Full wwPDB X-ray Structure Validation Report (i)

Oct 31, 2023 – 07:31 AM EDT

PDB ID	:	3KZI
Title	:	Crystal Structure of Monomeric Form of Cyanobacterial Photosystem II
Authors	:	Gabdulkhakov, A.; Guskov, A.; Broser, M.; Kern, J.; Zouni, A.; Saenger, W.
Deposited on	:	2009-12-08
Resolution	:	3.60 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

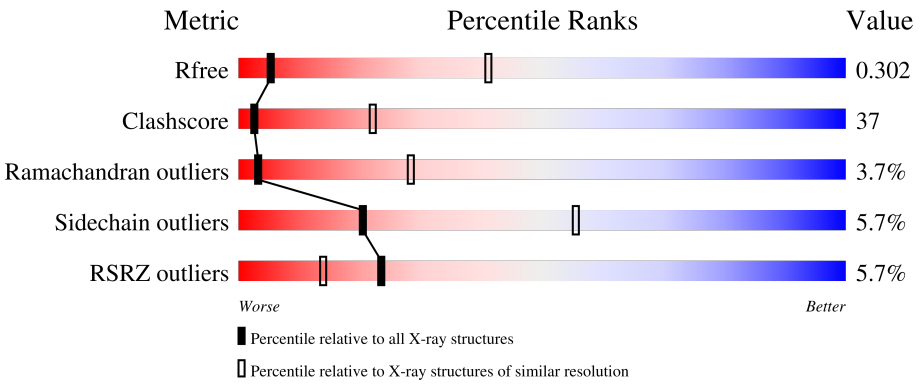
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	344	5%; 47%; 46%; 5% •
2	B	510	3%; 53%; 38%; • 5%
3	C	461	5%; 41%; 50%; 6% •
4	D	352	7%; 51%; 39%; 7% •
5	E	83	2%; 28%; 57%; 7% • 7%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	F	44	11% 25% 50% 11% 14%
7	H	65	3% 38% 49% 11%
8	I	38	11% 47% 45% 8%
9	J	40	20% 58% 8% 15%
10	K	37	3% 11% 78% 11%
11	L	37	8% 54% 32% 14%
12	M	36	22% 39% 56% 6%
13	O	246	8% 50% 45%
14	T	32	6% 56% 34% 6%
15	U	104	4% 55% 34% 7%
16	V	137	4% 60% 36%
17	y	46	4% 48% 13% 39%
18	X	40	10% 48% 25% 12% 12%
19	Z	62	8% 37% 53% 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
21	CLA	A	362	X	-	-	-
21	CLA	A	363	X	-	-	X
21	CLA	A	364	X	-	-	-
21	CLA	A	366	X	-	-	-
21	CLA	B	511	X	-	-	X
21	CLA	B	512	X	-	-	-
21	CLA	B	513	X	-	X	-
21	CLA	B	514	X	-	-	-
21	CLA	B	515	X	-	-	-
21	CLA	B	516	X	-	-	-
21	CLA	B	517	X	-	-	-
21	CLA	B	518	X	-	-	-
21	CLA	B	519	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	B	520	X	-	-	-
21	CLA	B	521	X	-	-	-
21	CLA	B	522	X	-	-	-
21	CLA	B	523	X	-	-	-
21	CLA	B	524	X	-	-	-
21	CLA	B	525	X	-	-	-
21	CLA	B	526	X	-	-	X
21	CLA	C	477	X	-	-	-
21	CLA	C	478	X	-	-	-
21	CLA	C	479	X	-	-	-
21	CLA	C	480	X	-	-	-
21	CLA	C	481	X	-	-	-
21	CLA	C	482	X	-	-	X
21	CLA	C	483	X	-	-	-
21	CLA	C	484	X	-	-	-
21	CLA	C	485	X	-	-	-
21	CLA	C	486	X	-	X	-
21	CLA	C	487	X	-	-	-
21	CLA	C	488	X	-	-	-
21	CLA	D	354	X	-	-	-
21	CLA	D	356	X	-	-	-
21	CLA	K	483	X	-	-	-
22	PHO	A	365	X	-	-	-
22	PHO	D	355	X	-	-	-
23	MES	A	367	-	-	X	-
25	BCR	B	527	-	-	-	X
25	BCR	B	529	-	-	-	X
25	BCR	B	530	-	-	-	X
25	BCR	C	490	-	-	-	X
25	BCR	J	115	-	-	-	X
25	BCR	X	107	-	-	-	X
25	BCR	Z	116	-	-	-	X
26	LHG	C	476	-	-	-	X
27	LMG	A	373	-	-	X	X
27	LMG	C	494	-	-	-	X
27	LMG	D	360	-	-	X	X
27	LMG	I	220	-	-	-	X
27	LMG	J	492	-	-	-	X
27	LMG	M	217	-	-	-	X
28	DGD	A	375	-	-	-	X
28	DGD	B	528	-	-	X	-
28	DGD	C	474	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
28	DGD	C	492	X	-	-	-
28	DGD	C	493	X	-	X	-
28	DGD	D	362	-	-	-	X
29	LMT	A	376	-	-	-	X
29	LMT	B	535	-	-	-	X
29	LMT	D	363	-	-	-	X
29	LMT	I	274	-	-	-	X
29	LMT	T	226	-	-	-	X
30	SQD	C	475	-	-	-	X
30	SQD	F	224	-	-	-	X
30	SQD	L	213	-	-	-	X
32	PL9	D	357	-	-	X	X
34	CA	O	273	-	-	-	X

2 Entry composition (i)

There are 34 unique types of molecules in this entry. The entry contains 24678 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Q(B) protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	335	2628	1720	432	461	15	0	0	0

- Molecule 2 is a protein called Photosystem II core light harvesting protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	485	3812	2505	635	659	13	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	448	3455	2262	580	600	13	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	340	2706	1794	440	460	12	0	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	H	65	507	338	81	86	2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	I	35	286	195	45	45	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	J	34	249	170	38	40	1	0	0	0

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

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

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

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

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

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

- Molecule 13 is a protein called Photosystem II manganese-stabilizing polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	O	243	1845	1154	308	379	4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	T	30	256	180	36	38	2	0	0	0

- Molecule 15 is a protein called Photosystem II 12 kDa extrinsic protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
15	U	97	774	491	129	154	0	0	0

- Molecule 16 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
16	V	137	1060	673	177	206	4	0	0	0

- Molecule 17 is a protein called Photosystem II reaction center protein ycf12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
17	y	28	201	134	33	31	3	0	0	0

- Molecule 18 is a protein called Photosystem II reaction center X protein.

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

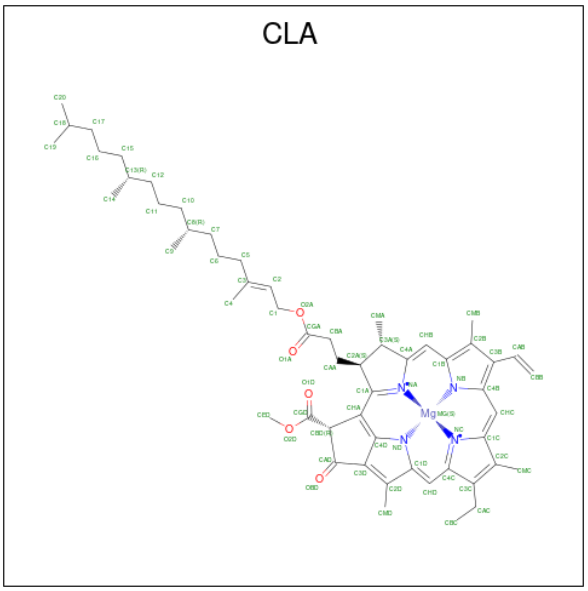
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
19	Z	62	479	328	72	77	2	0	0	0

- Molecule 20 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
20	A	1	1	1	0	0

- Molecule 21 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



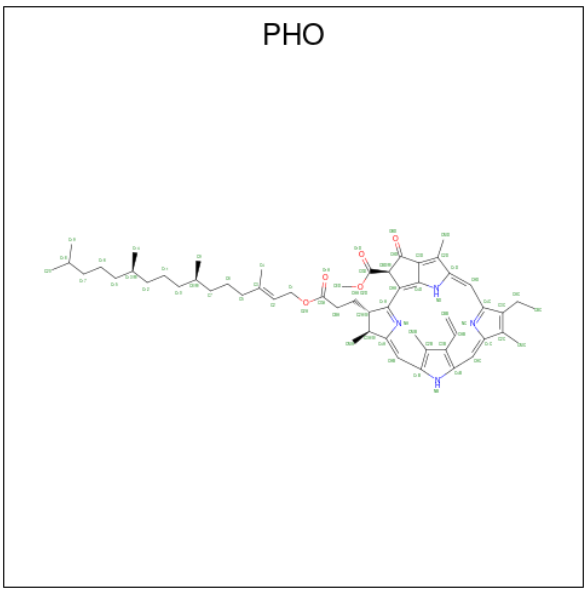
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
21	A	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
21	A	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
21	A	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
21	A	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
21	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
21	B	1	65	55	1	4	5	0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

Continued on next page...

Continued from previous page...

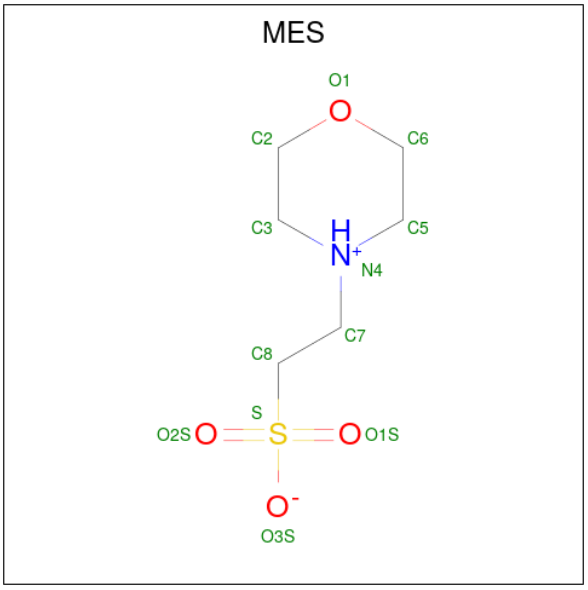
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
21	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
21	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
21	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
21	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
21	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
21	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
21	C	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
21	C	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
21	C	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
21	C	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
21	C	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
21	C	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
21	C	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
21	C	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
21	C	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
21	C	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
21	C	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
21	D	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
21	D	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
21	K	1	65	55	1	4	5	0	0

- Molecule 22 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



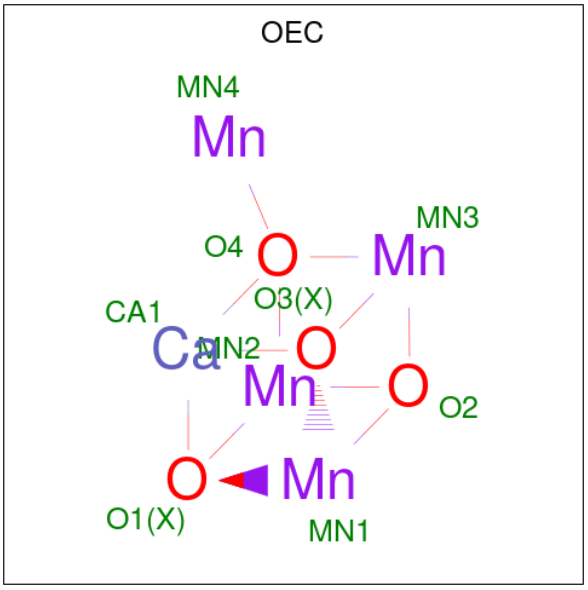
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
22	A	1	64	55	4	5	0	0
			Total	C	N	O		
22	D	1	64	55	4	5	0	0

- Molecule 23 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



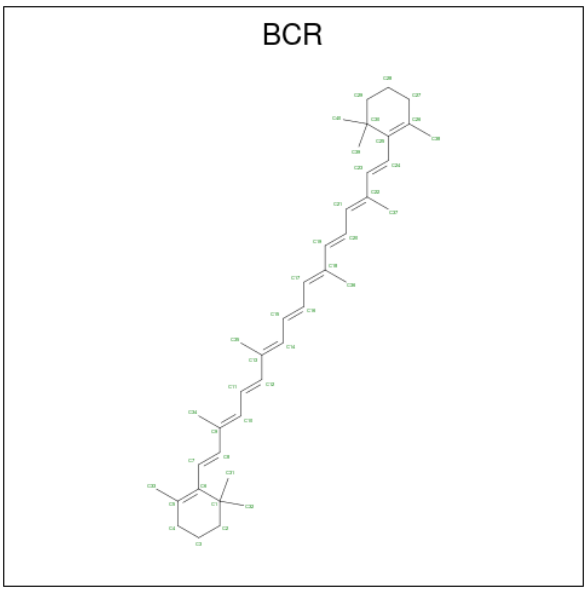
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
23	A	1	12	6	1	4	1	0	0

- Molecule 24 is OXYGEN EVOLVING SYSTEM (three-letter code: OEC) (formula: $CaMn_4O_4$).



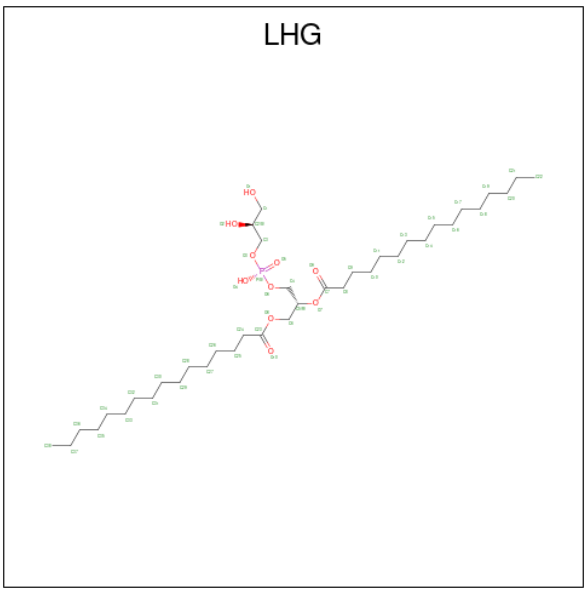
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Ca	Mn		
24	A	1	5	1	4	0	0

- Molecule 25 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



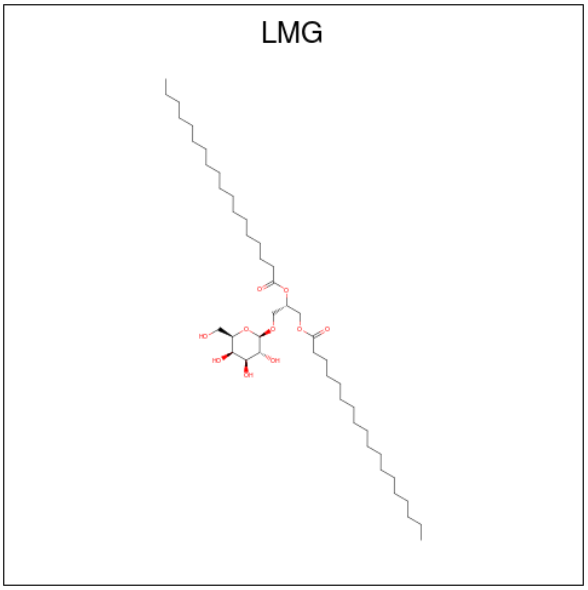
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	C		
25	A	1	40	40	0	0
			Total	C		
25	B	1	40	40	0	0
			Total	C		
25	B	1	40	40	0	0
			Total	C		
25	B	1	40	40	0	0
			Total	C		
25	C	1	40	40	0	0
			Total	C		
25	C	1	40	40	0	0
			Total	C		
25	D	1	40	40	0	0
			Total	C		
25	J	1	40	40	0	0
			Total	C		
25	J	1	40	40	0	0
			Total	C		
25	X	1	40	40	0	0
			Total	C		
25	Z	1	40	40	0	0

- Molecule 26 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



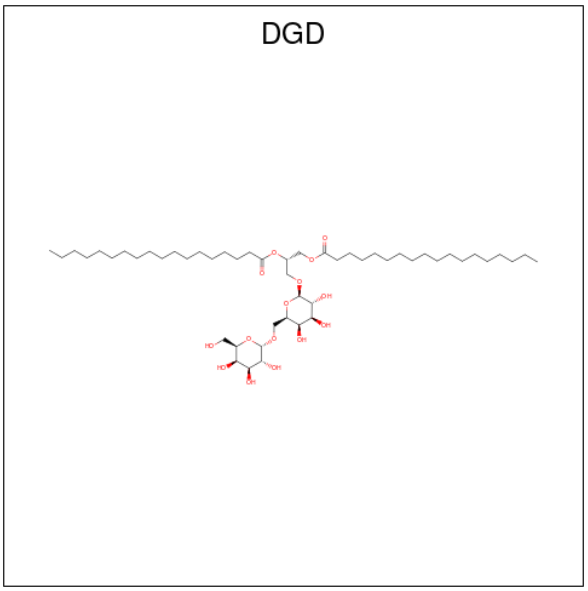
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
26	A	1	39	28	10	1	0	0
			Total	C	O	P		
26	C	1	37	26	10	1	0	0

- Molecule 27 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



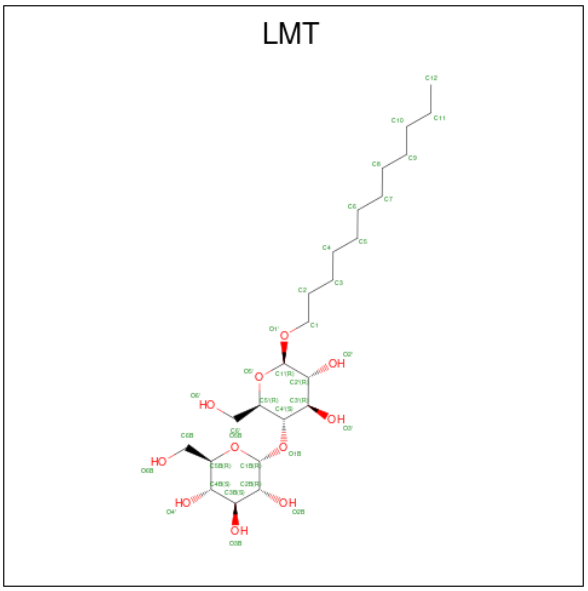
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
27	A	1	51	41	10	0	0
			Total	C	O		
27	B	1	49	39	10	0	0
			Total	C	O		
27	C	1	45	35	10	0	0
			Total	C	O		
27	D	1	46	36	10	0	0
			Total	C	O		
27	D	1	48	38	10	0	0
			Total	C	O		
27	I	1	43	33	10	0	0
			Total	C	O		
27	J	1	48	38	10	0	0
			Total	C	O		
27	M	1	42	32	10	0	0

- Molecule 28 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



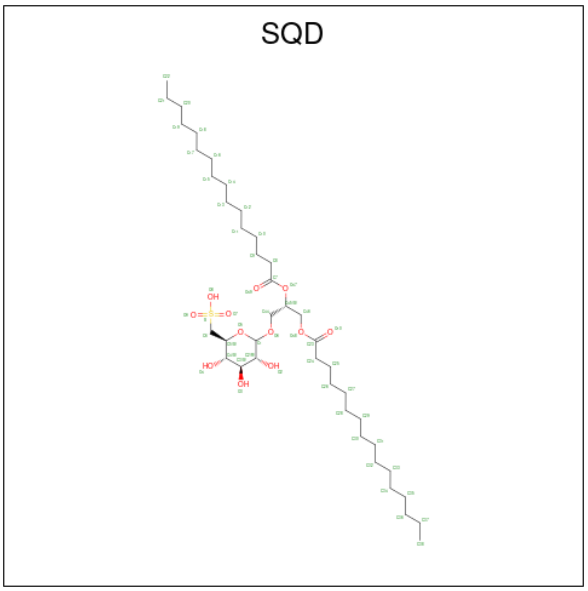
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
28	A	1	52	37	15	0	0
			Total	C	O		
28	B	1	66	51	15	0	0
			Total	C	O		
28	B	1	58	43	15	0	0
			Total	C	O		
28	C	1	56	41	15	0	0
			Total	C	O		
28	C	1	53	38	15	0	0
			Total	C	O		
28	C	1	62	47	15	0	0
			Total	C	O		
28	C	1	66	51	15	0	0
			Total	C	O		
28	D	1	63	48	15	0	0

- Molecule 29 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



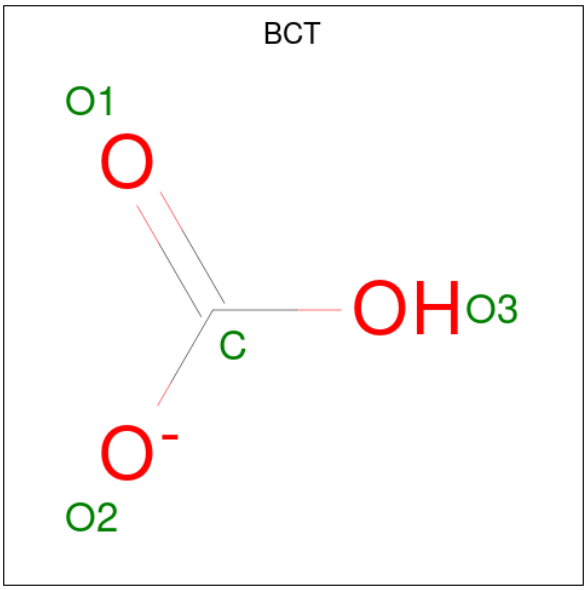
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
29	A	1	35	24	11	0	0
			Total	C	O		
29	B	1	35	24	11	0	0
			Total	C	O		
29	D	1	35	24	11	0	0
			Total	C	O		
29	D	1	31	20	11	0	0
			Total	C	O		
29	I	1	35	24	11	0	0
			Total	C	O		
29	O	1	35	24	11	0	0
			Total	C	O		
29	T	1	35	24	11	0	0

- Molecule 30 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



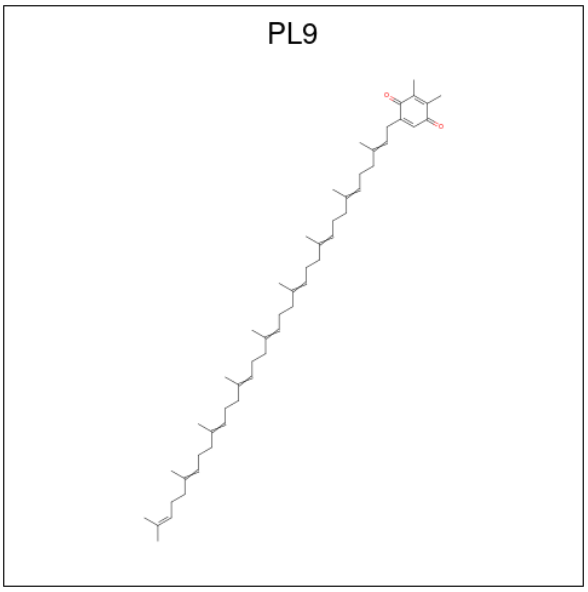
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	C	1	Total	C	O	S	0	0
			51	38	12	1		
30	D	1	Total	C	O	S	0	0
			43	30	12	1		
30	F	1	Total	C	O	S	0	0
			45	32	12	1		
30	L	1	Total	C	O	S	0	0
			47	34	12	1		

- Molecule 31 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



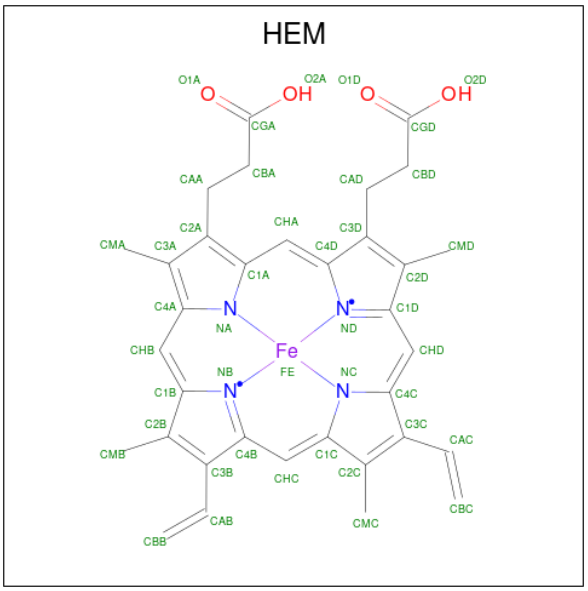
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
31	D	1	4	1	3	0	0

- Molecule 32 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			ZeroOcc	AltConf
			Total	C	O		
32	D	1	55	53	2	0	0

- Molecule 33 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
33	F	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
33	V	1	43	34	1	4	4	0	0

- Molecule 34 is CALCIUM ION (three-letter code: CA) (formula: Ca).

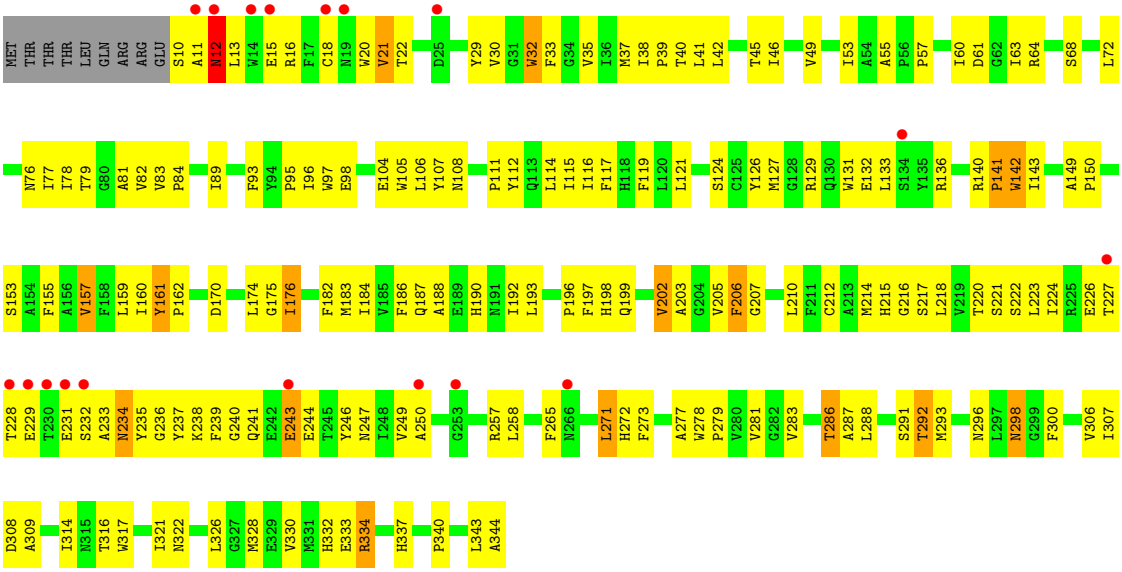
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
34	F	1	1	1	0	0
			Total	Ca		
34	K	1	1	1	0	0
			Total	Ca		
34	O	1	1	1	0	0

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 electron 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 dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

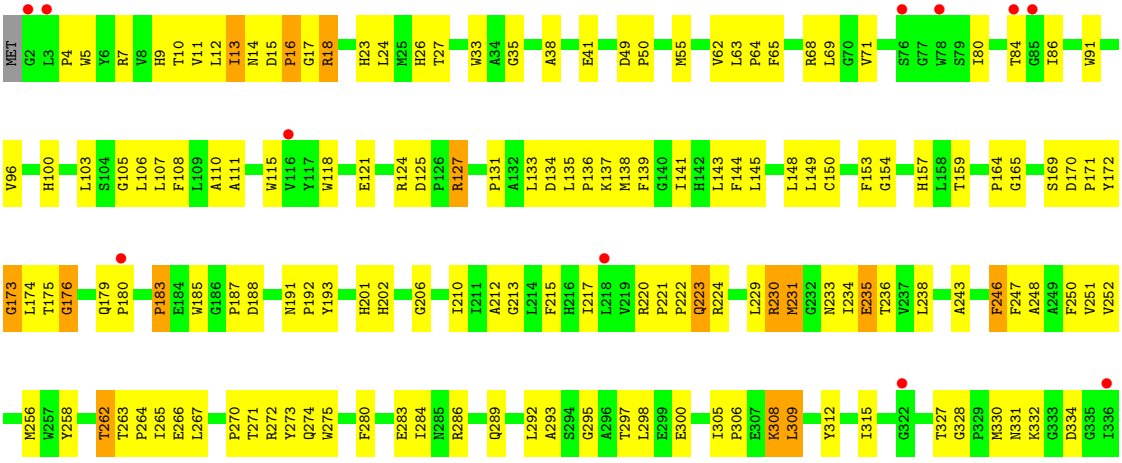
• Molecule 1: Photosystem Q(B) protein 1

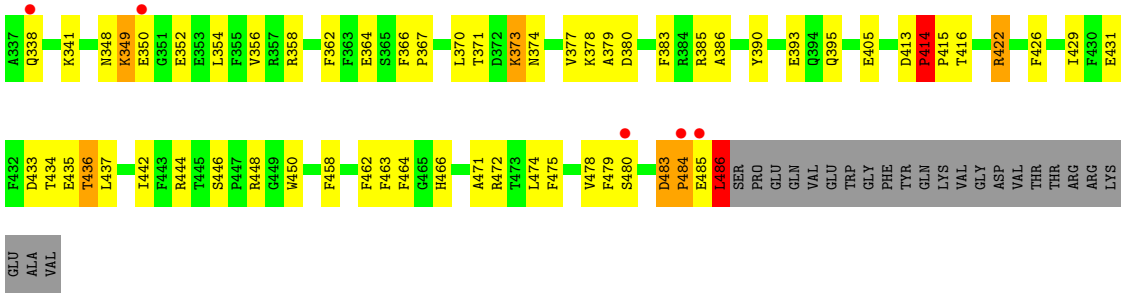
Chain A:



• Molecule 2: Photosystem II core light harvesting protein

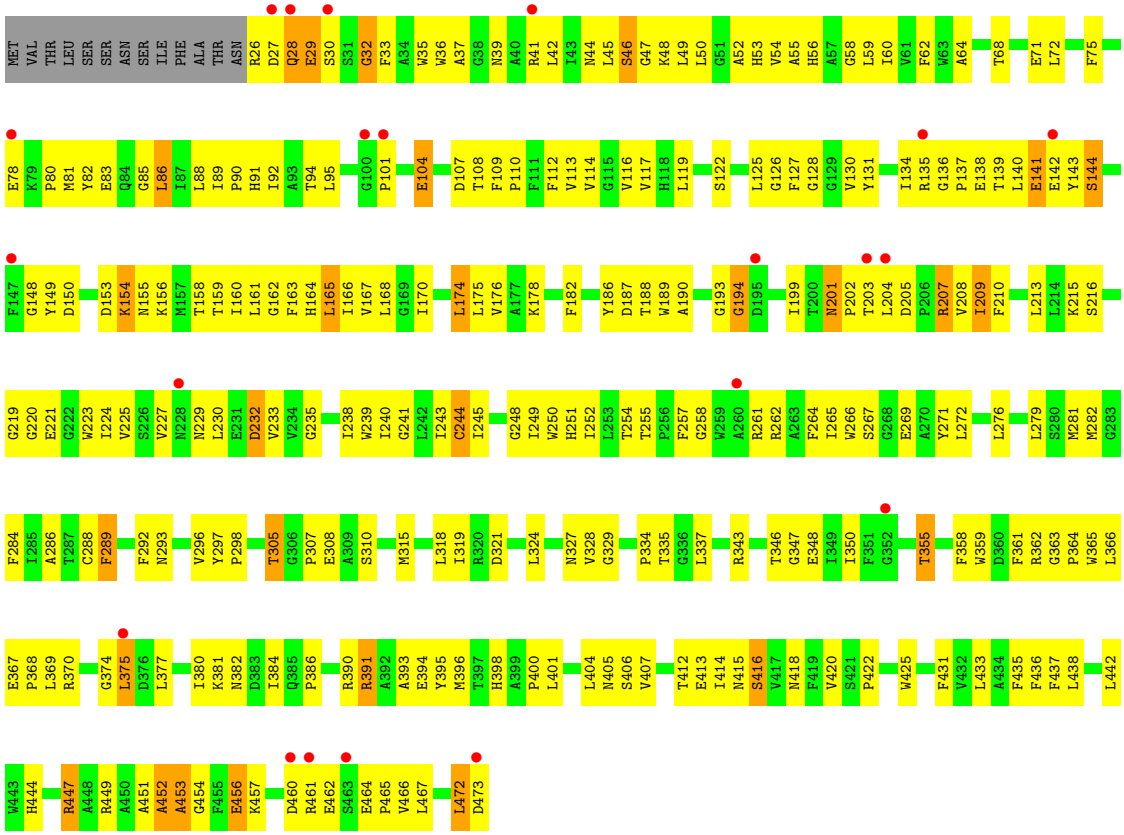
Chain B:





