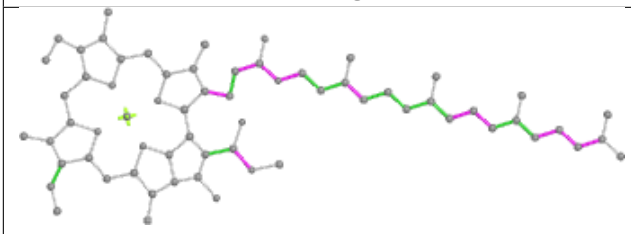
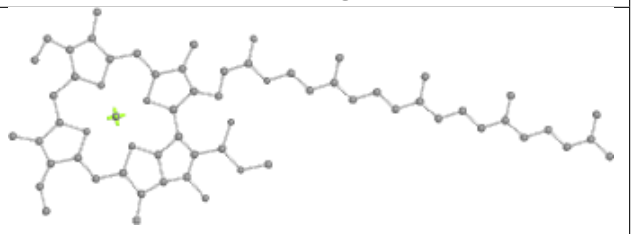


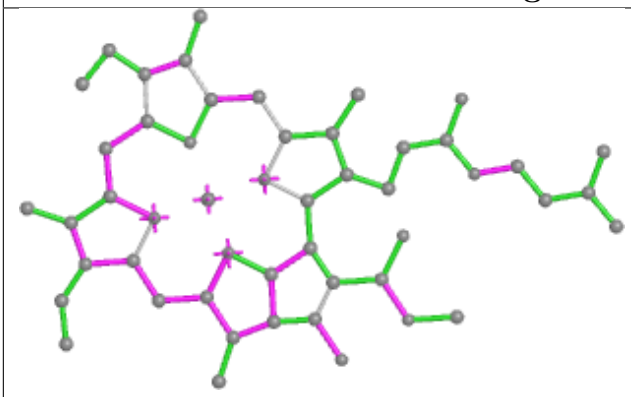
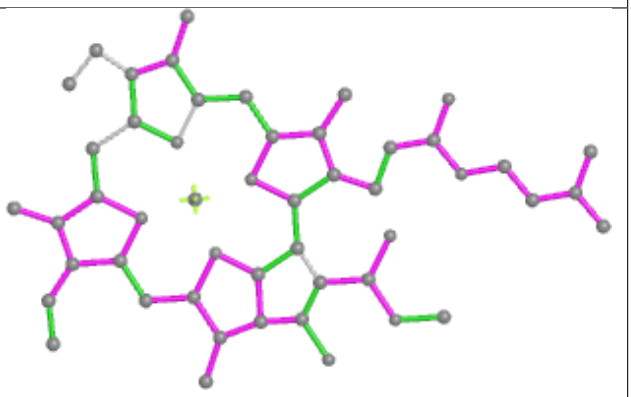
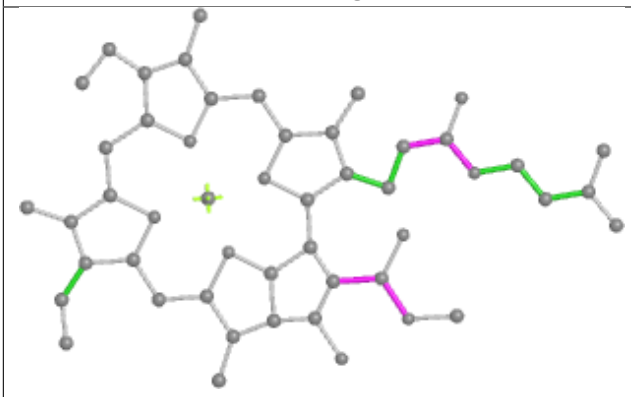
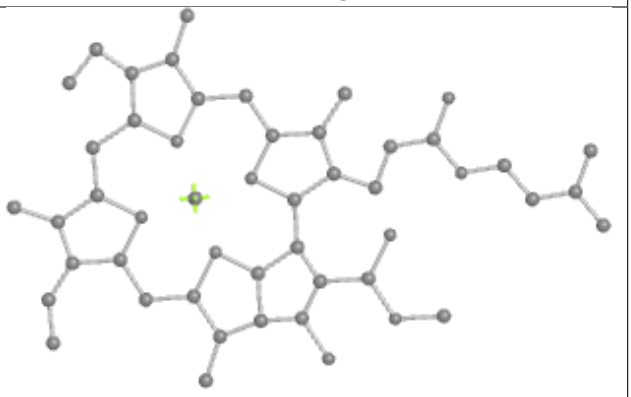
Torsions

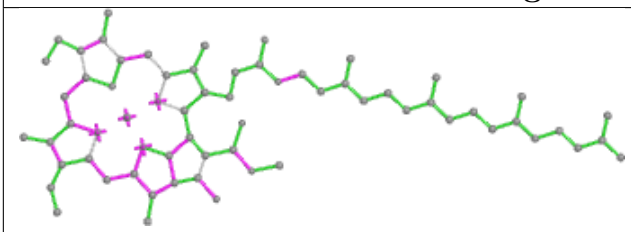
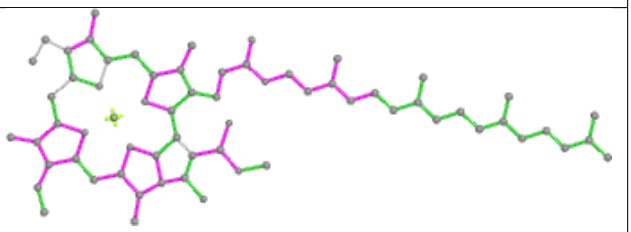
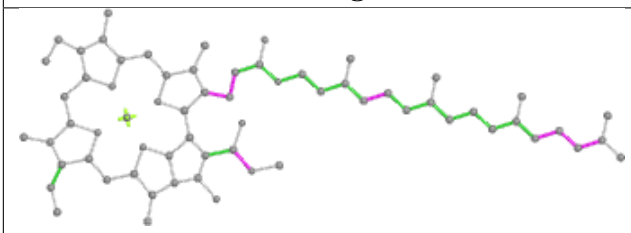
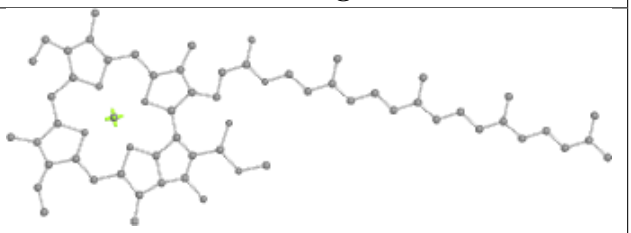


Rings

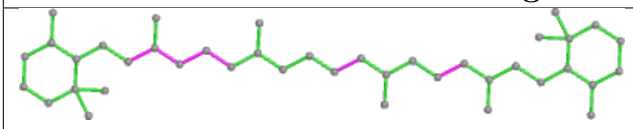
Ligand CLA D 406	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA D 405	
 Bond lengths	 Bond angles
 Torsions	 Rings

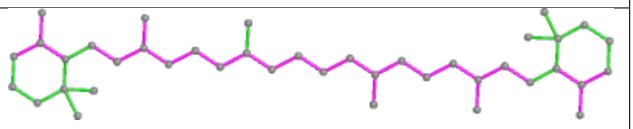
Ligand CLA A 405	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 402	
 Bond lengths	 Bond angles
 Torsions	 Rings