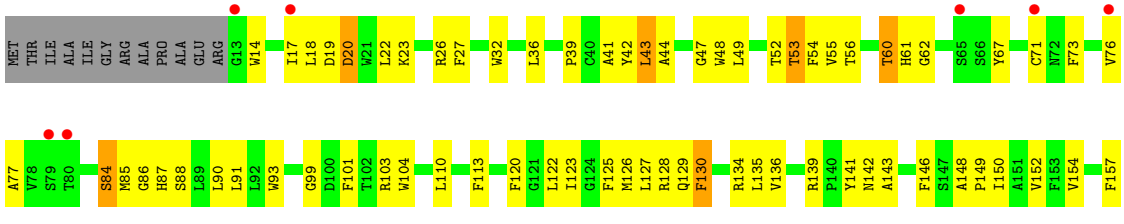
- Molecule 3: Photosystem II CP43 protein

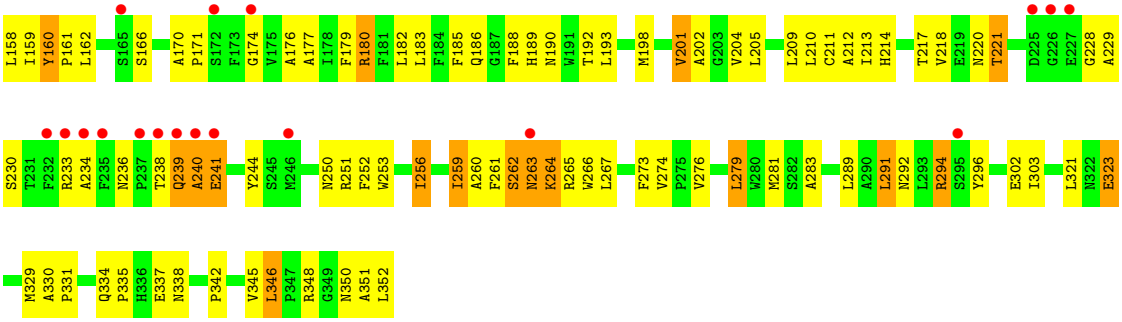
Chain C:



- Molecule 4: Photosystem II D2 protein

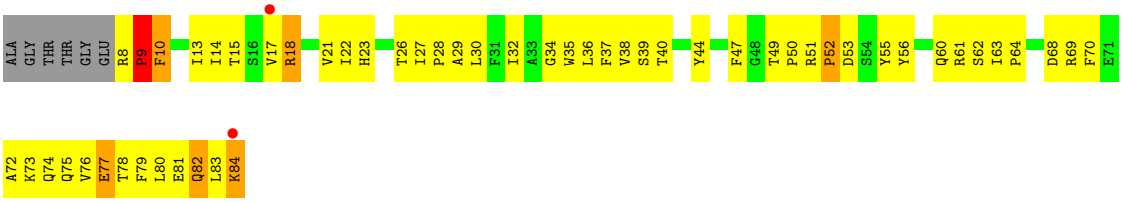
Chain D:





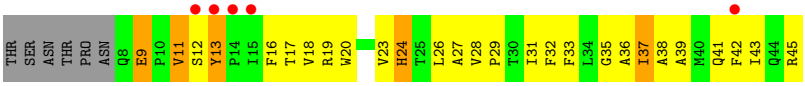
• Molecule 5: Cytochrome b559 subunit alpha

Chain E: 2% 28% 57% 7% • 7%



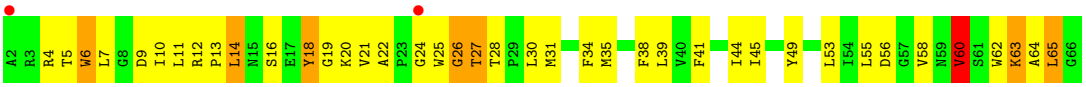
• Molecule 6: Cytochrome b559 subunit beta

Chain F: 11% 25% 50% 11% 14%



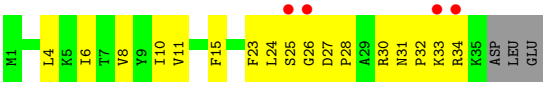
• Molecule 7: Photosystem II reaction center protein H

Chain H: 3% 38% 49% 11% •



• Molecule 8: Photosystem II reaction center protein I

Chain I: 11% 47% 45% 8%



• Molecule 9: Photosystem II reaction center protein J

Chain J: 20% 58% 8% 15%

• Molecule 10: Photosystem II reaction center protein K

Chain K: 3% 11% 78% 11%

K10 L11 P12 E13 A16 I17 F18 D19 P20 L21 V22 D23 V24 L25 P26 V27 I28 P29 V30 L31 F32 L33 A34 L35 A36 F37 V38 W39 Q40 A41 A42 V43 G44 F45 R46

• Molecule 11: Photosystem II reaction center protein L

Chain L: 8% 54% 32% 14%

M1 E2 P3 N4 P5 N6 R7 Q8 P9 V10 E11 L12 N13 R14 T15 L19 G20 L21 L22 L23 I24 L25 V26 F31 F35 F36 N37

• Molecule 12: Photosystem II reaction center protein M

Chain M: 22% 39% 56% 6%

M1 E2 V3 L6 G7 L8 I9 A10 L13 F14 V17 P18 S19 V20 F21 L22 I23 I24 L25 Q28 T29 E30 S31 Q32 Q33 K34 SER SER

• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O: 8% 50% 45%

ALA LYS GLN T30 L31 T32 Y33 D34 D35 I36 V37 G38 T39 G40 L41 A42 N43 T47 T51 A52 R53 G54 A55 Y56 D59 S60 S61 Q62 I66 L69 C70 L71 Q72 P73 L77 V78 K79 E80 E81 P82 K83 N84 K85 R86 Q87 E88 A89 E90 F91 V92 P93 T94 K95 L96

V97 T98 R99 T102 S103 Q106 I107 Q108 G109 K112 V113 N114 S115 D116 G117 S118 L119 T120 F121 V122 E123 E124 D125 G126 I127 D128 P131 V132 Q135 G138 R141 L144 T147 V148 V152 A153 S154 T155 Q156 P157 N158 V159 T160 S161 S165 T166 D167 F168

E171 F172 N173 R178 T179 A180 N181 F182 L183 D184 P185 K186 G187 R188 G189 L190 A191 S192 G193 Y194 I198 A199 L200 P201 Q202 A203 K204 E205 E206 K214 R215 L218 T219 K220 G221 Q222 I223 S224 L225 N226 V227 A228 K229 V230 D231 G232 R233 T234 G235 E236 T240 S243 V259

G263 V264 F265 P271 A272

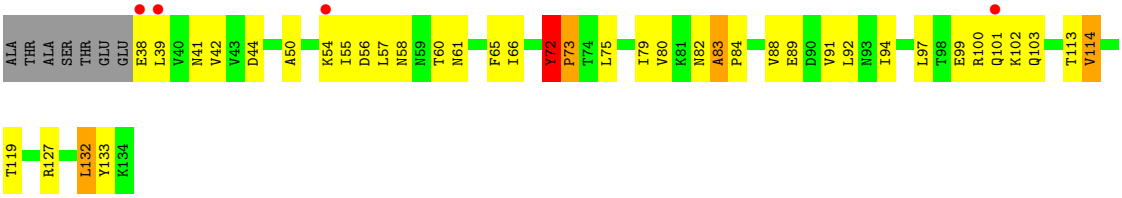
• Molecule 14: Photosystem II reaction center protein T

Chain T: 6% 56% 34% 6%

M1 E2 T3 Y6 I13 F17 I21 F22 F23 R24 E25 P26 P27 R28 I29 T30 LYS LYS

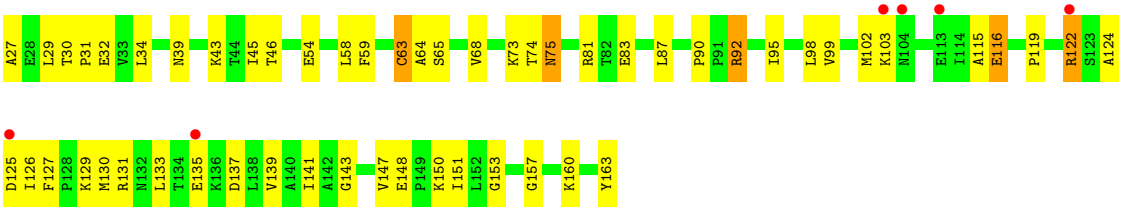
• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U: 4% 55% 34% 7%



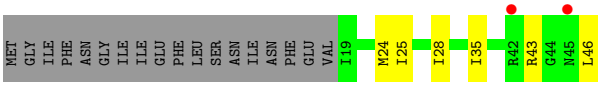
• Molecule 16: Cytochrome c-550

Chain V:



• Molecule 17: Photosystem II reaction center protein ycf12

Chain y:

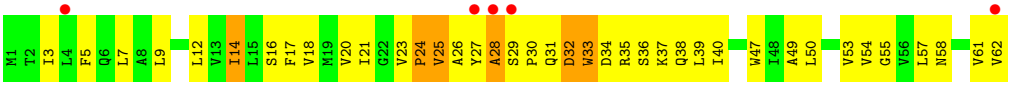


• Molecule 18: Photosystem II reaction center X protein

Chain X:

• Molecule 19: Photosystem II reaction center protein Z

Chain Z:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	119.89Å 224.69Å 337.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.87 – 3.60 29.87 – 3.60	Depositor EDS
% Data completeness (in resolution range)	89.2 (29.87-3.60) 99.3 (29.87-3.60)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	1.24 (at 3.56Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.297 , 0.308 0.294 , 0.302	Depositor DCC
R_{free} test set	1054 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å^2)	153.9	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 84.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	24678	wwPDB-VP
Average B, all atoms (Å^2)	163.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.50% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: CA, HEM, FE2, MES, BCT, PHO, BCR, LMT, PL9, LHG, CLA, OEC, DGD, SQD, LMG

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	0.44	0/2713	0.66	0/3700
2	B	0.43	0/3947	0.66	1/5379 (0.0%)
3	C	0.41	0/3567	0.64	1/4856 (0.0%)
4	D	0.47	0/2801	0.65	0/3818
5	E	0.43	0/654	0.69	0/891
6	F	0.62	0/317	0.71	0/433
7	H	0.38	0/520	0.67	0/709
8	I	0.51	0/293	0.68	0/395
9	J	0.41	0/255	0.68	0/346
10	K	0.41	0/303	0.62	0/416
11	L	0.37	0/311	0.65	0/422
12	M	0.44	0/270	0.70	0/367
13	O	0.44	0/1876	0.70	0/2548
14	T	0.49	0/265	0.63	0/359
15	U	0.42	0/785	0.73	1/1064 (0.1%)
16	V	0.39	0/1081	0.65	0/1468
17	y	0.46	0/202	0.73	0/272
18	X	0.42	0/257	0.59	0/348
19	Z	0.45	0/490	0.69	0/669
All	All	0.43	0/20907	0.66	3/28460 (0.0%)

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.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	486	LEU	CA-CB-CG	6.98	131.36	115.30
3	C	32	GLY	N-CA-C	-5.55	99.23	113.10
15	U	72	TYR	N-CA-C	5.05	124.64	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	161	TYR	Sidechain

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	2628	0	2524	244	0
2	B	3812	0	3683	272	0
3	C	3455	0	3378	373	0
4	D	2706	0	2608	238	0
5	E	635	0	625	82	0
6	F	307	0	312	49	0
7	H	507	0	521	67	0
8	I	286	0	308	18	0
9	J	249	0	262	50	0
10	K	293	0	305	56	0
11	L	304	0	316	28	0
12	M	267	0	289	34	0
13	O	1845	0	1801	119	0
14	T	256	0	262	24	0
15	U	774	0	773	47	0
16	V	1060	0	1068	49	0
17	y	201	0	226	0	0
18	X	254	0	282	28	0
19	Z	479	0	516	64	0
20	A	1	0	0	0	0
21	A	260	0	288	49	0
21	B	1040	0	1152	151	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	C	780	0	864	143	0
21	D	130	0	144	20	0
21	K	65	0	72	15	0
22	A	64	0	74	8	0
22	D	64	0	74	12	0
23	A	12	0	13	13	0
24	A	5	0	0	0	0
25	A	40	0	56	8	0
25	B	120	0	168	7	0
25	C	80	0	112	26	0
25	D	40	0	56	8	0
25	J	80	0	112	19	0
25	X	40	0	56	6	0
25	Z	40	0	56	4	0
26	A	39	0	51	7	0
26	C	37	0	44	5	0
27	A	51	0	72	40	0
27	B	49	0	68	6	0
27	C	45	0	60	6	0
27	D	94	0	127	36	0
27	I	43	0	56	0	0
27	J	48	0	66	4	0
27	M	42	0	54	3	0
28	A	52	0	62	1	0
28	B	124	0	170	42	0
28	C	237	0	311	76	0
28	D	63	0	87	0	0
29	A	35	0	46	0	0
29	B	35	0	46	2	0
29	D	66	0	81	3	0
29	I	35	0	46	2	0
29	O	35	0	46	1	0
29	T	35	0	46	1	0
30	C	51	0	68	5	0
30	D	43	0	49	9	0
30	F	45	0	53	0	0
30	L	47	0	60	2	0
31	D	4	0	0	0	0
32	D	55	0	80	31	0
33	F	43	0	30	6	0
33	V	43	0	30	5	0
34	F	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	K	1	0	0	0	0
34	O	1	0	0	0	0
All	All	24678	0	25265	1799	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 37.

All (1799) 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)
30:C:475:SQD:C3	30:C:475:SQD:C4	1.74	1.58
16:V:63:CYS:SG	33:V:164:HEM:HAB	1.65	1.35
27:A:373:LMG:H112	4:D:266:TRP:CH2	1.77	1.19
1:A:271:LEU:HD11	23:A:367:MES:C8	1.73	1.17
28:B:533:DGD:HAH1	12:M:17:VAL:HG21	1.21	1.14
2:B:121:GLU:HG2	7:H:4:ARG:HG2	1.25	1.13
9:J:15:THR:HG21	10:K:38:VAL:HG13	1.18	1.13
2:B:327:THR:HA	21:B:517:CLA:O1A	1.49	1.12
15:U:83:ALA:HB1	15:U:84:PRO:HD2	1.23	1.11
1:A:271:LEU:CD1	23:A:367:MES:H82	1.80	1.11
3:C:174:LEU:HD22	21:C:478:CLA:H161	1.21	1.10
10:K:10:LYS:O	10:K:10:LYS:HG2	1.44	1.10
3:C:293:ASN:HA	28:C:491:DGD:O2E	1.53	1.09
27:A:373:LMG:H332	12:M:22:LEU:HD21	1.27	1.08
3:C:174:LEU:CD2	21:C:478:CLA:H161	1.84	1.07
21:B:518:CLA:H42	4:D:127:LEU:HD11	1.07	1.05
5:E:15:THR:HG22	9:J:7:ARG:CG	1.85	1.05
3:C:473:ASP:HB2	14:T:26:PRO:HB3	1.31	1.05
28:B:528:DGD:O1B	28:B:528:DGD:HG12	1.57	1.04
1:A:129:ARG:HH21	4:D:256:ILE:HD12	1.20	1.04
5:E:15:THR:CG2	9:J:7:ARG:HG2	1.86	1.04
3:C:254:THR:HG22	3:C:255:THR:H	1.18	1.04
4:D:23:LYS:HZ1	30:D:361:SQD:H462	1.22	1.04
13:O:178:ARG:HH11	13:O:178:ARG:HG3	1.18	1.04
28:B:528:DGD:O2D	4:D:87:HIS:HB2	1.58	1.03
27:D:360:LMG:O6	11:L:15:THR:HG21	1.62	1.00
27:A:373:LMG:H112	4:D:266:TRP:HH2	0.85	1.00
2:B:250:PHE:HD1	28:B:528:DGD:HB92	1.22	1.00
2:B:149:LEU:HG	21:B:513:CLA:HBC1	1.41	1.00
27:A:373:LMG:H372	12:M:18:PRO:CB	1.91	0.98
1:A:317:TRP:CZ3	4:D:180:ARG:HD3	2.00	0.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:373:LMG:C37	12:M:18:PRO:HB3	1.93	0.96
27:A:373:LMG:H372	12:M:18:PRO:HB3	0.97	0.96
13:O:69:LEU:HB3	13:O:107:ILE:HB	1.49	0.95
13:O:230:VAL:HG12	13:O:231:ASP:H	1.30	0.94
14:T:29:ILE:H	14:T:29:ILE:HD12	1.33	0.94
15:U:83:ALA:HB1	15:U:84:PRO:CD	1.98	0.93
25:C:489:BCR:H312	19:Z:9:LEU:HD11	1.51	0.93
1:A:11:ALA:O	1:A:12:ASN:HB2	1.67	0.93
27:A:373:LMG:C11	4:D:266:TRP:HH2	1.80	0.92
2:B:332:LYS:HE3	28:B:533:DGD:O4D	1.68	0.92
11:L:1:MET:HG2	11:L:1:MET:O	1.70	0.92
3:C:407:VAL:HA	28:C:493:DGD:O2E	1.70	0.91
21:B:517:CLA:H202	4:D:281:MET:SD	2.11	0.91
4:D:186:GLN:HB2	21:D:354:CLA:HBC1	1.52	0.91
21:C:477:CLA:HMB3	25:C:490:BCR:H403	1.51	0.90
3:C:52:ALA:HA	21:C:486:CLA:HMB3	1.53	0.90
3:C:225:VAL:HG21	28:C:491:DGD:HG11	1.52	0.90
1:A:286:THR:HG23	21:A:362:CLA:HED3	1.50	0.90
27:D:360:LMG:O7	11:L:19:LEU:HD21	1.71	0.89
27:D:360:LMG:H212	14:T:17:PHE:HZ	1.36	0.89
21:B:524:CLA:H18	28:B:533:DGD:HAS1	1.53	0.89
5:E:15:THR:CG2	9:J:7:ARG:CG	2.48	0.89
28:B:528:DGD:HO2D	4:D:87:HIS:CG	1.90	0.89
3:C:224:ILE:O	3:C:227:VAL:HG23	1.73	0.89
2:B:414:PRO:HB2	2:B:415:PRO:HD3	1.55	0.88
2:B:434:THR:HG23	13:O:204:LYS:HE3	1.54	0.88
21:B:514:CLA:H11	21:B:522:CLA:H152	1.54	0.88
28:C:493:DGD:HE62	9:J:40:LEU:HD21	1.54	0.88
2:B:271:THR:HG22	2:B:273:TYR:H	1.39	0.88
5:E:15:THR:HG21	9:J:7:ARG:HG2	1.56	0.87
3:C:305:THR:HG22	3:C:308:GLU:H	1.40	0.87
13:O:218:LEU:HD22	15:U:119:THR:HG21	1.57	0.87
18:X:12:ILE:HG12	18:X:16:LEU:HD12	1.56	0.87
13:O:69:LEU:HD12	13:O:70:CYS:H	1.39	0.87
27:A:373:LMG:H231	27:D:360:LMG:H202	1.54	0.87
3:C:155:ASN:HD21	3:C:255:THR:HB	1.40	0.87
28:B:528:DGD:HBE1	4:D:159:ILE:HG23	1.57	0.87
3:C:447:ARG:HG2	3:C:447:ARG:HH11	1.40	0.86
2:B:250:PHE:HD1	28:B:528:DGD:C9B	1.88	0.86
16:V:30:THR:HB	16:V:31:PRO:HD2	1.54	0.86
4:D:259:ILE:HG12	27:D:360:LMG:H301	1.57	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:5:PRO:HA	11:L:7:ARG:HH22	1.40	0.86
25:C:489:BCR:H353	25:J:112:BCR:H321	1.56	0.85
13:O:178:ARG:HH11	13:O:178:ARG:CG	1.88	0.85
1:A:121:LEU:HD21	21:A:366:CLA:HMB3	1.58	0.85
4:D:129:GLN:NE2	4:D:143:ALA:HA	1.92	0.85
21:B:513:CLA:HBB1	21:B:515:CLA:H171	1.59	0.85
7:H:12:ARG:O	7:H:12:ARG:HD3	1.76	0.85
11:L:8:GLN:N	11:L:8:GLN:HE21	1.75	0.85
5:E:18:ARG:HD2	5:E:22:ILE:HD11	1.60	0.84
15:U:72:TYR:HB3	15:U:73:PRO:HD3	1.57	0.84
2:B:250:PHE:CD1	28:B:528:DGD:HB92	2.12	0.84
3:C:305:THR:HG23	3:C:307:PRO:HD2	1.60	0.83
1:A:39:PRO:HG3	25:A:369:BCR:HC8	1.58	0.83
28:B:533:DGD:HG31	12:M:6:LEU:HD12	1.59	0.83
3:C:437:PHE:CZ	21:K:483:CLA:HMB3	2.14	0.83
1:A:317:TRP:HZ3	4:D:180:ARG:HD3	1.39	0.83
2:B:124:ARG:HE	2:B:131:PRO:HD3	1.43	0.83
27:D:360:LMG:H221	14:T:13:ILE:HG21	1.60	0.83
3:C:166:ILE:HG23	3:C:245:ILE:HG23	1.61	0.83
21:C:478:CLA:H12	21:C:479:CLA:H42	1.61	0.82
28:B:528:DGD:O2D	4:D:87:HIS:CB	2.27	0.82
1:A:214:MET:HB3	23:A:367:MES:H61	1.59	0.82
4:D:135:LEU:HD23	30:D:361:SQD:O2	1.78	0.82
3:C:407:VAL:HA	28:C:493:DGD:HO2E	1.45	0.82
21:B:518:CLA:CBB	4:D:123:ILE:HG12	2.10	0.81
3:C:407:VAL:HG22	28:C:493:DGD:O2E	1.81	0.81
21:C:487:CLA:H172	21:C:487:CLA:HMA2	1.61	0.81
3:C:28:GLN:OE1	3:C:28:GLN:HA	1.78	0.81
27:D:360:LMG:H341	14:T:21:ILE:HD11	1.62	0.81
2:B:247:PHE:HE1	21:B:512:CLA:H8	1.46	0.81
3:C:254:THR:HG22	3:C:255:THR:N	1.96	0.81
4:D:23:LYS:NZ	30:D:361:SQD:H462	1.97	0.80
4:D:148:ALA:HB3	4:D:149:PRO:HD3	1.63	0.80
4:D:323:GLU:HG2	13:O:194:TYR:OH	1.81	0.80
1:A:192:ILE:HA	1:A:293:MET:HE3	1.64	0.80
5:E:84:LYS:HB2	5:E:84:LYS:NZ	1.97	0.80
27:A:373:LMG:C20	32:D:357:PL9:H212	2.13	0.79
25:C:489:BCR:HC22	10:K:18:PHE:HD1	1.46	0.79
3:C:473:ASP:HB2	14:T:26:PRO:CB	2.11	0.79
30:C:475:SQD:C3	30:C:475:SQD:C5	2.60	0.79
28:B:533:DGD:HAH1	12:M:17:VAL:CG2	2.08	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:10:LYS:O	10:K:10:LYS:CG	2.30	0.78
2:B:238:LEU:HB2	21:B:522:CLA:HMD3	1.65	0.78
13:O:230:VAL:HG12	13:O:231:ASP:N	1.98	0.78
2:B:434:THR:CG2	13:O:204:LYS:HE3	2.12	0.78
21:C:484:CLA:H141	21:K:483:CLA:H162	1.64	0.78
19:Z:36:SER:HA	19:Z:39:LEU:HG	1.64	0.78
1:A:215:HIS:HA	23:A:367:MES:H51	1.63	0.78
2:B:383:PHE:O	13:O:192:SER:HA	1.84	0.78
3:C:110:PRO:HG3	27:C:494:LMG:H141	1.65	0.78
21:C:480:CLA:H143	21:C:484:CLA:H152	1.66	0.77
2:B:348:ASN:HB3	2:B:354:LEU:HD21	1.65	0.77
1:A:218:LEU:HD22	23:A:367:MES:H52	1.66	0.77
3:C:233:VAL:HA	25:C:490:BCR:H281	1.65	0.77
4:D:152:VAL:HG11	21:D:354:CLA:H11	1.67	0.77
7:H:35:MET:HE2	25:X:107:BCR:HC21	1.65	0.77
13:O:31:LEU:HB2	13:O:36:ILE:HD11	1.67	0.77
1:A:271:LEU:HD21	23:A:367:MES:HN4	1.50	0.77
27:D:360:LMG:H201	11:L:22:LEU:HD11	1.66	0.77
27:A:373:LMG:H332	12:M:22:LEU:CD2	2.12	0.77
3:C:284:PHE:HB3	28:C:491:DGD:HA52	1.66	0.77
3:C:135:ARG:HE	19:Z:33:TRP:HE1	1.30	0.76
2:B:134:ASP:OD2	2:B:137:LYS:HE3	1.86	0.76
1:A:131:TRP:CH2	21:C:481:CLA:HBA2	2.20	0.76
4:D:192:THR:HG23	21:D:354:CLA:HBC2	1.68	0.76
5:E:35:TRP:CD2	6:F:39:ALA:HB2	2.20	0.76
2:B:271:THR:HG22	2:B:273:TYR:N	1.98	0.76
3:C:209:ILE:HG23	25:C:490:BCR:H382	1.65	0.76
19:Z:49:ALA:O	19:Z:53:VAL:HG23	1.86	0.76
11:L:5:PRO:HA	11:L:7:ARG:NH2	2.00	0.75
1:A:46:ILE:HD13	28:A:375:DGD:HBE2	1.68	0.75
1:A:93:PHE:CZ	21:A:366:CLA:HBA1	2.20	0.75
3:C:473:ASP:CB	14:T:26:PRO:HB3	2.14	0.75
30:C:475:SQD:H251	26:C:476:LHG:H102	1.66	0.75
18:X:12:ILE:O	18:X:12:ILE:HG23	1.85	0.75
1:A:258:LEU:HD12	4:D:128:ARG:HD3	1.66	0.75
2:B:483:ASP:CG	2:B:484:PRO:HD2	2.07	0.75
3:C:391:ARG:NH1	3:C:391:ARG:HB2	2.02	0.75
3:C:437:PHE:HZ	21:K:483:CLA:HMB3	1.50	0.75
1:A:57:PRO:HG3	1:A:68:SER:HB3	1.67	0.75
8:I:4:LEU:HD22	29:I:274:LMT:H52	1.69	0.75
4:D:279:LEU:HG	22:D:355:PHO:HBC3	1.67	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:28:VAL:HB	6:F:29:PRO:HD3	1.68	0.75
21:B:523:CLA:HED3	21:B:523:CLA:H2	1.68	0.74
16:V:63:CYS:SG	33:V:164:HEM:CAB	2.61	0.74
21:B:518:CLA:H42	4:D:127:LEU:CD1	2.03	0.74
1:A:214:MET:CB	23:A:367:MES:H61	2.16	0.74
27:A:373:LMG:H192	32:D:357:PL9:H221	1.69	0.74
3:C:135:ARG:NE	19:Z:33:TRP:HE1	1.85	0.74
3:C:223:TRP:CZ2	28:C:474:DGD:HA62	2.23	0.74
2:B:483:ASP:CB	2:B:484:PRO:HD2	2.17	0.74
19:Z:32:ASP:HB2	19:Z:35:ARG:HG2	1.67	0.74
4:D:244:TYR:OH	4:D:264:LYS:HE3	1.88	0.74
5:E:18:ARG:HB3	5:E:18:ARG:HH11	1.52	0.74
27:A:373:LMG:C33	12:M:22:LEU:HD21	2.14	0.74
16:V:31:PRO:HA	16:V:34:LEU:HD12	1.68	0.74
3:C:418:ASN:HB2	28:C:493:DGD:O4E	1.88	0.73
2:B:234:ILE:HD11	21:B:520:CLA:H191	1.70	0.73
3:C:29:GLU:HB3	10:K:46:ARG:NH1	2.03	0.73
3:C:135:ARG:HB2	19:Z:27:TYR:HB3	1.69	0.73
3:C:155:ASN:HA	3:C:158:THR:HG22	1.69	0.73
4:D:41:ALA:HB2	22:D:355:PHO:H43	1.70	0.73
19:Z:32:ASP:CG	19:Z:33:TRP:H	1.90	0.73
4:D:262:SER:HG	27:D:360:LMG:HO3	1.33	0.73
21:B:518:CLA:H102	21:B:518:CLA:H142	1.69	0.73
1:A:214:MET:HA	1:A:214:MET:CE	2.17	0.73
1:A:41:LEU:O	1:A:45:THR:HG22	1.89	0.73
5:E:15:THR:HG22	9:J:7:ARG:HG3	1.71	0.73
30:C:475:SQD:C4	30:C:475:SQD:C2	2.66	0.73
18:X:34:PHE:O	18:X:38:ILE:HG12	1.88	0.73
1:A:42:LEU:HD12	25:A:369:BCR:C11	2.18	0.73
3:C:85:GLY:O	21:C:480:CLA:HED1	1.89	0.73
3:C:241:GLY:O	3:C:245:ILE:HG13	1.88	0.73
4:D:60:THR:HG23	4:D:61:HIS:CD2	2.23	0.73
5:E:17:VAL:O	5:E:21:VAL:HG23	1.88	0.73
27:A:373:LMG:H202	32:D:357:PL9:H212	1.70	0.72
3:C:225:VAL:CG2	28:C:491:DGD:HG11	2.20	0.72
1:A:35:VAL:HA	25:A:369:BCR:H333	1.70	0.72
3:C:168:LEU:HD13	21:C:483:CLA:H43	1.71	0.72
4:D:148:ALA:HB2	4:D:276:VAL:HG13	1.70	0.72
2:B:27:THR:HG22	2:B:107:LEU:HD13	1.72	0.72
4:D:261:PHE:HB2	32:D:357:PL9:H522	1.71	0.72
2:B:124:ARG:HH11	2:B:124:ARG:HG3	1.55	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:305:THR:CG2	3:C:308:GLU:H	2.02	0.72
2:B:450:TRP:HB3	21:B:517:CLA:HMB2	1.71	0.72
3:C:240:ILE:O	3:C:244:CYS:HB2	1.88	0.72
3:C:254:THR:CG2	3:C:255:THR:H	2.00	0.72
3:C:415:ASN:O	3:C:416:SER:HB3	1.89	0.72
25:C:489:BCR:H11C	25:J:112:BCR:H322	1.69	0.71
3:C:91:HIS:CD2	21:C:478:CLA:HBA1	2.25	0.71
3:C:404:LEU:HG	28:C:493:DGD:O1A	1.90	0.71
27:D:360:LMG:H192	11:L:22:LEU:HD21	1.71	0.71
2:B:68:ARG:NH1	2:B:262:THR:HG23	2.04	0.71
2:B:327:THR:CA	21:B:517:CLA:O1A	2.36	0.71
1:A:40:THR:HG21	1:A:121:LEU:HD23	1.73	0.71
21:B:513:CLA:H161	7:H:38:PHE:HE2	1.54	0.71
13:O:92:VAL:CG1	13:O:93:PRO:HD2	2.19	0.71
3:C:391:ARG:HB2	3:C:391:ARG:HH11	1.56	0.71
1:A:93:PHE:HZ	21:A:366:CLA:HBA1	1.54	0.71
2:B:250:PHE:CD1	28:B:528:DGD:C9B	2.72	0.71
4:D:44:ALA:HB3	22:D:355:PHO:H92	1.72	0.71
4:D:129:GLN:HE22	4:D:143:ALA:HA	1.55	0.71
1:A:22:THR:HG21	8:I:30:ARG:HD3	1.72	0.71
3:C:348:GLU:OE2	13:O:37:VAL:HA	1.91	0.70
3:C:187:ASP:HB2	3:C:230:LEU:HD12	1.74	0.70
1:A:129:ARG:NH2	4:D:256:ILE:HD12	2.02	0.70
2:B:135:LEU:HA	2:B:138:MET:HE3	1.72	0.70
3:C:116:VAL:HG12	25:C:489:BCR:H332	1.72	0.70
2:B:224:ARG:HG2	7:H:24:GLY:O	1.91	0.70
13:O:33:TYR:O	13:O:37:VAL:HG23	1.92	0.70
13:O:77:LEU:HD23	13:O:93:PRO:HA	1.74	0.70
13:O:69:LEU:HD12	13:O:70:CYS:N	2.05	0.70
1:A:93:PHE:CD2	1:A:95:PRO:HD3	2.26	0.70
2:B:222:PRO:HG3	7:H:27:THR:H	1.57	0.70
1:A:332:HIS:CD2	1:A:333:GLU:HG3	2.27	0.70
13:O:35:ASP:C	13:O:36:ILE:HD12	2.12	0.70
16:V:115:ALA:CB	16:V:122:ARG:HD2	2.22	0.70
3:C:219:GLY:HA2	28:C:491:DGD:O3D	1.92	0.70
4:D:55:VAL:HG21	4:D:110:LEU:HD12	1.74	0.70
28:B:533:DGD:CDA	12:M:17:VAL:HG21	2.12	0.69
4:D:88:SER:HB2	5:E:69:ARG:NH2	2.06	0.69
3:C:54:VAL:HG13	21:C:487:CLA:HED1	1.74	0.69
4:D:259:ILE:HG12	27:D:360:LMG:C30	2.21	0.69
15:U:38:GLU:HG2	15:U:39:LEU:N	2.05	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:65:PHE:O	21:B:515:CLA:HBA1	1.92	0.69
21:B:521:CLA:H193	21:B:523:CLA:H92	1.74	0.69
2:B:137:LYS:HD2	7:H:14:LEU:O	1.93	0.69
2:B:284:ILE:HG12	2:B:309:LEU:CD1	2.22	0.69
4:D:39:PRO:O	4:D:43:LEU:HD22	1.93	0.69
21:B:513:CLA:H161	7:H:38:PHE:CE2	2.28	0.69
3:C:404:LEU:HD21	28:C:493:DGD:HA31	1.73	0.69
7:H:6:TRP:CE2	7:H:10:ILE:HD11	2.27	0.69
1:A:119:PHE:HZ	21:A:362:CLA:H101	1.58	0.69
2:B:4:PRO:HD2	2:B:7:ARG:HD2	1.74	0.69
3:C:284:PHE:CB	28:C:491:DGD:HA52	2.23	0.69
21:C:478:CLA:O1A	21:C:479:CLA:H11	1.92	0.69
4:D:41:ALA:CB	22:D:355:PHO:H43	2.23	0.69
9:J:22:ILE:HG21	27:J:492:LMG:H202	1.75	0.69
19:Z:30:PRO:HG3	19:Z:33:TRP:HZ3	1.58	0.69
2:B:222:PRO:HG3	7:H:26:GLY:HA3	1.74	0.69
3:C:60:ILE:HG21	21:C:479:CLA:H191	1.75	0.69
3:C:158:THR:O	3:C:251:HIS:HB3	1.92	0.69
27:J:492:LMG:O8	27:J:492:LMG:O9	2.11	0.69
19:Z:28:ALA:O	19:Z:30:PRO:HD3	1.93	0.69
3:C:68:THR:OG1	21:C:479:CLA:HED1	1.92	0.69
5:E:81:GLU:C	5:E:83:LEU:H	1.96	0.69
1:A:77:ILE:HD11	14:T:6:TYR:HB3	1.76	0.68
2:B:264:PRO:HG2	2:B:267:LEU:HD12	1.75	0.68
21:B:524:CLA:OBD	11:L:10:VAL:HG21	1.93	0.68
5:E:81:GLU:O	5:E:83:LEU:N	2.24	0.68
3:C:130:VAL:HG13	21:C:486:CLA:H92	1.74	0.68
4:D:152:VAL:HG21	4:D:279:LEU:HD12	1.72	0.68
19:Z:32:ASP:HB3	19:Z:35:ARG:NH1	2.07	0.68
21:B:521:CLA:H52	21:B:524:CLA:HBC3	1.74	0.68
27:A:373:LMG:HC92	2:B:5:TRP:HE1	1.59	0.68
28:C:493:DGD:HD3	9:J:32:ALA:O	1.93	0.68
25:D:358:BCR:H403	9:J:25:VAL:HG21	1.75	0.68
2:B:188:ASP:HA	7:H:58:VAL:HG23	1.76	0.68
16:V:29:LEU:HD13	16:V:151:ILE:HD11	1.75	0.68
3:C:166:ILE:O	3:C:170:ILE:HG13	1.94	0.68
10:K:19:ASP:N	10:K:20:PRO:HD2	2.09	0.68
2:B:270:PRO:HG3	2:B:312:TYR:HD2	1.59	0.68
3:C:405:ASN:HA	28:C:493:DGD:HG12	1.75	0.68
2:B:471:ALA:HB2	4:D:130:PHE:CZ	2.29	0.68
1:A:271:LEU:HD11	23:A:367:MES:H82	0.83	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:ILE:HG13	6:F:45:ARG:HD2	1.76	0.68
2:B:133:LEU:HB3	2:B:138:MET:CE	2.24	0.68
2:B:328:GLY:O	21:B:517:CLA:HBA1	1.94	0.67
2:B:332:LYS:HE3	28:B:533:DGD:C4D	2.24	0.67
2:B:464:PHE:HD2	21:B:521:CLA:HAC2	1.58	0.67
4:D:152:VAL:CG1	21:D:354:CLA:H11	2.24	0.67
6:F:18:VAL:HG13	6:F:19:ARG:H	1.59	0.67
3:C:30:SER:HB2	10:K:46:ARG:O	1.94	0.67
3:C:472:LEU:HD12	3:C:473:ASP:H	1.59	0.67
3:C:113:VAL:HG12	27:C:494:LMG:H192	1.76	0.67
4:D:27:PHE:CD2	6:F:19:ARG:HD3	2.29	0.67
5:E:78:THR:O	5:E:81:GLU:HB2	1.94	0.67
1:A:39:PRO:HB2	21:A:366:CLA:HBB1	1.75	0.67
7:H:63:LYS:C	7:H:65:LEU:H	1.98	0.67
1:A:183:MET:HG2	21:A:363:CLA:HBC1	1.77	0.67
3:C:75:PHE:HD1	3:C:86:LEU:HD21	1.59	0.67
28:B:533:DGD:HA81	12:M:14:PHE:HA	1.75	0.67
3:C:215:LYS:HB3	3:C:223:TRP:HA	1.77	0.67
4:D:87:HIS:HD2	4:D:162:LEU:HD23	1.58	0.67
4:D:180:ARG:HH11	4:D:180:ARG:CG	2.08	0.67
2:B:135:LEU:HD23	2:B:138:MET:CE	2.25	0.67
21:C:479:CLA:H171	21:K:483:CLA:HBB2	1.77	0.67
28:C:492:DGD:O3D	25:J:115:BCR:H382	1.94	0.67
1:A:45:THR:HB	22:A:365:PHO:H8	1.77	0.67
1:A:278:TRP:HA	28:C:493:DGD:HAG1	1.76	0.67
3:C:161:LEU:HG	3:C:165:LEU:HD12	1.78	0.67
1:A:129:ARG:NH2	4:D:256:ILE:HA	2.08	0.66
2:B:356:VAL:HG22	2:B:370:LEU:CD2	2.26	0.66
25:C:489:BCR:HC22	10:K:18:PHE:CD1	2.31	0.66
2:B:133:LEU:HB3	2:B:138:MET:HE2	1.78	0.66
2:B:483:ASP:OD2	2:B:484:PRO:HD2	1.94	0.66
3:C:150:ASP:HB3	3:C:153:ASP:HB2	1.77	0.66
3:C:155:ASN:HD21	3:C:255:THR:CB	2.07	0.66
3:C:377:LEU:O	3:C:381:LYS:HB2	1.95	0.66
28:C:493:DGD:HBF1	27:D:359:LMG:H211	1.77	0.66
2:B:62:VAL:CG1	21:B:515:CLA:HED3	2.26	0.66
3:C:305:THR:HG22	3:C:308:GLU:CB	2.26	0.66
19:Z:33:TRP:O	19:Z:33:TRP:CD1	2.48	0.66
1:A:161:TYR:HB3	1:A:162:PRO:HD3	1.77	0.66
27:A:373:LMG:C11	4:D:266:TRP:CH2	2.66	0.66
2:B:271:THR:CG2	2:B:273:TYR:H	2.08	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:15:THR:HG22	9:J:7:ARG:CB	2.25	0.66
19:Z:33:TRP:O	19:Z:37:LYS:HB2	1.95	0.66
1:A:119:PHE:CZ	21:A:362:CLA:H101	2.30	0.66
28:C:492:DGD:HB52	25:J:115:BCR:H352	1.78	0.66
2:B:385:ARG:HD3	13:O:191:ALA:O	1.96	0.65
4:D:192:THR:CG2	21:D:354:CLA:HBC2	2.26	0.65
13:O:206:GLU:CD	13:O:206:GLU:H	1.97	0.65
4:D:250:ASN:HD22	4:D:262:SER:HB3	1.62	0.65
2:B:271:THR:HB	2:B:274:GLN:HG3	1.78	0.65
27:D:360:LMG:O9	27:D:360:LMG:C7	2.43	0.65
3:C:437:PHE:HA	21:C:484:CLA:CMC	2.26	0.65
21:C:486:CLA:H151	19:Z:24:PRO:HG3	1.79	0.65
1:A:121:LEU:CD2	21:A:366:CLA:HMB3	2.25	0.65
21:B:517:CLA:H141	21:B:517:CLA:H172	1.79	0.65
3:C:453:ALA:O	8:I:34:ARG:HB2	1.97	0.65
3:C:165:LEU:HD21	21:C:482:CLA:HHC	1.78	0.65
3:C:220:GLY:N	28:C:491:DGD:O3D	2.29	0.65
13:O:92:VAL:HG12	13:O:93:PRO:HD2	1.78	0.65
15:U:83:ALA:CB	15:U:84:PRO:HD2	2.14	0.65
2:B:86:ILE:HD12	2:B:86:ILE:O	1.97	0.65
1:A:64:ARG:NH1	13:O:98:THR:HG21	2.12	0.65
3:C:89:ILE:N	3:C:90:PRO:HD2	2.11	0.65
21:B:513:CLA:H3A	21:B:513:CLA:O2A	1.97	0.64
16:V:143:GLY:O	16:V:147:VAL:HG23	1.97	0.64
2:B:135:LEU:HB2	2:B:136:PRO:HD3	1.79	0.64
2:B:442:ILE:HD11	13:O:200:LEU:HD23	1.76	0.64
32:D:357:PL9:H262	32:D:357:PL9:C30	2.27	0.64
21:D:356:CLA:H42	18:X:26:GLY:HA3	1.79	0.64
2:B:7:ARG:HA	21:B:521:CLA:HBA1	1.78	0.64
2:B:139:PHE:CZ	2:B:143:LEU:HD22	2.32	0.64
1:A:81:ALA:HB2	1:A:175:GLY:HA3	1.78	0.64
2:B:250:PHE:HB3	28:B:528:DGD:HB82	1.78	0.64
11:L:7:ARG:O	11:L:7:ARG:HD2	1.97	0.64
2:B:331:ASN:HB3	2:B:437:LEU:HD12	1.79	0.64
21:C:483:CLA:OBD	21:C:485:CLA:H152	1.96	0.64
2:B:286:ARG:HG2	2:B:286:ARG:HH11	1.63	0.64
3:C:281:MET:HE2	28:C:474:DGD:HAE1	1.79	0.64
13:O:120:THR:HG22	13:O:154:SER:OG	1.96	0.64
13:O:144:LEU:HD13	13:O:259:VAL:HG11	1.78	0.64
2:B:135:LEU:HD23	2:B:138:MET:HE3	1.77	0.64
3:C:186:TYR:HE2	3:C:188:THR:HG22	1.62	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:36:LEU:O	5:E:40:THR:HG23	1.98	0.64
2:B:284:ILE:HG23	2:B:305:ILE:HD12	1.80	0.63
19:Z:55:GLY:HA2	25:Z:116:BCR:H312	1.80	0.63
1:A:32:TRP:HA	1:A:32:TRP:CE3	2.32	0.63
1:A:57:PRO:HG3	1:A:68:SER:CB	2.28	0.63
14:T:29:ILE:H	14:T:29:ILE:CD1	1.95	0.63
5:E:27:ILE:HB	5:E:28:PRO:HD3	1.80	0.63
2:B:297:THR:OG1	2:B:300:GLU:HG3	1.98	0.63
2:B:486:LEU:O	2:B:486:LEU:HD13	1.98	0.63
3:C:310:SER:OG	3:C:355:THR:HG23	1.98	0.63
32:D:357:PL9:H262	32:D:357:PL9:H302	1.80	0.63
2:B:187:PRO:HB3	21:B:511:CLA:HMB2	1.81	0.63
6:F:19:ARG:NH2	33:F:85:HEM:O2D	2.32	0.63
5:E:26:THR:O	5:E:29:ALA:HB3	1.98	0.63
2:B:247:PHE:HB2	21:B:518:CLA:HBC1	1.80	0.63
1:A:300:PHE:CZ	3:C:404:LEU:HD23	2.33	0.62
21:B:513:CLA:H3A	21:B:513:CLA:CGA	2.29	0.62
21:B:517:CLA:H11	28:B:533:DGD:HB32	1.79	0.62
3:C:407:VAL:CA	28:C:493:DGD:O2E	2.45	0.62
1:A:136:ARG:NH2	8:I:27:ASP:OD1	2.32	0.62
1:A:22:THR:HG21	8:I:30:ARG:CD	2.29	0.62
27:A:373:LMG:H201	32:D:357:PL9:H212	1.80	0.62
3:C:135:ARG:NE	19:Z:33:TRP:NE1	2.47	0.62
3:C:293:ASN:CA	28:C:491:DGD:O2E	2.40	0.62
3:C:305:THR:HG22	3:C:308:GLU:HB2	1.82	0.62
1:A:18:CYS:O	1:A:22:THR:HG22	2.00	0.62
3:C:44:ASN:C	3:C:45:LEU:HD12	2.20	0.62
13:O:117:GLY:O	13:O:159:VAL:HG12	1.98	0.62
5:E:23:HIS:HA	5:E:26:THR:OG1	2.00	0.62
1:A:29:TYR:CG	1:A:133:LEU:HD13	2.34	0.62
13:O:36:ILE:HG23	13:O:41:LEU:HB3	1.80	0.62
1:A:343:LEU:O	1:A:344:ALA:HB2	2.00	0.62
3:C:107:ASP:OD2	3:C:110:PRO:HD3	1.99	0.62
21:C:486:CLA:H141	19:Z:20:VAL:O	2.00	0.62
13:O:234:THR:OG1	13:O:236:GLU:HG2	2.00	0.62
15:U:54:LYS:HB2	15:U:113:THR:HG23	1.82	0.62
1:A:228:THR:HG22	1:A:229:GLU:H	1.65	0.62
2:B:379:ALA:HA	2:B:390:TYR:HB3	1.80	0.62
28:B:528:DGD:HE5	28:B:528:DGD:HD61	1.82	0.62
3:C:418:ASN:HA	28:C:493:DGD:HE2	1.81	0.62
10:K:18:PHE:HD2	10:K:18:PHE:N	1.97	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:LEU:HD12	25:A:369:BCR:H11C	1.81	0.62
2:B:371:THR:HG22	2:B:377:VAL:HA	1.81	0.62
3:C:286:ALA:HB2	21:C:478:CLA:CMD	2.30	0.62
5:E:10:PHE:CE2	6:F:19:ARG:NH1	2.67	0.62
2:B:356:VAL:HG22	2:B:370:LEU:HD21	1.81	0.61
3:C:44:ASN:O	3:C:45:LEU:HD12	1.99	0.61
3:C:119:LEU:HG	25:C:489:BCR:H10C	1.82	0.61
5:E:18:ARG:O	5:E:22:ILE:HG13	2.00	0.61
2:B:69:LEU:HD11	21:B:513:CLA:OBD	2.00	0.61
3:C:41:ARG:NH1	21:C:486:CLA:HMD1	2.14	0.61
26:C:476:LHG:H171	28:C:492:DGD:HBG2	1.82	0.61
4:D:160:TYR:HB3	4:D:161:PRO:CD	2.30	0.61
5:E:64:PRO:HB3	5:E:84:LYS:HE2	1.82	0.61
19:Z:32:ASP:CB	19:Z:35:ARG:HG2	2.30	0.61
1:A:218:LEU:CD2	23:A:367:MES:H52	2.30	0.61
2:B:69:LEU:HD12	21:B:515:CLA:HBA2	1.82	0.61
2:B:462:PHE:CE1	21:B:523:CLA:HMB3	2.36	0.61
3:C:41:ARG:NH1	21:C:486:CLA:OBD	2.33	0.61
28:C:492:DGD:HB42	28:C:493:DGD:HA21	1.81	0.61
4:D:267:LEU:HD23	4:D:267:LEU:C	2.20	0.61
15:U:66:ILE:O	15:U:66:ILE:HG22	1.98	0.61
18:X:11:THR:HG23	18:X:12:ILE:HG22	1.81	0.61
3:C:113:VAL:HG11	27:C:494:LMG:H172	1.81	0.61
3:C:461:ARG:HH11	3:C:461:ARG:HG3	1.65	0.61
4:D:342:PRO:O	4:D:345:VAL:HG12	2.01	0.61
2:B:264:PRO:CG	2:B:267:LEU:HD12	2.31	0.61
27:B:531:LMG:HC2	4:D:141:TYR:OH	2.00	0.61
3:C:224:ILE:HD11	21:C:477:CLA:H93	1.81	0.61
3:C:248:GLY:O	3:C:252:ILE:HG12	2.00	0.61
6:F:31:ILE:HD12	6:F:31:ILE:N	2.16	0.61
14:T:29:ILE:HD12	14:T:29:ILE:N	2.10	0.61
15:U:58:ASN:ND2	15:U:114:VAL:HG13	2.15	0.61
15:U:94:ILE:O	15:U:97:LEU:HG	2.00	0.61
21:B:517:CLA:HBC3	25:B:529:BCR:H10C	1.83	0.61
3:C:318:LEU:HG	3:C:328:VAL:HG11	1.82	0.61
3:C:405:ASN:HB2	28:C:493:DGD:HG32	1.82	0.61
1:A:53:ILE:HD11	32:D:357:PL9:H501	1.82	0.61
3:C:114:VAL:HG22	27:C:494:LMG:H211	1.83	0.61
4:D:49:LEU:O	4:D:53:THR:HG23	2.01	0.61
5:E:15:THR:CG2	9:J:8:ILE:H	2.13	0.61
5:E:79:PHE:O	5:E:84:LYS:HB3	2.01	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:19:GLY:O	7:H:21:VAL:HG13	1.99	0.61
13:O:39:THR:OG1	13:O:41:LEU:HB2	2.01	0.61
27:A:373:LMG:H331	11:L:24:ILE:HD11	1.81	0.61
4:D:209:LEU:HD23	4:D:209:LEU:C	2.22	0.61
10:K:18:PHE:N	10:K:18:PHE:CD2	2.68	0.61
1:A:89:ILE:HD11	1:A:108:ASN:HB3	1.81	0.61
3:C:88:LEU:HB3	21:C:479:CLA:HED3	1.83	0.61
9:J:18:GLY:HA3	25:J:112:BCR:H371	1.82	0.61
21:B:518:CLA:HBB2	4:D:123:ILE:HG12	1.82	0.60
3:C:143:TYR:O	3:C:144:SER:HB2	2.00	0.60
21:C:480:CLA:H93	28:C:492:DGD:HAT2	1.83	0.60
16:V:90:PRO:O	16:V:92:ARG:HD3	2.01	0.60
1:A:322:ASN:OD1	3:C:412:THR:HA	2.01	0.60
21:A:362:CLA:H111	22:A:365:PHO:H3A	1.83	0.60
27:A:373:LMG:H192	32:D:357:PL9:C22	2.31	0.60
3:C:223:TRP:CD2	3:C:224:ILE:HG13	2.36	0.60
6:F:38:ALA:O	6:F:41:GLN:HG2	2.01	0.60
13:O:86:ARG:HG3	13:O:86:ARG:HH11	1.66	0.60
15:U:97:LEU:O	15:U:102:LYS:HE2	2.01	0.60
2:B:315:ILE:HG22	2:B:426:PHE:HB3	1.82	0.60
10:K:17:ILE:HD12	10:K:17:ILE:N	2.17	0.60
2:B:124:ARG:NE	2:B:131:PRO:HD3	2.13	0.60
3:C:204:LEU:HD21	3:C:238:ILE:HG21	1.84	0.60
3:C:391:ARG:HD2	3:C:395:TYR:CE2	2.36	0.60
13:O:230:VAL:CG1	13:O:231:ASP:H	2.10	0.60
1:A:153:SER:HB2	21:A:362:CLA:H43	1.83	0.60
7:H:58:VAL:HG13	7:H:58:VAL:O	2.00	0.60
4:D:47:GLY:HA2	25:D:358:BCR:H332	1.83	0.60
10:K:40:GLN:HA	10:K:43:VAL:HG12	1.83	0.60
18:X:12:ILE:HG12	18:X:16:LEU:CD1	2.30	0.60
19:Z:33:TRP:O	19:Z:33:TRP:HD1	1.84	0.60
1:A:107:TYR:CD1	13:O:141:ARG:NH1	2.69	0.60
2:B:41:GLU:OE1	2:B:63:LEU:HB2	2.02	0.60
3:C:264:PHE:HE2	21:C:482:CLA:O1A	1.85	0.60
27:A:373:LMG:H311	11:L:20:GLY:HA2	1.82	0.60
3:C:178:LYS:HB2	21:C:478:CLA:H162	1.83	0.60
1:A:60:ILE:HD12	1:A:84:PRO:HD2	1.83	0.60
1:A:306:VAL:HG13	1:A:314:ILE:O	2.01	0.60
2:B:143:LEU:HA	21:B:520:CLA:HED1	1.83	0.60
2:B:238:LEU:HD13	21:B:522:CLA:C1D	2.32	0.60
5:E:18:ARG:HB3	5:E:18:ARG:NH1	2.17	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:213:GLY:O	2:B:217:ILE:HG13	2.02	0.60
2:B:462:PHE:HA	21:B:521:CLA:HMC1	1.84	0.60
3:C:39:ASN:OD1	21:C:485:CLA:HBB2	2.02	0.59
3:C:141:GLU:CD	3:C:141:GLU:H	2.05	0.59
4:D:56:THR:HG21	5:E:50:PRO:HD3	1.82	0.59
13:O:87:GLN:O	13:O:88:GLU:HB3	2.02	0.59
15:U:113:THR:O	15:U:114:VAL:HG23	2.02	0.59
1:A:22:THR:HG21	8:I:30:ARG:NE	2.16	0.59
21:B:517:CLA:H142	27:B:531:LMG:H382	1.84	0.59
21:C:477:CLA:H151	21:C:483:CLA:HMB3	1.84	0.59
5:E:15:THR:HG23	9:J:8:ILE:O	2.01	0.59
1:A:257:ARG:HG3	1:A:257:ARG:HH11	1.66	0.59
27:B:531:LMG:H201	27:B:531:LMG:H291	1.83	0.59
3:C:292:PHE:O	28:C:491:DGD:O2E	2.20	0.59
13:O:31:LEU:HD12	13:O:31:LEU:N	2.17	0.59
1:A:309:ALA:HB3	16:V:27:ALA:O	2.03	0.59
21:B:520:CLA:HHC	21:B:520:CLA:HBB1	1.83	0.59
3:C:233:VAL:HA	25:C:490:BCR:C28	2.32	0.59
16:V:102:MET:HE3	16:V:141:ILE:HG21	1.83	0.59
1:A:214:MET:HA	1:A:214:MET:HE3	1.85	0.59
2:B:172:TYR:O	2:B:174:LEU:HG	2.02	0.59
4:D:87:HIS:CD2	4:D:162:LEU:HD23	2.37	0.59
6:F:16:PHE:HE2	33:F:85:HEM:HMA2	1.66	0.59
21:A:363:CLA:H42	22:A:365:PHO:HMB3	1.85	0.59
2:B:149:LEU:CG	21:B:513:CLA:HBC1	2.26	0.59
10:K:33:LEU:HD23	21:K:483:CLA:OBD	2.03	0.59
1:A:22:THR:HG21	8:I:30:ARG:HE	1.67	0.59
21:B:512:CLA:C4	7:H:45:ILE:HD11	2.33	0.59
6:F:27:ALA:HB1	33:F:85:HEM:HBC2	1.82	0.59
5:E:56:TYR:O	16:V:27:ALA:HB2	2.02	0.59
21:B:511:CLA:HHC	21:B:511:CLA:HBB1	1.84	0.59
3:C:418:ASN:CB	28:C:493:DGD:HE2	2.32	0.59
21:C:480:CLA:H42	28:C:493:DGD:HA32	1.84	0.59
6:F:41:GLN:OE1	9:J:31:GLY:HA3	2.01	0.59
2:B:458:PHE:HB3	21:B:514:CLA:HBC2	1.84	0.59
3:C:37:ALA:C	21:C:484:CLA:HBA1	2.23	0.59
3:C:318:LEU:HD23	3:C:318:LEU:C	2.24	0.59
21:C:480:CLA:H43	28:C:492:DGD:HA91	1.85	0.59
6:F:23:VAL:O	6:F:27:ALA:HB2	2.03	0.59
3:C:112:PHE:O	3:C:116:VAL:HG13	2.03	0.58
3:C:186:TYR:CE2	3:C:188:THR:HG22	2.37	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:437:PHE:HA	21:C:484:CLA:HMC3	1.86	0.58
2:B:68:ARG:HH11	2:B:262:THR:HG23	1.68	0.58
3:C:369:LEU:HD21	3:C:384:ILE:HD13	1.85	0.58
21:C:481:CLA:H12	8:I:23:PHE:CD2	2.38	0.58
4:D:55:VAL:HG21	4:D:110:LEU:CD1	2.33	0.58
9:J:22:ILE:HG13	25:J:115:BCR:H10C	1.85	0.58
13:O:80:GLU:O	13:O:89:ALA:HB1	2.03	0.58
1:A:238:LYS:O	1:A:241:GLN:HG3	2.03	0.58
3:C:95:LEU:HD11	21:C:479:CLA:HBA2	1.83	0.58
3:C:380:ILE:HA	3:C:384:ILE:HD11	1.85	0.58
3:C:418:ASN:CA	28:C:493:DGD:HE2	2.34	0.58
27:D:360:LMG:O9	27:D:360:LMG:HC72	2.03	0.58
5:E:8:ARG:N	6:F:13:TYR:CE1	2.71	0.58
1:A:240:GLY:HA3	14:T:29:ILE:HG22	1.86	0.58
3:C:28:GLN:HB2	21:C:486:CLA:HED2	1.86	0.58
4:D:32:TRP:CG	30:D:361:SQD:H251	2.38	0.58
10:K:17:ILE:HD12	10:K:17:ILE:H	1.69	0.58
2:B:188:ASP:OD1	7:H:58:VAL:HA	2.04	0.58
5:E:15:THR:HG23	9:J:8:ILE:H	1.68	0.58
5:E:76:VAL:O	5:E:80:LEU:HD22	2.03	0.58
1:A:190:HIS:HB3	1:A:293:MET:HE2	1.86	0.58
2:B:262:THR:HG21	21:B:513:CLA:HBA2	1.86	0.58
21:B:516:CLA:H161	21:B:526:CLA:H161	1.84	0.58
3:C:131:TYR:HE1	3:C:135:ARG:HD2	1.67	0.58
2:B:150:CYS:HA	21:B:513:CLA:HBC2	1.85	0.58
3:C:156:LYS:O	3:C:160:ILE:HG13	2.03	0.58
4:D:279:LEU:HD13	21:D:354:CLA:HBA2	1.86	0.58
1:A:142:TRP:HB2	4:D:220:ASN:OD1	2.03	0.58
1:A:205:VAL:HG21	21:A:362:CLA:HMA1	1.86	0.58
3:C:52:ALA:HA	21:C:486:CLA:CMB	2.31	0.58
3:C:130:VAL:O	3:C:134:ILE:HG12	2.04	0.58
13:O:123:GLU:HG2	13:O:124:GLU:N	2.18	0.58
15:U:38:GLU:HG2	15:U:39:LEU:H	1.68	0.58
16:V:81:ARG:CZ	16:V:157:GLY:HA3	2.34	0.58
19:Z:14:ILE:O	19:Z:18:VAL:HG23	2.04	0.58
2:B:462:PHE:HA	21:B:521:CLA:CMC	2.33	0.58
3:C:122:SER:OG	25:C:489:BCR:H14C	2.04	0.58
3:C:305:THR:HG23	3:C:307:PRO:CD	2.32	0.58
4:D:239:GLN:O	4:D:240:ALA:HB3	2.03	0.58
1:A:203:ALA:HB1	28:C:493:DGD:HBV2	1.86	0.57
1:A:272:HIS:CD2	4:D:218:VAL:HG21	2.39	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:80:PRO:HD2	16:V:129:LYS:HZ1	1.69	0.57
11:L:7:ARG:C	11:L:8:GLN:HE21	2.06	0.57
3:C:60:ILE:HG21	21:C:479:CLA:C19	2.34	0.57
32:D:357:PL9:H43	27:D:360:LMG:C25	2.34	0.57
9:J:14:ALA:HB1	25:J:112:BCR:C38	2.34	0.57
2:B:12:LEU:HD22	2:B:18:ARG:HB2	1.87	0.57
3:C:289:PHE:CD1	21:C:477:CLA:H12	2.38	0.57
3:C:447:ARG:HH11	3:C:447:ARG:CG	2.14	0.57
32:D:357:PL9:H23	32:D:357:PL9:H303	1.87	0.57
5:E:15:THR:O	9:J:8:ILE:HD12	2.03	0.57
2:B:393:GLU:HG2	15:U:44:ASP:O	2.03	0.57
3:C:272:LEU:HA	21:C:485:CLA:HMD3	1.86	0.57
3:C:362:ARG:HG2	28:C:491:DGD:HE61	1.86	0.57
28:C:493:DGD:O3D	9:J:37:GLY:O	2.22	0.57
19:Z:55:GLY:CA	25:Z:116:BCR:H312	2.34	0.57
2:B:150:CYS:CA	21:B:513:CLA:HBC2	2.35	0.57
2:B:224:ARG:NE	7:H:25:TRP:NE1	2.52	0.57
4:D:252:PHE:O	4:D:256:ILE:HG22	2.05	0.57
4:D:279:LEU:CD1	21:D:354:CLA:HBA2	2.35	0.57
6:F:20:TRP:O	6:F:24:HIS:HB2	2.04	0.57
1:A:234:ASN:HB2	27:A:373:LMG:HC3	1.87	0.57
3:C:39:ASN:HB2	21:C:484:CLA:HBA2	1.85	0.57
4:D:122:LEU:HD21	22:D:355:PHO:H62	1.86	0.57
4:D:188:PHE:HE2	4:D:329:MET:CE	2.17	0.57
7:H:63:LYS:O	7:H:65:LEU:N	2.37	0.57
16:V:74:THR:O	16:V:75:ASN:HB2	2.04	0.57
21:B:511:CLA:H152	21:B:511:CLA:HMD2	1.87	0.57
21:B:521:CLA:OBD	27:B:531:LMG:HC8	2.05	0.57
1:A:214:MET:HB3	23:A:367:MES:C6	2.33	0.57
1:A:233:ALA:HB3	27:B:531:LMG:HC4	1.86	0.57
27:D:360:LMG:C20	11:L:22:LEU:HD11	2.34	0.57
12:M:29:THR:O	12:M:32:GLN:HG3	2.05	0.57
1:A:38:ILE:O	1:A:42:LEU:HG	2.05	0.57
1:A:244:GLU:HG3	1:A:246:TYR:H	1.70	0.57
2:B:230:ARG:O	2:B:233:ASN:HB3	2.05	0.57
2:B:262:THR:HG21	21:B:513:CLA:CBA	2.35	0.57
3:C:343:ARG:NH1	3:C:347:GLY:O	2.38	0.57