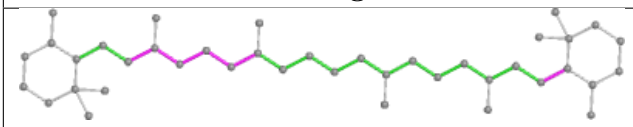
Ligand BCR B 618



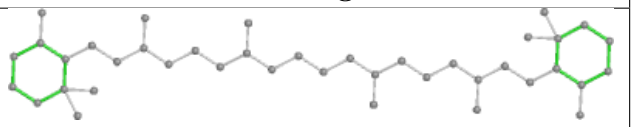
Bond lengths



Bond angles

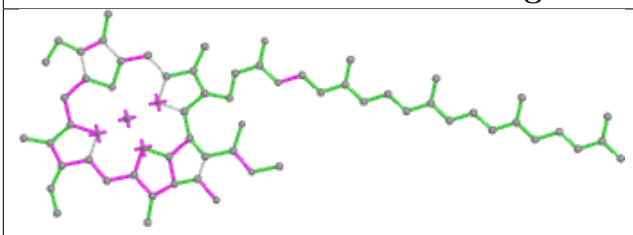


Torsions

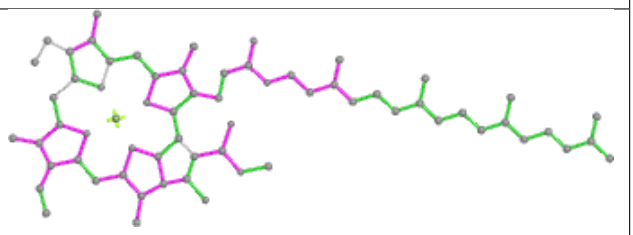


Rings

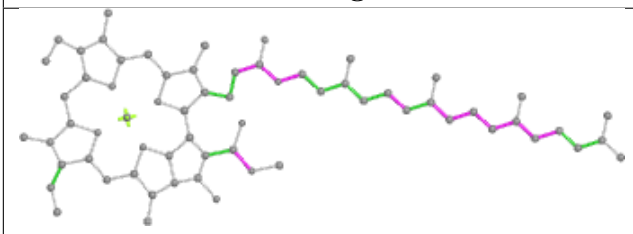
Ligand CLA C 514



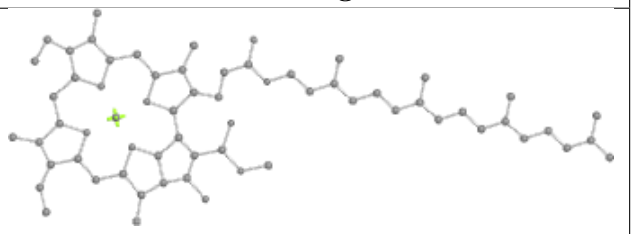
Bond lengths



Bond angles

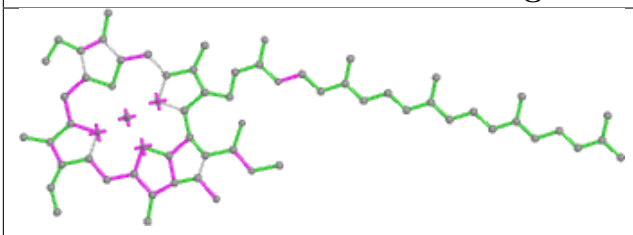


Torsions

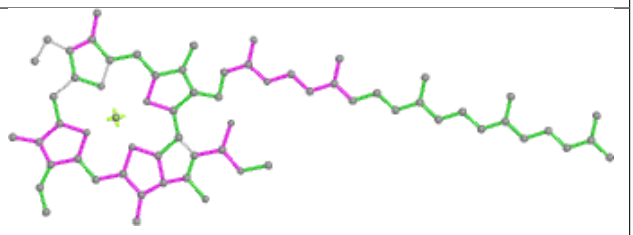


Rings

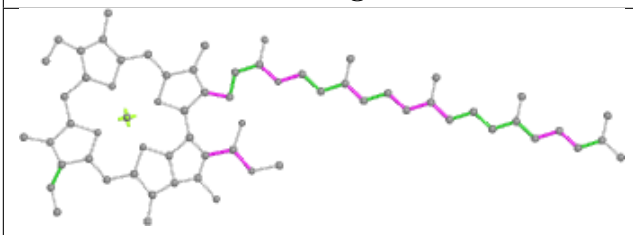
Ligand CLA B 609



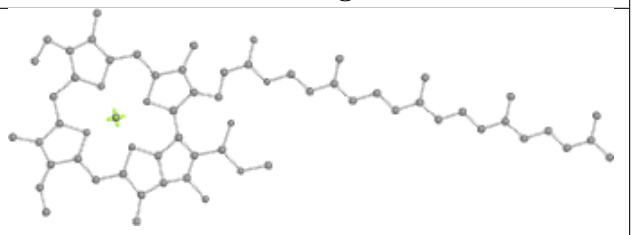
Bond lengths



Bond angles

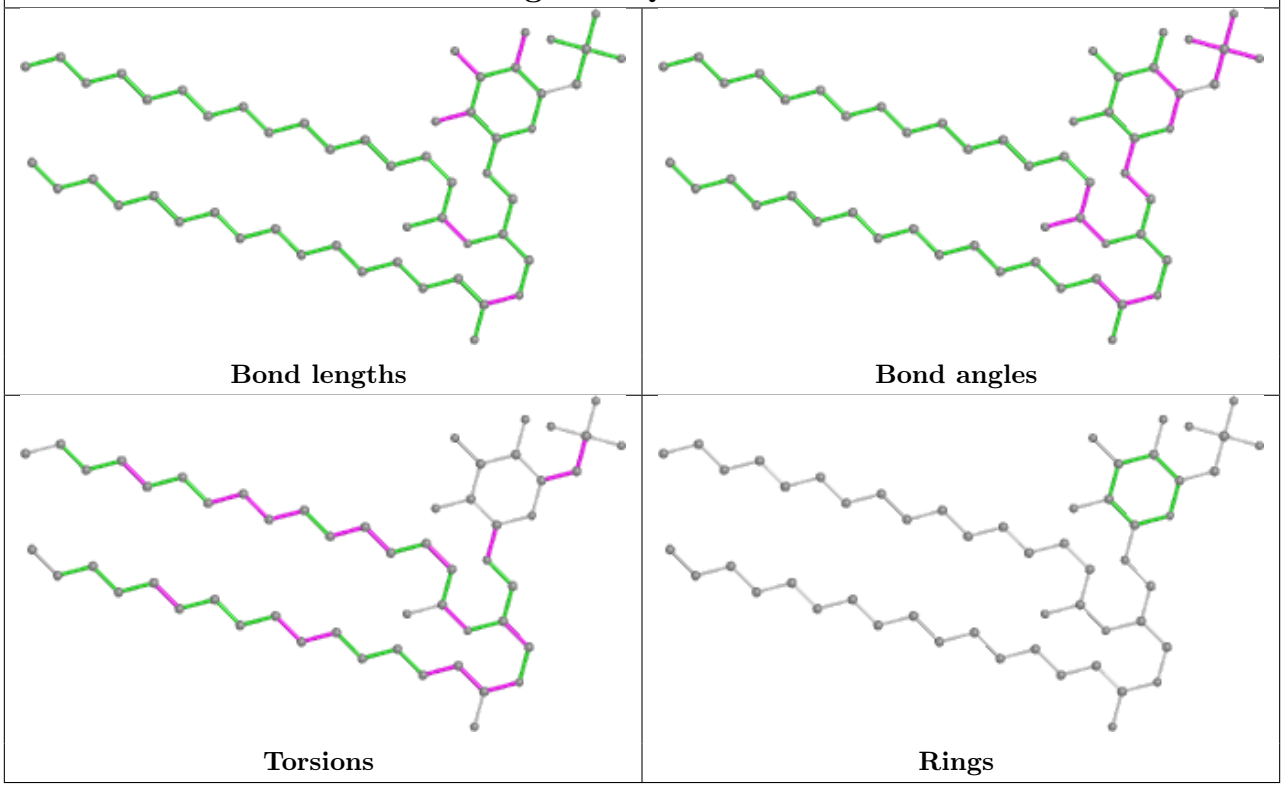


Torsions

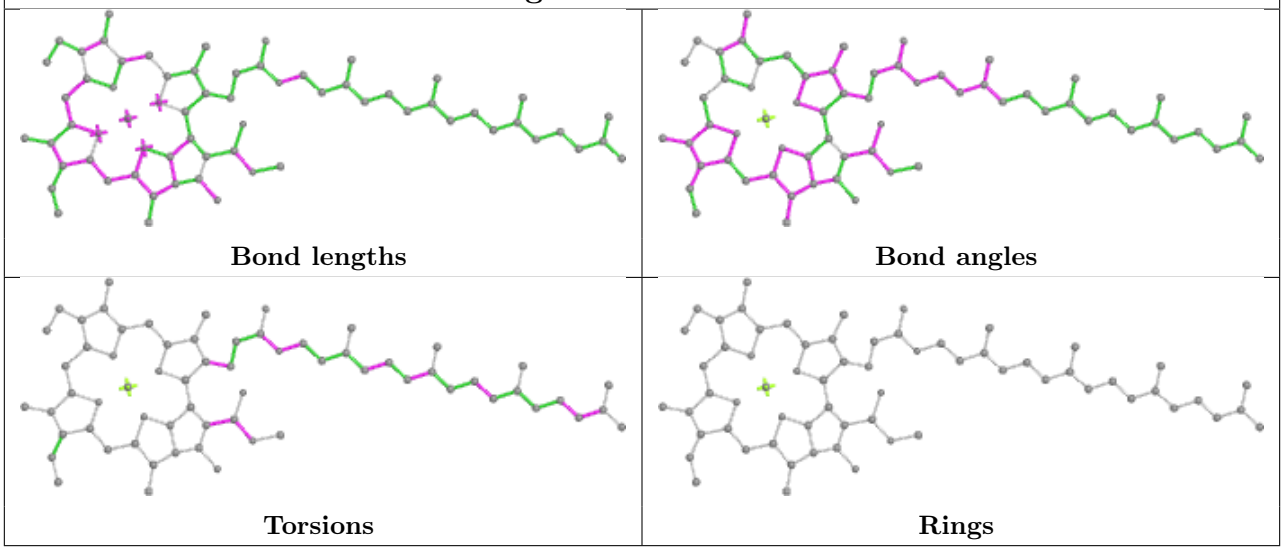


Rings

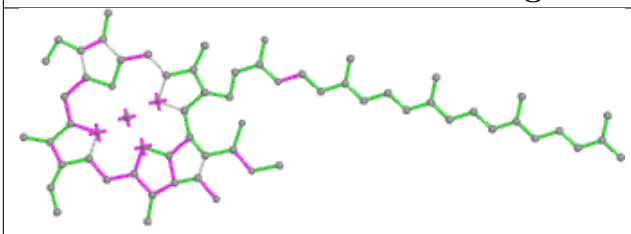
Ligand SQD A 409



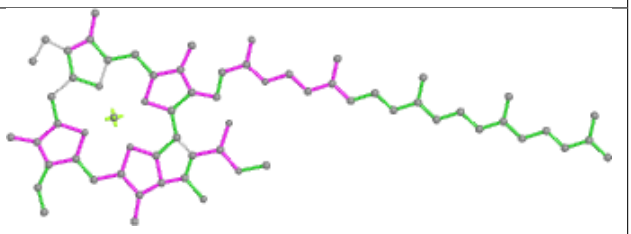
Ligand CLA B 604



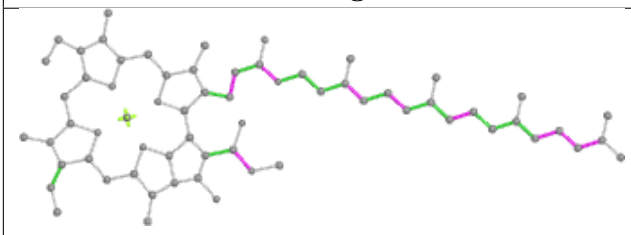
Ligand CLA C 511



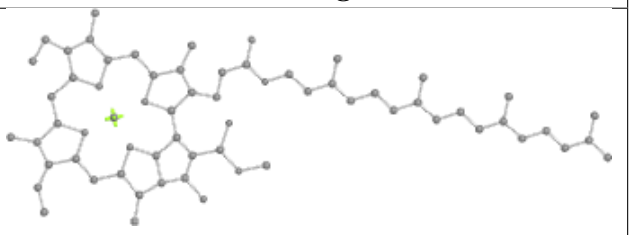
Bond lengths



Bond angles

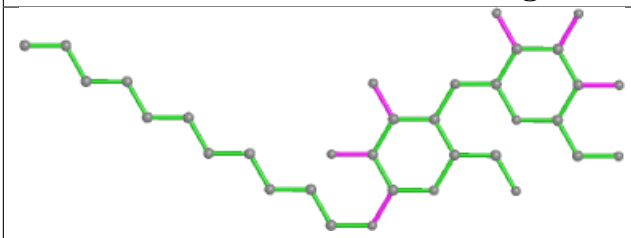


Torsions

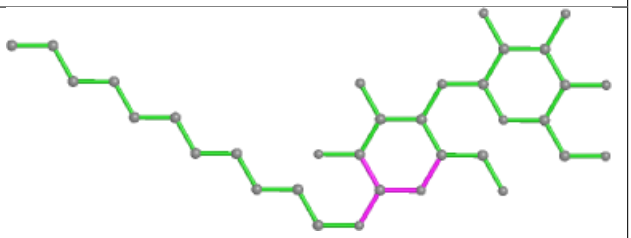


Rings

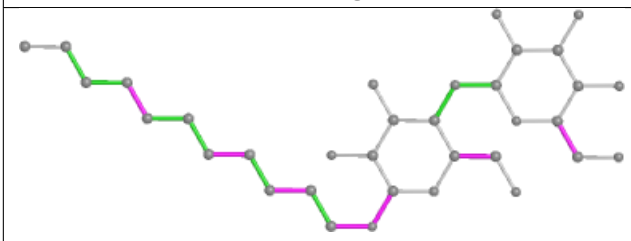
Ligand LMT B 623



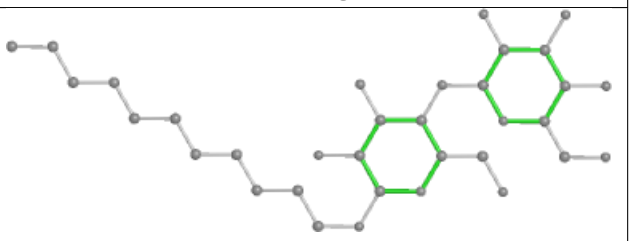
Bond lengths



Bond angles

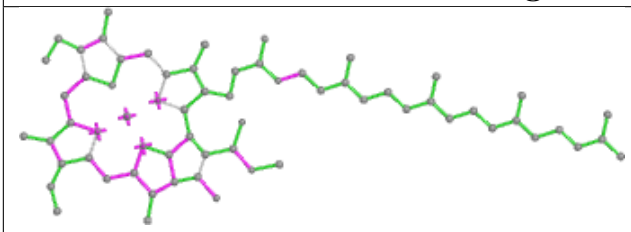


Torsions

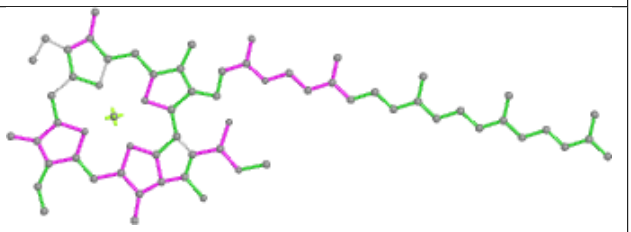


Rings

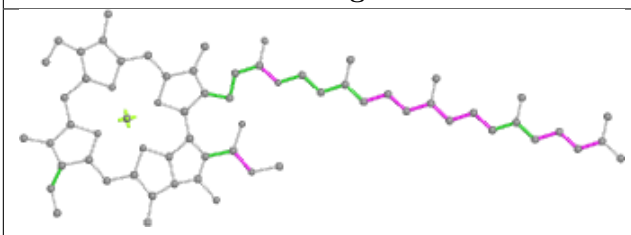
Ligand CLA B 613



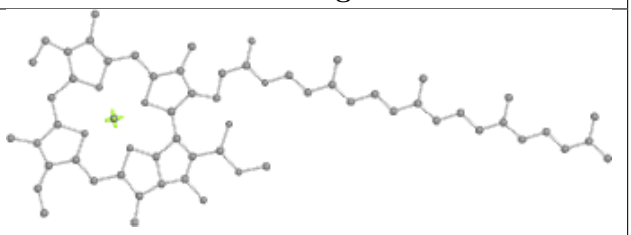
Bond lengths



Bond angles

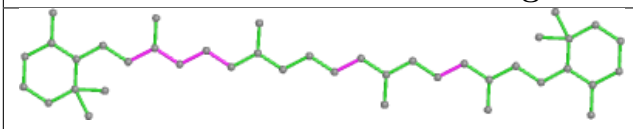


Torsions

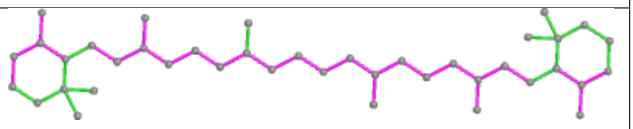


Rings

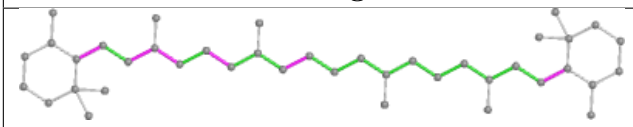
Ligand BCR X 102