5:E:84:LYS:HB2	5:E:84:LYS:HZ3	1.70	0.57
10:K:31:LEU:O	10:K:34:ALA:HB3	2.04	0.57
15:U:72:TYR:HB3	15:U:73:PRO:CD	2.34	0.57
18:X:45:LYS:HD3	18:X:45:LYS:N	2.20	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:ILE:HD11	28:C:491:DGD:HA91	1.86	0.56
2:B:256:MET:HA	2:B:263:THR:HG21	1.87	0.56
2:B:110:ALA:CB	21:B:526:CLA:HMB2	2.34	0.56
28:B:528:DGD:HO2D	4:D:87:HIS:CB	2.09	0.56
3:C:350:ILE:HG21	3:C:359:TRP:HB2	1.88	0.56
4:D:113:PHE:CE2	25:D:358:BCR:HC41	2.40	0.56
4:D:152:VAL:HG21	4:D:279:LEU:CD1	2.35	0.56
10:K:26:PRO:O	10:K:29:PRO:HD2	2.05	0.56
1:A:13:LEU:H	1:A:13:LEU:HD12	1.69	0.56
27:A:373:LMG:H202	32:D:357:PL9:H201	1.86	0.56
2:B:174:LEU:HD23	2:B:308:LYS:HG2	1.87	0.56
2:B:191:ASN:HB2	7:H:58:VAL:CG2	2.35	0.56
2:B:192:PRO:HD2	7:H:60:VAL:HG12	1.88	0.56
3:C:305:THR:HG22	3:C:308:GLU:N	2.16	0.56
3:C:374:GLY:O	3:C:375:LEU:C	2.44	0.56
21:C:477:CLA:H141	21:C:483:CLA:HMA1	1.87	0.56
4:D:36:LEU:O	4:D:39:PRO:HD2	2.05	0.56
7:H:12:ARG:HD3	7:H:12:ARG:C	2.24	0.56
16:V:125:ASP:HA	16:V:131:ARG:HH21	1.70	0.56
18:X:12:ILE:CG1	18:X:16:LEU:HD12	2.33	0.56
1:A:77:ILE:HG12	14:T:6:TYR:CD1	2.40	0.56
1:A:84:PRO:HA	1:A:112:TYR:CG	2.40	0.56
1:A:193:LEU:HD21	21:A:362:CLA:C2C	2.36	0.56
1:A:265:PHE:CD1	1:A:271:LEU:HA	2.41	0.56
27:A:373:LMG:C25	27:D:360:LMG:C22	2.83	0.56
19:Z:16:SER:O	19:Z:20:VAL:HG23	2.04	0.56
4:D:18:LEU:O	4:D:22:LEU:HG	2.05	0.56
13:O:178:ARG:CG	13:O:178:ARG:NH1	2.55	0.56
3:C:149:TYR:HA	3:C:156:LYS:HD3	1.88	0.56
4:D:18:LEU:HD22	18:X:38:ILE:HD13	1.86	0.56
7:H:58:VAL:O	7:H:58:VAL:CG1	2.53	0.56
11:L:11:GLU:HG2	11:L:12:LEU:N	2.19	0.56
3:C:113:VAL:CG1	27:C:494:LMG:H192	2.36	0.56
2:B:224:ARG:HG3	7:H:25:TRP:CD1	2.41	0.56
4:D:157:PHE:CE1	4:D:171:PRO:HG2	2.41	0.56
10:K:10:LYS:O	10:K:11:LEU:C	2.43	0.56
13:O:31:LEU:HD12	13:O:31:LEU:H	1.71	0.56
4:D:85:MET:CE	5:E:69:ARG:HA	2.36	0.56
4:D:267:LEU:HD23	4:D:267:LEU:O	2.06	0.56
13:O:88:GLU:OE2	13:O:90:GLU:HG2	2.06	0.56
1:A:292:THR:OG1	28:C:492:DGD:CEA	2.54	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:113:PHE:CZ	25:D:358:BCR:HC41	2.41	0.56
6:F:18:VAL:HG13	6:F:19:ARG:N	2.21	0.56
15:U:89:GLU:CD	15:U:89:GLU:H	2.09	0.56
16:V:87:LEU:HD12	16:V:87:LEU:N	2.20	0.56
1:A:187:GLN:HB2	21:A:362:CLA:HAC2	1.88	0.55
19:Z:26:ALA:CB	19:Z:40:ILE:HD11	2.36	0.55
21:A:362:CLA:H202	21:A:363:CLA:H112	1.88	0.55
3:C:135:ARG:HG2	19:Z:33:TRP:CE2	2.41	0.55
3:C:167:VAL:CG1	21:C:487:CLA:H11	2.36	0.55
19:Z:21:ILE:O	19:Z:25:VAL:HG22	2.07	0.55
1:A:136:ARG:HH22	8:I:27:ASP:CG	2.08	0.55
3:C:107:ASP:OD2	3:C:109:PHE:HB3	2.06	0.55
4:D:189:HIS:HA	4:D:294:ARG:HD2	1.88	0.55
1:A:37:MET:HG2	1:A:41:LEU:HD12	1.89	0.55
21:B:512:CLA:H203	28:B:528:DGD:HB91	1.88	0.55
25:J:112:BCR:HC31	10:K:21:LEU:HD21	1.89	0.55
1:A:217:SER:HA	1:A:220:THR:HG22	1.88	0.55
3:C:199:ILE:N	3:C:199:ILE:HD12	2.22	0.55
4:D:48:TRP:CE2	22:D:355:PHO:H161	2.42	0.55
5:E:30:LEU:HD12	33:F:85:HEM:HMC1	1.88	0.55
13:O:66:ILE:HD12	13:O:121:PHE:CD1	2.42	0.55
15:U:57:LEU:HD22	15:U:79:ILE:HG21	1.87	0.55
1:A:29:TYR:CD2	1:A:133:LEU:HD13	2.41	0.55
2:B:191:ASN:HD21	7:H:60:VAL:HA	1.72	0.55
2:B:386:ALA:HB3	15:U:132:LEU:HD11	1.88	0.55
3:C:239:TRP:CE3	3:C:243:ILE:HD11	2.42	0.55
3:C:286:ALA:HB2	21:C:478:CLA:HMD1	1.88	0.55
3:C:337:LEU:HD12	13:O:131:PRO:HG3	1.88	0.55
4:D:54:PHE:HB3	5:E:47:PHE:CD2	2.42	0.55
16:V:59:PHE:HA	16:V:63:CYS:SG	2.47	0.55
3:C:135:ARG:HG2	19:Z:33:TRP:CZ2	2.42	0.55
21:C:478:CLA:H122	21:C:479:CLA:HMB2	1.89	0.55
8:I:11:VAL:O	8:I:15:PHE:HD2	1.89	0.55
13:O:227:VAL:HG12	13:O:228:ALA:N	2.22	0.55
18:X:32:LEU:HD23	18:X:32:LEU:N	2.22	0.55
19:Z:29:SER:HB2	19:Z:31:GLN:HG3	1.88	0.55
2:B:100:HIS:CE1	21:B:516:CLA:H11	2.42	0.55
21:C:477:CLA:HMB3	25:C:490:BCR:C40	2.30	0.55
5:E:8:ARG:NE	5:E:13:ILE:HG12	2.22	0.55
13:O:180:ALA:HB1	13:O:191:ALA:HB2	1.89	0.55
19:Z:23:VAL:O	19:Z:26:ALA:HB3	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:371:LHG:HC2	4:D:229:ALA:HB1	1.87	0.55
3:C:29:GLU:HB3	10:K:46:ARG:HH11	1.70	0.55
19:Z:36:SER:OG	19:Z:39:LEU:HD12	2.07	0.55
2:B:170:ASP:HB2	2:B:171:PRO:CD	2.36	0.54
4:D:85:MET:HE2	5:E:69:ARG:HA	1.89	0.54
4:D:250:ASN:ND2	4:D:262:SER:HB3	2.22	0.54
1:A:76:ASN:OD1	1:A:79:THR:HG23	2.07	0.54
1:A:82:VAL:HB	1:A:174:LEU:HB2	1.88	0.54
1:A:131:TRP:CE3	1:A:132:GLU:N	2.75	0.54
21:B:520:CLA:H111	21:B:525:CLA:HAA1	1.88	0.54
3:C:55:ALA:HB1	25:C:489:BCR:H373	1.89	0.54
3:C:127:PHE:HE1	19:Z:23:VAL:HG21	1.72	0.54
3:C:178:LYS:HA	3:C:182:PHE:HB2	1.90	0.54
5:E:55:TYR:O	5:E:84:LYS:HE3	2.07	0.54
13:O:141:ARG:HG2	13:O:141:ARG:HH11	1.71	0.54
13:O:154:SER:O	13:O:168:PHE:HA	2.07	0.54
27:A:373:LMG:C25	27:D:360:LMG:H222	2.37	0.54
3:C:54:VAL:CG1	21:C:488:CLA:HMC3	2.36	0.54
2:B:169:SER:O	7:H:65:LEU:HD13	2.06	0.54
2:B:238:LEU:CB	21:B:522:CLA:HMD3	2.37	0.54
3:C:45:LEU:HD23	3:C:48:LYS:HD2	1.89	0.54
3:C:155:ASN:O	3:C:158:THR:HG22	2.07	0.54
4:D:152:VAL:HG11	21:D:354:CLA:C1	2.34	0.54
4:D:152:VAL:HG11	21:D:354:CLA:HBA1	1.88	0.54
30:L:213:SQD:H261	27:M:217:LMG:H191	1.90	0.54
15:U:66:ILE:O	15:U:66:ILE:CG2	2.56	0.54
1:A:197:PHE:CE2	28:C:492:DGD:CEA	2.90	0.54
21:C:477:CLA:H3A	21:C:477:CLA:O2A	2.08	0.54
15:U:58:ASN:OD1	15:U:84:PRO:HA	2.07	0.54
19:Z:36:SER:HA	19:Z:39:LEU:CG	2.35	0.54
2:B:247:PHE:CE1	21:B:512:CLA:H8	2.33	0.54
21:B:518:CLA:H111	4:D:120:PHE:CE1	2.42	0.54
4:D:180:ARG:HG3	4:D:180:ARG:NH1	2.23	0.54
5:E:84:LYS:HB2	5:E:84:LYS:HZ2	1.68	0.54
1:A:45:THR:OG1	21:A:363:CLA:H141	2.08	0.54
3:C:386:PRO:HB3	16:V:116:GLU:HG2	1.89	0.54
21:C:477:CLA:C3D	21:C:479:CLA:H2	2.38	0.54
15:U:100:ARG:O	15:U:103:GLN:HB3	2.07	0.54
21:B:519:CLA:HAC2	7:H:34:PHE:CE2	2.43	0.54
3:C:53:HIS:CB	21:C:487:CLA:HMD1	2.38	0.54
13:O:92:VAL:HG13	13:O:93:PRO:HD2	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V:135:GLU:O	16:V:139:VAL:HG23	2.08	0.54
4:D:303:ILE:HD13	12:M:2:GLU:HG2	1.88	0.54
6:F:43:ILE:HG22	9:J:36:LEU:HD21	1.90	0.54
13:O:218:LEU:HD22	15:U:119:THR:CG2	2.35	0.54
1:A:183:MET:HE1	21:A:363:CLA:HMD3	1.90	0.54
21:A:364:CLA:H203	27:D:359:LMG:H402	1.89	0.54
2:B:474:LEU:O	4:D:134:ARG:NH1	2.41	0.54
21:B:511:CLA:HBB2	7:H:44:ILE:HG21	1.90	0.54
19:Z:35:ARG:O	19:Z:38:GLN:HB3	2.07	0.54
3:C:125:LEU:HD22	21:C:487:CLA:CED	2.37	0.53
7:H:12:ARG:N	7:H:13:PRO:HD2	2.23	0.53
3:C:80:PRO:HB2	3:C:83:GLU:HG3	1.90	0.53
4:D:86:GLY:O	4:D:166:SER:HB2	2.08	0.53
4:D:239:GLN:O	4:D:240:ALA:CB	2.55	0.53
5:E:15:THR:O	9:J:8:ILE:CD1	2.56	0.53
3:C:165:LEU:HD21	21:C:482:CLA:HBB1	1.89	0.53
3:C:418:ASN:HB2	28:C:493:DGD:HE2	1.89	0.53
28:C:492:DGD:HG11	27:J:492:LMG:H301	1.91	0.53
4:D:103:ARG:HG3	5:E:73:LYS:HG3	1.90	0.53
32:D:357:PL9:H352	11:L:26:VAL:HB	1.90	0.53
2:B:235:GLU:HG2	2:B:235:GLU:O	2.08	0.53
21:B:521:CLA:H52	21:B:524:CLA:CBC	2.38	0.53
25:B:530:BCR:HC31	29:B:535:LMT:H72	1.90	0.53
3:C:174:LEU:HD12	21:C:487:CLA:H51	1.89	0.53
3:C:223:TRP:CH2	28:C:474:DGD:HA62	2.44	0.53
4:D:330:ALA:HB3	4:D:331:PRO:HD3	1.91	0.53
10:K:43:VAL:O	10:K:43:VAL:HG13	2.09	0.53
2:B:10:THR:C	2:B:12:LEU:H	2.12	0.53
2:B:150:CYS:N	21:B:513:CLA:HBC2	2.23	0.53
2:B:471:ALA:HB2	4:D:130:PHE:CE2	2.44	0.53
9:J:15:THR:O	9:J:19:MET:HG3	2.08	0.53
1:A:160:ILE:HD11	28:C:491:DGD:HA81	1.90	0.53
21:B:512:CLA:H201	4:D:159:ILE:HG12	1.89	0.53
3:C:407:VAL:CG2	28:C:493:DGD:O2E	2.55	0.53
3:C:416:SER:H	28:C:493:DGD:C3E	2.22	0.53
3:C:425:TRP:CZ2	21:C:480:CLA:HBA2	2.44	0.53
12:M:25:LEU:O	12:M:28:GLN:HG3	2.08	0.53
13:O:82:PRO:HB3	13:O:87:GLN:HG3	1.89	0.53
16:V:116:GLU:HG3	16:V:116:GLU:O	2.08	0.53
1:A:81:ALA:CB	1:A:175:GLY:HA3	2.37	0.53
2:B:106:LEU:HD22	21:B:516:CLA:H193	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:54:VAL:HA	21:C:487:CLA:CED	2.39	0.53
3:C:404:LEU:CD2	28:C:493:DGD:HA31	2.37	0.53
1:A:193:LEU:HD11	21:A:362:CLA:HMC3	1.91	0.53
21:A:363:CLA:H101	27:D:360:LMG:C25	2.39	0.53
3:C:406:SER:O	28:C:493:DGD:O2E	2.23	0.53
4:D:77:ALA:HB2	4:D:174:GLY:HA3	1.91	0.53
7:H:55:LEU:O	7:H:58:VAL:HG12	2.09	0.53
1:A:196:PRO:HA	1:A:199:GLN:OE1	2.09	0.53
3:C:53:HIS:HB3	21:C:487:CLA:OBD	2.09	0.53
25:C:489:BCR:C11	25:J:112:BCR:H322	2.38	0.53
4:D:18:LEU:HD22	18:X:38:ILE:CD1	2.38	0.53
32:D:357:PL9:C35	11:L:26:VAL:HB	2.38	0.53
13:O:190:LEU:HB2	13:O:214:LYS:HB2	1.90	0.53
33:V:164:HEM:HMA2	33:V:164:HEM:HBA1	1.90	0.53
1:A:107:TYR:HD1	13:O:141:ARG:NH1	2.05	0.53
21:B:515:CLA:H92	21:B:522:CLA:H18	1.91	0.53
4:D:238:THR:O	4:D:239:GLN:O	2.27	0.53
4:D:261:PHE:CB	32:D:357:PL9:H522	2.39	0.53
19:Z:30:PRO:C	19:Z:32:ASP:H	2.12	0.53
21:B:520:CLA:H121	21:B:520:CLA:O1D	2.09	0.52
3:C:449:ARG:HG2	21:C:481:CLA:HED3	1.91	0.52
28:C:493:DGD:O2D	9:J:32:ALA:HB1	2.10	0.52
25:D:358:BCR:H391	9:J:21:VAL:HG11	1.91	0.52
10:K:24:VAL:O	10:K:27:VAL:HG12	2.10	0.52
1:A:140:ARG:NH2	1:A:142:TRP:HZ3	2.07	0.52
1:A:278:TRP:HA	28:C:493:DGD:CIA	2.38	0.52
3:C:216:SER:HB3	3:C:221:GLU:HB2	1.90	0.52
3:C:239:TRP:HE3	3:C:243:ILE:HD11	1.74	0.52
3:C:391:ARG:HH11	3:C:391:ARG:CB	2.19	0.52
21:C:484:CLA:H43	21:C:486:CLA:HAC1	1.90	0.52
4:D:44:ALA:CB	22:D:355:PHO:H92	2.39	0.52
13:O:190:LEU:HD12	15:U:41:ASN:ND2	2.24	0.52
15:U:100:ARG:HH11	15:U:103:GLN:HG2	1.73	0.52
19:Z:3:ILE:O	19:Z:7:LEU:HG	2.09	0.52
3:C:216:SER:HB2	28:C:474:DGD:HG31	1.91	0.52
26:C:476:LHG:H142	25:J:115:BCR:HC21	1.89	0.52
4:D:71:CYS:HB2	4:D:76:VAL:HG12	1.91	0.52
1:A:279:PRO:CG	4:D:212:ALA:HB2	2.40	0.52
2:B:7:ARG:HE	21:B:521:CLA:HED1	1.74	0.52
2:B:143:LEU:CA	21:B:520:CLA:HED1	2.39	0.52
2:B:464:PHE:CD2	21:B:521:CLA:HAC2	2.44	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:B:528:DGD:HE5	28:B:528:DGD:C6D	2.39	0.52
3:C:276:LEU:HD11	3:C:444:HIS:HD2	1.73	0.52
4:D:76:VAL:O	4:D:77:ALA:HB2	2.10	0.52
13:O:31:LEU:HB2	13:O:36:ILE:CD1	2.38	0.52
13:O:223:ILE:HG13	13:O:243:SER:HB3	1.92	0.52
19:Z:55:GLY:N	25:Z:116:BCR:H312	2.23	0.52
1:A:218:LEU:HD23	23:A:367:MES:H72	1.90	0.52
21:C:480:CLA:H193	28:C:492:DGD:HBV1	1.91	0.52
1:A:232:SER:HB3	1:A:235:TYR:CD1	2.45	0.52
1:A:334:ARG:HD2	13:O:183:LEU:HB2	1.92	0.52
1:A:334:ARG:NH1	13:O:183:LEU:O	2.42	0.52
2:B:191:ASN:ND2	7:H:60:VAL:HA	2.24	0.52
28:B:533:DGD:HAE1	12:M:17:VAL:HG21	1.92	0.52
3:C:405:ASN:CB	28:C:493:DGD:HG32	2.40	0.52
3:C:452:ALA:O	3:C:454:GLY:N	2.42	0.52
27:D:360:LMG:H212	14:T:17:PHE:CZ	2.28	0.52
13:O:240:THR:HA	13:O:264:VAL:HA	1.92	0.52
15:U:72:TYR:CB	15:U:73:PRO:HD3	2.34	0.52
21:C:486:CLA:HMB2	25:C:489:BCR:H382	1.92	0.52
9:J:11:TRP:CG	10:K:42:ALA:HA	2.45	0.52
15:U:83:ALA:CB	15:U:84:PRO:CD	2.77	0.52
1:A:232:SER:HB3	1:A:235:TYR:HD1	1.75	0.52
2:B:341:LYS:HD2	2:B:429:ILE:HG22	1.90	0.52
3:C:47:GLY:O	3:C:50:LEU:HB3	2.10	0.52
3:C:193:GLY:O	3:C:194:GLY:C	2.48	0.52
3:C:393:ALA:HB1	33:V:164:HEM:HBC1	1.91	0.52
3:C:447:ARG:HG2	3:C:447:ARG:NH1	2.16	0.52
4:D:221:THR:O	4:D:221:THR:HG23	2.10	0.52
5:E:61:ARG:HH22	16:V:153:GLY:HA3	1.74	0.52
13:O:141:ARG:NH1	13:O:141:ARG:HG2	2.24	0.52
15:U:66:ILE:HG13	15:U:72:TYR:CD1	2.44	0.52
19:Z:31:GLN:O	19:Z:32:ASP:HB3	2.10	0.52
1:A:49:VAL:O	1:A:53:ILE:HG13	2.10	0.52
3:C:271:TYR:CE1	21:C:483:CLA:HAC1	2.44	0.52
3:C:281:MET:CE	21:C:481:CLA:HAC2	2.40	0.52
4:D:161:PRO:HG3	4:D:170:ALA:HB2	1.91	0.52
11:L:1:MET:O	11:L:1:MET:CG	2.48	0.52
2:B:12:LEU:CD2	2:B:18:ARG:HB2	2.40	0.52
13:O:178:ARG:HD2	13:O:182:PHE:CD1	2.45	0.52
19:Z:32:ASP:C	19:Z:34:ASP:N	2.60	0.52
1:A:228:THR:HG22	1:A:229:GLU:N	2.25	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:334:GLN:N	4:D:335:PRO:HD3	2.25	0.51
5:E:61:ARG:NH2	16:V:153:GLY:HA3	2.25	0.51
2:B:222:PRO:CG	7:H:27:THR:H	2.21	0.51
4:D:42:TYR:HE1	6:F:26:LEU:HD23	1.75	0.51
4:D:87:HIS:CD2	4:D:162:LEU:HA	2.45	0.51
4:D:136:VAL:O	4:D:136:VAL:HG12	2.10	0.51
4:D:346:LEU:O	4:D:348:ARG:HG3	2.10	0.51
25:D:358:BCR:H391	25:J:115:BCR:H332	1.91	0.51
10:K:30:VAL:HA	21:K:483:CLA:H191	1.93	0.51
19:Z:32:ASP:OD1	19:Z:36:SER:HB2	2.11	0.51
1:A:202:VAL:HG11	21:A:364:CLA:OBD	2.09	0.51
3:C:346:THR:O	13:O:40:GLY:HA2	2.10	0.51
7:H:38:PHE:HB2	25:X:107:BCR:H10C	1.92	0.51
16:V:147:VAL:O	16:V:150:LYS:HB2	2.10	0.51
18:X:12:ILE:O	18:X:12:ILE:CG2	2.58	0.51
1:A:334:ARG:NH1	13:O:184:ASP:C	2.64	0.51
2:B:334:ASP:HB3	13:O:202:GLN:HG3	1.92	0.51
2:B:383:PHE:CZ	13:O:193:GLY:HA2	2.45	0.51
3:C:95:LEU:CD1	21:C:479:CLA:HBA2	2.40	0.51
3:C:227:VAL:HG11	25:C:490:BCR:H282	1.93	0.51
5:E:36:LEU:HA	5:E:39:SER:OG	2.11	0.51
2:B:149:LEU:HD22	21:B:514:CLA:H161	1.92	0.51
21:B:518:CLA:H143	21:D:356:CLA:HMB2	1.93	0.51
1:A:78:ILE:O	1:A:176:ILE:HB	2.10	0.51
1:A:150:PRO:O	21:A:362:CLA:H43	2.11	0.51
1:A:183:MET:HB3	21:A:362:CLA:HBC2	1.92	0.51
21:A:363:CLA:HED2	4:D:198:MET:SD	2.50	0.51
3:C:60:ILE:HG23	21:K:483:CLA:HMC2	1.92	0.51
3:C:128:GLY:HA3	21:C:488:CLA:C3C	2.40	0.51
3:C:269:GLU:OE1	3:C:447:ARG:HG2	2.10	0.51
5:E:15:THR:CG2	9:J:7:ARG:CB	2.85	0.51
25:J:112:BCR:C15	10:K:31:LEU:HB3	2.41	0.51
2:B:327:THR:HG22	21:B:517:CLA:H12	1.92	0.51
2:B:414:PRO:HB2	2:B:415:PRO:CD	2.35	0.51
3:C:415:ASN:O	3:C:416:SER:CB	2.57	0.51
5:E:81:GLU:C	5:E:83:LEU:N	2.64	0.51
13:O:118:SER:HB3	13:O:157:PRO:HA	1.93	0.51
19:Z:47:TRP:O	19:Z:50:LEU:HB2	2.11	0.51
1:A:188:ALA:HB2	1:A:328:MET:HB2	1.92	0.51
3:C:266:TRP:HB3	3:C:271:TYR:OH	2.11	0.51
10:K:17:ILE:H	10:K:17:ILE:CD1	2.24	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:ALA:HB3	1:A:150:PRO:CD	2.41	0.51
2:B:229:LEU:O	2:B:231:MET:N	2.43	0.51
3:C:158:THR:HG21	3:C:254:THR:O	2.10	0.51
4:D:221:THR:HG23	4:D:244:TYR:HB2	1.91	0.51
13:O:59:ASP:C	13:O:61:SER:H	2.14	0.51
18:X:17:LYS:O	18:X:21:ILE:HG13	2.10	0.51
27:A:373:LMG:O4	11:L:13:ASN:ND2	2.44	0.51
2:B:91:TRP:HE1	29:B:535:LMT:H41	1.75	0.51
2:B:293:ALA:C	2:B:295:GLY:H	2.14	0.51
10:K:25:LEU:HB2	10:K:26:PRO:HD3	1.93	0.51
15:U:72:TYR:O	15:U:73:PRO:C	2.48	0.51
16:V:30:THR:HB	16:V:31:PRO:CD	2.35	0.51
4:D:53:THR:HG22	4:D:67:TYR:CD2	2.46	0.50
19:Z:17:PHE:CE2	19:Z:21:ILE:HD11	2.45	0.50
1:A:227:THR:HA	1:A:231:GLU:OE2	2.10	0.50
21:A:364:CLA:HBB1	4:D:157:PHE:CE2	2.45	0.50
2:B:55:MET:CE	2:B:80:ILE:HD12	2.42	0.50
21:B:518:CLA:HBA1	30:D:361:SQD:H101	1.93	0.50
21:B:518:CLA:HMB2	4:D:127:LEU:HG	1.93	0.50
4:D:86:GLY:HA2	4:D:166:SER:HB3	1.93	0.50
19:Z:5:PHE:HA	19:Z:57:LEU:CD2	2.40	0.50
21:A:364:CLA:HED1	28:C:493:DGD:HBW2	1.93	0.50
2:B:125:ASP:OD2	2:B:127:ARG:HB3	2.11	0.50
3:C:81:MET:CE	3:C:89:ILE:HG22	2.41	0.50
3:C:137:PRO:HB2	3:C:139:THR:O	2.12	0.50
3:C:250:TRP:CD1	3:C:250:TRP:C	2.84	0.50
21:C:481:CLA:O1A	8:I:23:PHE:CZ	2.64	0.50
4:D:88:SER:HB2	5:E:69:ARG:CZ	2.40	0.50
4:D:99:GLY:HA3	29:D:363:LMT:H2'	1.94	0.50
8:I:27:ASP:N	8:I:28:PRO:CD	2.74	0.50
13:O:271:PRO:HG2	13:O:272:ALA:H	1.76	0.50
1:A:20:TRP:O	1:A:21:VAL:C	2.50	0.50
27:A:373:LMG:C25	27:D:360:LMG:H231	2.41	0.50
2:B:137:LYS:O	2:B:141:ILE:HG13	2.11	0.50
28:C:493:DGD:HG31	9:J:33:TYR:CZ	2.47	0.50
28:C:493:DGD:HB51	27:D:359:LMG:H121	1.94	0.50
18:X:16:LEU:HD13	18:X:16:LEU:C	2.31	0.50
1:A:283:VAL:O	1:A:286:THR:HG22	2.11	0.50
27:A:373:LMG:HC61	11:L:11:GLU:OE2	2.11	0.50
2:B:250:PHE:O	28:B:528:DGD:HB82	2.11	0.50
4:D:53:THR:HG22	4:D:67:TYR:CE2	2.47	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:55:LEU:HB2	7:H:58:VAL:HG12	1.92	0.50
7:H:62:TRP:O	7:H:63:LYS:O	2.30	0.50
2:B:220:ARG:HB3	2:B:221:PRO:HD2	1.93	0.50
3:C:155:ASN:CA	3:C:158:THR:HG22	2.39	0.50
3:C:159:THR:HG23	3:C:252:ILE:HD13	1.93	0.50
32:D:357:PL9:H33	32:D:357:PL9:H301	1.93	0.50
29:D:363:LMT:O2'	18:X:21:ILE:HD12	2.11	0.50
13:O:94:THR:HB	13:O:135:GLN:O	2.12	0.50
2:B:173:GLY:HA3	2:B:265:ILE:HD11	1.93	0.50
2:B:377:VAL:HG11	4:D:342:PRO:HG2	1.93	0.50
21:B:512:CLA:HBD	21:B:512:CLA:H43	1.92	0.50
21:C:481:CLA:HAA2	21:C:481:CLA:HBD	1.92	0.50
21:C:486:CLA:H13	19:Z:20:VAL:HG13	1.93	0.50
4:D:180:ARG:CG	4:D:180:ARG:NH1	2.70	0.50
1:A:126:TYR:OH	22:A:365:PHO:O1D	2.23	0.50
3:C:72:LEU:HD11	3:C:108:THR:HB	1.93	0.50
3:C:116:VAL:CG1	25:C:489:BCR:H332	2.40	0.50
3:C:405:ASN:HA	28:C:493:DGD:C1G	2.40	0.50
4:D:302:GLU:OE1	13:O:186:LYS:NZ	2.34	0.50
13:O:43:ASN:OD1	13:O:103:SER:HB2	2.12	0.50
1:A:249:VAL:HG11	2:B:486:LEU:HD23	1.92	0.50
2:B:27:THR:HG22	2:B:107:LEU:CD1	2.40	0.50
3:C:224:ILE:CD1	21:C:477:CLA:H93	2.42	0.50
19:Z:5:PHE:CE1	19:Z:54:VAL:HG13	2.46	0.50
1:A:106:LEU:HD11	25:A:369:BCR:H402	1.94	0.49
1:A:239:PHE:O	14:T:29:ILE:HA	2.12	0.49
2:B:23:HIS:C	21:B:525:CLA:HED1	2.33	0.49
28:B:533:DGD:HAW2	12:M:13:LEU:HD13	1.93	0.49
3:C:155:ASN:HA	3:C:158:THR:CG2	2.38	0.49
7:H:63:LYS:C	7:H:65:LEU:N	2.65	0.49
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.47	0.49
21:B:511:CLA:HMC1	21:B:511:CLA:HBC3	1.92	0.49
3:C:90:PRO:O	3:C:94:THR:HG23	2.12	0.49
3:C:126:GLY:O	3:C:130:VAL:HG23	2.12	0.49
3:C:391:ARG:HD2	3:C:395:TYR:CZ	2.47	0.49
18:X:43:ILE:HG22	18:X:43:ILE:O	2.12	0.49
1:A:215:HIS:N	23:A:367:MES:H61	2.27	0.49
27:A:373:LMG:H202	32:D:357:PL9:C21	2.40	0.49
3:C:33:PHE:CE1	4:D:229:ALA:CB	2.96	0.49
3:C:264:PHE:CE1	21:C:483:CLA:HBB1	2.48	0.49
3:C:405:ASN:CA	28:C:493:DGD:HG12	2.42	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:449:ARG:HG2	21:C:481:CLA:CED	2.42	0.49
21:C:484:CLA:C4	21:C:486:CLA:HAC1	2.42	0.49
27:D:360:LMG:H192	11:L:22:LEU:CD2	2.42	0.49
2:B:256:MET:O	2:B:448:ARG:NH1	2.42	0.49
13:O:178:ARG:HG3	13:O:178:ARG:NH1	2.01	0.49
19:Z:12:LEU:HB2	19:Z:50:LEU:HD22	1.93	0.49
3:C:165:LEU:HD21	21:C:482:CLA:CHC	2.43	0.49
4:D:192:THR:HG23	21:D:354:CLA:CBC	2.39	0.49
1:A:143:ILE:HD11	4:D:217:THR:HA	1.93	0.49
2:B:134:ASP:OD2	2:B:137:LYS:HB2	2.12	0.49
2:B:183:PRO:HB2	2:B:185:TRP:CH2	2.46	0.49
2:B:286:ARG:HG2	2:B:286:ARG:NH1	2.26	0.49
4:D:210:LEU:HA	4:D:213:ILE:HG22	1.95	0.49
5:E:30:LEU:CD1	6:F:28:VAL:HG13	2.41	0.49
7:H:53:LEU:HD12	18:X:19:PHE:CD1	2.47	0.49
13:O:59:ASP:HB3	13:O:62:GLN:HB3	1.93	0.49
13:O:159:VAL:HG13	13:O:159:VAL:O	2.13	0.49
19:Z:5:PHE:HA	19:Z:57:LEU:HD21	1.95	0.49
2:B:349:LYS:HG3	2:B:350:GLU:OE1	2.12	0.49
21:B:526:CLA:HMD1	7:H:5:THR:OG1	2.12	0.49
3:C:281:MET:HE1	21:C:481:CLA:HAC2	1.94	0.49
6:F:45:ARG:NH1	9:J:40:LEU:OXT	2.46	0.49
2:B:26:HIS:HB2	21:B:522:CLA:HMB2	1.93	0.49
21:B:518:CLA:H161	21:B:519:CLA:H203	1.95	0.49
4:D:283:ALA:HA	21:D:354:CLA:CED	2.43	0.49
9:J:34:ALA:O	9:J:35:GLY:O	2.31	0.49
1:A:190:HIS:O	1:A:298:ASN:HB3	2.13	0.49
3:C:89:ILE:N	3:C:90:PRO:CD	2.75	0.49
27:A:373:LMG:H192	32:D:357:PL9:C23	2.43	0.49
2:B:471:ALA:HB2	4:D:130:PHE:HZ	1.73	0.49
28:B:533:DGD:C3G	12:M:6:LEU:HD12	2.38	0.49
3:C:109:PHE:HB3	3:C:110:PRO:HD3	1.94	0.49
3:C:367:GLU:HB2	3:C:368:PRO:HD3	1.95	0.49
21:C:478:CLA:CGA	21:C:479:CLA:H11	2.43	0.49
21:C:481:CLA:HAA2	21:C:481:CLA:CBD	2.41	0.49
4:D:126:MET:CE	4:D:150:ILE:HG13	2.43	0.49
6:F:9:GLU:C	6:F:11:VAL:H	2.15	0.49
10:K:11:LEU:HD11	10:K:22:VAL:HG21	1.93	0.49
11:L:12:LEU:HD22	12:M:25:LEU:HD12	1.93	0.49
13:O:126:GLY:O	13:O:128:ASP:N	2.45	0.49
1:A:328:MET:HE1	4:D:183:LEU:HD22	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:C:486:CLA:H111	10:K:32:PHE:HE1	1.77	0.48
10:K:30:VAL:HA	21:K:483:CLA:H201	1.94	0.48
16:V:95:ILE:O	16:V:99:VAL:HG23	2.12	0.48
1:A:13:LEU:H	1:A:13:LEU:CD1	2.27	0.48
1:A:235:TYR:C	1:A:237:TYR:H	2.16	0.48
21:B:520:CLA:H11	21:B:522:CLA:H201	1.95	0.48
3:C:48:LYS:HD2	3:C:138:GLU:HG3	1.94	0.48
3:C:116:VAL:HG23	3:C:117:VAL:N	2.28	0.48
5:E:28:PRO:O	5:E:32:ILE:HG13	2.13	0.48
9:J:14:ALA:HB1	25:J:112:BCR:H382	1.94	0.48
13:O:226:ASN:HD22	13:O:226:ASN:N	2.11	0.48
18:X:42:GLN:O	18:X:43:ILE:HG13	2.12	0.48
1:A:224:ILE:O	1:A:226:GLU:OE2	2.30	0.48
3:C:167:VAL:HG13	21:C:487:CLA:H11	1.96	0.48
3:C:315:MET:O	3:C:319:ILE:HG13	2.12	0.48
3:C:390:ARG:NH2	16:V:126:ILE:HD13	2.29	0.48
21:C:486:CLA:H161	19:Z:20:VAL:HG13	1.94	0.48
4:D:210:LEU:HD21	32:D:357:PL9:H13	1.95	0.48
6:F:31:ILE:N	6:F:31:ILE:CD1	2.76	0.48
13:O:223:ILE:HG12	13:O:224:SER:N	2.27	0.48
33:V:164:HEM:HBA1	33:V:164:HEM:CMA	2.42	0.48
18:X:32:LEU:O	18:X:36:VAL:HG23	2.13	0.48
1:A:193:LEU:HD21	21:A:362:CLA:HMC3	1.94	0.48
2:B:35:GLY:O	2:B:38:ALA:HB3	2.13	0.48
2:B:118:TRP:CH2	11:L:5:PRO:HD2	2.48	0.48
4:D:60:THR:HG23	4:D:61:HIS:HD2	1.75	0.48
13:O:86:ARG:HG3	13:O:86:ARG:NH1	2.26	0.48
2:B:154:GLY:O	2:B:159:THR:HG23	2.13	0.48
21:B:519:CLA:HMD1	7:H:27:THR:HB	1.95	0.48
3:C:296:VAL:HG23	3:C:297:TYR:CD2	2.49	0.48
4:D:193:LEU:O	4:D:193:LEU:HG	2.14	0.48
27:D:360:LMG:C22	14:T:13:ILE:HG21	2.36	0.48
1:A:13:LEU:HD12	1:A:13:LEU:N	2.28	0.48
1:A:193:LEU:HD11	21:A:362:CLA:CMC	2.43	0.48
1:A:199:GLN:NE2	21:A:364:CLA:HED2	2.29	0.48
21:A:366:CLA:C1	28:C:474:DGD:HB22	2.44	0.48
28:B:528:DGD:HD3	4:D:87:HIS:ND1	2.29	0.48
3:C:91:HIS:NE2	21:C:478:CLA:HBA1	2.28	0.48
3:C:315:MET:CE	3:C:366:LEU:HD13	2.44	0.48
4:D:274:VAL:HA	32:D:357:PL9:H253	1.95	0.48
4:D:303:ILE:CD1	12:M:2:GLU:HG2	2.44	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:6:ILE:O	8:I:10:ILE:HG12	2.13	0.48
21:K:483:CLA:HMD3	21:K:483:CLA:H192	1.96	0.48
27:A:373:LMG:H312	12:M:22:LEU:HD11	1.95	0.48
21:B:516:CLA:H62	25:B:530:BCR:H342	1.95	0.48
2:B:458:PHE:CG	21:B:514:CLA:HMC3	2.49	0.48
3:C:71:GLU:OE1	3:C:89:ILE:HG13	2.13	0.48
3:C:135:ARG:HB2	19:Z:27:TYR:CB	2.42	0.48
21:C:480:CLA:C4	28:C:493:DGD:HA32	2.43	0.48
21:C:486:CLA:C4D	10:K:39:TRP:HH2	2.26	0.48
4:D:180:ARG:HH11	4:D:180:ARG:HG3	1.79	0.48
21:B:513:CLA:H52	21:B:513:CLA:HMB2	1.94	0.48
21:B:523:CLA:H161	25:B:529:BCR:H312	1.96	0.48
3:C:154:LYS:HE2	3:C:261:ARG:HD2	1.94	0.48
3:C:413:GLU:HG3	3:C:414:ILE:H	1.78	0.48
4:D:26:ARG:HD3	6:F:18:VAL:HG21	1.95	0.48
4:D:201:VAL:O	4:D:205:LEU:HB2	2.13	0.48
10:K:11:LEU:HD12	10:K:19:ASP:HA	1.96	0.48
2:B:9:HIS:HB2	21:B:521:CLA:O1A	2.13	0.48
2:B:328:GLY:C	21:B:517:CLA:HBA1	2.34	0.48
21:B:512:CLA:H42	7:H:45:ILE:CD1	2.44	0.48
21:B:523:CLA:H61	21:B:523:CLA:H41	1.59	0.48
3:C:413:GLU:HG3	3:C:414:ILE:N	2.28	0.48
4:D:146:PHE:O	4:D:150:ILE:HG12	2.14	0.48
10:K:20:PRO:O	10:K:23:ASP:HB2	2.13	0.48
13:O:36:ILE:HD12	13:O:36:ILE:N	2.29	0.48
19:Z:32:ASP:C	19:Z:34:ASP:H	2.17	0.48
1:A:10:SER:C	1:A:12:ASN:H	2.16	0.47
1:A:114:LEU:HD23	1:A:114:LEU:C	2.34	0.47
2:B:133:LEU:HB3	2:B:138:MET:HE1	1.95	0.47
2:B:175:THR:O	2:B:176:GLY:O	2.31	0.47
2:B:221:PRO:HA	21:B:519:CLA:HED3	1.95	0.47
2:B:364:GLU:HG3	4:D:296:TYR:CE2	2.48	0.47
3:C:457:LYS:HE3	4:D:228:GLY:O	2.13	0.47
30:C:475:SQD:O8	4:D:233:ARG:HG3	2.14	0.47
4:D:337:GLU:O	4:D:338:ASN:C	2.51	0.47
7:H:30:LEU:HD11	7:H:34:PHE:HE1	1.78	0.47
8:I:24:LEU:O	8:I:26:GLY:N	2.41	0.47
12:M:8:LEU:HD21	29:T:226:LMT:H81	1.95	0.47
1:A:111:PRO:O	1:A:115:ILE:HG13	2.14	0.47
1:A:287:ALA:HA	21:A:362:CLA:HED2	1.96	0.47
1:A:330:VAL:HG11	4:D:348:ARG:HG2	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:106:LEU:CD2	21:B:516:CLA:H193	2.44	0.47
2:B:135:LEU:HD23	2:B:138:MET:HE1	1.95	0.47
3:C:30:SER:OG	4:D:233:ARG:NH2	2.47	0.47
3:C:466:VAL:HG13	4:D:251:ARG:HD2	1.95	0.47
21:C:487:CLA:H121	21:C:488:CLA:H202	1.96	0.47
4:D:93:TRP:HA	4:D:99:GLY:H	1.80	0.47
4:D:135:LEU:HD23	30:D:361:SQD:HO2	1.78	0.47
5:E:22:ILE:O	5:E:26:THR:HG23	2.14	0.47
13:O:79:LYS:HE2	13:O:89:ALA:HB3	1.95	0.47
1:A:190:HIS:HB3	1:A:293:MET:CE	2.43	0.47
1:A:281:VAL:HB	28:C:493:DGD:HAG3	1.96	0.47
21:B:517:CLA:H61	21:B:517:CLA:H41	1.67	0.47
3:C:94:THR:HG22	3:C:298:PRO:HD2	1.96	0.47
3:C:437:PHE:CE1	21:K:483:CLA:HMB3	2.48	0.47
2:B:124:ARG:HG3	2:B:124:ARG:NH1	2.26	0.47
2:B:124:ARG:HD3	2:B:131:PRO:N	2.30	0.47
2:B:235:GLU:OE1	2:B:472:ARG:NH1	2.47	0.47
3:C:272:LEU:CA	21:C:485:CLA:HMD3	2.43	0.47
21:C:487:CLA:H172	21:C:487:CLA:CMA	2.37	0.47
32:D:357:PL9:H301	32:D:357:PL9:C33	2.45	0.47
5:E:77:GLU:HA	5:E:80:LEU:HD23	1.95	0.47
16:V:45:ILE:HG12	16:V:46:THR:N	2.28	0.47
1:A:287:ALA:HA	21:A:362:CLA:CED	2.44	0.47
26:A:371:LHG:H341	21:C:480:CLA:H203	1.96	0.47
2:B:250:PHE:CB	28:B:528:DGD:HB82	2.45	0.47
2:B:265:ILE:HG13	2:B:266:GLU:N	2.30	0.47
2:B:373:LYS:HA	2:B:373:LYS:HD2	1.55	0.47
4:D:23:LYS:HZ1	30:D:361:SQD:C46	2.10	0.47
4:D:176:ALA:HA	4:D:179:PHE:CD2	2.49	0.47
4:D:350:ASN:O	4:D:352:LEU:N	2.42	0.47
1:A:124:SER:O	1:A:127:MET:HB3	2.15	0.47
1:A:183:MET:CE	21:A:363:CLA:HMD3	2.44	0.47
1:A:212:CYS:HB2	4:D:211:CYS:HB2	1.96	0.47
1:A:243:GLU:HA	4:D:241:GLU:HA	1.97	0.47
2:B:258:TYR:CE2	28:B:528:DGD:O1B	2.67	0.47
2:B:274:GLN:NE2	7:H:62:TRP:NE1	2.63	0.47
3:C:29:GLU:HA	10:K:46:ARG:HH12	1.79	0.47
4:D:32:TRP:CZ3	30:D:361:SQD:H282	2.49	0.47
27:D:360:LMG:H361	14:T:21:ILE:HD11	1.97	0.47
6:F:20:TRP:NE1	6:F:24:HIS:CE1	2.83	0.47
10:K:35:LEU:HA	10:K:38:VAL:HG23	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:77:LEU:HB3	13:O:91:PHE:HB3	1.96	0.47
19:Z:32:ASP:CG	19:Z:33:TRP:N	2.60	0.47
1:A:22:THR:CG2	8:I:30:ARG:HD3	2.42	0.47
2:B:24:LEU:HD21	21:B:526:CLA:CAB	2.44	0.47
2:B:68:ARG:HH22	21:B:514:CLA:HED3	1.80	0.47
2:B:248:ALA:HA	21:B:513:CLA:H42	1.97	0.47
3:C:288:CYS:SG	28:C:491:DGD:HA21	2.55	0.47
3:C:447:ARG:CG	3:C:447:ARG:NH1	2.74	0.47
4:D:122:LEU:CD2	22:D:355:PHO:H62	2.44	0.47
4:D:259:ILE:HG12	27:D:360:LMG:C29	2.44	0.47
7:H:25:TRP:O	7:H:26:GLY:C	2.53	0.47
8:I:30:ARG:O	8:I:31:ASN:HB3	2.14	0.47
11:L:24:ILE:HD12	11:L:24:ILE:N	2.29	0.47
13:O:194:TYR:CE1	13:O:198:ILE:HD13	2.49	0.47
19:Z:29:SER:C	19:Z:31:GLN:H	2.17	0.47
1:A:214:MET:HA	1:A:214:MET:HE2	1.95	0.47
3:C:135:ARG:HB2	19:Z:27:TYR:CG	2.50	0.47
4:D:134:ARG:HA	4:D:134:ARG:HE	1.78	0.47
1:A:176:ILE:HG23	21:A:363:CLA:O1D	2.14	0.47
2:B:110:ALA:HB2	21:B:526:CLA:HMB2	1.97	0.47
21:B:517:CLA:HBC3	25:B:529:BCR:HC8	1.97	0.47
21:C:477:CLA:H171	21:C:483:CLA:HMB3	1.97	0.47
13:O:225:LEU:C	13:O:226:ASN:HD22	2.17	0.47
21:B:522:CLA:H12	21:B:525:CLA:HAA2	1.96	0.47
3:C:365:TRP:CB	3:C:391:ARG:HG2	2.45	0.47
4:D:202:ALA:HB3	32:D:357:PL9:C30	2.44	0.47
4:D:261:PHE:HB2	32:D:357:PL9:C52	2.43	0.47
13:O:135:GLN:HG2	13:O:141:ARG:HG3	1.97	0.47
26:A:371:LHG:O4	4:D:230:SER:HA	2.14	0.46
5:E:8:ARG:HA	6:F:13:TYR:CE2	2.50	0.46
13:O:184:ASP:OD2	13:O:188:ARG:HB2	2.15	0.46
1:A:10:SER:C	1:A:12:ASN:N	2.69	0.46
2:B:270:PRO:HG3	2:B:312:TYR:CD2	2.43	0.46
21:B:519:CLA:OBD	7:H:27:THR:HB	2.15	0.46
3:C:52:ALA:CA	21:C:486:CLA:HMB3	2.37	0.46
3:C:127:PHE:HA	21:C:486:CLA:H192	1.96	0.46
3:C:436:PHE:O	21:C:484:CLA:HAC1	2.14	0.46
29:D:536:LMT:H5'	30:D:361:SQD:H5	1.97	0.46
5:E:9:PRO:O	5:E:10:PHE:C	2.53	0.46
13:O:113:VAL:HA	13:O:119:LEU:HD23	1.97	0.46
16:V:68:VAL:O	16:V:68:VAL:HG13	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Z:23:VAL:HB	19:Z:24:PRO:HD3	1.97	0.46
1:A:105:TRP:CZ3	25:A:369:BCR:H371	2.49	0.46
1:A:214:MET:HE1	4:D:142:ASN:HD21	1.81	0.46
28:B:528:DGD:O2D	4:D:87:HIS:CG	2.54	0.46
3:C:193:GLY:O	3:C:194:GLY:O	2.33	0.46
4:D:261:PHE:O	4:D:262:SER:HB3	2.14	0.46
14:T:25:GLU:O	14:T:26:PRO:C	2.54	0.46
16:V:148:GLU:OE1	16:V:148:GLU:HA	2.14	0.46
1:A:215:HIS:O	1:A:216:GLY:C	2.53	0.46
28:B:533:DGD:HA81	12:M:14:PHE:CA	2.42	0.46
4:D:27:PHE:CD2	6:F:19:ARG:CD	2.97	0.46
1:A:12:ASN:O	1:A:16:ARG:HG3	2.15	0.46
21:A:363:CLA:H43	22:A:365:PHO:HMA1	1.98	0.46
2:B:63:LEU:N	2:B:64:PRO:HD2	2.30	0.46
2:B:138:MET:SD	21:B:525:CLA:HAC1	2.55	0.46
2:B:246:PHE:CD1	2:B:246:PHE:C	2.88	0.46
2:B:252:VAL:HG13	21:B:513:CLA:H12	1.97	0.46
2:B:462:PHE:CZ	21:B:523:CLA:HMB3	2.51	0.46
3:C:265:ILE:HG13	21:C:481:CLA:HED1	1.97	0.46
4:D:274:VAL:HG13	32:D:357:PL9:H253	1.97	0.46
13:O:82:PRO:O	13:O:83:LYS:CB	2.64	0.46
1:A:157:VAL:HG21	21:A:363:CLA:CMC	2.45	0.46
1:A:216:GLY:O	1:A:220:THR:HG22	2.16	0.46
1:A:278:TRP:HB3	1:A:279:PRO:CD	2.46	0.46
2:B:172:TYR:O	2:B:173:GLY:C	2.52	0.46
3:C:213:LEU:HD21	25:C:490:BCR:C20	2.46	0.46
4:D:122:LEU:HB3	4:D:150:ILE:CD1	2.45	0.46
11:L:31:PHE:HB3	11:L:35:PHE:CE1	2.51	0.46