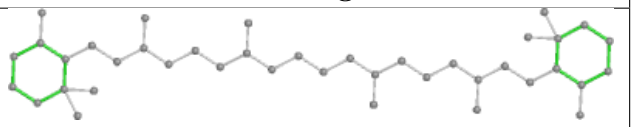
Bond lengths



Bond angles

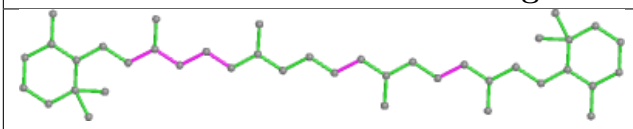


Torsions

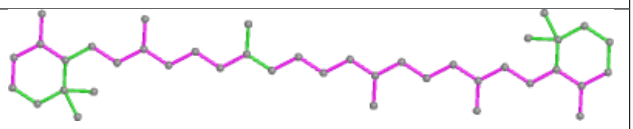


Rings

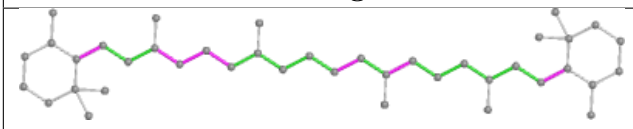
Ligand BCR D 407



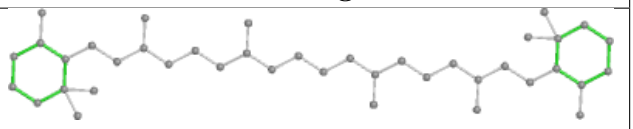
Bond lengths



Bond angles

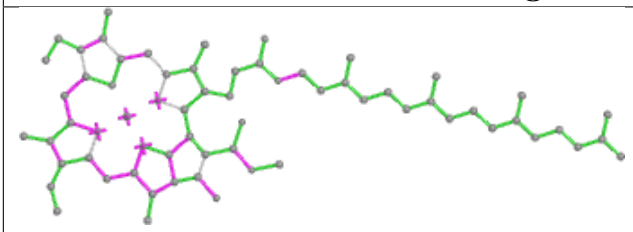


Torsions

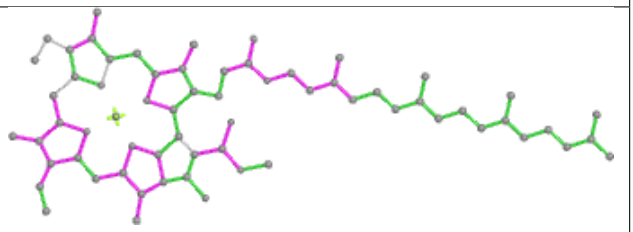


Rings

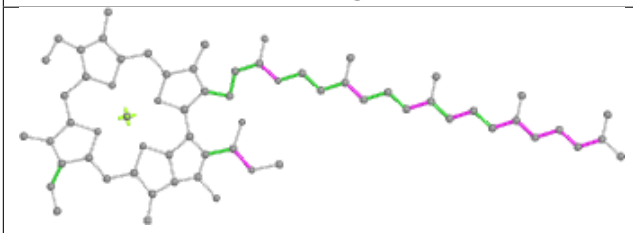
Ligand CLA B 611



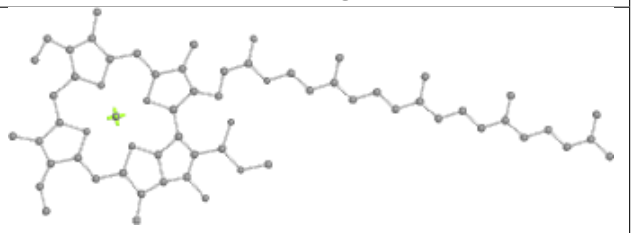
Bond lengths



Bond angles

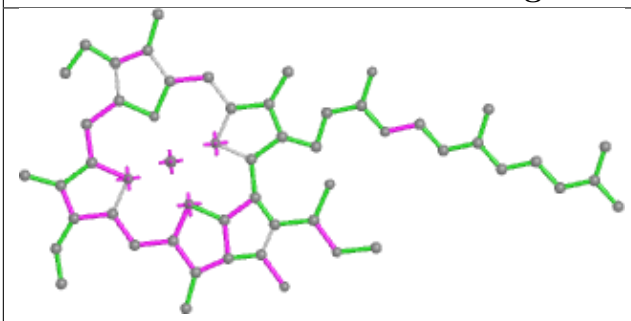


Torsions

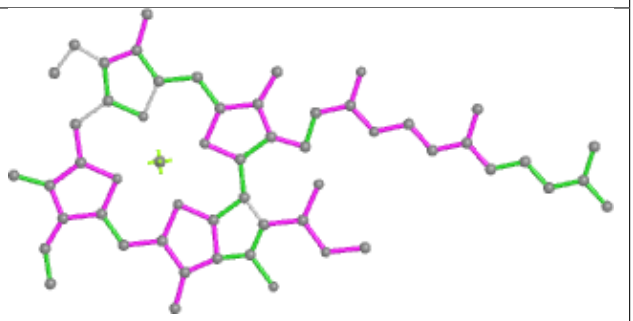


Rings

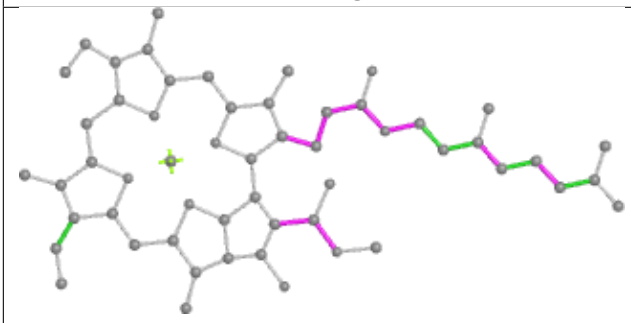
Ligand CLA C 509



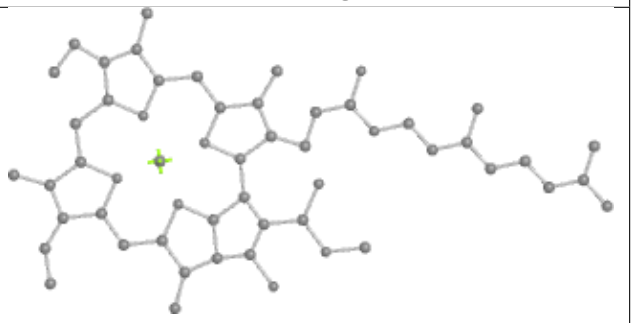
Bond lengths



Bond angles

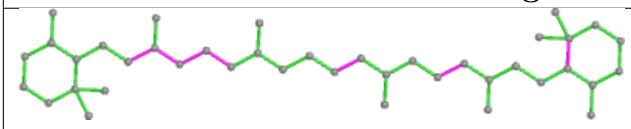


Torsions

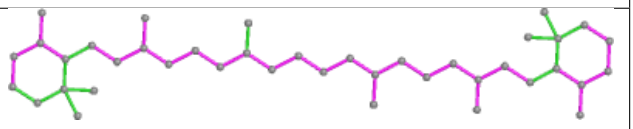


Rings

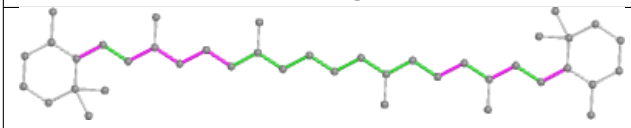
Ligand BCR C 515



Bond lengths



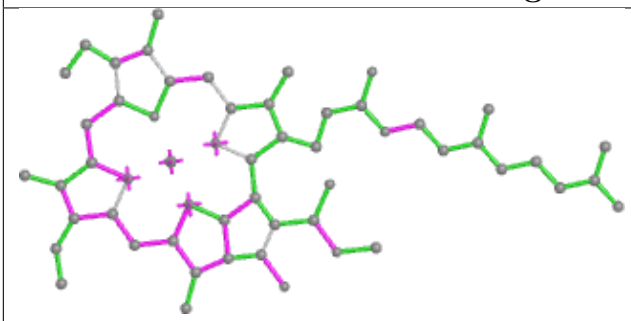
Bond angles



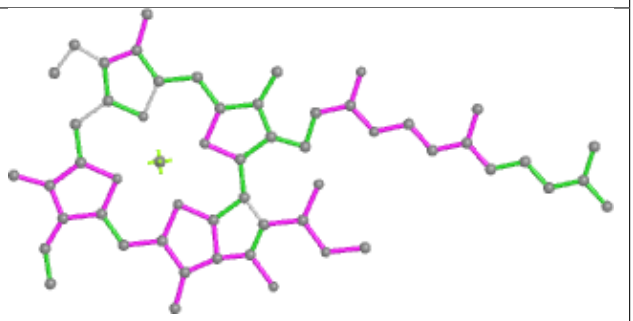
Torsions

Rings

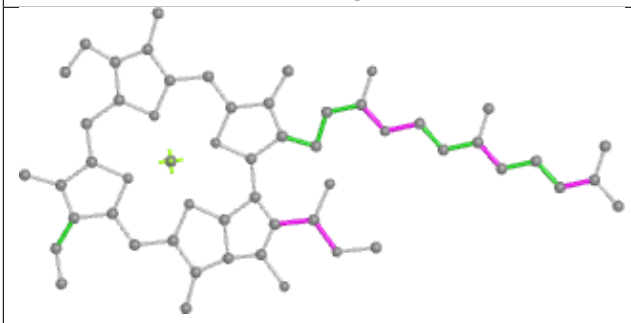
Ligand CLA B 614



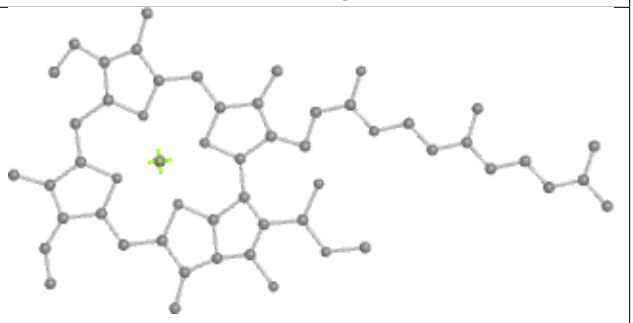
Bond lengths



Bond angles

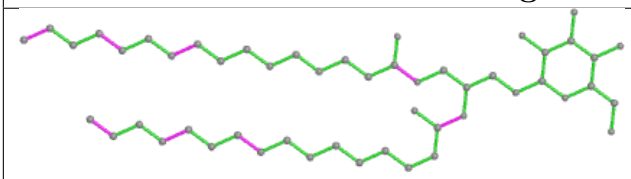


Torsions

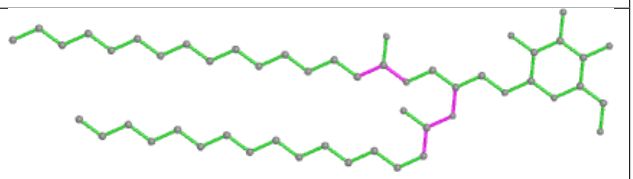


Rings

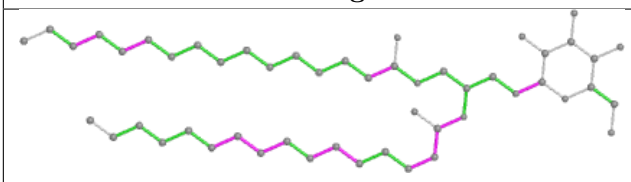
Ligand LMG C 501



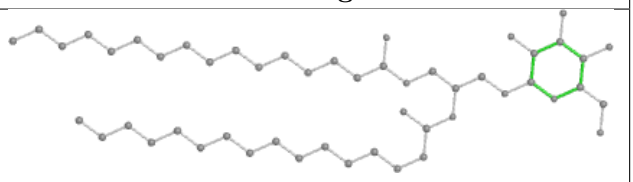
Bond lengths



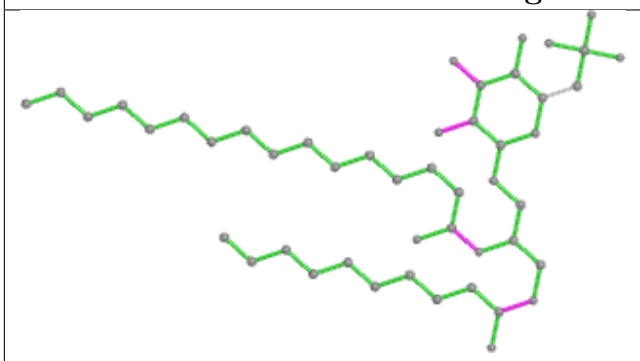
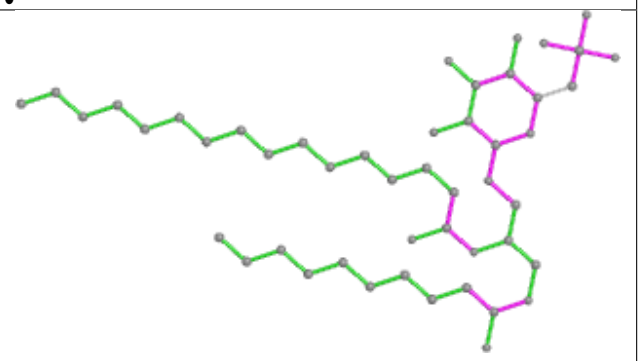
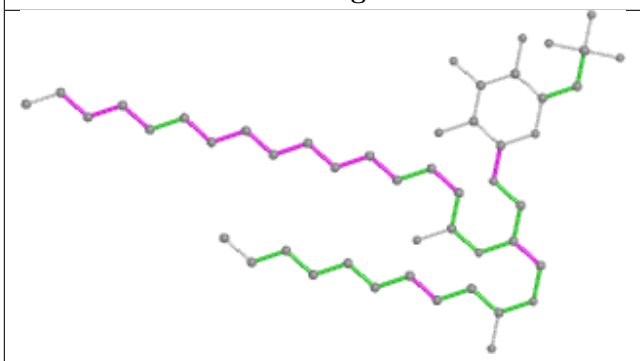
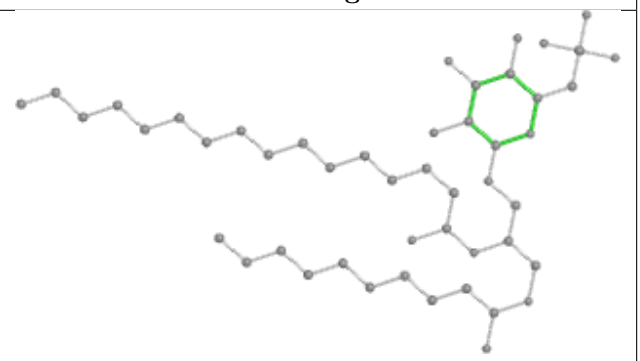
Bond angles



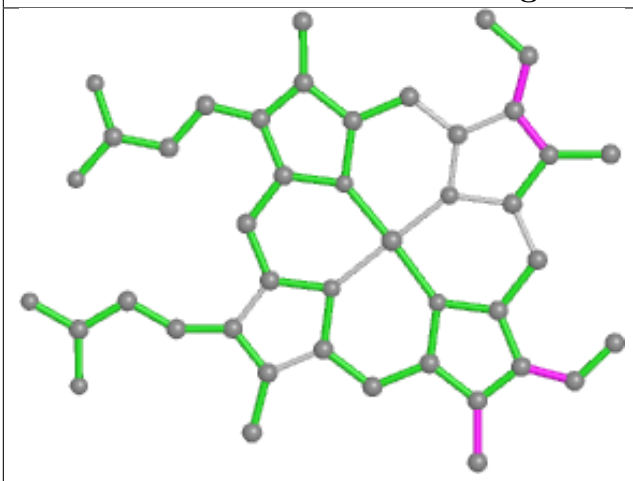
Torsions



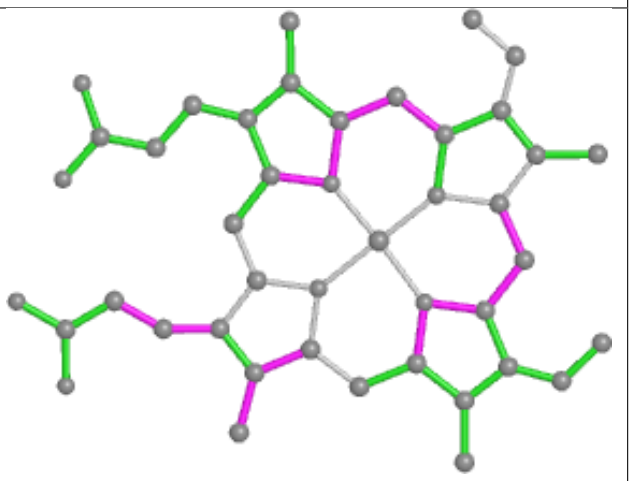
Rings

Ligand SQD A 407	
 Bond lengths	 Bond angles
 Torsions	 Rings

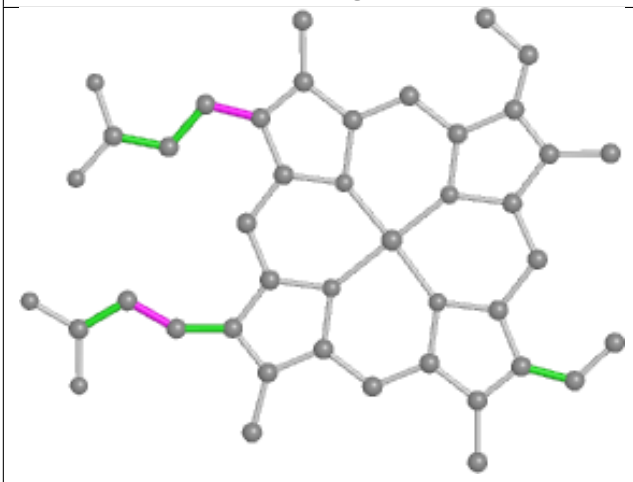
Ligand HEM E 101



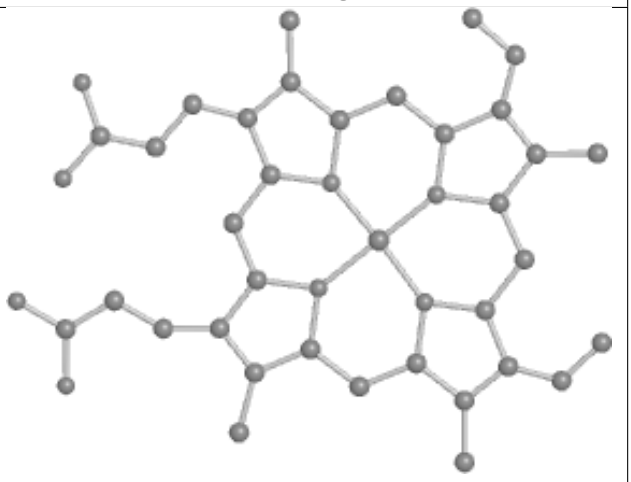
Bond lengths



Bond angles

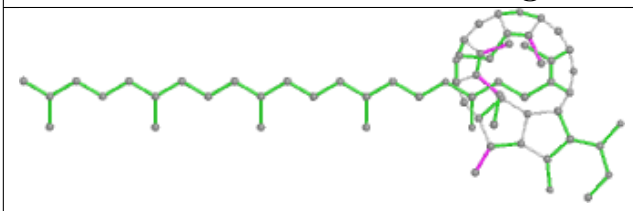


Torsions

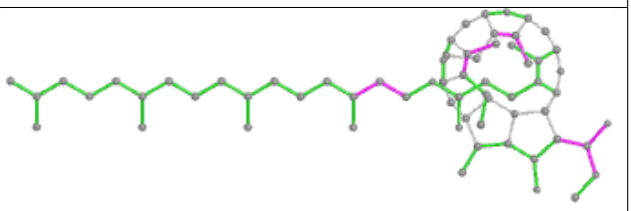


Rings

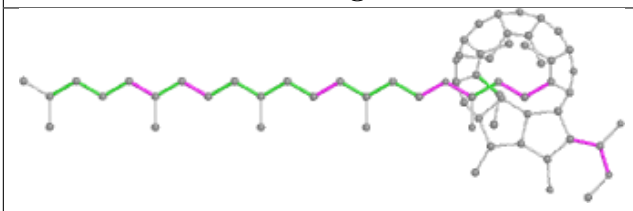
Ligand PHO A 404



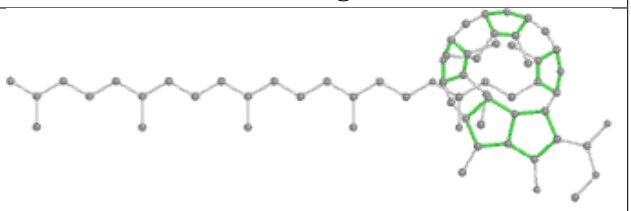
Bond lengths



Bond angles

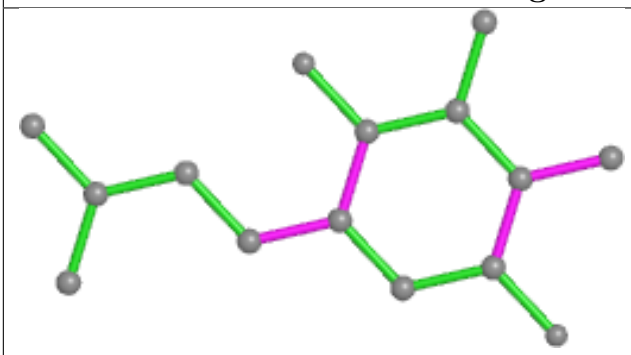


Torsions

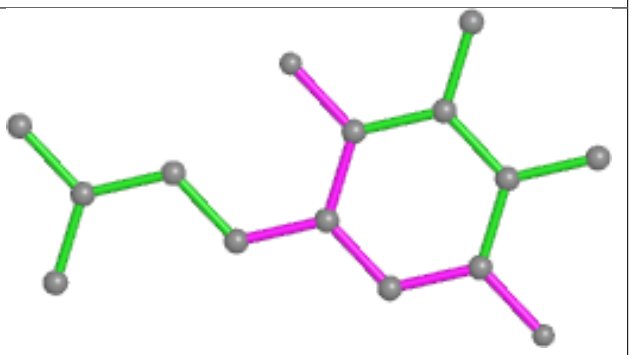


Rings

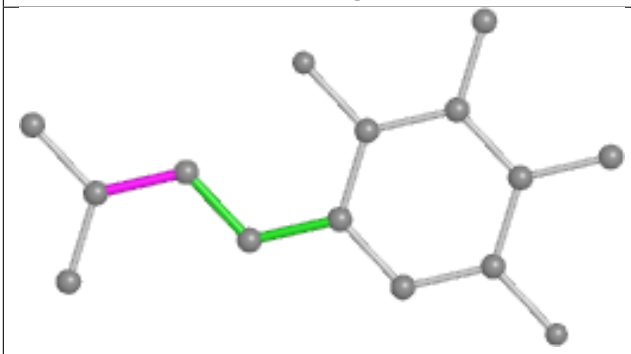
Ligand PL9 A 408



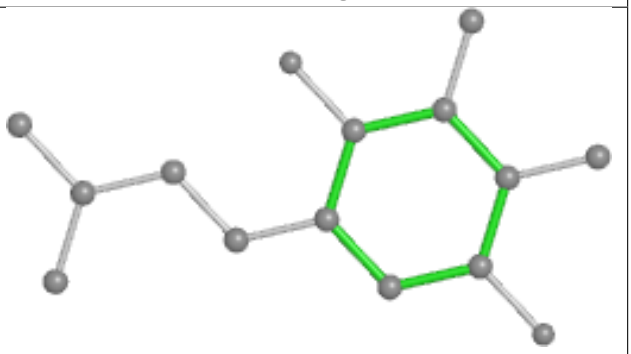
Bond lengths



Bond angles

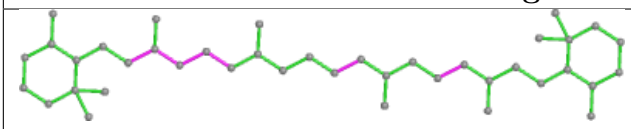


Torsions

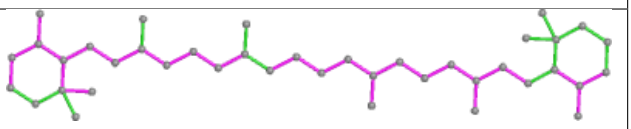


Rings

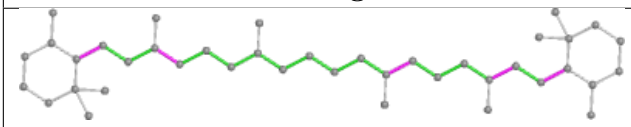
Ligand BCR B 617



Bond lengths



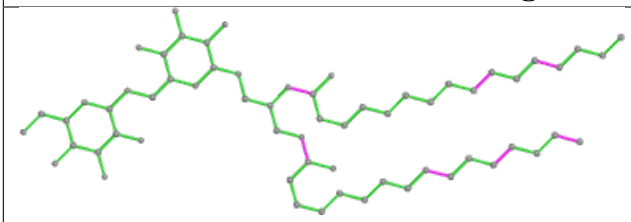
Bond angles



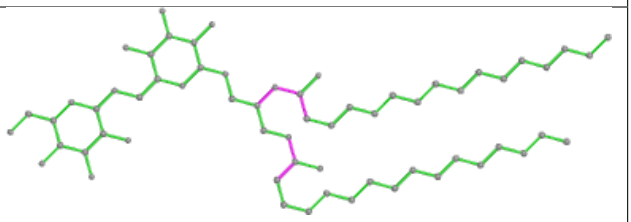
Torsions

Rings

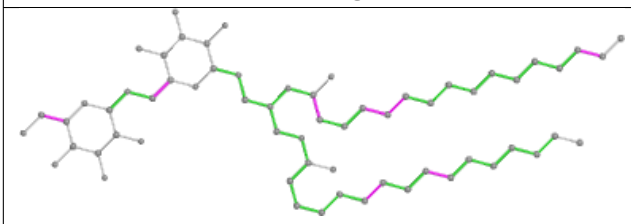
Ligand DGD C 517



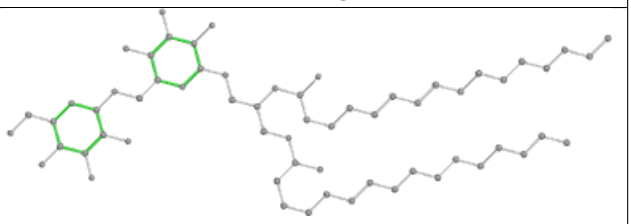
Bond lengths



Bond angles

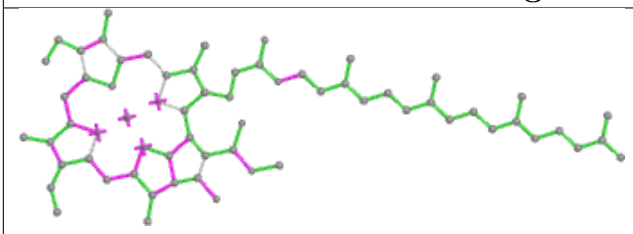


Torsions

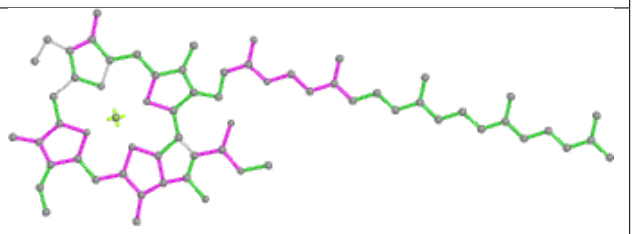


Rings

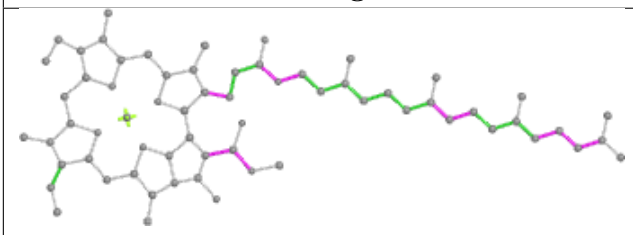
Ligand CLA B 612



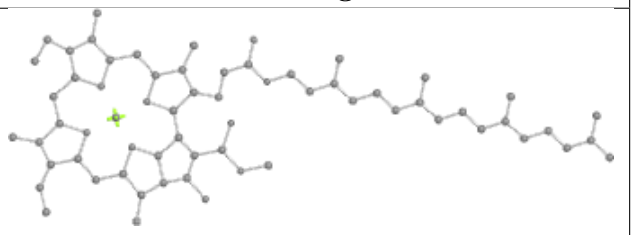
Bond lengths



Bond angles

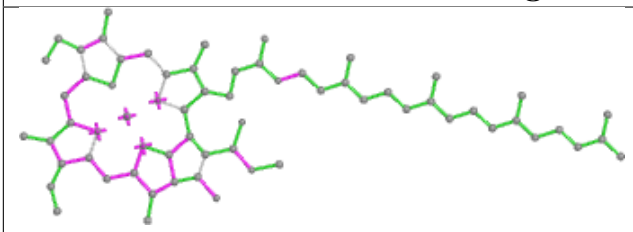


Torsions