16:V:98:LEU:O	16:V:102:MET:HG3	2.15	0.46
1:A:221:SER:HB2	4:D:139:ARG:O	2.16	0.46
2:B:238:LEU:CA	21:B:522:CLA:HMD3	2.45	0.46
3:C:390:ARG:CZ	16:V:126:ILE:HD13	2.46	0.46
3:C:396:MET:HE1	16:V:73:LYS:O	2.16	0.46
7:H:35:MET:HE2	25:X:107:BCR:H322	1.97	0.46
9:J:15:THR:HA	25:J:112:BCR:C37	2.46	0.46
19:Z:5:PHE:HE1	19:Z:54:VAL:HG13	1.80	0.46
19:Z:36:SER:C	19:Z:38:GLN:N	2.69	0.46
1:A:45:THR:HG23	1:A:46:ILE:N	2.31	0.46
1:A:330:VAL:HG12	4:D:348:ARG:HA	1.97	0.46
2:B:24:LEU:HB3	2:B:111:ALA:HB2	1.96	0.46
3:C:42:LEU:CD2	21:C:486:CLA:HED3	2.44	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:229:ASN:ND2	3:C:232:ASP:OD1	2.44	0.46
3:C:276:LEU:HD21	21:C:484:CLA:CBB	2.46	0.46
3:C:370:ARG:HD3	13:O:33:TYR:CE2	2.51	0.46
3:C:472:LEU:HD12	3:C:473:ASP:N	2.28	0.46
4:D:217:THR:O	4:D:221:THR:HB	2.15	0.46
7:H:35:MET:HG3	25:X:107:BCR:H323	1.98	0.46
12:M:18:PRO:O	12:M:21:PHE:HB3	2.16	0.46
16:V:54:GLU:OE1	16:V:54:GLU:HA	2.16	0.46
1:A:121:LEU:HD11	21:C:481:CLA:H171	1.98	0.46
2:B:298:LEU:HD12	2:B:298:LEU:HA	1.75	0.46
3:C:125:LEU:HA	21:C:488:CLA:HMC1	1.98	0.46
3:C:308:GLU:HB2	3:C:361:PHE:CE1	2.51	0.46
28:C:492:DGD:HBE2	28:C:493:DGD:HA92	1.97	0.46
1:A:64:ARG:O	13:O:178:ARG:NH2	2.49	0.46
1:A:306:VAL:HG11	1:A:316:THR:HG23	1.97	0.46
3:C:39:ASN:HD21	21:C:486:CLA:C1C	2.29	0.46
3:C:49:LEU:O	3:C:53:HIS:ND1	2.43	0.46
3:C:56:HIS:C	3:C:58:GLY:N	2.68	0.46
3:C:143:TYR:O	3:C:144:SER:CB	2.64	0.46
3:C:452:ALA:C	3:C:454:GLY:N	2.68	0.46
4:D:201:VAL:HA	21:D:354:CLA:HMB3	1.97	0.46
21:D:354:CLA:H101	22:D:355:PHO:H2	1.98	0.46
5:E:51:ARG:O	5:E:53:ASP:N	2.49	0.46
1:A:32:TRP:HA	1:A:32:TRP:HE3	1.76	0.45
1:A:72:LEU:CD2	14:T:3:THR:HG21	2.46	0.45
1:A:214:MET:O	1:A:215:HIS:C	2.54	0.45
1:A:317:TRP:CD1	4:D:177:ALA:HB2	2.51	0.45
1:A:326:LEU:HD21	3:C:412:THR:HB	1.98	0.45
2:B:341:LYS:HA	2:B:405:GLU:HB2	1.98	0.45
3:C:435:PHE:O	3:C:438:LEU:N	2.49	0.45
21:C:486:CLA:H8	25:C:489:BCR:H402	1.97	0.45
4:D:41:ALA:HB2	22:D:355:PHO:C4	2.44	0.45
27:D:359:LMG:O3	9:J:32:ALA:HA	2.16	0.45
1:A:131:TRP:CZ3	21:C:481:CLA:HBA2	2.51	0.45
21:A:366:CLA:H12	28:C:474:DGD:HB22	1.98	0.45
2:B:27:THR:CG2	2:B:107:LEU:HD13	2.45	0.45
2:B:229:LEU:O	2:B:230:ARG:C	2.54	0.45
21:B:519:CLA:C3D	7:H:31:MET:HB2	2.45	0.45
3:C:328:VAL:HG23	3:C:329:GLY:N	2.31	0.45
5:E:64:PRO:HD3	5:E:84:LYS:HE2	1.98	0.45
10:K:18:PHE:O	10:K:22:VAL:HG23	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:PRO:HB2	21:A:366:CLA:CBB	2.44	0.45
1:A:202:VAL:O	1:A:206:PHE:HB2	2.17	0.45
2:B:15:ASP:O	2:B:17:GLY:N	2.50	0.45
2:B:68:ARG:HH12	21:B:514:CLA:CED	2.30	0.45
2:B:212:ALA:HB2	21:B:519:CLA:HMC3	1.99	0.45
3:C:54:VAL:HG22	21:C:487:CLA:HED1	1.99	0.45
3:C:176:VAL:HG11	3:C:238:ILE:HG12	1.99	0.45
3:C:210:PHE:HZ	3:C:243:ILE:HD11	1.81	0.45
3:C:223:TRP:CH2	28:C:474:DGD:HA82	2.51	0.45
3:C:282:MET:O	21:C:478:CLA:HMD3	2.16	0.45
6:F:12:SER:O	6:F:13:TYR:HB2	2.16	0.45
13:O:144:LEU:CD1	13:O:259:VAL:HG11	2.45	0.45
15:U:56:ASP:HB3	15:U:60:THR:H	1.80	0.45
2:B:68:ARG:HH12	21:B:514:CLA:HED1	1.81	0.45
21:B:518:CLA:H102	21:B:518:CLA:C14	2.41	0.45
28:B:528:DGD:C6D	28:B:528:DGD:C5E	2.94	0.45
3:C:276:LEU:CD1	3:C:444:HIS:HD2	2.30	0.45
4:D:14:TRP:CE3	18:X:38:ILE:HD12	2.52	0.45
6:F:23:VAL:O	6:F:23:VAL:HG22	2.17	0.45
19:Z:35:ARG:HG3	19:Z:36:SER:N	2.30	0.45
1:A:243:GLU:H	1:A:243:GLU:CD	2.16	0.45
2:B:306:PRO:HG2	2:B:309:LEU:HB2	1.97	0.45
21:B:515:CLA:H41	21:B:515:CLA:H61	1.51	0.45
3:C:35:TRP:CG	3:C:36:TRP:N	2.84	0.45
3:C:245:ILE:O	3:C:249:ILE:HG12	2.16	0.45
3:C:258:GLY:CA	3:C:262:ARG:HH12	2.28	0.45
4:D:126:MET:HE3	4:D:150:ILE:HG13	1.99	0.45
5:E:10:PHE:CZ	6:F:19:ARG:HD2	2.51	0.45
9:J:14:ALA:HB1	25:J:112:BCR:C26	2.46	0.45
13:O:56:TYR:O	13:O:161:SER:HA	2.17	0.45
13:O:88:GLU:HG2	13:O:89:ALA:N	2.31	0.45
15:U:99:GLU:HA	15:U:102:LYS:HE3	1.99	0.45
16:V:30:THR:O	16:V:34:LEU:HG	2.17	0.45
26:A:371:LHG:HC11	3:C:447:ARG:CZ	2.46	0.45
21:B:516:CLA:HBB1	21:B:516:CLA:HHC	1.99	0.45
21:B:517:CLA:C1	28:B:533:DGD:HB32	2.46	0.45
3:C:168:LEU:HD13	21:C:483:CLA:C4	2.45	0.45
3:C:318:LEU:HD23	3:C:318:LEU:O	2.16	0.45
4:D:36:LEU:C	4:D:39:PRO:HD2	2.37	0.45
15:U:80:VAL:HG22	15:U:127:ARG:HH21	1.82	0.45
15:U:80:VAL:HG22	15:U:127:ARG:NH2	2.31	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:ILE:HB	25:A:369:BCR:H331	1.99	0.45
2:B:364:GLU:HG3	4:D:296:TYR:CD2	2.52	0.45
3:C:460:ASP:O	3:C:461:ARG:C	2.55	0.45
7:H:21:VAL:HG23	7:H:22:ALA:O	2.16	0.45
1:A:221:SER:HB3	4:D:141:TYR:HB2	1.98	0.45
21:A:363:CLA:H2	27:A:373:LMG:H242	1.99	0.45
2:B:62:VAL:HG11	21:B:515:CLA:HED3	1.99	0.45
2:B:145:LEU:CD1	21:B:525:CLA:HMB2	2.46	0.45
4:D:56:THR:HB	5:E:49:THR:HG23	1.97	0.45
4:D:213:ILE:HG23	4:D:214:HIS:N	2.30	0.45
13:O:92:VAL:HG12	13:O:93:PRO:CD	2.43	0.45
1:A:11:ALA:HB1	1:A:15:GLU:OE1	2.17	0.45
1:A:214:MET:CE	4:D:142:ASN:ND2	2.80	0.45
27:A:373:LMG:O10	27:A:373:LMG:O9	2.34	0.45
2:B:10:THR:O	2:B:13:ILE:HG13	2.16	0.45
2:B:422:ARG:HG2	2:B:422:ARG:HH11	1.82	0.45
3:C:33:PHE:HE1	4:D:229:ALA:CB	2.29	0.45
3:C:258:GLY:HA3	3:C:262:ARG:HH12	1.81	0.45
13:O:69:LEU:HB3	13:O:107:ILE:CB	2.35	0.45
13:O:132:VAL:O	13:O:144:LEU:HD23	2.17	0.45
2:B:71:VAL:HG21	2:B:96:VAL:CG2	2.47	0.45
2:B:247:PHE:CD2	21:B:513:CLA:H111	2.52	0.45
3:C:163:PHE:CD1	3:C:252:ILE:HD11	2.52	0.45
3:C:225:VAL:HG13	3:C:289:PHE:HA	1.99	0.45
21:C:479:CLA:H61	21:C:479:CLA:H41	1.58	0.45
4:D:67:TYR:CE1	4:D:76:VAL:HG11	2.51	0.45
15:U:100:ARG:NH1	15:U:103:GLN:HG2	2.31	0.45
16:V:119:PRO:HG3	16:V:127:PHE:CD1	2.52	0.45
1:A:39:PRO:HB3	21:A:366:CLA:HMC3	1.99	0.44
27:A:373:LMG:H171	11:L:23:LEU:HD13	1.99	0.44
2:B:141:ILE:O	2:B:144:PHE:HB3	2.17	0.44
25:B:529:BCR:H361	25:B:529:BCR:H20C	1.80	0.44
3:C:68:THR:OG1	21:C:479:CLA:CED	2.63	0.44
3:C:110:PRO:O	3:C:114:VAL:HG23	2.17	0.44
3:C:337:LEU:CD1	13:O:131:PRO:HG3	2.47	0.44
5:E:14:ILE:CG2	9:J:13:VAL:HG11	2.47	0.44
13:O:173:ASN:ND2	13:O:220:LYS:HD3	2.32	0.44
1:A:214:MET:HE1	4:D:142:ASN:ND2	2.33	0.44
2:B:18:ARG:HD2	2:B:115:TRP:CE3	2.52	0.44
4:D:19:ASP:O	4:D:20:ASP:C	2.55	0.44
4:D:122:LEU:CG	22:D:355:PHO:H62	2.47	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:34:GLY:HA2	6:F:32:PHE:CE2	2.53	0.44
7:H:9:ASP:O	7:H:12:ARG:HB3	2.17	0.44
7:H:28:THR:O	7:H:31:MET:HB3	2.18	0.44
8:I:4:LEU:O	8:I:8:VAL:HG23	2.17	0.44
2:B:148:LEU:HG	21:B:514:CLA:H193	1.99	0.44
3:C:334:PRO:HA	13:O:179:THR:OG1	2.17	0.44
3:C:436:PHE:HB3	21:K:483:CLA:H93	1.99	0.44
25:D:358:BCR:H331	25:D:358:BCR:C8	2.47	0.44
27:D:360:LMG:H221	14:T:13:ILE:CG2	2.38	0.44
6:F:36:ALA:O	6:F:38:ALA:N	2.50	0.44
18:X:16:LEU:HD11	18:X:20:PHE:CE2	2.53	0.44
3:C:264:PHE:CE2	21:C:482:CLA:O1A	2.66	0.44
3:C:269:GLU:O	3:C:272:LEU:HB3	2.18	0.44
3:C:452:ALA:O	3:C:453:ALA:C	2.55	0.44
9:J:22:ILE:HG21	27:J:492:LMG:C20	2.45	0.44
10:K:17:ILE:N	10:K:17:ILE:CD1	2.81	0.44
10:K:17:ILE:C	10:K:18:PHE:HD2	2.21	0.44
1:A:182:PHE:O	1:A:186:PHE:HB2	2.18	0.44
2:B:71:VAL:HG21	2:B:96:VAL:HG21	1.99	0.44
21:B:512:CLA:C20	28:B:528:DGD:HB91	2.48	0.44
3:C:28:GLN:CB	21:C:486:CLA:HED2	2.47	0.44
3:C:276:LEU:HD21	21:C:484:CLA:HBB1	1.99	0.44
4:D:190:ASN:HB2	4:D:296:TYR:CD1	2.52	0.44
4:D:253:TRP:HB2	4:D:260:ALA:HB2	2.00	0.44
15:U:72:TYR:CB	15:U:73:PRO:CD	2.92	0.44
16:V:59:PHE:CD1	16:V:63:CYS:SG	3.08	0.44
16:V:81:ARG:HG2	16:V:81:ARG:HH11	1.83	0.44
1:A:60:ILE:HG23	1:A:61:ASP:N	2.32	0.44
2:B:86:ILE:HD12	2:B:86:ILE:C	2.38	0.44
2:B:201:HIS:HD2	2:B:202:HIS:ND1	2.16	0.44
2:B:435:GLU:O	2:B:436:THR:C	2.56	0.44
3:C:281:MET:CE	21:C:481:CLA:HMC1	2.47	0.44
5:E:15:THR:CG2	9:J:7:ARG:HB3	2.47	0.44
6:F:36:ALA:O	6:F:39:ALA:N	2.51	0.44
1:A:159:LEU:C	1:A:162:PRO:HD2	2.38	0.44
1:A:333:GLU:HB2	1:A:337:HIS:HE1	1.83	0.44
4:D:185:PHE:CE2	4:D:289:LEU:HD12	2.52	0.44
4:D:209:LEU:O	4:D:213:ILE:HG22	2.18	0.44
7:H:41:PHE:O	7:H:45:ILE:HG23	2.18	0.44
2:B:444:ARG:HH11	2:B:444:ARG:HG3	1.82	0.44
3:C:394:GLU:OE2	3:C:398:HIS:CD2	2.71	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:202:ALA:HB3	32:D:357:PL9:H302	2.00	0.44
32:D:357:PL9:C43	27:D:360:LMG:C25	2.95	0.44
13:O:120:THR:HG22	13:O:154:SER:CB	2.47	0.44
18:X:44:ASP:O	18:X:45:LYS:HB3	2.17	0.44
1:A:184:ILE:HD11	4:D:186:GLN:CD	2.38	0.44
1:A:220:THR:O	1:A:223:LEU:HG	2.18	0.44
2:B:366:PHE:CD1	2:B:367:PRO:HD2	2.53	0.44
21:B:517:CLA:CBC	25:B:529:BCR:H10C	2.48	0.44
3:C:54:VAL:HA	21:C:487:CLA:HED1	2.00	0.44
3:C:82:TYR:HA	3:C:422:PRO:HG2	2.00	0.44
3:C:92:ILE:HD11	21:C:479:CLA:HED2	1.99	0.44
4:D:154:VAL:O	4:D:158:LEU:HB2	2.18	0.44
4:D:221:THR:CG2	4:D:244:TYR:HB2	2.48	0.44
25:D:358:BCR:C39	9:J:21:VAL:HG11	2.48	0.44
27:D:360:LMG:H111	27:D:360:LMG:H292	1.98	0.44
5:E:63:ILE:HG23	5:E:64:PRO:HD2	1.99	0.44
7:H:44:ILE:HG12	18:X:19:PHE:CZ	2.52	0.44
1:A:217:SER:O	1:A:220:THR:HG22	2.18	0.43
2:B:283:GLU:OE1	2:B:283:GLU:HA	2.17	0.43
21:C:487:CLA:HBB1	21:C:487:CLA:HHC	2.00	0.43
21:C:488:CLA:C1	21:C:488:CLA:HAA1	2.47	0.43
4:D:67:TYR:OH	27:D:359:LMG:H291	2.18	0.43
5:E:74:GLN:HG3	5:E:75:GLN:N	2.31	0.43
6:F:45:ARG:NH2	6:F:45:ARG:HB3	2.33	0.43
10:K:17:ILE:O	10:K:17:ILE:HG22	2.17	0.43
26:A:371:LHG:HC32	4:D:229:ALA:O	2.18	0.43
2:B:10:THR:C	2:B:12:LEU:N	2.71	0.43
2:B:206:GLY:O	2:B:210:ILE:HG13	2.18	0.43
2:B:238:LEU:N	21:B:522:CLA:HMD3	2.32	0.43
2:B:271:THR:CG2	2:B:273:TYR:HB2	2.48	0.43
2:B:484:PRO:O	2:B:485:GLU:HG2	2.18	0.43
21:B:518:CLA:C1	4:D:127:LEU:HD21	2.48	0.43
28:B:533:DGD:HA32	12:M:10:ALA:HB1	2.00	0.43
3:C:235:GLY:O	3:C:238:ILE:HB	2.18	0.43
4:D:101:PHE:O	4:D:104:TRP:HB3	2.18	0.43
21:D:356:CLA:C4	18:X:26:GLY:HA3	2.47	0.43
13:O:116:ASP:OD1	13:O:157:PRO:HB3	2.18	0.43
13:O:225:LEU:N	13:O:225:LEU:HD12	2.33	0.43
16:V:39:ASN:HD21	16:V:43:LYS:HB3	1.82	0.43
1:A:29:TYR:OH	1:A:132:GLU:OE2	2.26	0.43
1:A:198:HIS:O	1:A:202:VAL:HG12	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:164:PRO:HG2	2:B:165:GLY:H	1.82	0.43
2:B:434:THR:HG21	13:O:204:LYS:HE3	1.97	0.43
2:B:463:PHE:CE1	28:B:528:DGD:CFA	3.01	0.43
3:C:168:LEU:O	21:C:477:CLA:HMC1	2.18	0.43
3:C:390:ARG:NE	16:V:126:ILE:CG2	2.82	0.43
3:C:416:SER:OG	16:V:68:VAL:HG23	2.17	0.43
5:E:72:ALA:O	5:E:76:VAL:HG23	2.18	0.43
16:V:63:CYS:O	16:V:64:ALA:C	2.55	0.43
19:Z:5:PHE:CG	19:Z:61:VAL:HG21	2.53	0.43
19:Z:17:PHE:HE2	19:Z:21:ILE:HD11	1.84	0.43
2:B:327:THR:HG22	21:B:517:CLA:C1	2.49	0.43
2:B:348:ASN:OD1	2:B:352:GLU:HB2	2.18	0.43
21:B:514:CLA:H142	21:B:525:CLA:H52	2.01	0.43
28:B:533:DGD:HA32	12:M:10:ALA:CB	2.49	0.43
3:C:33:PHE:CD1	4:D:229:ALA:HB3	2.54	0.43
3:C:362:ARG:CG	28:C:491:DGD:HE61	2.48	0.43
3:C:370:ARG:HD3	13:O:33:TYR:CD2	2.54	0.43
10:K:18:PHE:CE1	19:Z:9:LEU:HG	2.53	0.43
10:K:30:VAL:N	21:K:483:CLA:H191	2.34	0.43
13:O:72:GLN:O	13:O:263:GLY:HA3	2.17	0.43
15:U:54:LYS:HD2	15:U:113:THR:CG2	2.49	0.43
1:A:309:ALA:HB3	5:E:53:ASP:HA	2.00	0.43
2:B:247:PHE:HD2	21:B:513:CLA:H111	1.83	0.43
21:B:512:CLA:CAA	7:H:45:ILE:HD12	2.48	0.43
21:B:518:CLA:C14	21:D:356:CLA:HMB2	2.48	0.43
3:C:72:LEU:HG	10:K:10:LYS:N	2.33	0.43
21:C:486:CLA:H122	10:K:32:PHE:CE1	2.53	0.43
5:E:38:VAL:CG2	6:F:36:ALA:HB1	2.47	0.43
13:O:70:CYS:O	13:O:265:PHE:HB2	2.18	0.43
16:V:64:ALA:O	16:V:65:SER:C	2.56	0.43
19:Z:36:SER:HA	19:Z:39:LEU:CD1	2.48	0.43
1:A:63:ILE:HB	3:C:335:THR:HG21	1.99	0.43
3:C:160:ILE:HA	3:C:163:PHE:CD2	2.53	0.43
3:C:437:PHE:HA	21:C:484:CLA:HMC1	2.00	0.43
5:E:8:ARG:HA	6:F:13:TYR:CZ	2.52	0.43
1:A:42:LEU:HA	1:A:45:THR:HG22	2.00	0.43
1:A:187:GLN:HB2	21:A:362:CLA:CAC	2.48	0.43
27:A:373:LMG:H301	12:M:22:LEU:HD22	1.99	0.43
2:B:252:VAL:HG11	21:B:514:CLA:OBD	2.18	0.43
2:B:284:ILE:HG23	2:B:305:ILE:CD1	2.48	0.43
2:B:450:TRP:HB3	21:B:517:CLA:CMB	2.47	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:128:GLY:N	21:C:488:CLA:HAC2	2.33	0.43
4:D:62:GLY:HA3	5:E:63:ILE:HD13	2.00	0.43
4:D:253:TRP:HA	4:D:256:ILE:HG23	2.01	0.43
29:I:274:LMT:H6D	13:O:95:LYS:NZ	2.34	0.43
10:K:46:ARG:NH1	10:K:46:ARG:HB2	2.34	0.43
21:A:363:CLA:HMB3	22:A:365:PHO:H172	2.01	0.43
2:B:263:THR:HB	2:B:448:ARG:HH12	1.82	0.43
2:B:289:GLN:OE1	2:B:292:LEU:HD12	2.19	0.43
3:C:50:LEU:O	3:C:54:VAL:HG23	2.17	0.43
3:C:433:LEU:HD13	21:C:478:CLA:CHC	2.49	0.43
3:C:473:ASP:HA	14:T:27:PRO:HD2	2.01	0.43
4:D:263:ASN:O	4:D:265:ARG:N	2.52	0.43
4:D:291:LEU:O	4:D:292:ASN:HB2	2.18	0.43
13:O:109:GLY:HA3	13:O:122:VAL:O	2.18	0.43
13:O:171:GLU:HA	13:O:221:GLY:O	2.19	0.43
2:B:327:THR:O	2:B:444:ARG:NE	2.46	0.43
3:C:55:ALA:C	25:C:489:BCR:H373	2.39	0.43
4:D:161:PRO:HB3	4:D:170:ALA:HB2	2.01	0.43
6:F:33:PHE:C	6:F:35:GLY:H	2.22	0.43
7:H:55:LEU:HB2	7:H:58:VAL:CG1	2.49	0.43
12:M:33:GLN:HG2	12:M:34:LYS:N	2.33	0.43
18:X:32:LEU:HD23	18:X:32:LEU:H	1.83	0.43
2:B:103:LEU:HD21	21:B:515:CLA:HMC3	2.01	0.43
21:B:517:CLA:HMB1	21:B:517:CLA:HAB	1.85	0.43
3:C:33:PHE:CE1	4:D:229:ALA:HB3	2.54	0.43
3:C:48:LYS:CD	3:C:138:GLU:HG3	2.49	0.43
3:C:55:ALA:HB1	25:C:489:BCR:C37	2.49	0.43
28:C:492:DGD:HB41	9:J:29:PHE:CZ	2.54	0.43
10:K:43:VAL:O	10:K:46:ARG:HG3	2.19	0.43
12:M:1:MET:HG2	12:M:2:GLU:H	1.84	0.43
16:V:103:LYS:O	16:V:122:ARG:HG2	2.19	0.43
1:A:45:THR:CB	22:A:365:PHO:H8	2.48	0.42
1:A:247:ASN:HB3	1:A:250:ALA:HB3	2.00	0.42
1:A:286:THR:CG2	21:A:362:CLA:HED3	2.35	0.42
2:B:222:PRO:HG3	7:H:27:THR:N	2.28	0.42
2:B:275:TRP:CH2	2:B:358:ARG:HD3	2.54	0.42
2:B:413:ASP:OD1	2:B:416:THR:HB	2.19	0.42
21:C:484:CLA:H41	21:C:484:CLA:H62	1.64	0.42
4:D:125:PHE:O	4:D:128:ARG:HB3	2.19	0.42
5:E:34:GLY:O	5:E:37:PHE:HB3	2.19	0.42
9:J:12:ILE:O	9:J:16:VAL:HG23	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:U:91:VAL:HG13	15:U:92:LEU:N	2.33	0.42
1:A:55:ALA:HA	25:A:369:BCR:C27	2.50	0.42
1:A:340:PRO:HG3	15:U:133:TYR:CG	2.55	0.42
2:B:215:PHE:C	2:B:215:PHE:CD2	2.93	0.42
28:B:528:DGD:HD61	28:B:528:DGD:C5E	2.48	0.42
3:C:164:HIS:CB	21:C:483:CLA:HED3	2.49	0.42
3:C:164:HIS:HB2	21:C:483:CLA:HED3	2.00	0.42
3:C:318:LEU:HG	3:C:328:VAL:CG1	2.48	0.42
5:E:35:TRP:C	5:E:35:TRP:CD1	2.93	0.42
12:M:33:GLN:CG	12:M:34:LYS:N	2.82	0.42
19:Z:30:PRO:C	19:Z:32:ASP:N	2.72	0.42
1:A:239:PHE:HB3	14:T:28:ARG:O	2.19	0.42
1:A:291:SER:HB3	3:C:431:PHE:CE2	2.54	0.42
2:B:33:TRP:HZ3	21:B:515:CLA:HMD1	1.83	0.42
2:B:105:GLY:O	2:B:108:PHE:HB3	2.19	0.42
2:B:348:ASN:O	2:B:349:LYS:C	2.57	0.42
2:B:349:LYS:HG2	2:B:395:GLN:O	2.19	0.42
3:C:29:GLU:CB	10:K:46:ARG:NH1	2.80	0.42
3:C:101:PRO:O	3:C:104:GLU:HB2	2.19	0.42
3:C:203:THR:O	3:C:235:GLY:HA3	2.20	0.42
3:C:363:GLY:O	3:C:364:PRO:C	2.56	0.42
3:C:406:SER:HA	3:C:420:VAL:CG2	2.49	0.42
9:J:14:ALA:C	25:J:112:BCR:H382	2.40	0.42
26:A:371:LHG:H351	21:K:483:CLA:H71	2.01	0.42
27:A:373:LMG:HC92	2:B:5:TRP:NE1	2.32	0.42
2:B:150:CYS:HB2	21:B:513:CLA:HMC3	2.01	0.42
2:B:251:VAL:HB	21:B:513:CLA:C4	2.50	0.42
3:C:37:ALA:O	21:C:484:CLA:HBA1	2.19	0.42
3:C:202:PRO:HB2	3:C:235:GLY:HA2	2.01	0.42
3:C:436:PHE:O	21:C:484:CLA:HMC1	2.19	0.42
21:C:483:CLA:H61	21:C:483:CLA:H41	1.92	0.42
5:E:60:GLN:HG2	5:E:62:SER:H	1.84	0.42
12:M:19:SER:O	12:M:23:ILE:HG13	2.18	0.42
13:O:59:ASP:O	13:O:61:SER:N	2.53	0.42
13:O:230:VAL:CG1	13:O:231:ASP:N	2.70	0.42
16:V:130:MET:SD	16:V:133:LEU:HD12	2.60	0.42
1:A:207:GLY:O	1:A:210:LEU:HB3	2.20	0.42
2:B:234:ILE:C	2:B:236:THR:H	2.23	0.42
2:B:413:ASP:O	2:B:414:PRO:C	2.57	0.42
3:C:162:GLY:O	3:C:166:ILE:HG13	2.18	0.42
3:C:223:TRP:CE3	3:C:224:ILE:HG13	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:16:ALA:O	10:K:19:ASP:HB2	2.20	0.42
1:A:33:PHE:CE2	21:C:481:CLA:O1A	2.73	0.42
1:A:160:ILE:HD11	28:C:491:DGD:C9A	2.50	0.42
1:A:222:SER:O	1:A:246:TYR:HB2	2.19	0.42
2:B:330:MET:SD	2:B:446:SER:HB3	2.59	0.42
21:B:524:CLA:H41	21:B:524:CLA:H61	1.85	0.42
21:B:526:CLA:C1D	7:H:7:LEU:HD23	2.50	0.42
3:C:205:ASP:OD1	3:C:207:ARG:HB3	2.19	0.42
3:C:464:GLU:HA	3:C:465:PRO:HD2	1.72	0.42
21:C:477:CLA:C2D	21:C:479:CLA:H2	2.50	0.42
5:E:69:ARG:HG3	5:E:70:PHE:N	2.34	0.42
13:O:168:PHE:O	13:O:224:SER:HA	2.19	0.42
3:C:414:ILE:HG22	3:C:415:ASN:N	2.35	0.42
3:C:442:LEU:HD21	21:C:481:CLA:HMB3	2.02	0.42
28:C:493:DGD:HBW1	27:D:359:LMG:H181	2.02	0.42
5:E:35:TRP:CG	6:F:39:ALA:HB2	2.55	0.42
10:K:44:GLY:O	10:K:45:PHE:C	2.57	0.42
16:V:83:GLU:CD	16:V:83:GLU:H	2.23	0.42
1:A:21:VAL:HG11	1:A:32:TRP:CE3	2.55	0.42
1:A:39:PRO:CB	21:A:366:CLA:HBB1	2.45	0.42
1:A:273:PHE:CD1	26:A:371:LHG:H242	2.55	0.42
1:A:328:MET:CE	4:D:183:LEU:HD22	2.49	0.42
2:B:16:PRO:HB3	2:B:133:LEU:HD21	2.02	0.42
2:B:179:GLN:HA	2:B:180:PRO:HD3	1.92	0.42
2:B:222:PRO:HB3	7:H:26:GLY:N	2.34	0.42
3:C:365:TRP:HB3	3:C:391:ARG:HG2	2.02	0.42
26:C:476:LHG:H171	28:C:492:DGD:HBN1	2.00	0.42
4:D:52:THR:HG22	4:D:67:TYR:CE2	2.54	0.42
5:E:78:THR:HA	5:E:81:GLU:HG2	2.02	0.42
7:H:39:LEU:C	7:H:39:LEU:HD23	2.39	0.42
10:K:43:VAL:CG2	10:K:46:ARG:HE	2.33	0.42
30:L:213:SQD:H82	27:M:217:LMG:H152	2.01	0.42
1:A:42:LEU:HA	1:A:45:THR:CG2	2.49	0.42
1:A:129:ARG:C	1:A:131:TRP:H	2.23	0.42
1:A:234:ASN:CB	27:A:373:LMG:HC3	2.48	0.42
1:A:317:TRP:O	1:A:321:ILE:HG13	2.20	0.42
2:B:191:ASN:HB2	7:H:58:VAL:HG22	2.00	0.42
2:B:448:ARG:HH11	2:B:448:ARG:HG3	1.84	0.42
3:C:125:LEU:HG	25:Z:116:BCR:C36	2.49	0.42
28:C:492:DGD:HB52	25:J:115:BCR:C35	2.47	0.42
5:E:15:THR:HG23	9:J:8:ILE:N	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:35:MET:HA	25:X:107:BCR:C32	2.50	0.42
29:O:274:LMT:H5'	29:O:274:LMT:H1B	1.92	0.42
22:A:365:PHO:HAC2	4:D:212:ALA:HB3	2.01	0.42
27:A:373:LMG:C31	12:M:22:LEU:HD21	2.50	0.42
2:B:243:ALA:HB2	2:B:466:HIS:CE1	2.54	0.42
2:B:338:GLN:HB2	2:B:431:GLU:O	2.20	0.42
2:B:472:ARG:HG2	2:B:472:ARG:HH11	1.84	0.42
3:C:140:LEU:HB2	3:C:148:GLY:HA2	2.02	0.42
3:C:148:GLY:O	3:C:156:LYS:NZ	2.51	0.42
3:C:461:ARG:HG3	3:C:461:ARG:NH1	2.32	0.42
4:D:261:PHE:N	32:D:357:PL9:O1	2.51	0.42
7:H:18:TYR:CG	7:H:19:GLY:N	2.85	0.42
10:K:30:VAL:CA	21:K:483:CLA:H191	2.50	0.42
18:X:12:ILE:HD13	18:X:12:ILE:C	2.40	0.42
27:A:373:LMG:C25	27:D:360:LMG:C21	2.97	0.41
27:A:373:LMG:C31	11:L:20:GLY:HA2	2.49	0.41
27:A:373:LMG:H131	4:D:273:PHE:CE2	2.55	0.41
2:B:18:ARG:HD3	2:B:118:TRP:HB3	2.01	0.41
2:B:280:PHE:O	2:B:284:ILE:HG13	2.20	0.41
28:B:533:DGD:HG11	12:M:6:LEU:HD12	2.02	0.41
21:C:486:CLA:H122	10:K:32:PHE:HE1	1.85	0.41
4:D:204:VAL:HG22	4:D:279:LEU:HD21	2.01	0.41
6:F:45:ARG:CZ	9:J:40:LEU:OXT	2.68	0.41
9:J:15:THR:O	25:J:112:BCR:H372	2.19	0.41
13:O:227:VAL:CG1	13:O:228:ALA:N	2.82	0.41
14:T:22:PHE:C	14:T:23:PHE:CD2	2.93	0.41
15:U:72:TYR:CG	15:U:73:PRO:N	2.87	0.41
16:V:119:PRO:HA	16:V:127:PHE:CD2	2.55	0.41
1:A:104:GLU:OE2	13:O:99:ARG:HD3	2.20	0.41
1:A:131:TRP:CH2	21:C:481:CLA:CBA	2.99	0.41
1:A:228:THR:HB	1:A:231:GLU:HB3	2.01	0.41
21:A:362:CLA:HMC3	4:D:182:LEU:HD13	2.02	0.41
3:C:208:VAL:O	3:C:209:ILE:C	2.57	0.41
3:C:405:ASN:HB2	28:C:493:DGD:O6D	2.20	0.41
21:C:478:CLA:O1A	21:C:479:CLA:HBD	2.19	0.41
4:D:122:LEU:HG	22:D:355:PHO:H62	2.02	0.41
10:K:11:LEU:O	10:K:12:PRO:C	2.57	0.41
1:A:236:GLY:HA3	4:D:265:ARG:NH1	2.35	0.41
1:A:332:HIS:HB3	4:D:321:LEU:HD21	2.01	0.41
2:B:462:PHE:HE1	21:B:523:CLA:HMB3	1.82	0.41
3:C:125:LEU:HD22	21:C:487:CLA:HED3	2.00	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:128:ARG:O	4:D:129:GLN:C	2.59	0.41
4:D:302:GLU:OE1	4:D:302:GLU:HA	2.20	0.41
15:U:50:ALA:HB1	15:U:113:THR:HG21	2.01	0.41
15:U:75:LEU:O	15:U:79:ILE:HG13	2.20	0.41
15:U:82:ASN:ND2	15:U:94:ILE:HG23	2.34	0.41
1:A:10:SER:OG	1:A:13:LEU:HD12	2.20	0.41
1:A:193:LEU:HD21	21:A:362:CLA:CMC	2.50	0.41
2:B:170:ASP:HB2	2:B:171:PRO:HD2	2.02	0.41
21:B:513:CLA:H203	21:B:519:CLA:H92	2.02	0.41
3:C:72:LEU:O	10:K:10:LYS:N	2.52	0.41
3:C:109:PHE:CD2	27:C:494:LMG:H112	2.55	0.41
3:C:264:PHE:HE2	21:C:482:CLA:CGA	2.33	0.41
3:C:292:PHE:CD2	28:C:491:DGD:HG31	2.55	0.41
3:C:456:GLU:N	3:C:456:GLU:OE1	2.53	0.41
4:D:274:VAL:HG13	32:D:357:PL9:H222	2.02	0.41
9:J:36:LEU:C	9:J:38:SER:H	2.23	0.41
15:U:55:ILE:HG21	15:U:65:PHE:CE1	2.56	0.41
19:Z:5:PHE:CD2	19:Z:61:VAL:HG21	2.54	0.41
21:B:511:CLA:H152	21:B:511:CLA:CMD	2.49	0.41
27:B:531:LMG:C2	4:D:141:TYR:OH	2.67	0.41
3:C:55:ALA:CB	25:C:489:BCR:H373	2.51	0.41
3:C:272:LEU:N	21:C:485:CLA:HMD3	2.36	0.41
26:C:476:LHG:H242	26:C:476:LHG:H121	2.02	0.41
4:D:205:LEU:HD12	4:D:205:LEU:HA	1.71	0.41
4:D:259:ILE:HG21	27:D:360:LMG:H292	2.01	0.41
6:F:28:VAL:CB	6:F:29:PRO:HD3	2.46	0.41
9:J:11:TRP:CE2	9:J:12:ILE:HG12	2.55	0.41
11:L:22:LEU:O	11:L:26:VAL:HG13	2.21	0.41
13:O:215:ARG:NE	15:U:39:LEU:HD22	2.34	0.41
1:A:296:ASN:HB2	3:C:400:PRO:O	2.20	0.41
1:A:307:ILE:HG13	6:F:45:ARG:CD	2.49	0.41
2:B:328:GLY:N	21:B:517:CLA:O1A	2.54	0.41
3:C:45:LEU:O	3:C:46:SER:C	2.58	0.41
3:C:75:PHE:CD1	3:C:86:LEU:HD21	2.48	0.41
3:C:189:TRP:O	3:C:190:ALA:C	2.58	0.41
3:C:464:GLU:O	3:C:467:LEU:HB2	2.19	0.41
4:D:161:PRO:CB	4:D:170:ALA:HB2	2.51	0.41
5:E:14:ILE:HG22	5:E:14:ILE:O	2.20	0.41
10:K:28:ILE:O	10:K:31:LEU:HB2	2.21	0.41
1:A:12:ASN:O	1:A:15:GLU:HB3	2.20	0.41
1:A:96:ILE:C	1:A:98:GLU:H	2.23	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:TRP:CZ3	1:A:111:PRO:HG3	2.55	0.41
1:A:155:PHE:CD1	28:C:491:DGD:HAE2	2.56	0.41
2:B:12:LEU:O	2:B:14:ASN:N	2.54	0.41
2:B:222:PRO:O	2:B:223:GLN:C	2.59	0.41
2:B:289:GLN:OE1	2:B:289:GLN:HA	2.21	0.41
2:B:479:PHE:O	2:B:480:SER:CB	2.68	0.41
3:C:187:ASP:HB2	3:C:230:LEU:CD1	2.48	0.41
3:C:321:ASP:HA	3:C:324:LEU:HD23	2.01	0.41
4:D:263:ASN:O	4:D:266:TRP:N	2.50	0.41
15:U:58:ASN:HD22	15:U:114:VAL:HG13	1.84	0.41
1:A:83:VAL:HA	1:A:84:PRO:HD3	1.85	0.41
1:A:277:ALA:O	1:A:281:VAL:HG23	2.21	0.41
2:B:49:ASP:HA	2:B:50:PRO:HD2	1.88	0.41
2:B:220:ARG:NH1	7:H:20:LYS:O	2.51	0.41
21:C:480:CLA:HHC	21:C:480:CLA:HBB1	2.03	0.41
5:E:44:TYR:OH	6:F:43:ILE:HD13	2.21	0.41
6:F:24:HIS:HE1	33:F:85:HEM:ND	2.19	0.41
6:F:38:ALA:HB1	9:J:27:LEU:CD2	2.50	0.41
7:H:13:PRO:HG2	7:H:14:LEU:H	1.85	0.41
9:J:9:PRO:HB2	9:J:12:ILE:HG13	2.03	0.41
13:O:120:THR:HA	13:O:153:ALA:O	2.21	0.41
15:U:75:LEU:HD21	15:U:101:GLN:HB3	2.03	0.41
16:V:124:ALA:HB1	16:V:131:ARG:CG	2.51	0.41
19:Z:36:SER:C	19:Z:38:GLN:H	2.24	0.41
1:A:114:LEU:HD23	1:A:114:LEU:O	2.21	0.41
1:A:279:PRO:HG2	4:D:212:ALA:HB2	2.01	0.41
2:B:305:ILE:HA	2:B:306:PRO:HD2	1.88	0.41
2:B:354:LEU:HD12	2:B:378:LYS:HB2	2.02	0.41
2:B:475:PHE:HB3	2:B:478:VAL:CG2	2.51	0.41
3:C:142:GLU:C	3:C:144:SER:H	2.24	0.41
3:C:175:LEU:HA	21:C:478:CLA:H141	2.02	0.41
3:C:199:ILE:N	3:C:199:ILE:CD1	2.83	0.41
3:C:451:ALA:HA	3:C:456:GLU:CD	2.41	0.41
21:C:478:CLA:HMB1	21:C:480:CLA:HMC3	2.03	0.41
25:C:489:BCR:H20C	25:C:489:BCR:H361	1.87	0.41
16:V:58:LEU:HD13	16:V:137:ASP:HB3	2.02	0.41
1:A:18:CYS:O	1:A:22:THR:CG2	2.69	0.41
1:A:131:TRP:CE3	1:A:132:GLU:CA	3.03	0.41
1:A:278:TRP:CH2	28:C:493:DGD:HBV1	2.56	0.41
21:A:364:CLA:H91	21:D:354:CLA:H203	2.02	0.41
2:B:191:ASN:OD1	2:B:193:TYR:N	2.52	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:380:ASP:OD1	2:B:380:ASP:C	2.60	0.41
3:C:62:PHE:HE2	10:K:29:PRO:HD3	1.86	0.41
3:C:267:SER:O	3:C:271:TYR:CD2	2.74	0.41
5:E:64:PRO:HB3	5:E:84:LYS:CD	2.51	0.41
6:F:31:ILE:HG12	33:F:85:HEM:HMC2	2.03	0.41
6:F:37:ILE:O	6:F:37:ILE:HG22	2.20	0.41
7:H:10:ILE:H	7:H:10:ILE:HG13	1.70	0.41
13:O:73:PRO:HG2	13:O:102:THR:HB	2.03	0.41
13:O:147:THR:OG1	13:O:148:VAL:N	2.54	0.41
16:V:160:LYS:HA	16:V:163:TYR:CD2	2.57	0.41
1:A:234:ASN:HD22	1:A:234:ASN:HA	1.66	0.40
21:A:363:CLA:H92	32:D:357:PL9:H422	2.02	0.40
2:B:238:LEU:HD13	21:B:522:CLA:C2D	2.51	0.40
2:B:414:PRO:CB	2:B:415:PRO:HD3	2.40	0.40
3:C:64:ALA:HB2	21:C:479:CLA:C2D	2.51	0.40
3:C:216:SER:HA	28:C:474:DGD:HG12	2.03	0.40
3:C:271:TYR:CE1	21:C:483:CLA:CAC	3.04	0.40
3:C:279:LEU:HD23	3:C:282:MET:HE3	2.02	0.40
3:C:307:PRO:HG3	3:C:358:PHE:CD1	2.56	0.40
3:C:308:GLU:HG3	3:C:361:PHE:CZ	2.56	0.40
3:C:327:ASN:HB3	13:O:125:ASP:OD1	2.21	0.40
3:C:369:LEU:CD2	3:C:384:ILE:HD13	2.51	0.40
4:D:190:ASN:HB2	4:D:296:TYR:CE1	2.55	0.40
4:D:274:VAL:HG22	32:D:357:PL9:H253	2.03	0.40
12:M:10:ALA:O	12:M:14:PHE:HB2	2.21	0.40
12:M:31:SER:HA	27:M:217:LMG:HC72	2.03	0.40
13:O:190:LEU:HD12	15:U:41:ASN:CG	2.41	0.40
1:A:141:PRO:O	1:A:143:ILE:N	2.53	0.40
1:A:288:LEU:O	1:A:292:THR:HB	2.21	0.40
2:B:224:ARG:NE	7:H:25:TRP:HE1	2.19	0.40
2:B:472:ARG:HE	21:B:521:CLA:HED2	1.86	0.40
21:B:518:CLA:H11	4:D:127:LEU:HD21	2.04	0.40
21:B:525:CLA:H62	21:B:525:CLA:H41	1.72	0.40
3:C:116:VAL:CG2	3:C:117:VAL:N	2.84	0.40
3:C:188:THR:CG2	3:C:298:PRO:HB3	2.50	0.40
4:D:90:LEU:O	21:D:356:CLA:HED1	2.21	0.40
5:E:15:THR:HG22	9:J:8:ILE:H	1.83	0.40
6:F:45:ARG:CB	6:F:45:ARG:HH21	2.35	0.40
25:J:115:BCR:H20C	25:J:115:BCR:H361	1.96	0.40
13:O:226:ASN:N	13:O:226:ASN:ND2	2.68	0.40
1:A:217:SER:HA	1:A:220:THR:CG2	2.51	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:ALA:HB2	5:E:52:PRO:C	2.42	0.40
27:A:373:LMG:C20	32:D:357:PL9:C21	2.92	0.40
2:B:327:THR:HG1	28:B:533:DGD:HO2D	1.70	0.40
21:B:513:CLA:CBB	21:B:515:CLA:H171	2.42	0.40
21:B:517:CLA:C2	28:B:533:DGD:HB52	2.52	0.40
3:C:54:VAL:HG11	21:C:488:CLA:HMC3	2.02	0.40
3:C:59:LEU:HD11	25:C:489:BCR:H372	2.03	0.40
3:C:350:ILE:CG2	3:C:359:TRP:HB2	2.51	0.40
7:H:53:LEU:HD21	7:H:55:LEU:HD21	2.03	0.40
9:J:24:ILE:HG23	9:J:25:VAL:N	2.37	0.40
10:K:18:PHE:O	10:K:19:ASP:C	2.60	0.40
10:K:34:ALA:O	10:K:37:PHE:HB2	2.20	0.40
13:O:157:PRO:O	13:O:158:ASN:O	2.38	0.40
18:X:11:THR:OG1	25:X:107:BCR:H282	2.21	0.40
1:A:258:LEU:O	4:D:128:ARG:NH1	2.55	0.40
2:B:150:CYS:HA	21:B:513:CLA:CBC	2.52	0.40
2:B:272:ARG:HG3	2:B:273:TYR:N	2.36	0.40
21:B:522:CLA:H102	21:B:522:CLA:H13	1.86	0.40
3:C:127:PHE:CE1	19:Z:23:VAL:HG21	2.54	0.40
3:C:258:GLY:C	3:C:262:ARG:NH1	2.74	0.40
21:C:483:CLA:H121	25:C:490:BCR:H362	2.04	0.40
21:C:486:CLA:C14	19:Z:24:PRO:HG2	2.51	0.40
4:D:84:SER:HB3	5:E:68:ASP:HA	2.04	0.40
4:D:185:PHE:HE2	4:D:289:LEU:HD12	1.87	0.40
4:D:239:GLN:HB3	4:D:240:ALA:H	1.33	0.40
27:D:360:LMG:H361	14:T:21:ILE:CD1	2.51	0.40
5:E:30:LEU:CD2	6:F:28:VAL:HG13	2.51	0.40
6:F:33:PHE:C	6:F:35:GLY:N	2.74	0.40
21:K:483:CLA:HHC	21:K:483:CLA:HBB1	2.03	0.40
1:A:72:LEU:HD23	14:T:3:THR:HG21	2.03	0.40
1:A:116:ILE:HG13	1:A:117:PHE:N	2.37	0.40
1:A:214:MET:HB2	23:A:367:MES:H61	1.99	0.40
1:A:238:LYS:HA	1:A:238:LYS:HD3	1.86	0.40
2:B:26:HIS:CE1	21:B:522:CLA:HMA1	2.57	0.40
2:B:153:PHE:O	2:B:157:HIS:HB3	2.22	0.40
2:B:262:THR:HG21	21:B:513:CLA:HBA1	2.03	0.40
2:B:463:PHE:CD2	2:B:463:PHE:C	2.94	0.40
2:B:483:ASP:CB	2:B:484:PRO:CD	2.97	0.40
3:C:141:GLU:HA	3:C:148:GLY:HA3	2.04	0.40
21:C:481:CLA:O1A	8:I:23:PHE:CE1	2.74	0.40
4:D:17:ILE:HG21	18:X:42:GLN:HG3	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:279:LEU:CD1	21:D:354:CLA:CBA	3.00	0.40
6:F:42:PHE:N	6:F:42:PHE:CD1	2.90	0.40
7:H:7:LEU:HG	7:H:11:LEU:CD1	2.52	0.40
7:H:11:LEU:C	7:H:13:PRO:HD2	2.41	0.40
13:O:215:ARG:HD2	15:U:39:LEU:HD22	2.04	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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	333/344 (97%)	285 (86%)	41 (12%)	7 (2%)	7	40
2	B	483/510 (95%)	416 (86%)	54 (11%)	13 (3%)	5	35
3	C	446/461 (97%)	370 (83%)	60 (14%)	16 (4%)	3	29
4	D	338/352 (96%)	286 (85%)	43 (13%)	9 (3%)	5	35
5	E	75/83 (90%)	66 (88%)	5 (7%)	4 (5%)	2	19
6	F	36/44 (82%)	22 (61%)	9 (25%)	5 (14%)	0	4
7	H	63/65 (97%)	45 (71%)	9 (14%)	9 (14%)	0	4
8	I	33/38 (87%)	20 (61%)	11 (33%)	2 (6%)	1	17
9	J	32/40 (80%)	26 (81%)	4 (12%)	2 (6%)	1	17
10	K	35/37 (95%)	26 (74%)	7 (20%)	2 (6%)	1	18
11	L	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
12	M	32/36 (89%)	23 (72%)	9 (28%)	0	100	100
13	O	241/246 (98%)	201 (83%)	29 (12%)	11 (5%)	2	23
14	T	28/32 (88%)	25 (89%)	3 (11%)	0	100	100
15	U	95/104 (91%)	79 (83%)	12 (13%)	4 (4%)	3	25
16	V	135/137 (98%)	111 (82%)	23 (17%)	1 (1%)	22	61