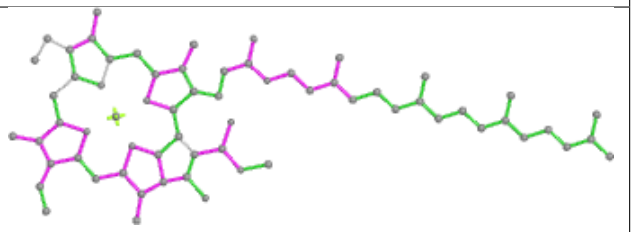


Rings

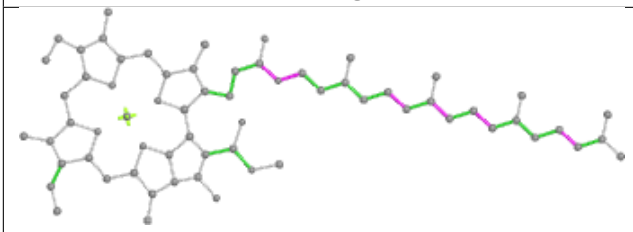
Ligand CLA B 615



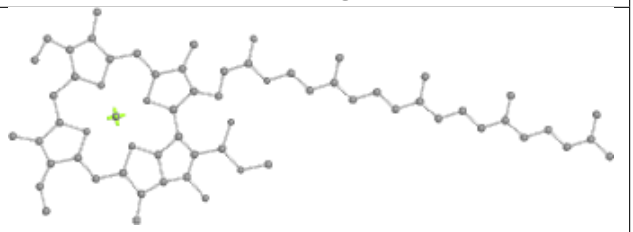
Bond lengths



Bond angles

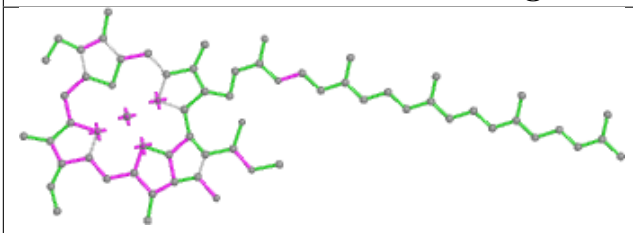


Torsions

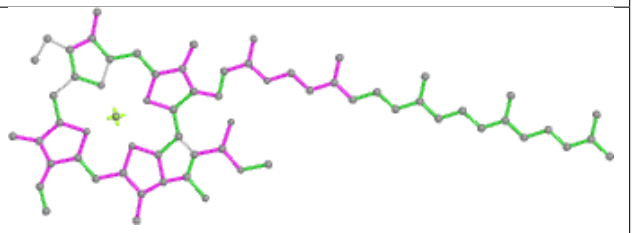


Rings

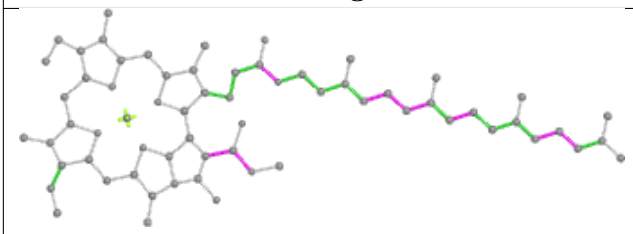
Ligand CLA C 505



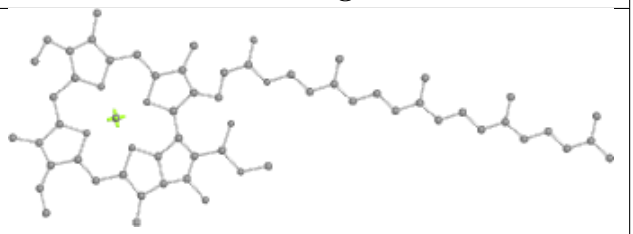
Bond lengths



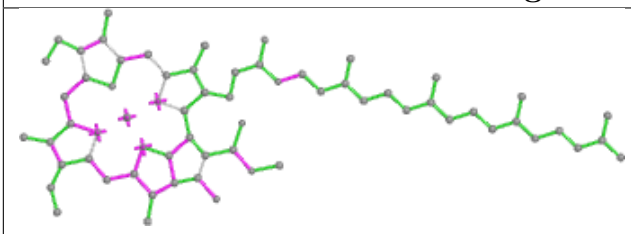
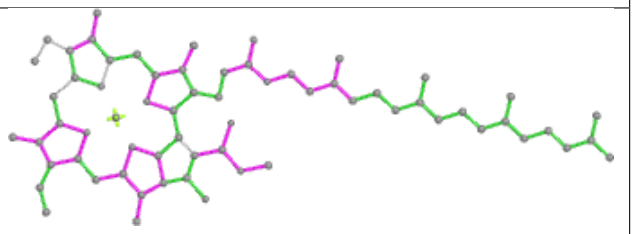
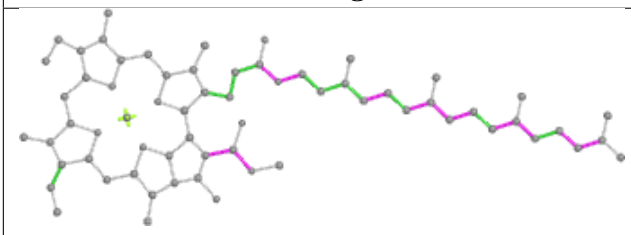
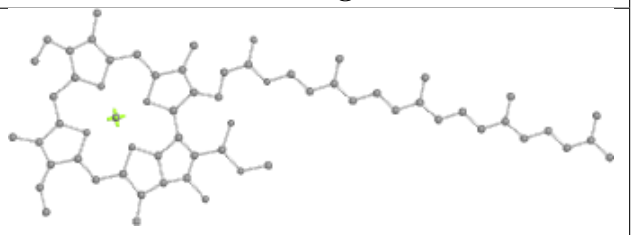
Bond angles

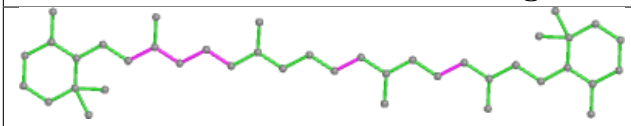
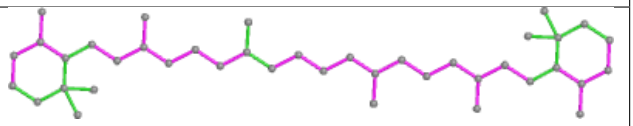
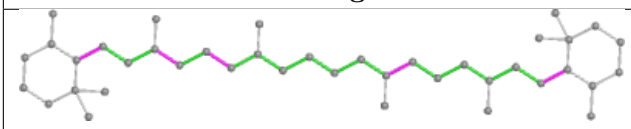
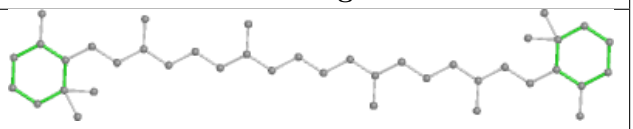


Torsions

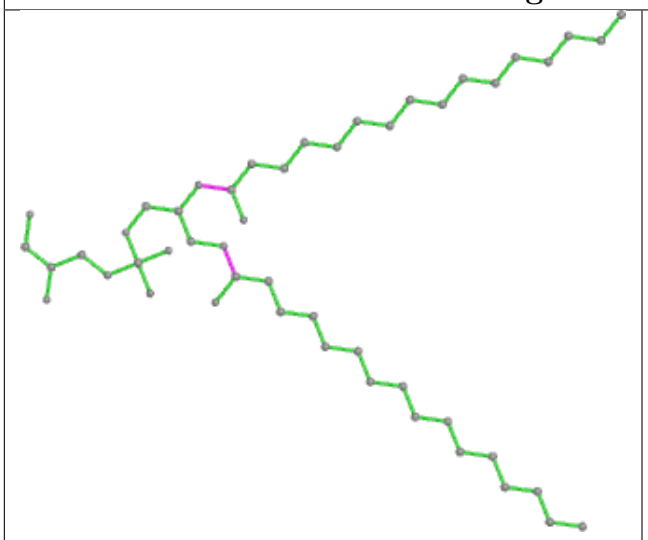


Rings

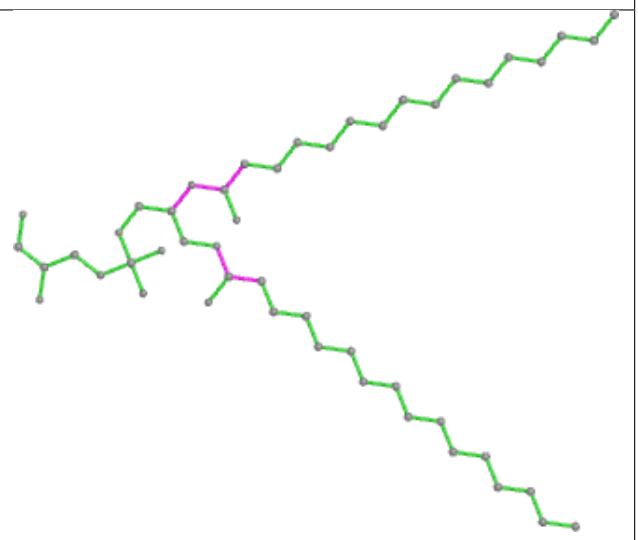
Ligand CLA C 510	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR C 519	
 Bond lengths	 Bond angles
 Torsions	 Rings

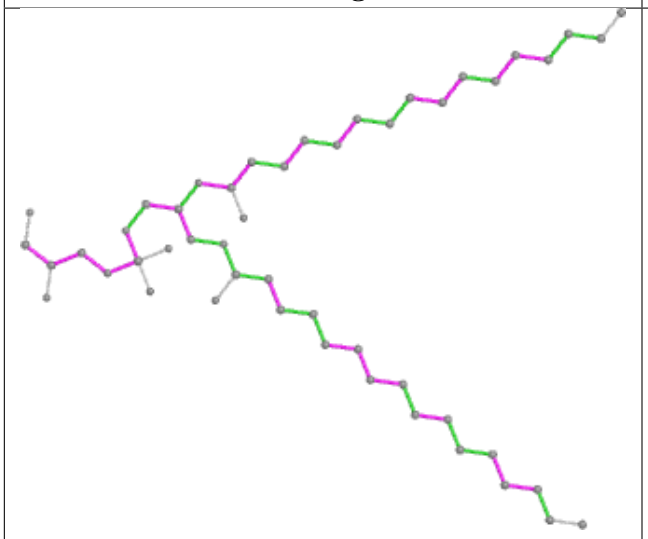
Ligand LHG L 101



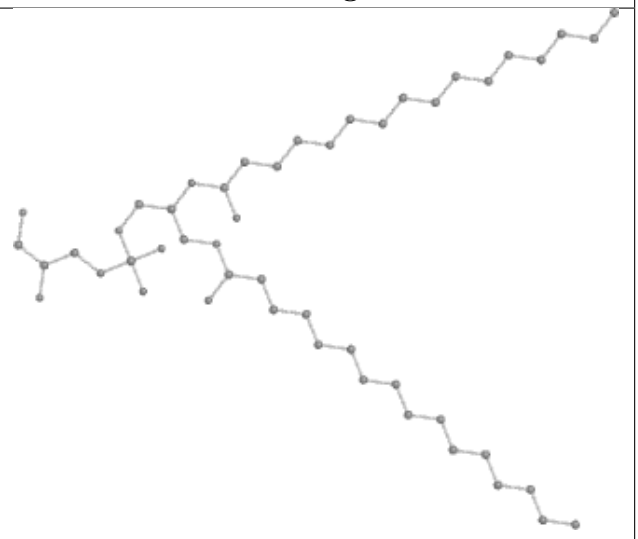
Bond lengths



Bond angles

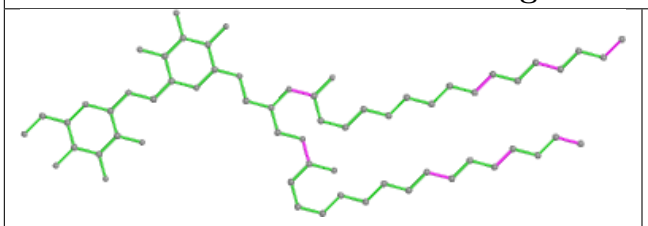


Torsions

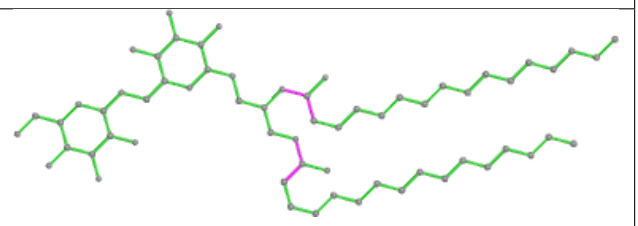


Rings

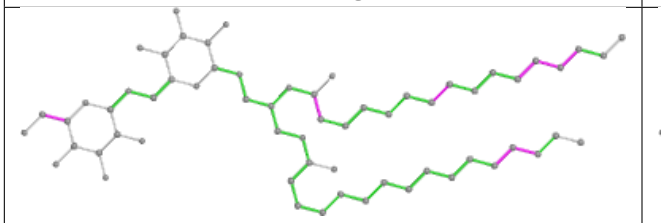
Ligand DGD H 101



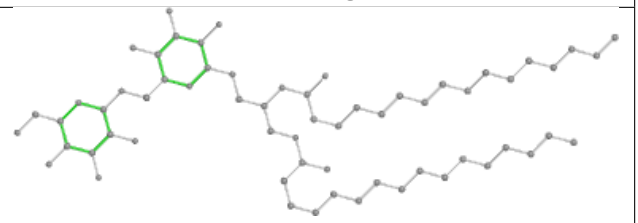
Bond lengths



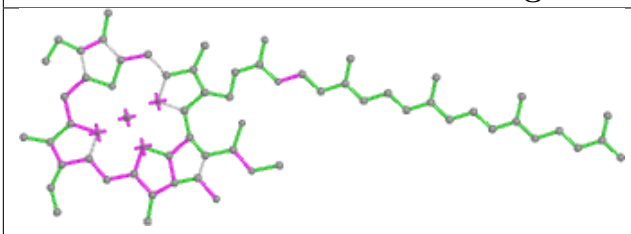
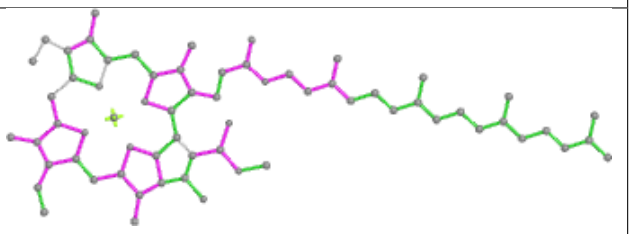
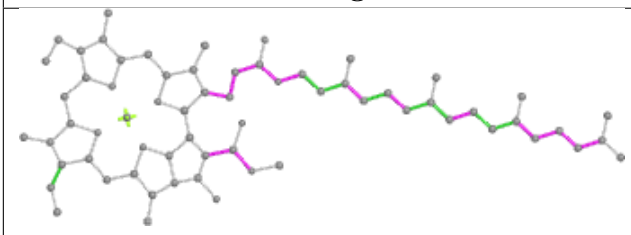
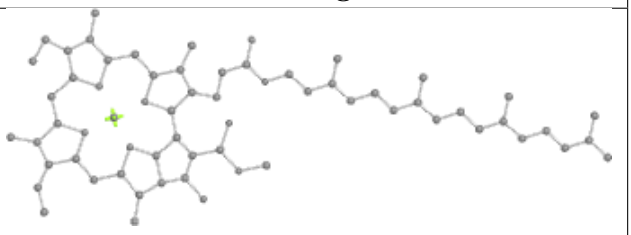
Bond angles

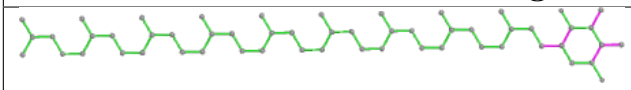
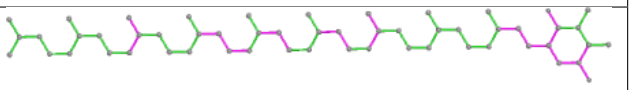
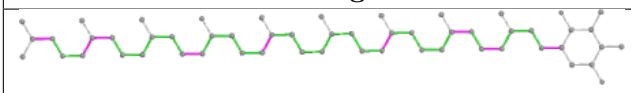
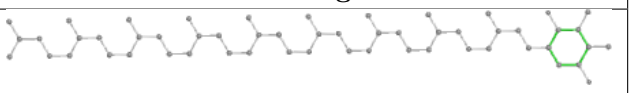


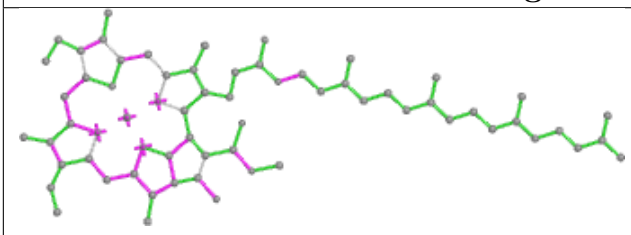
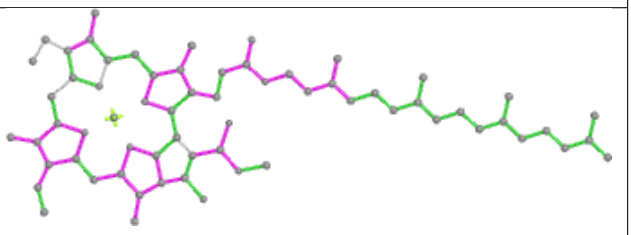
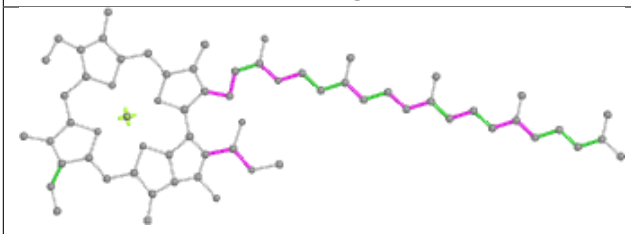
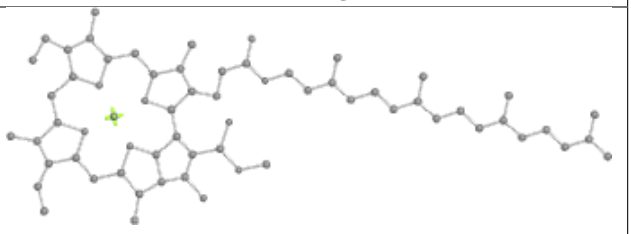
Torsions



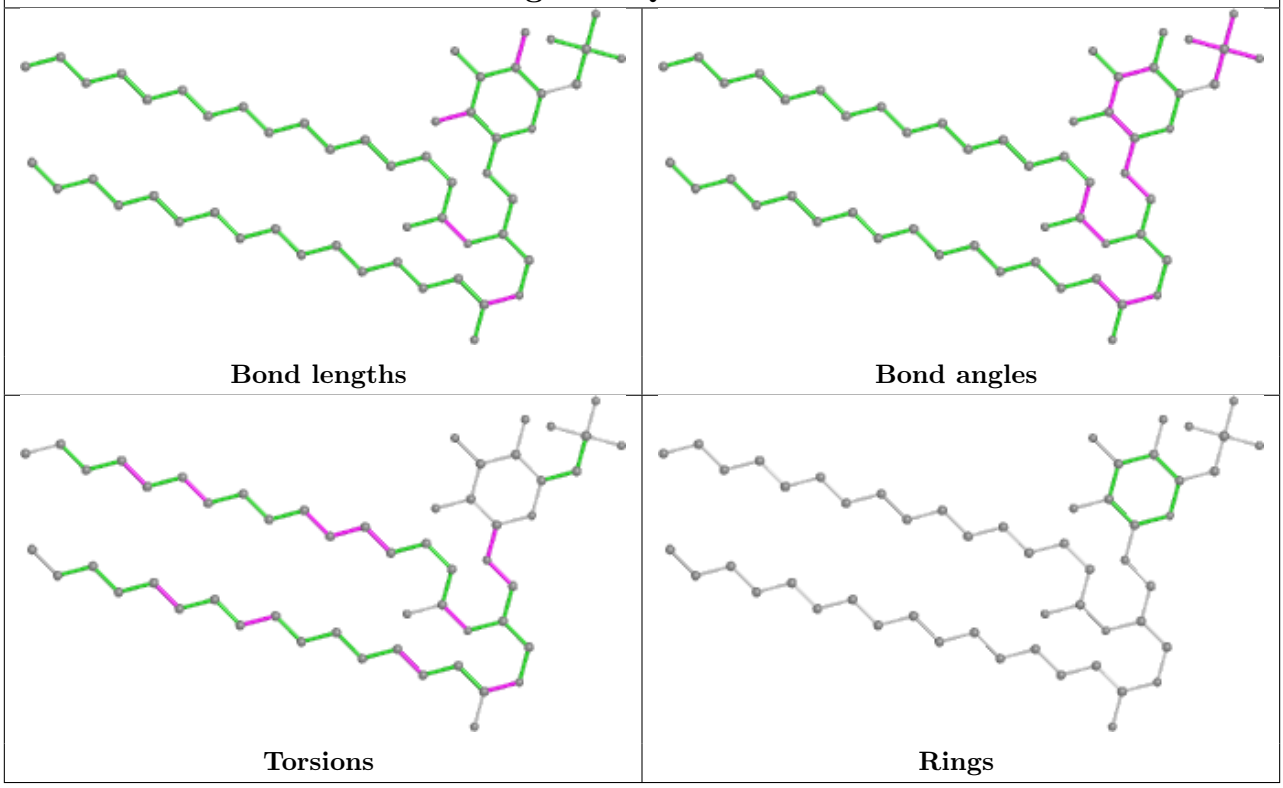
Rings

Ligand CLA C 507	
 Bond lengths	 Bond angles
 Torsions	 Rings

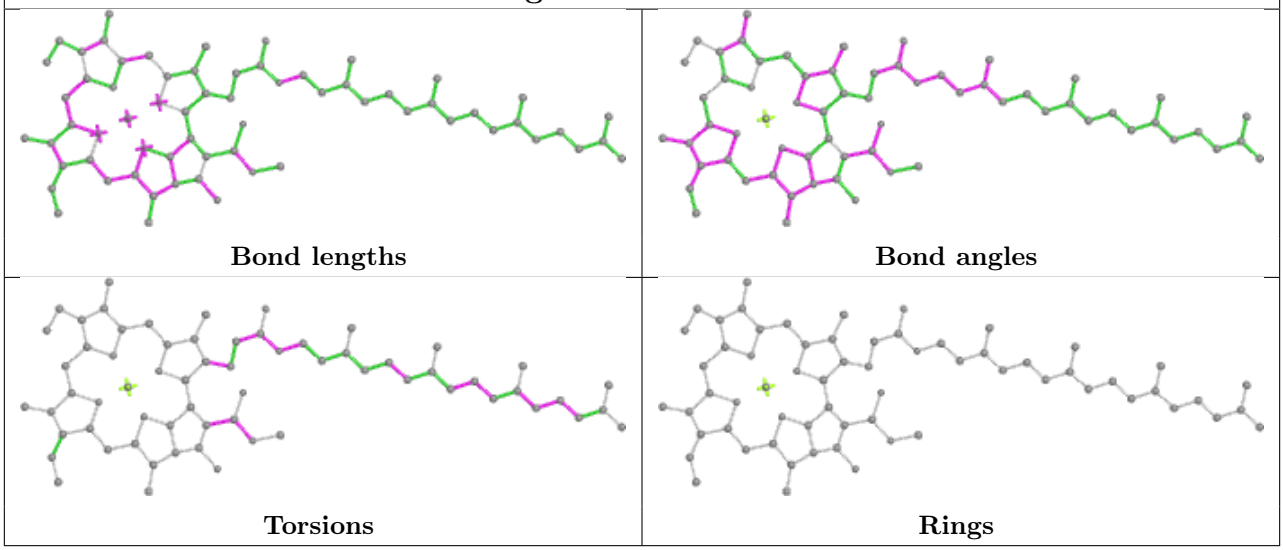
Ligand PL9 D 408	
 Bond lengths	 Bond angles
 Torsions	 Rings

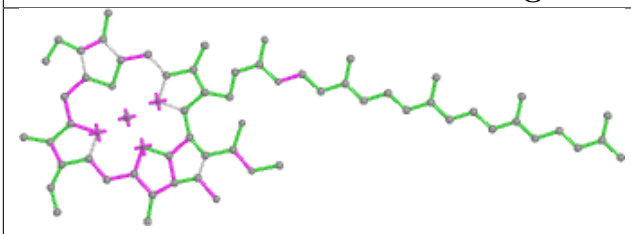
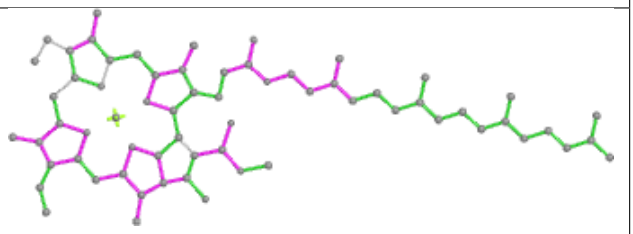
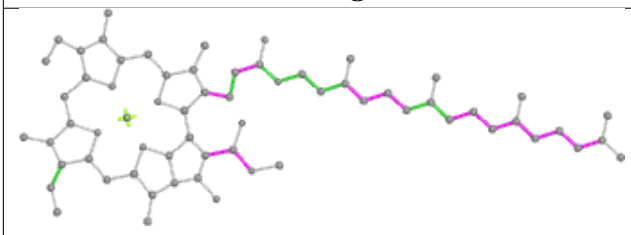
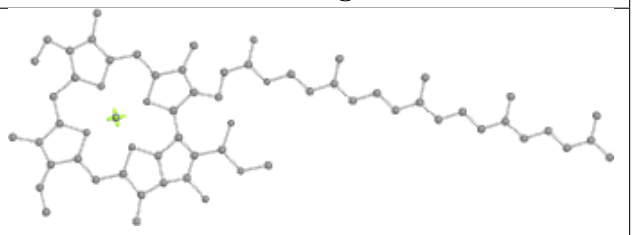
Ligand CLA B 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SQD C 518



Ligand CLA C 504



Ligand CLA B 608	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

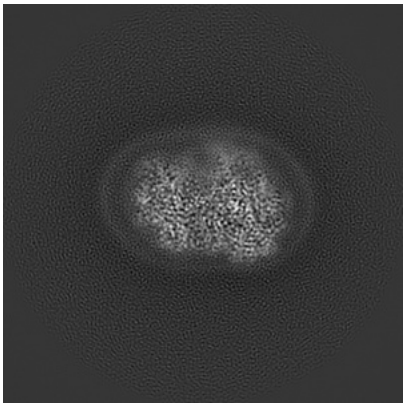
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-21690. These allow visual inspection of the internal detail of the map and identification of artifacts.

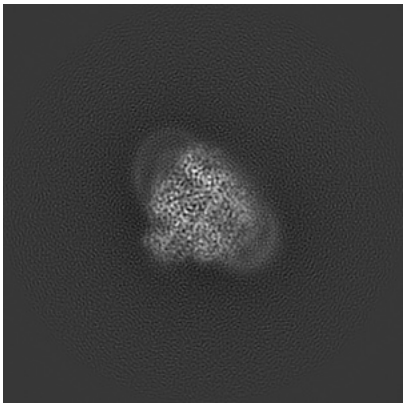
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

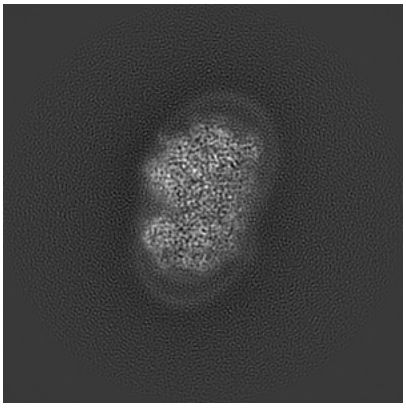
6.1.1 Primary map



X



Y

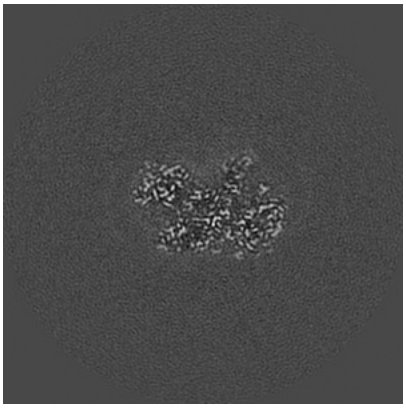


Z

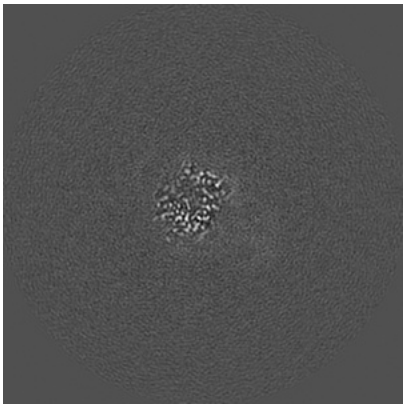
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