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
17	y	26/46 (56%)	14 (54%)	8 (31%)	4 (15%)	0 3
18	X	33/40 (82%)	25 (76%)	5 (15%)	3 (9%)	1 9
19	Z	60/62 (97%)	48 (80%)	9 (15%)	3 (5%)	2 21
All	All	2559/2714 (94%)	2121 (83%)	343 (13%)	95 (4%)	3 28

All (95) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	141	PRO
1	A	142	TRP
2	B	176	GLY
2	B	230	ARG
2	B	484	PRO
3	C	144	SER
3	C	257	PHE
3	C	416	SER
3	C	452	ALA
4	D	239	GLN
4	D	240	ALA
4	D	262	SER
5	E	82	GLN
7	H	18	TYR
7	H	63	LYS
8	I	25	SER
9	J	35	GLY
13	O	52	ALA
15	U	72	TYR
15	U	83	ALA
16	V	75	ASN
17	y	43	ARG
19	Z	32	ASP
2	B	349	LYS
3	C	46	SER
3	C	136	GLY
3	C	194	GLY
3	C	209	ILE
3	C	456	GLU
4	D	234	ALA
4	D	264	LYS
6	F	37	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	H	26	GLY
9	J	38	SER
13	O	83	LYS
13	O	231	ASP
15	U	73	PRO
17	y	25	ILE
18	X	43	ILE
2	B	13	ILE
2	B	127	ARG
2	B	183	PRO
2	B	414	PRO
2	B	436	THR
3	C	32	GLY
3	C	141	GLU
3	C	375	LEU
3	C	453	ALA
4	D	263	ASN
5	E	9	PRO
6	F	17	THR
7	H	16	SER
7	H	64	ALA
10	K	13	GLU
10	K	45	PHE
13	O	60	SER
13	O	158	ASN
13	O	165	SER
19	Z	24	PRO
19	Z	28	ALA
2	B	173	GLY
2	B	231	MET
2	B	235	GLU
3	C	154	LYS
4	D	73	PHE
5	E	10	PHE
13	O	51	THR
17	y	24	MET
18	X	44	ASP
1	A	97	TRP
3	C	462	GLU
6	F	13	TYR
7	H	6	TRP
7	H	65	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	U	42	VAL
18	X	12	ILE
1	A	334	ARG
4	D	351	ALA
7	H	14	LEU
1	A	21	VAL
2	B	16	PRO
13	O	159	VAL
3	C	201	ASN
6	F	9	GLU
6	F	11	VAL
17	y	35	ILE
5	E	52	PRO
7	H	60	VAL
8	I	32	PRO
13	O	232	GLY
1	A	176	ILE
4	D	160	TYR
13	O	127	ILE
13	O	152	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	271/280 (97%)	257 (95%)	14 (5%)	23	58
2	B	385/407 (95%)	369 (96%)	16 (4%)	30	63
3	C	348/362 (96%)	327 (94%)	21 (6%)	19	54
4	D	275/283 (97%)	256 (93%)	19 (7%)	15	49
5	E	69/72 (96%)	64 (93%)	5 (7%)	14	47
6	F	32/38 (84%)	31 (97%)	1 (3%)	40	71
7	H	53/54 (98%)	49 (92%)	4 (8%)	13	45
8	I	32/35 (91%)	31 (97%)	1 (3%)	40	71