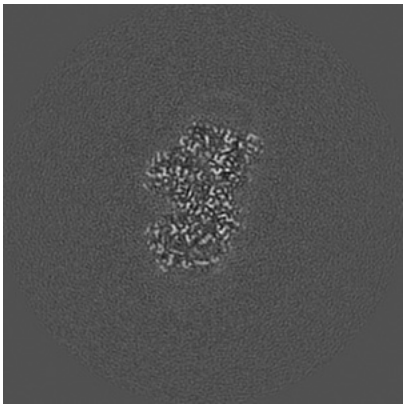
6.2.1 Primary map



X Index: 128



Y Index: 128

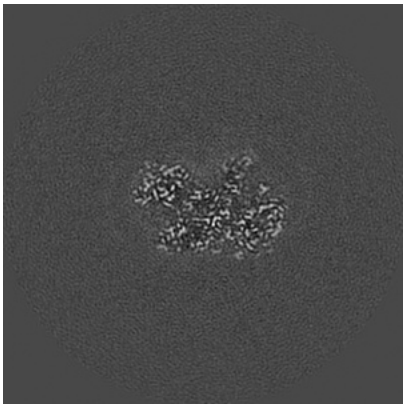


Z Index: 128

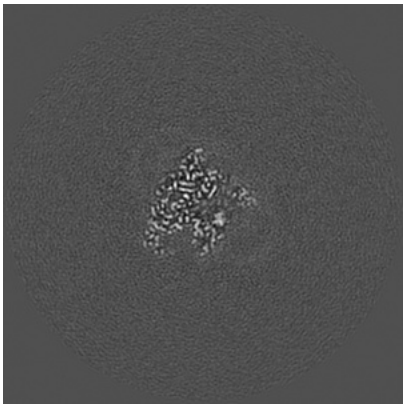
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

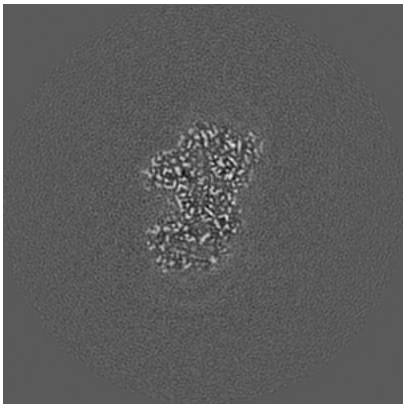
6.3.1 Primary map



X Index: 128



Y Index: 155

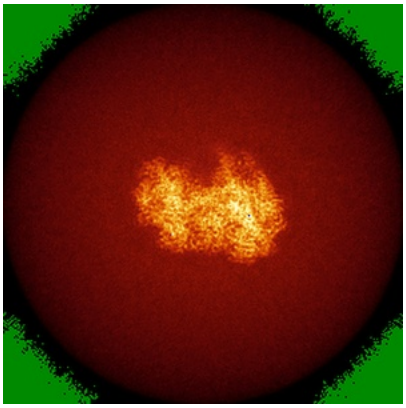


Z Index: 127

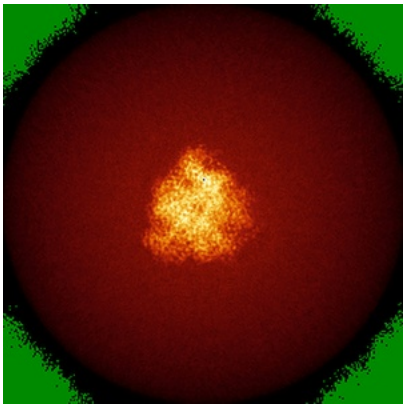
The images above show the largest variance slices of the map in three orthogonal directions.

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

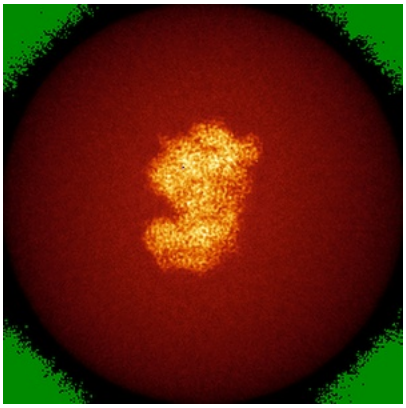
6.4.1 Primary map



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 0.0394. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

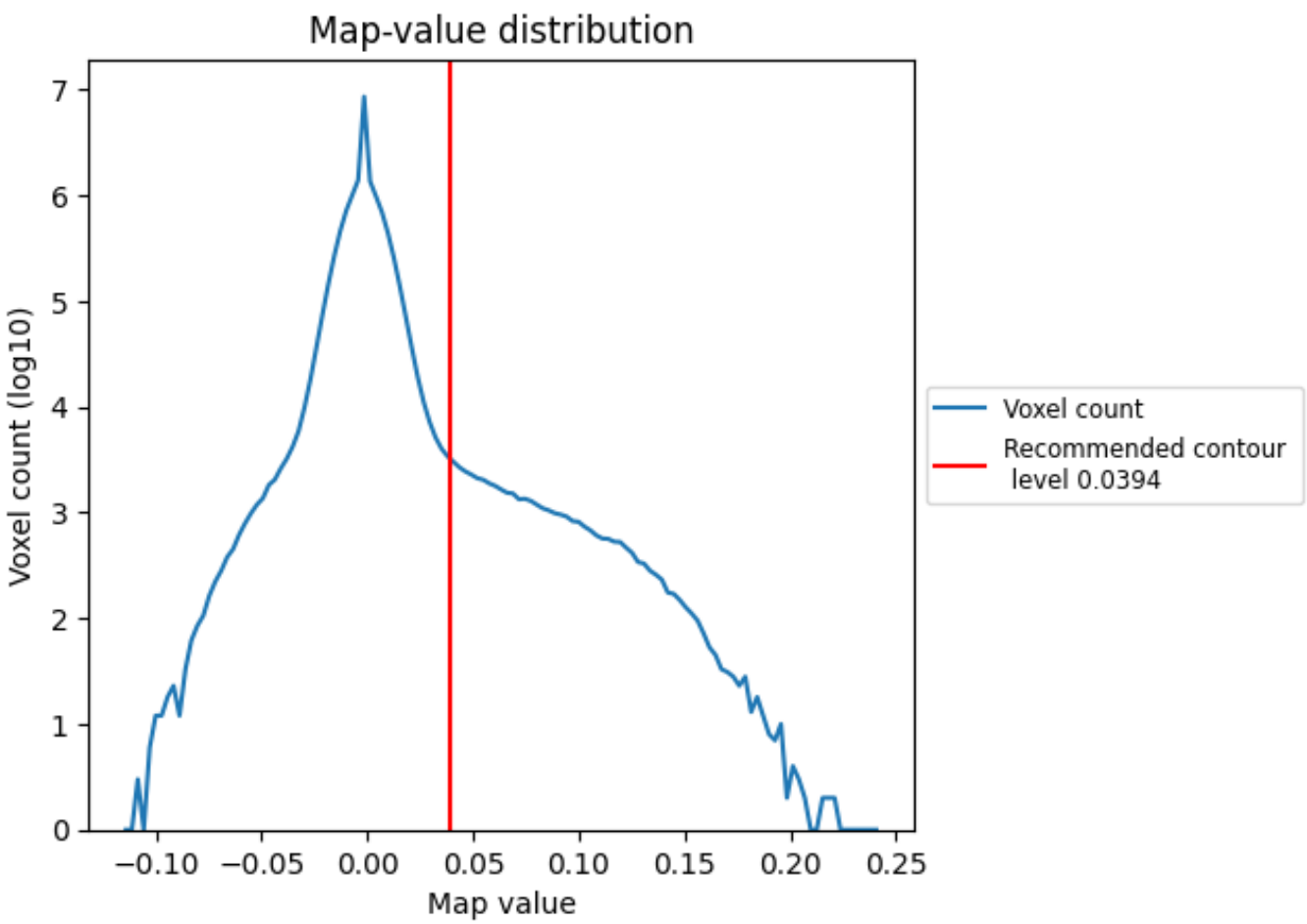
6.6 Mask visualisation (i)

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

7 Map analysis (i)

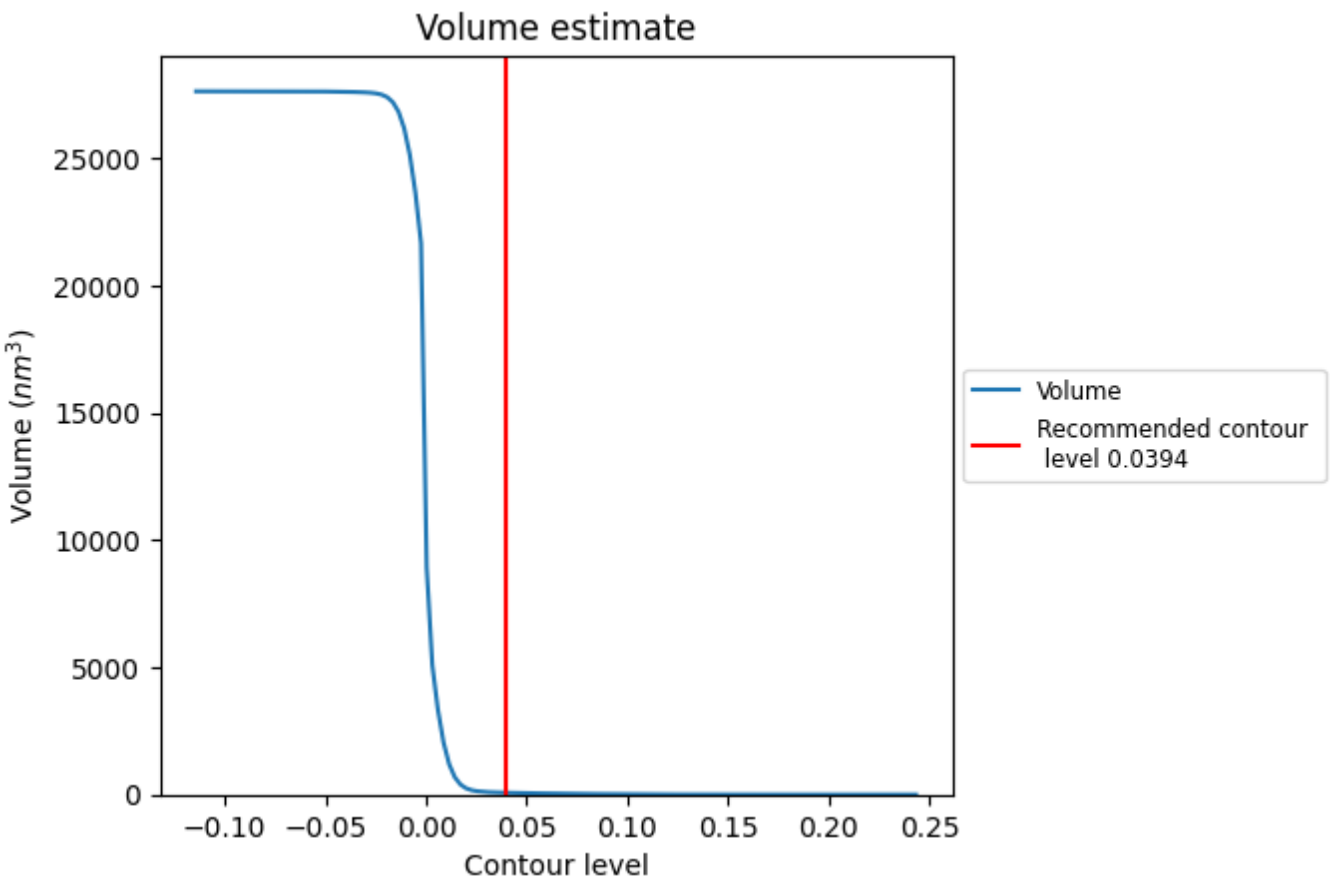
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

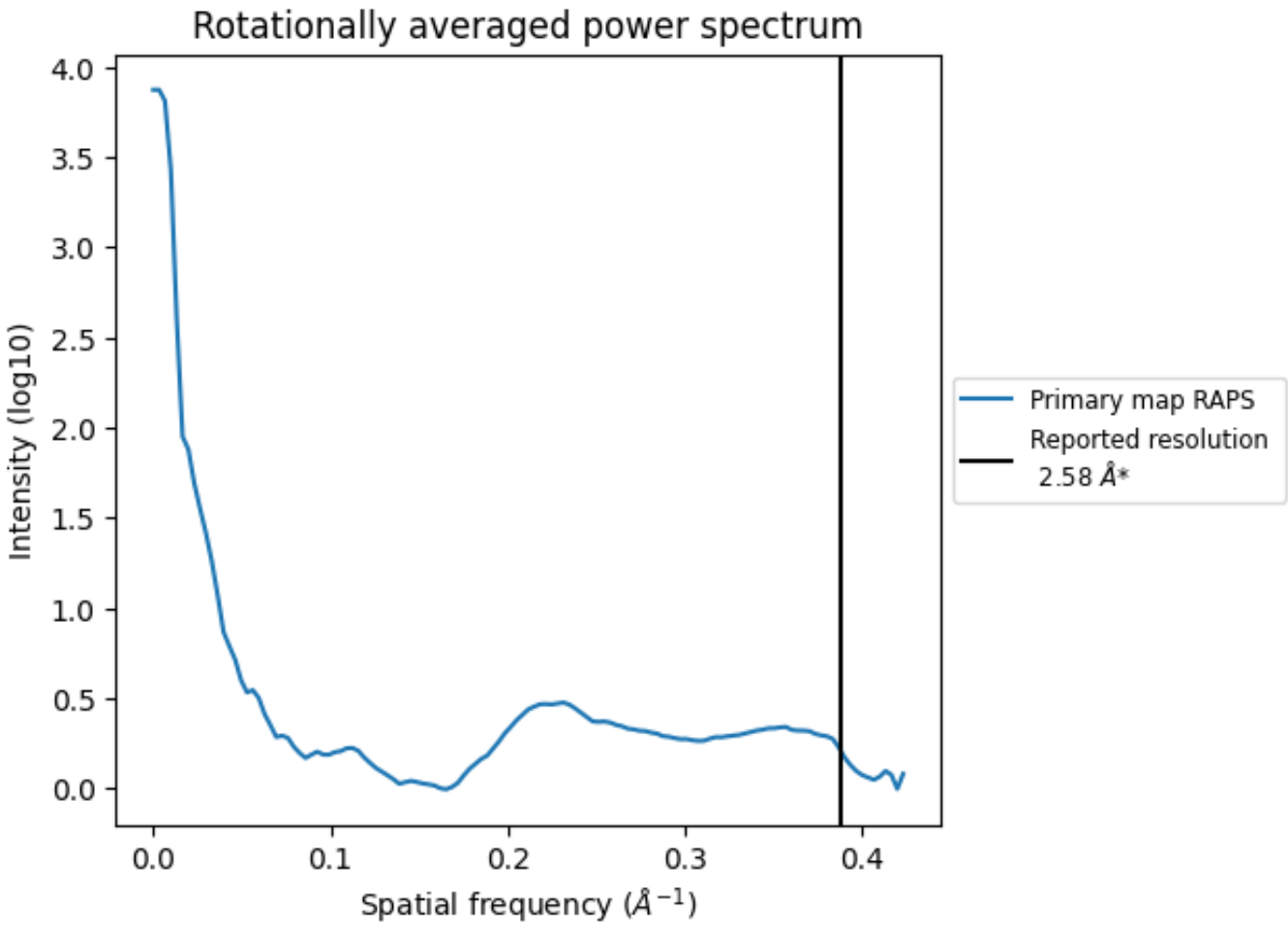
7.2 Volume estimate (i)