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	J	24/28 (86%)	23 (96%)	1 (4%)	30	63
10	K	30/30 (100%)	27 (90%)	3 (10%)	7	35
11	L	35/35 (100%)	30 (86%)	5 (14%)	3	21
12	M	31/33 (94%)	31 (100%)	0	100	100
13	O	202/208 (97%)	193 (96%)	9 (4%)	27	62
14	T	27/29 (93%)	26 (96%)	1 (4%)	34	66
15	U	84/89 (94%)	80 (95%)	4 (5%)	25	60
16	V	116/117 (99%)	111 (96%)	5 (4%)	29	63
17	y	20/37 (54%)	18 (90%)	2 (10%)	7	35
18	X	28/33 (85%)	24 (86%)	4 (14%)	3	21
19	Z	52/52 (100%)	47 (90%)	5 (10%)	8	37
All	All	2114/2222 (95%)	1994 (94%)	120 (6%)	20	55

All (120) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	30	VAL
1	A	32	TRP
1	A	157	VAL
1	A	170	ASP
1	A	202	VAL
1	A	206	PHE
1	A	234	ASN
1	A	243	GLU
1	A	271	LEU
1	A	286	THR
1	A	292	THR
1	A	298	ASN
1	A	308	ASP
2	B	11	VAL
2	B	18	ARG
2	B	84	THR
2	B	223	GLN
2	B	246	PHE
2	B	262	THR
2	B	308	LYS
2	B	309	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	362	PHE
2	B	373	LYS
2	B	374	ASN
2	B	414	PRO
2	B	422	ARG
2	B	433	ASP
2	B	483	ASP
2	B	486	LEU
3	C	26	ARG
3	C	27	ASP
3	C	28	GLN
3	C	29	GLU
3	C	78	GLU
3	C	86	LEU
3	C	104	GLU
3	C	165	LEU
3	C	174	LEU
3	C	201	ASN
3	C	207	ARG
3	C	232	ASP
3	C	244	CYS
3	C	289	PHE
3	C	305	THR
3	C	355	THR
3	C	382	ASN
3	C	391	ARG
3	C	401	LEU
3	C	447	ARG
3	C	472	LEU
4	D	20	ASP
4	D	43	LEU
4	D	53	THR
4	D	60	THR
4	D	84	SER
4	D	91	LEU
4	D	130	PHE
4	D	180	ARG
4	D	201	VAL
4	D	221	THR
4	D	236	ASN
4	D	241	GLU
4	D	256	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	259	ILE
4	D	279	LEU
4	D	291	LEU
4	D	294	ARG
4	D	323	GLU
4	D	346	LEU
5	E	9	PRO
5	E	18	ARG
5	E	77	GLU
5	E	82	GLN
5	E	84	LYS
6	F	24	HIS
7	H	27	THR
7	H	49	TYR
7	H	56	ASP
7	H	60	VAL
8	I	33	LYS
9	J	7	ARG
10	K	10	LYS
10	K	18	PHE
10	K	19	ASP
11	L	1	MET
11	L	7	ARG
11	L	8	GLN
11	L	11	GLU
11	L	15	THR
13	O	31	LEU
13	O	87	GLN
13	O	88	GLU
13	O	97	VAL
13	O	106	GLN
13	O	114	ASN
13	O	141	ARG
13	O	178	ARG
13	O	219	THR
14	T	29	ILE
15	U	61	ASN
15	U	88	VAL
15	U	114	VAL
15	U	132	LEU
16	V	32	GLU
16	V	63	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	V	92	ARG
16	V	116	GLU
16	V	122	ARG
17	y	28	ILE
17	y	46	LEU
18	X	11	THR
18	X	12	ILE
18	X	42	GLN
18	X	45	LYS
19	Z	14	ILE
19	Z	25	VAL
19	Z	33	TRP
19	Z	58	ASN
19	Z	62	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	241	GLN
1	A	261	GLN
2	B	201	HIS
2	B	216	HIS
2	B	374	ASN
3	C	155	ASN
3	C	251	HIS
3	C	398	HIS
3	C	418	ASN
3	C	444	HIS
4	D	98	GLN
4	D	117	HIS
4	D	129	GLN
4	D	142	ASN
4	D	239	GLN
4	D	250	ASN
5	E	74	GLN
6	F	44	GLN
7	H	59	ASN
11	L	6	ASN
11	L	8	GLN
12	M	33	GLN
13	O	106	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	O	135	GLN
13	O	150	ASN
13	O	173	ASN
13	O	222	GLN
13	O	226	ASN
15	U	82	ASN
18	X	42	GLN
19	Z	6	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 87 ligands modelled in this entry, 4 are monoatomic - leaving 83 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	$\#\|Z\| > 2$
21	CLA	C	483	-	65,73,73	2.93	21 (32%)	76,113,113	1.78	13 (17%)
21	CLA	A	363	-	65,73,73	2.42	19 (29%)	76,113,113	1.90	15 (19%)
30	SQD	D	361	-	42,43,54	2.57	19 (45%)	51,54,65	2.94	15 (29%)
21	CLA	C	477	-	65,73,73	2.54	17 (26%)	76,113,113	1.92	14 (18%)
21	CLA	B	518	-	65,73,73	2.72	20 (30%)	76,113,113	2.17	20 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
25	BCR	Z	116	-	41,41,41	1.95	8 (19%)	56,56,56	2.08	19 (33%)
30	SQD	F	224	-	44,45,54	2.65	21 (47%)	53,56,65	2.85	19 (35%)
30	SQD	L	213	-	46,47,54	2.60	24 (52%)	55,58,65	2.88	19 (34%)
29	LMT	D	536	-	36,36,36	1.70	10 (27%)	47,47,47	1.58	8 (17%)
29	LMT	T	226	-	36,36,36	1.79	9 (25%)	47,47,47	0.98	2 (4%)
23	MES	A	367	-	12,12,12	1.49	1 (8%)	14,16,16	1.21	3 (21%)
33	HEM	V	164	16	41,50,50	2.53	14 (34%)	45,82,82	3.01	16 (35%)
21	CLA	D	356	-	65,73,73	2.59	20 (30%)	76,113,113	1.88	13 (17%)
21	CLA	A	366	-	65,73,73	2.67	19 (29%)	76,113,113	1.75	11 (14%)
21	CLA	B	520	-	65,73,73	2.54	18 (27%)	76,113,113	1.72	11 (14%)
21	CLA	B	512	-	65,73,73	2.38	18 (27%)	76,113,113	1.61	9 (11%)
25	BCR	D	358	-	41,41,41	1.72	7 (17%)	56,56,56	2.29	20 (35%)
22	PHO	A	365	-	51,69,69	3.42	10 (19%)	47,99,99	1.69	6 (12%)
25	BCR	X	107	-	41,41,41	1.55	6 (14%)	56,56,56	2.40	20 (35%)
21	CLA	C	487	-	65,73,73	3.11	22 (33%)	76,113,113	1.85	10 (13%)
21	CLA	B	522	-	65,73,73	2.39	18 (27%)	76,113,113	1.67	11 (14%)
28	DGD	C	492	-	63,63,67	1.36	10 (15%)	77,77,81	2.78	21 (27%)
21	CLA	B	526	-	65,73,73	2.98	20 (30%)	76,113,113	1.77	11 (14%)
21	CLA	B	521	-	65,73,73	2.63	18 (27%)	76,113,113	1.95	19 (25%)
21	CLA	B	523	-	65,73,73	2.52	18 (27%)	76,113,113	1.63	15 (19%)
21	CLA	B	524	-	65,73,73	2.76	21 (32%)	76,113,113	1.84	15 (19%)
21	CLA	C	479	-	65,73,73	2.75	20 (30%)	76,113,113	1.94	14 (18%)
21	CLA	C	484	-	65,73,73	2.74	18 (27%)	76,113,113	1.81	16 (21%)
22	PHO	D	355	-	51,69,69	3.23	11 (21%)	47,99,99	1.69	6 (12%)
21	CLA	C	480	-	65,73,73	2.74	19 (29%)	76,113,113	2.00	13 (17%)
21	CLA	C	482	-	65,73,73	3.25	22 (33%)	76,113,113	1.86	17 (22%)
29	LMT	A	376	-	36,36,36	1.99	11 (30%)	47,47,47	1.45	8 (17%)
27	LMG	M	217	-	42,42,55	1.95	8 (19%)	50,50,63	1.47	7 (14%)
28	DGD	C	491	-	54,54,67	1.63	9 (16%)	68,68,81	2.98	23 (33%)
21	CLA	C	488	-	65,73,73	2.88	19 (29%)	76,113,113	1.86	16 (21%)
28	DGD	A	375	-	53,53,67	2.05	13 (24%)	67,67,81	2.50	22 (32%)
33	HEM	F	85	5	41,50,50	2.78	17 (41%)	45,82,82	3.03	16 (35%)
25	BCR	C	489	-	41,41,41	1.90	9 (21%)	56,56,56	2.09	16 (28%)
25	BCR	B	530	-	41,41,41	2.51	11 (26%)	56,56,56	2.22	23 (41%)
26	LHG	A	371	-	38,38,48	2.22	5 (13%)	41,44,54	1.41	4 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
25	BCR	J	112	-	41,41,41	1.90	8 (19%)	56,56,56	2.41	24 (42%)
21	CLA	B	516	-	65,73,73	2.80	20 (30%)	76,113,113	1.98	17 (22%)
21	CLA	C	485	-	65,73,73	2.75	19 (29%)	76,113,113	1.75	12 (15%)
21	CLA	B	515	-	65,73,73	2.66	18 (27%)	76,113,113	1.79	12 (15%)
29	LMT	I	274	-	36,36,36	1.87	12 (33%)	47,47,47	1.33	7 (14%)
29	LMT	B	535	-	36,36,36	1.87	10 (27%)	47,47,47	1.15	2 (4%)
21	CLA	C	486	3	65,73,73	3.25	22 (33%)	76,113,113	1.77	16 (21%)
27	LMG	I	220	-	43,43,55	2.02	12 (27%)	51,51,63	2.17	14 (27%)
28	DGD	C	493	-	67,67,67	1.44	16 (23%)	81,81,81	3.04	28 (34%)
27	LMG	B	531	-	49,49,55	1.66	6 (12%)	57,57,63	2.81	18 (31%)
27	LMG	J	492	-	48,48,55	1.95	9 (18%)	56,56,63	1.87	17 (30%)
27	LMG	D	359	-	46,46,55	1.72	6 (13%)	54,54,63	2.55	17 (31%)
25	BCR	J	115	-	41,41,41	2.24	11 (26%)	56,56,56	3.20	17 (30%)
21	CLA	A	362	-	65,73,73	2.36	19 (29%)	76,113,113	1.78	13 (17%)
27	LMG	C	494	-	45,45,55	1.91	8 (17%)	53,53,63	2.19	16 (30%)
28	DGD	B	533	-	67,67,67	1.49	13 (19%)	81,81,81	1.83	19 (23%)
21	CLA	B	511	-	65,73,73	3.30	26 (40%)	76,113,113	1.81	15 (19%)
21	CLA	D	354	-	65,73,73	2.83	19 (29%)	76,113,113	1.64	12 (15%)
31	BCT	D	353	20	2,3,3	0.65	0	2,3,3	0.40	0
25	BCR	B	529	-	41,41,41	2.17	9 (21%)	56,56,56	2.16	19 (33%)
28	DGD	C	474	-	57,57,67	2.08	15 (26%)	71,71,81	3.57	24 (33%)
21	CLA	C	481	-	65,73,73	3.16	20 (30%)	76,113,113	2.03	15 (19%)
21	CLA	B	513	-	65,73,73	2.40	18 (27%)	76,113,113	1.87	14 (18%)
25	BCR	A	369	-	41,41,41	1.91	6 (14%)	56,56,56	2.08	18 (32%)
28	DGD	B	528	-	59,59,67	0.60	2 (3%)	73,73,81	1.07	8 (10%)
29	LMT	D	363	-	32,32,36	1.82	7 (21%)	43,43,47	1.49	6 (13%)
26	LHG	C	476	-	36,36,48	2.39	6 (16%)	39,42,54	1.50	4 (10%)
21	CLA	B	517	-	65,73,73	2.86	21 (32%)	76,113,113	2.04	22 (28%)
25	BCR	C	490	-	41,41,41	1.98	8 (19%)	56,56,56	2.21	21 (37%)
30	SQD	C	475	-	50,51,54	2.59	26 (52%)	59,62,65	2.75	18 (30%)
25	BCR	B	527	-	41,41,41	1.79	7 (17%)	56,56,56	2.34	21 (37%)
21	CLA	K	483	-	65,73,73	2.51	17 (26%)	76,113,113	1.76	11 (14%)
27	LMG	A	373	-	51,51,55	0.55	1 (1%)	59,59,63	1.09	6 (10%)
27	LMG	D	360	-	48,48,55	0.56	1 (2%)	56,56,63	1.11	6 (10%)
32	PL9	D	357	-	55,55,55	3.11	23 (41%)	68,69,69	2.92	26 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
29	LMT	O	274	-	36,36,36	2.00	12 (33%)	47,47,47	1.39	7 (14%)
21	CLA	B	514	-	65,73,73	2.60	17 (26%)	76,113,113	1.60	14 (18%)
21	CLA	A	364	-	65,73,73	2.57	21 (32%)	76,113,113	1.91	15 (19%)
21	CLA	C	478	-	65,73,73	2.52	18 (27%)	76,113,113	1.73	14 (18%)
21	CLA	B	525	-	65,73,73	2.75	19 (29%)	76,113,113	1.83	11 (14%)
28	DGD	D	362	-	64,64,67	2.09	22 (34%)	78,78,81	2.55	21 (26%)
21	CLA	B	519	-	65,73,73	2.61	17 (26%)	76,113,113	1.84	15 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	C	483	-	2/2/15/20	11/37/115/115	-
21	CLA	A	363	-	2/2/15/20	8/37/115/115	-
30	SQD	D	361	-	-	15/38/58/69	0/1/1/1
21	CLA	C	477	-	2/2/15/20	8/37/115/115	-
21	CLA	B	518	-	2/2/15/20	10/37/115/115	-
25	BCR	Z	116	-	-	2/29/63/63	0/2/2/2
30	SQD	F	224	-	-	19/40/60/69	0/1/1/1
30	SQD	L	213	-	-	17/42/62/69	0/1/1/1
29	LMT	D	536	-	-	1/21/61/61	0/2/2/2
29	LMT	T	226	-	-	1/21/61/61	0/2/2/2
23	MES	A	367	-	-	3/6/14/14	0/1/1/1
33	HEM	V	164	16	-	8/12/54/54	-
21	CLA	D	356	-	2/2/15/20	8/37/115/115	-
21	CLA	A	366	-	2/2/15/20	10/37/115/115	-
21	CLA	B	520	-	2/2/15/20	14/37/115/115	-
21	CLA	B	512	-	2/2/15/20	9/37/115/115	-
25	BCR	D	358	-	-	3/29/63/63	0/2/2/2
22	PHO	A	365	-	1/1/17/22	8/37/103/103	0/5/6/6
25	BCR	X	107	-	-	3/29/63/63	0/2/2/2
21	CLA	C	487	-	2/2/15/20	9/37/115/115	-
21	CLA	B	522	-	2/2/15/20	16/37/115/115	-
28	DGD	C	492	-	1/1/13/13	8/51/91/95	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	B	526	-	2/2/15/20	11/37/115/115	-
21	CLA	B	521	-	2/2/15/20	11/37/115/115	-
21	CLA	B	523	-	2/2/15/20	10/37/115/115	-
21	CLA	B	524	-	2/2/15/20	14/37/115/115	-
21	CLA	C	479	-	2/2/15/20	11/37/115/115	-
21	CLA	C	484	-	2/2/15/20	11/37/115/115	-
22	PHO	D	355	-	1/1/17/22	17/37/103/103	0/5/6/6
21	CLA	C	480	-	2/2/15/20	13/37/115/115	-
21	CLA	C	482	-	2/2/15/20	12/37/115/115	-
29	LMT	A	376	-	-	3/21/61/61	0/2/2/2
27	LMG	M	217	-	-	3/37/57/70	0/1/1/1
28	DGD	C	491	-	-	5/42/82/95	0/2/2/2
21	CLA	C	488	-	2/2/15/20	9/37/115/115	-
28	DGD	A	375	-	-	6/41/81/95	0/2/2/2
33	HEM	F	85	5	-	6/12/54/54	-
25	BCR	C	489	-	-	5/29/63/63	0/2/2/2
25	BCR	B	530	-	-	4/29/63/63	0/2/2/2
26	LHG	A	371	-	-	17/43/43/53	-
25	BCR	J	112	-	-	1/29/63/63	0/2/2/2
21	CLA	B	516	-	2/2/15/20	9/37/115/115	-
21	CLA	C	485	-	2/2/15/20	11/37/115/115	-
21	CLA	B	515	-	2/2/15/20	8/37/115/115	-
29	LMT	I	274	-	-	2/21/61/61	0/2/2/2
29	LMT	B	535	-	-	3/21/61/61	0/2/2/2
21	CLA	C	486	3	2/2/15/20	8/37/115/115	-
27	LMG	I	220	-	-	4/38/58/70	0/1/1/1
28	DGD	C	493	-	1/1/13/13	9/55/95/95	0/2/2/2
27	LMG	B	531	-	-	4/44/64/70	0/1/1/1
27	LMG	J	492	-	-	5/43/63/70	0/1/1/1
27	LMG	D	359	-	-	5/41/61/70	0/1/1/1
25	BCR	J	115	-	-	4/29/63/63	0/2/2/2
21	CLA	A	362	-	2/2/15/20	10/37/115/115	-
27	LMG	C	494	-	-	3/40/60/70	0/1/1/1
28	DGD	B	533	-	-	9/55/95/95	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	B	511	-	2/2/15/20	16/37/115/115	-
21	CLA	D	354	-	2/2/15/20	10/37/115/115	-
25	BCR	B	529	-	-	0/29/63/63	0/2/2/2
28	DGD	C	474	-	-	7/45/85/95	0/2/2/2
21	CLA	C	481	-	2/2/15/20	10/37/115/115	-
21	CLA	B	513	-	2/2/15/20	12/37/115/115	-
25	BCR	A	369	-	-	5/29/63/63	0/2/2/2
28	DGD	B	528	-	-	19/47/87/95	0/2/2/2
29	LMT	D	363	-	-	1/17/57/61	0/2/2/2
26	LHG	C	476	-	-	18/41/41/53	-
21	CLA	B	517	-	2/2/15/20	8/37/115/115	-
25	BCR	C	490	-	-	3/29/63/63	0/2/2/2
30	SQD	C	475	-	-	22/46/66/69	0/1/1/1
25	BCR	B	527	-	-	4/29/63/63	0/2/2/2
21	CLA	K	483	-	2/2/15/20	7/37/115/115	-
27	LMG	A	373	-	-	20/46/66/70	0/1/1/1
27	LMG	D	360	-	-	19/43/63/70	0/1/1/1
32	PL9	D	357	-	-	17/53/73/73	0/1/1/1
29	LMT	O	274	-	-	3/21/61/61	0/2/2/2
21	CLA	B	514	-	2/2/15/20	10/37/115/115	-
21	CLA	A	364	-	2/2/15/20	14/37/115/115	-
21	CLA	C	478	-	2/2/15/20	7/37/115/115	-
21	CLA	B	525	-	2/2/15/20	11/37/115/115	-
28	DGD	D	362	-	-	10/52/92/95	0/2/2/2
21	CLA	B	519	-	2/2/15/20	9/37/115/115	-