The volume at the recommended contour level is 73 nm^3; this corresponds to an approximate mass of 66 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)

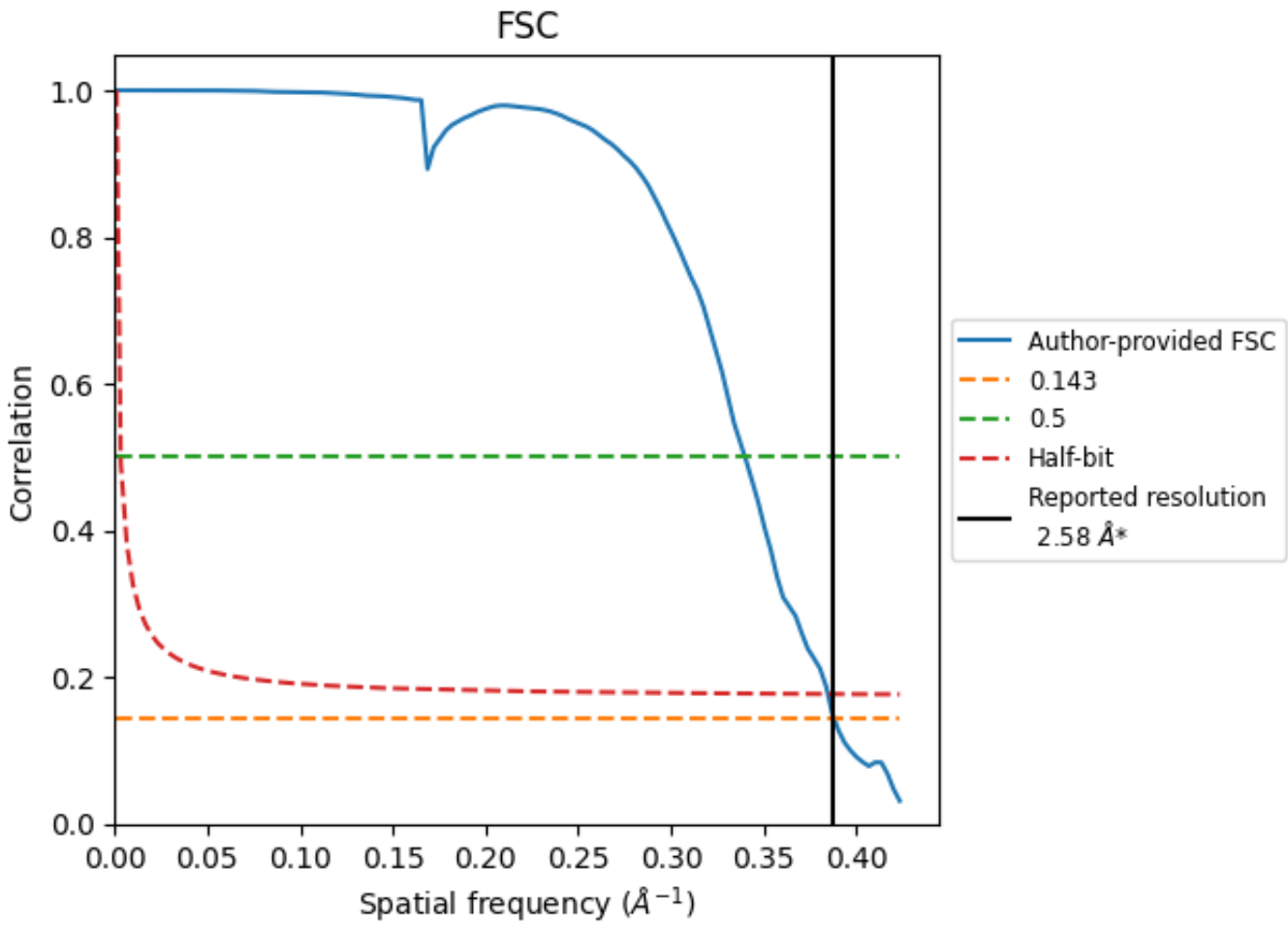


*Reported resolution corresponds to spatial frequency of 0.388 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.388 Å^{-1}

8.2 Resolution estimates (i)

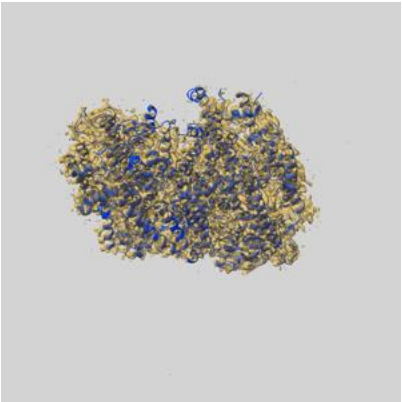
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.58	-	-
Author-provided FSC curve	2.58	2.94	2.60
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

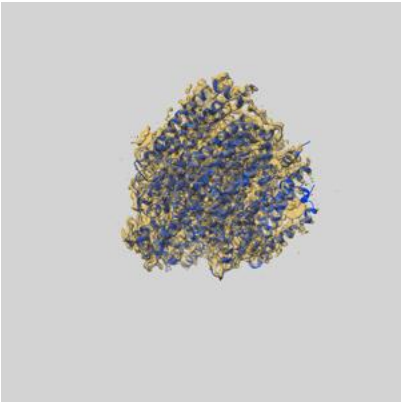
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-21690 and PDB model 6WJ6. Per-residue inclusion information can be found in section 3 on page 18.

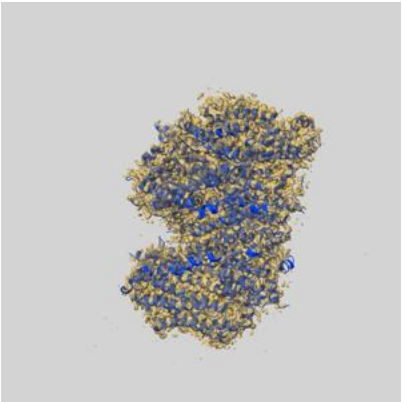
9.1 Map-model overlay (i)



X



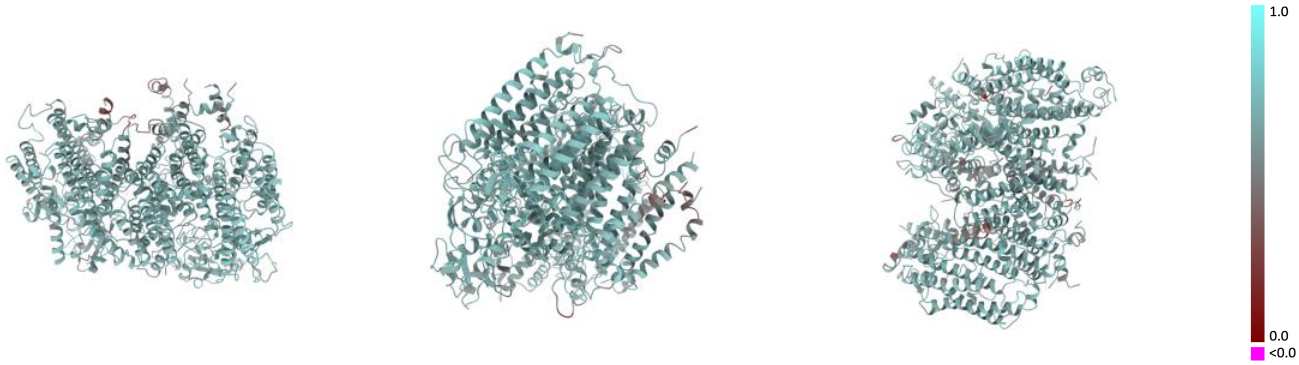
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0394 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.

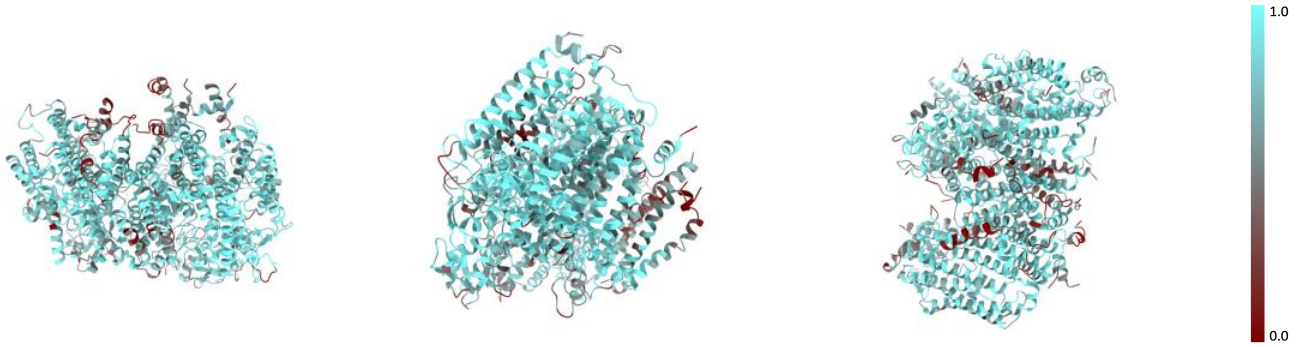
9.2 Q-score mapped to coordinate model (i)



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.

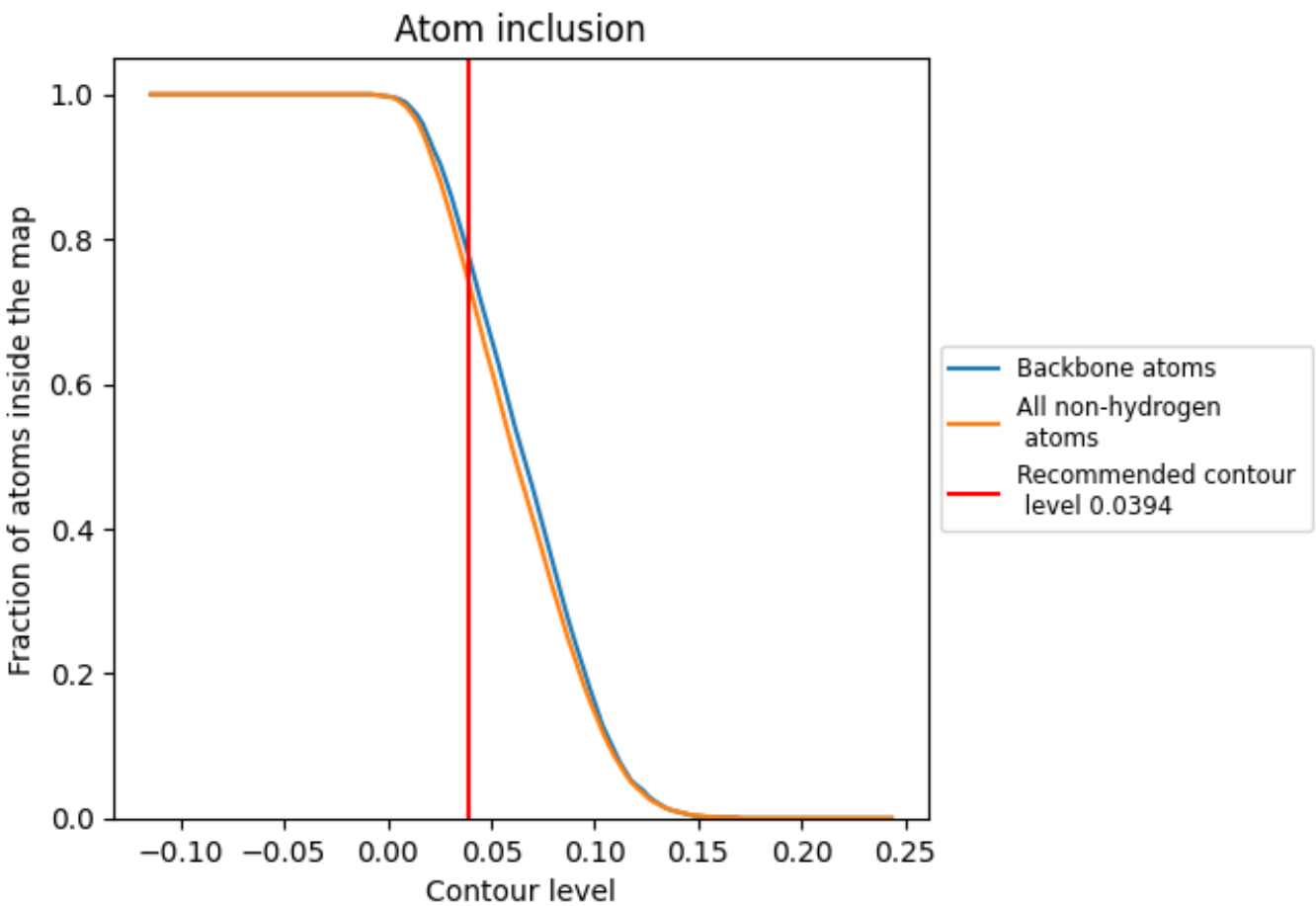
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0394).

9.4 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 74% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0394) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7390	0.6280
A	0.7490	0.6320
B	0.8000	0.6430
C	0.7270	0.6230
D	0.8010	0.6470
E	0.6080	0.5650
F	0.5880	0.5810
H	0.7380	0.6190
I	0.6480	0.6150
K	0.3260	0.4860
L	0.7050	0.6530
M	0.5850	0.6200
T	0.4160	0.5800
X	0.5100	0.5860