All (1167) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	365	PHO	C3A-C2A	-16.73	1.39	1.54
22	D	355	PHO	C3A-C2A	-16.66	1.39	1.54
21	B	511	CLA	C3B-C2B	11.81	1.56	1.40
21	C	486	CLA	MG-NA	11.31	2.33	2.06
32	D	357	PL9	C28-C29	11.30	1.60	1.33
21	B	524	CLA	C2-C3	10.83	1.58	1.33
21	C	482	CLA	C2-C3	10.57	1.58	1.33
21	B	521	CLA	C2-C3	10.49	1.58	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	517	CLA	C2-C3	10.37	1.57	1.33
21	B	518	CLA	C2-C3	10.24	1.57	1.33
21	C	487	CLA	C2-C3	10.20	1.57	1.33
21	B	514	CLA	C2-C3	9.76	1.56	1.33
27	B	531	LMG	O1-C1	-9.72	1.23	1.40
21	C	477	CLA	C2-C3	9.72	1.56	1.33
27	M	217	LMG	O1-C1	-9.69	1.23	1.40
32	D	357	PL9	C13-C14	9.69	1.56	1.33
21	B	526	CLA	C2-C3	9.67	1.56	1.33
21	D	354	CLA	MG-NA	9.67	2.29	2.06
21	B	515	CLA	C2-C3	9.66	1.56	1.33
27	I	220	LMG	O1-C1	-9.64	1.23	1.40
21	B	516	CLA	C2-C3	9.63	1.56	1.33
21	C	486	CLA	C2-C3	9.62	1.56	1.33
27	C	494	LMG	O1-C1	-9.62	1.23	1.40
27	J	492	LMG	O1-C1	-9.60	1.23	1.40
27	D	359	LMG	O1-C1	-9.60	1.23	1.40
21	B	519	CLA	C2-C3	9.52	1.55	1.33
21	C	479	CLA	C2-C3	9.51	1.55	1.33
21	C	481	CLA	C3B-C2B	9.50	1.53	1.40
21	C	482	CLA	C3B-C2B	9.45	1.53	1.40
21	C	481	CLA	C2-C3	9.44	1.55	1.33
21	B	525	CLA	C2-C3	9.40	1.55	1.33
21	C	482	CLA	C1B-NB	9.38	1.43	1.35
21	C	481	CLA	MG-NA	9.27	2.28	2.06
21	C	480	CLA	C2-C3	9.20	1.55	1.33
21	B	511	CLA	C2-C3	9.17	1.55	1.33
21	B	520	CLA	C2-C3	9.15	1.54	1.33
21	C	483	CLA	C2-C3	9.06	1.54	1.33
21	A	364	CLA	C2-C3	8.93	1.54	1.33
21	D	356	CLA	C2-C3	8.88	1.54	1.33
21	C	487	CLA	C3B-C2B	8.87	1.52	1.40
26	C	476	LHG	P-O5	8.85	1.82	1.50
21	C	481	CLA	C1B-NB	8.84	1.43	1.35
21	B	522	CLA	C2-C3	8.78	1.54	1.33
21	C	485	CLA	C2-C3	8.77	1.54	1.33
30	C	475	SQD	C4-C3	8.76	1.74	1.52
21	B	523	CLA	C2-C3	8.75	1.54	1.33
21	C	478	CLA	C2-C3	8.73	1.53	1.33
21	B	526	CLA	C1B-NB	8.69	1.43	1.35
21	C	479	CLA	C3B-C2B	8.65	1.52	1.40
21	D	354	CLA	C2-C3	8.62	1.53	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	365	PHO	C2-C3	8.56	1.53	1.33
26	A	371	LHG	P-O5	8.56	1.81	1.50
21	K	483	CLA	C2-C3	8.54	1.53	1.33
21	C	484	CLA	C3B-C2B	8.48	1.52	1.40
21	C	488	CLA	C2-C3	8.46	1.53	1.33
21	C	484	CLA	C2-C3	8.44	1.53	1.33
32	D	357	PL9	C2-C3	8.44	1.56	1.34
21	C	480	CLA	C1B-NB	8.43	1.42	1.35
21	A	366	CLA	C3B-C2B	8.39	1.52	1.40
25	B	530	BCR	C30-C25	8.38	1.65	1.53
21	C	488	CLA	C3B-C2B	8.36	1.52	1.40
21	B	526	CLA	C3B-C2B	8.36	1.52	1.40
21	A	366	CLA	C2-C3	8.36	1.53	1.33
21	B	514	CLA	C3B-C2B	8.27	1.51	1.40
21	C	485	CLA	C1B-NB	8.26	1.42	1.35
22	D	355	PHO	C3B-C2B	8.25	1.51	1.40
21	B	513	CLA	C2-C3	8.22	1.52	1.33
21	B	519	CLA	C3B-C2B	8.20	1.51	1.40
21	A	363	CLA	C2-C3	8.19	1.52	1.33
30	F	224	SQD	C4-C3	8.17	1.73	1.52
22	A	365	PHO	CHA-CBD	8.14	1.61	1.52
21	C	483	CLA	C3B-C2B	8.08	1.51	1.40
21	B	512	CLA	C2-C3	8.06	1.52	1.33
21	B	525	CLA	C3B-C2B	8.03	1.51	1.40
30	D	361	SQD	C4-C3	7.94	1.72	1.52
21	B	511	CLA	C1B-NB	7.94	1.42	1.35
21	C	480	CLA	C3B-C2B	7.91	1.51	1.40
21	C	486	CLA	C1B-NB	7.84	1.42	1.35
21	C	486	CLA	C3B-C2B	7.83	1.51	1.40
21	C	488	CLA	MG-NA	7.80	2.24	2.06
21	B	516	CLA	C3B-C2B	7.80	1.51	1.40
21	B	518	CLA	O2A-CGA	7.78	1.56	1.33
22	A	365	PHO	C3B-C2B	7.62	1.50	1.40
21	B	520	CLA	C3B-C2B	7.58	1.50	1.40
21	C	484	CLA	C1B-NB	7.55	1.41	1.35
21	D	354	CLA	C3B-C2B	7.52	1.50	1.40
21	C	483	CLA	C1B-NB	7.46	1.41	1.35
33	F	85	HEM	O1D-CGD	7.42	1.46	1.22
30	L	213	SQD	C4-C3	7.36	1.71	1.52
21	B	512	CLA	C3B-C2B	7.35	1.50	1.40
21	B	515	CLA	C3B-C2B	7.35	1.50	1.40
33	V	164	HEM	O1D-CGD	7.34	1.46	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	C	488	CLA	C1B-NB	7.32	1.41	1.35
21	A	363	CLA	C3B-C2B	7.32	1.50	1.40
21	B	518	CLA	C3B-C2B	7.25	1.50	1.40
21	B	515	CLA	C1B-NB	7.18	1.41	1.35
21	K	483	CLA	C1B-NB	7.18	1.41	1.35
33	F	85	HEM	C3B-C2B	7.18	1.51	1.37
21	C	487	CLA	C1B-NB	7.17	1.41	1.35
21	C	485	CLA	C3B-C2B	7.12	1.50	1.40
22	D	355	PHO	C2-C3	7.06	1.49	1.33
21	B	523	CLA	C1B-NB	7.05	1.41	1.35
21	C	478	CLA	C3B-C2B	7.01	1.50	1.40
25	B	529	BCR	C30-C25	7.00	1.63	1.53
28	A	375	DGD	O3G-C1D	6.99	1.52	1.40
21	A	364	CLA	C3B-C2B	6.97	1.50	1.40
21	C	477	CLA	C3B-C2B	6.95	1.50	1.40
21	A	362	CLA	C3B-C2B	6.93	1.50	1.40
21	A	362	CLA	C2-C3	6.90	1.49	1.33
25	C	489	BCR	C1-C6	6.83	1.63	1.53
21	D	356	CLA	C3B-C2B	6.83	1.49	1.40
21	B	521	CLA	C3B-C2B	6.81	1.49	1.40
21	K	483	CLA	C3B-C2B	6.80	1.49	1.40
25	B	530	BCR	C1-C6	6.80	1.63	1.53
21	B	525	CLA	C1B-NB	6.77	1.41	1.35
21	B	511	CLA	C4C-C3C	6.70	1.56	1.45
21	A	366	CLA	C1B-NB	6.65	1.41	1.35
21	B	517	CLA	O2A-CGA	6.62	1.52	1.33
25	J	112	BCR	C30-C25	6.59	1.62	1.53
26	C	476	LHG	P-O3	6.53	1.85	1.59
21	B	524	CLA	C3B-C2B	6.52	1.49	1.40
21	B	524	CLA	O2A-CGA	6.51	1.52	1.33
25	J	115	BCR	C30-C25	6.49	1.62	1.53
21	B	511	CLA	O2D-CGD	6.44	1.48	1.33
28	C	474	DGD	O5D-C1E	6.36	1.51	1.40
28	D	362	DGD	O5D-C1E	6.36	1.51	1.40
21	C	487	CLA	O2A-CGA	6.35	1.51	1.33
21	C	484	CLA	O2D-CGD	6.32	1.48	1.33
21	B	523	CLA	C3B-C2B	6.31	1.49	1.40
21	B	524	CLA	C1B-NB	6.29	1.40	1.35
21	B	513	CLA	C3B-C2B	6.27	1.49	1.40
21	B	517	CLA	MG-NA	6.25	2.21	2.06
21	B	526	CLA	MG-NA	6.25	2.21	2.06
25	A	369	BCR	C30-C25	6.22	1.62	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	C	478	CLA	C1B-NB	6.19	1.40	1.35
21	C	482	CLA	O2D-CGD	6.14	1.48	1.33
21	B	515	CLA	O2A-CGA	6.12	1.51	1.33
21	C	486	CLA	C4B-NB	6.08	1.40	1.35
21	C	482	CLA	C1C-C2C	6.04	1.56	1.44
25	Z	116	BCR	C30-C25	6.03	1.62	1.53
21	C	482	CLA	C4B-NB	6.02	1.40	1.35
28	D	362	DGD	O3G-C1D	6.02	1.50	1.40
21	C	487	CLA	MG-NA	6.01	2.20	2.06
32	D	357	PL9	C3-C4	-5.99	1.39	1.49
21	B	520	CLA	C1B-NB	5.97	1.40	1.35
21	B	511	CLA	C4B-NB	5.96	1.40	1.35
21	C	483	CLA	C4B-NB	5.92	1.40	1.35
21	C	481	CLA	C4B-NB	5.91	1.40	1.35
21	B	511	CLA	O2A-CGA	5.89	1.50	1.33
25	J	115	BCR	C5-C6	5.85	1.44	1.34
25	C	490	BCR	C1-C6	5.83	1.61	1.53
21	B	526	CLA	O2A-CGA	5.81	1.50	1.33
21	B	516	CLA	O2A-CGA	5.80	1.50	1.33
21	C	479	CLA	C1B-NB	5.79	1.40	1.35
21	B	519	CLA	C1B-NB	5.79	1.40	1.35
21	C	477	CLA	O2D-CGD	5.78	1.47	1.33
21	C	486	CLA	O2A-CGA	5.76	1.50	1.33
25	Z	116	BCR	C1-C6	5.73	1.61	1.53
21	B	511	CLA	MG-NA	5.72	2.19	2.06
21	B	517	CLA	C3B-C2B	5.72	1.48	1.40
21	C	481	CLA	C1C-C2C	5.71	1.55	1.44
26	A	371	LHG	P-O3	5.68	1.82	1.59
21	B	513	CLA	O2A-CGA	5.68	1.49	1.33
21	A	364	CLA	O2A-CGA	5.67	1.49	1.33
21	D	354	CLA	C1B-NB	5.64	1.40	1.35
21	B	522	CLA	C3B-C2B	5.62	1.48	1.40
21	B	516	CLA	C1B-NB	5.61	1.40	1.35
21	C	482	CLA	O2A-CGA	5.59	1.49	1.33
25	C	490	BCR	C30-C25	5.58	1.61	1.53
21	C	477	CLA	O2A-CGA	5.57	1.49	1.33
21	C	482	CLA	C4C-C3C	5.55	1.54	1.45
21	C	481	CLA	O2A-CGA	5.54	1.49	1.33
28	C	491	DGD	O5D-C1E	5.47	1.49	1.40
33	V	164	HEM	C3B-C2B	5.47	1.48	1.37
21	B	525	CLA	O2A-CGA	5.44	1.49	1.33
33	F	85	HEM	C2C-C1C	5.43	1.54	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	516	CLA	C3A-C2A	-5.42	1.39	1.54
21	C	483	CLA	O2D-CGD	5.41	1.46	1.33
21	C	486	CLA	C1C-C2C	5.40	1.55	1.44
21	B	517	CLA	C3A-C2A	-5.40	1.39	1.54
21	C	477	CLA	C3A-C2A	-5.40	1.39	1.54
21	B	519	CLA	O2D-CGD	5.40	1.46	1.33
21	B	513	CLA	C3A-C2A	-5.39	1.39	1.54
21	B	523	CLA	C3A-C2A	-5.39	1.39	1.54
21	D	356	CLA	C3A-C2A	-5.39	1.39	1.54
21	B	521	CLA	C3A-C2A	-5.39	1.39	1.54
21	B	512	CLA	C3A-C2A	-5.39	1.39	1.54
21	A	366	CLA	C3A-C2A	-5.38	1.39	1.54
21	C	478	CLA	C3A-C2A	-5.38	1.39	1.54
21	C	485	CLA	C3A-C2A	-5.38	1.39	1.54
21	C	484	CLA	C3A-C2A	-5.38	1.39	1.54
21	B	514	CLA	C3A-C2A	-5.38	1.39	1.54
21	A	362	CLA	C3A-C2A	-5.38	1.39	1.54
21	A	364	CLA	C3A-C2A	-5.38	1.39	1.54
21	B	520	CLA	C4C-C3C	5.37	1.54	1.45
21	C	488	CLA	C3A-C2A	-5.37	1.39	1.54
21	B	518	CLA	C3A-C2A	-5.37	1.39	1.54
21	B	522	CLA	C3A-C2A	-5.36	1.39	1.54
21	B	520	CLA	C3A-C2A	-5.36	1.39	1.54
21	C	482	CLA	C3A-C2A	-5.36	1.39	1.54
21	B	519	CLA	C3A-C2A	-5.35	1.39	1.54
21	C	480	CLA	C3A-C2A	-5.35	1.39	1.54
21	C	479	CLA	C3A-C2A	-5.35	1.39	1.54
21	B	521	CLA	O2D-CGD	5.35	1.46	1.33
21	B	515	CLA	C3A-C2A	-5.35	1.39	1.54
21	C	481	CLA	C3A-C2A	-5.34	1.39	1.54
21	B	524	CLA	C3A-C2A	-5.34	1.39	1.54
21	C	487	CLA	C3A-C2A	-5.34	1.39	1.54
21	A	363	CLA	C1B-NB	5.34	1.40	1.35
21	K	483	CLA	C3A-C2A	-5.34	1.39	1.54
21	A	363	CLA	C3A-C2A	-5.33	1.39	1.54
21	B	525	CLA	C3A-C2A	-5.32	1.39	1.54
21	B	511	CLA	C3A-C2A	-5.32	1.39	1.54
21	C	486	CLA	C3A-C2A	-5.32	1.39	1.54
21	D	354	CLA	C3A-C2A	-5.31	1.39	1.54
21	B	517	CLA	C4B-NB	5.31	1.39	1.35
21	B	526	CLA	C3A-C2A	-5.30	1.39	1.54
21	D	354	CLA	O2A-CGA	5.29	1.48	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	C	483	CLA	C3A-C2A	-5.28	1.39	1.54
21	C	479	CLA	O2A-CGA	5.27	1.48	1.33
21	B	526	CLA	O2D-CGD	5.27	1.46	1.33
21	C	487	CLA	C4C-C3C	5.27	1.54	1.45
28	C	474	DGD	O6D-C1D	5.27	1.55	1.41
21	B	522	CLA	C1B-NB	5.26	1.39	1.35
30	D	361	SQD	O47-C7	5.26	1.49	1.34
25	A	369	BCR	C1-C6	5.24	1.61	1.53
21	A	362	CLA	C1B-NB	5.17	1.39	1.35
33	F	85	HEM	C4D-ND	-5.16	1.31	1.40
21	B	516	CLA	O2D-CGD	5.16	1.45	1.33
21	C	485	CLA	O2D-CGD	5.15	1.45	1.33
33	V	164	HEM	C2C-C1C	5.15	1.54	1.42
26	C	476	LHG	P-O6	5.14	1.80	1.59
21	B	525	CLA	O2D-CGD	5.14	1.45	1.33
21	C	487	CLA	C1C-C2C	5.13	1.54	1.44
25	J	115	BCR	C26-C25	5.12	1.43	1.34
21	B	514	CLA	C1B-NB	5.12	1.39	1.35
32	D	357	PL9	C6-C1	-5.12	1.39	1.48
21	C	485	CLA	C4C-C3C	5.10	1.53	1.45
21	A	364	CLA	C1B-NB	5.10	1.39	1.35
21	B	512	CLA	C1B-NB	5.09	1.39	1.35
21	C	486	CLA	O2D-CGD	5.09	1.45	1.33
21	C	478	CLA	O2A-CGA	5.09	1.48	1.33
30	L	213	SQD	O5-C5	5.08	1.56	1.44
21	C	483	CLA	MG-NA	5.08	2.18	2.06
21	D	356	CLA	C1B-NB	5.07	1.39	1.35
28	D	362	DGD	O6D-C1D	5.06	1.54	1.41
25	B	527	BCR	C1-C6	5.06	1.60	1.53
28	C	491	DGD	O6D-C1D	5.06	1.54	1.41
21	B	522	CLA	O2D-CGD	5.06	1.45	1.33
21	D	356	CLA	C1C-C2C	5.05	1.54	1.44
29	T	226	LMT	C4B-C3B	-5.04	1.39	1.52
21	B	515	CLA	C1C-C2C	5.04	1.54	1.44
29	O	274	LMT	C4B-C3B	-5.03	1.39	1.52
21	B	524	CLA	C1C-C2C	5.03	1.54	1.44
21	C	485	CLA	C1C-C2C	5.01	1.54	1.44
21	D	356	CLA	O2A-CGA	5.01	1.48	1.33
29	A	376	LMT	C4B-C3B	-5.00	1.39	1.52
21	C	488	CLA	C1C-C2C	5.00	1.54	1.44
29	D	363	LMT	C4B-C3B	-5.00	1.39	1.52
29	D	536	LMT	C4B-C3B	-4.98	1.39	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	525	CLA	MG-NA	4.98	2.18	2.06
29	B	535	LMT	C4B-C3B	-4.98	1.39	1.52
21	A	366	CLA	C4B-NB	4.97	1.39	1.35
29	I	274	LMT	C4B-C3B	-4.96	1.39	1.52
21	C	488	CLA	O2A-CGA	4.95	1.47	1.33
21	C	483	CLA	C1C-C2C	4.94	1.54	1.44
21	B	516	CLA	C4C-C3C	4.94	1.53	1.45
21	C	483	CLA	O2A-CGA	4.93	1.47	1.33
21	C	483	CLA	C4C-C3C	4.93	1.53	1.45
21	C	486	CLA	C4C-C3C	4.92	1.53	1.45
21	C	488	CLA	O2D-CGD	4.91	1.45	1.33
21	B	514	CLA	O2A-CGA	4.89	1.47	1.33
30	F	224	SQD	O47-C7	4.88	1.48	1.34
21	B	521	CLA	C1D-C2D	4.87	1.54	1.45
25	B	529	BCR	C5-C6	4.87	1.42	1.34
21	C	487	CLA	O2D-CGD	4.86	1.45	1.33
29	A	376	LMT	O5B-C1B	4.84	1.54	1.41
21	B	526	CLA	C4B-NB	4.82	1.39	1.35
25	B	529	BCR	C26-C25	4.82	1.42	1.34
21	A	366	CLA	C1C-C2C	4.81	1.53	1.44
21	B	512	CLA	O2A-CGA	4.80	1.47	1.33
28	C	491	DGD	O3G-C1D	4.79	1.48	1.40
21	C	487	CLA	C4B-NB	4.79	1.39	1.35
21	A	362	CLA	O2D-CGD	4.79	1.44	1.33
21	C	484	CLA	O2A-CGA	4.78	1.47	1.33
21	K	483	CLA	O2A-CGA	4.78	1.47	1.33
21	K	483	CLA	O2D-CGD	4.77	1.44	1.33
30	F	224	SQD	O48-C23	4.76	1.47	1.33
21	C	477	CLA	C1B-NB	4.75	1.39	1.35
21	C	480	CLA	O2A-CGA	4.73	1.47	1.33
21	B	526	CLA	C4C-C3C	4.73	1.53	1.45
28	B	533	DGD	O5D-C1E	4.73	1.48	1.40
30	L	213	SQD	O47-C7	4.72	1.47	1.34
25	B	527	BCR	C30-C25	4.72	1.60	1.53
21	B	521	CLA	C4C-C3C	4.72	1.53	1.45
22	A	365	PHO	O2D-CGD	4.72	1.44	1.33
21	C	479	CLA	C1C-C2C	4.71	1.53	1.44
21	C	484	CLA	C1C-C2C	4.71	1.53	1.44
21	C	482	CLA	MG-NC	4.71	2.17	2.06
21	C	479	CLA	C1D-C2D	4.70	1.54	1.45
30	L	213	SQD	O7-S	4.70	1.58	1.45
21	D	354	CLA	C4C-C3C	4.70	1.53	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	D	358	BCR	C26-C25	4.69	1.42	1.34
22	D	355	PHO	CHA-CBD	4.69	1.57	1.52
21	A	363	CLA	O2A-CGA	4.68	1.47	1.33
21	C	488	CLA	C4B-NB	4.67	1.39	1.35
21	A	366	CLA	O2A-CGA	4.64	1.46	1.33
21	B	522	CLA	O2A-CGA	4.63	1.46	1.33
21	B	523	CLA	C1C-C2C	4.63	1.53	1.44
26	A	371	LHG	P-O6	4.63	1.78	1.59
21	C	478	CLA	O2D-CGD	4.62	1.44	1.33
21	C	485	CLA	C1D-C2D	4.61	1.54	1.45
28	A	375	DGD	O6D-C1D	4.61	1.53	1.41
33	V	164	HEM	C3C-CAC	4.60	1.57	1.47
25	B	530	BCR	C26-C25	4.60	1.42	1.34
21	K	483	CLA	C1C-C2C	4.60	1.53	1.44
21	C	480	CLA	O2D-CGD	4.59	1.44	1.33
33	F	85	HEM	C3B-C4B	4.58	1.54	1.44
21	C	484	CLA	C4B-NB	4.58	1.39	1.35
21	C	478	CLA	C1C-C2C	4.57	1.53	1.44
21	A	362	CLA	MG-NA	4.56	2.17	2.06
21	A	366	CLA	O2D-CGD	4.56	1.44	1.33
28	A	375	DGD	O6D-C5D	4.56	1.55	1.44
21	C	486	CLA	CHC-C1C	4.56	1.46	1.35
21	D	356	CLA	C4C-C3C	4.55	1.52	1.45
30	C	475	SQD	O47-C7	4.53	1.47	1.34
29	O	274	LMT	O5B-C1B	4.53	1.53	1.41
21	B	517	CLA	C1C-C2C	4.52	1.53	1.44
21	B	513	CLA	O2D-CGD	4.52	1.44	1.33
25	B	530	BCR	C5-C6	4.50	1.42	1.34
21	D	354	CLA	C1C-C2C	4.50	1.53	1.44
21	B	525	CLA	C1C-C2C	4.49	1.53	1.44
30	D	361	SQD	O7-S	4.48	1.58	1.45
21	B	520	CLA	O2D-CGD	4.47	1.44	1.33
21	B	511	CLA	MG-NC	4.47	2.16	2.06
21	B	514	CLA	C4C-C3C	4.45	1.52	1.45
25	B	530	BCR	C2-C1	4.45	1.64	1.54
21	C	480	CLA	C4C-C3C	4.45	1.52	1.45
25	D	358	BCR	C30-C25	4.45	1.59	1.53
25	J	115	BCR	C29-C30	4.45	1.64	1.54
21	B	518	CLA	C4-C3	-4.44	1.39	1.50
21	C	481	CLA	CAA-CBA	-4.44	1.39	1.52
21	B	516	CLA	MG-NC	4.43	2.16	2.06
21	B	518	CLA	C1B-NB	4.43	1.39	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	520	CLA	C4-C3	-4.43	1.39	1.50
30	F	224	SQD	O5-C5	4.43	1.55	1.44
33	F	85	HEM	C3C-CAC	4.42	1.56	1.47
21	B	515	CLA	O2D-CGD	4.42	1.44	1.33
21	D	354	CLA	C4-C3	-4.42	1.39	1.50
21	A	362	CLA	C4-C3	-4.41	1.39	1.50
21	B	521	CLA	O2A-CGA	4.41	1.46	1.33
21	B	512	CLA	C4-C3	-4.41	1.39	1.50
28	C	492	DGD	O6D-C1D	4.41	1.53	1.41
21	B	517	CLA	C4-C3	-4.41	1.39	1.50
22	D	355	PHO	C4-C3	-4.41	1.39	1.50
21	B	516	CLA	C4-C3	-4.41	1.39	1.50
21	C	482	CLA	C4-C3	-4.40	1.39	1.50
21	B	522	CLA	C1C-C2C	4.40	1.53	1.44
22	A	365	PHO	C4-C3	-4.39	1.39	1.50
30	D	361	SQD	O5-C5	4.39	1.55	1.44
21	A	366	CLA	C4-C3	-4.39	1.39	1.50
21	B	519	CLA	C4-C3	-4.39	1.39	1.50
21	B	514	CLA	C4-C3	-4.38	1.39	1.50
21	D	356	CLA	C4-C3	-4.38	1.39	1.50
21	C	481	CLA	C4-C3	-4.38	1.39	1.50
21	B	513	CLA	C4-C3	-4.38	1.39	1.50
25	J	112	BCR	C5-C6	4.38	1.42	1.34
21	C	483	CLA	C4-C3	-4.38	1.39	1.50
21	B	515	CLA	C4-C3	-4.37	1.39	1.50
21	C	479	CLA	C4-C3	-4.37	1.39	1.50
21	B	518	CLA	C1C-C2C	4.37	1.53	1.44
21	C	484	CLA	C4-C3	-4.37	1.39	1.50
21	B	523	CLA	C4-C3	-4.37	1.39	1.50
21	B	524	CLA	C4-C3	-4.37	1.39	1.50
21	B	518	CLA	CAA-CBA	-4.37	1.39	1.52
21	A	363	CLA	C4-C3	-4.36	1.39	1.50
21	B	511	CLA	C4-C3	-4.36	1.39	1.50
21	A	364	CLA	C4-C3	-4.36	1.39	1.50
21	C	477	CLA	C4-C3	-4.36	1.39	1.50
21	C	480	CLA	C1C-C2C	4.36	1.53	1.44
21	C	480	CLA	C4-C3	-4.36	1.39	1.50
21	C	486	CLA	C4-C3	-4.36	1.39	1.50
21	C	485	CLA	C4-C3	-4.36	1.39	1.50
21	K	483	CLA	C4-C3	-4.36	1.39	1.50
21	C	487	CLA	C4-C3	-4.35	1.39	1.50
21	B	522	CLA	C4-C3	-4.35	1.39	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	517	CLA	CAA-CBA	-4.35	1.39	1.52
21	B	526	CLA	C4-C3	-4.35	1.39	1.50
21	B	515	CLA	CAA-CBA	-4.35	1.39	1.52
21	C	484	CLA	CAA-CBA	-4.35	1.39	1.52
21	C	488	CLA	C4-C3	-4.34	1.39	1.50
21	C	485	CLA	O2A-CGA	4.34	1.46	1.33
21	C	482	CLA	C1D-C2D	4.34	1.53	1.45
21	C	478	CLA	C4-C3	-4.34	1.39	1.50
29	D	363	LMT	O1'-C1'	4.34	1.47	1.40
21	B	519	CLA	CAA-CBA	-4.33	1.39	1.52
21	A	366	CLA	MG-NC	4.33	2.16	2.06
21	C	480	CLA	CAA-CBA	-4.33	1.39	1.52
21	B	525	CLA	C4-C3	-4.33	1.39	1.50
21	B	523	CLA	O2A-CGA	4.33	1.46	1.33
21	C	478	CLA	CAA-CBA	-4.32	1.39	1.52
28	C	493	DGD	O6D-C1D	4.32	1.52	1.41
21	B	521	CLA	C4-C3	-4.32	1.39	1.50
21	B	522	CLA	CAA-CBA	-4.31	1.39	1.52
21	B	520	CLA	CAA-CBA	-4.31	1.39	1.52
21	C	479	CLA	CAA-CBA	-4.31	1.39	1.52
21	C	488	CLA	CAA-CBA	-4.31	1.39	1.52
21	C	477	CLA	CAA-CBA	-4.31	1.39	1.52
21	A	363	CLA	C1C-C2C	4.30	1.52	1.44
22	A	365	PHO	CAA-CBA	-4.30	1.39	1.52
21	B	521	CLA	CAA-CBA	-4.30	1.39	1.52
21	B	512	CLA	CAA-CBA	-4.29	1.39	1.52
21	A	362	CLA	CAA-CBA	-4.29	1.39	1.52
21	K	483	CLA	CAA-CBA	-4.29	1.39	1.52
30	F	224	SQD	O7-S	4.29	1.57	1.45
21	B	524	CLA	CAA-CBA	-4.28	1.39	1.52
21	D	356	CLA	CAA-CBA	-4.28	1.39	1.52
21	B	514	CLA	CAA-CBA	-4.28	1.39	1.52
21	B	523	CLA	CAA-CBA	-4.28	1.39	1.52
21	C	481	CLA	C4C-C3C	4.27	1.52	1.45
21	B	523	CLA	O2D-CGD	4.27	1.43	1.33
30	C	475	SQD	O5-C5	4.27	1.54	1.44
21	D	354	CLA	CAA-CBA	-4.27	1.39	1.52
25	B	530	BCR	C29-C30	4.27	1.64	1.54
21	C	486	CLA	CAA-CBA	-4.27	1.39	1.52
21	C	478	CLA	C4C-C3C	4.27	1.52	1.45
21	K	483	CLA	C4C-C3C	4.27	1.52	1.45
21	B	517	CLA	C4C-C3C	4.26	1.52	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	512	CLA	O2D-CGD	4.26	1.43	1.33
21	B	517	CLA	O2D-CGD	4.26	1.43	1.33
21	A	364	CLA	CAA-CBA	-4.26	1.39	1.52
21	A	364	CLA	O2D-CGD	4.26	1.43	1.33
21	A	366	CLA	CAA-CBA	-4.25	1.39	1.52
21	B	513	CLA	CAA-CBA	-4.25	1.39	1.52
21	B	516	CLA	CAA-CBA	-4.25	1.39	1.52
21	C	485	CLA	C4B-NB	4.25	1.39	1.35
21	C	482	CLA	CAA-CBA	-4.25	1.39	1.52
25	C	489	BCR	C30-C25	4.25	1.59	1.53
21	C	485	CLA	CAA-CBA	-4.24	1.39	1.52
22	D	355	PHO	CAA-CBA	-4.24	1.39	1.52
21	C	483	CLA	CAA-CBA	-4.24	1.39	1.52
30	L	213	SQD	O48-C23	4.23	1.45	1.33
21	B	517	CLA	C1D-C2D	4.23	1.53	1.45
21	B	526	CLA	CAA-CBA	-4.23	1.39	1.52
23	A	367	MES	C8-S	4.23	1.83	1.77
21	B	519	CLA	O2A-CGA	4.23	1.45	1.33
21	A	363	CLA	CAA-CBA	-4.23	1.39	1.52
21	D	354	CLA	C4B-NB	4.23	1.39	1.35
21	B	516	CLA	C1C-C2C	4.22	1.52	1.44
21	C	479	CLA	O2D-CGD	4.21	1.43	1.33
21	B	525	CLA	CAA-CBA	-4.21	1.39	1.52
21	B	524	CLA	O2D-CGD	4.21	1.43	1.33
21	B	519	CLA	C1D-C2D	4.20	1.53	1.45
21	B	511	CLA	CAA-CBA	-4.19	1.39	1.52
25	C	490	BCR	C5-C6	4.19	1.41	1.34
28	C	474	DGD	O3G-C1D	4.19	1.47	1.40
25	B	529	BCR	C1-C6	4.19	1.59	1.53
21	B	519	CLA	C4C-C3C	4.18	1.52	1.45
21	B	518	CLA	O2D-CGD	4.18	1.43	1.33
21	C	487	CLA	CAA-CBA	-4.18	1.39	1.52
22	A	365	PHO	O2A-CGA	4.17	1.45	1.33
21	A	364	CLA	C4C-C3C	4.17	1.52	1.45
21	B	519	CLA	C1C-C2C	4.16	1.52	1.44
33	V	164	HEM	C4D-ND	-4.15	1.33	1.40
26	A	371	LHG	O7-C7	4.15	1.46	1.34
30	D	361	SQD	C1-C2	4.14	1.64	1.52
28	C	474	DGD	O1G-C1A	4.14	1.45	1.33
27	J	492	LMG	O7-C8	4.13	1.57	1.46
21	C	487	CLA	MG-NC	4.13	2.16	2.06
21	B	524	CLA	C1D-C2D	4.12	1.53	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	517	CLA	C1B-NB	4.12	1.38	1.35
21	D	354	CLA	O2D-CGD	4.12	1.43	1.33
21	B	513	CLA	C4B-NB	4.12	1.38	1.35
28	C	474	DGD	O6D-C5D	4.10	1.54	1.44
21	C	481	CLA	O2D-CGD	4.10	1.43	1.33
21	B	514	CLA	C1C-C2C	4.10	1.52	1.44
21	B	521	CLA	C1B-NB	4.09	1.38	1.35
21	B	524	CLA	C4C-C3C	4.08	1.52	1.45
21	B	520	CLA	C1C-C2C	4.08	1.52	1.44
30	L	213	SQD	C1-C2	4.07	1.64	1.52
21	C	479	CLA	C4C-C3C	4.07	1.52	1.45
21	C	479	CLA	MG-NC	4.06	2.15	2.06
28	A	375	DGD	O5D-C1E	4.05	1.47	1.40
21	B	513	CLA	C1C-C2C	4.05	1.52	1.44
21	C	479	CLA	C4B-NB	4.05	1.38	1.35
21	C	481	CLA	CHC-C1C	4.05	1.45	1.35
21	B	517	CLA	CHC-C1C	4.04	1.45	1.35
21	C	477	CLA	C4C-C3C	4.03	1.52	1.45
21	B	518	CLA	C1D-C2D	4.03	1.53	1.45
25	X	107	BCR	C26-C25	4.02	1.41	1.34
30	C	475	SQD	C1-C2	4.02	1.64	1.52
25	B	529	BCR	C29-C30	4.01	1.63	1.54
22	D	355	PHO	O2A-CGA	4.01	1.45	1.33
25	D	358	BCR	C29-C30	4.01	1.63	1.54
25	Z	116	BCR	C26-C25	4.01	1.41	1.34
21	A	364	CLA	C1C-C2C	3.99	1.52	1.44
21	B	516	CLA	CBA-CGA	3.99	1.62	1.50
21	C	488	CLA	C4C-C3C	3.98	1.51	1.45
21	B	512	CLA	C1C-C2C	3.98	1.52	1.44
21	C	483	CLA	C1D-C2D	3.97	1.53	1.45
30	L	213	SQD	O6-C1	3.97	1.47	1.40
28	C	474	DGD	O6E-C1E	3.97	1.51	1.41
21	C	483	CLA	MG-NC	3.96	2.15	2.06
21	B	526	CLA	C1D-C2D	3.96	1.53	1.45
21	B	518	CLA	C4C-C3C	3.94	1.51	1.45
28	C	474	DGD	C3G-C2G	3.94	1.62	1.50
21	D	356	CLA	O2D-CGD	3.94	1.42	1.33
21	B	520	CLA	O2A-CGA	3.93	1.44	1.33
29	B	535	LMT	O5B-C1B	3.93	1.51	1.41
28	A	375	DGD	C3G-C2G	3.92	1.62	1.50
21	C	485	CLA	MG-NA	3.91	2.15	2.06
28	B	533	DGD	O6D-C1D	3.90	1.51	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	V	164	HEM	O2D-CGD	3.90	1.43	1.30
21	A	362	CLA	C4C-C3C	3.90	1.51	1.45
22	D	355	PHO	O2D-CGD	3.89	1.42	1.33
21	B	514	CLA	O2D-CGD	3.89	1.42	1.33
21	A	366	CLA	C4C-C3C	3.88	1.51	1.45
21	C	480	CLA	C4B-NB	3.88	1.38	1.35
25	D	358	BCR	C1-C6	3.88	1.59	1.53
28	C	474	DGD	O2G-C1B	3.88	1.45	1.34
26	C	476	LHG	O8-C23	3.86	1.44	1.33
21	B	525	CLA	C4B-NB	3.86	1.38	1.35
21	B	521	CLA	C1C-C2C	3.85	1.52	1.44
21	B	520	CLA	MG-NC	3.83	2.15	2.06
21	A	363	CLA	O2D-CGD	3.83	1.42	1.33
21	A	364	CLA	C1D-C2D	3.82	1.52	1.45
28	B	533	DGD	O6E-C1E	3.81	1.51	1.41
21	C	487	CLA	C5-C3	3.81	1.59	1.51
21	K	483	CLA	MG-NC	3.81	2.15	2.06
21	B	523	CLA	C4C-C3C	3.80	1.51	1.45
21	C	484	CLA	CHC-C1C	3.80	1.44	1.35
25	A	369	BCR	C26-C25	3.80	1.41	1.34
21	B	511	CLA	C1D-C2D	3.80	1.52	1.45
21	C	486	CLA	C1D-C2D	3.79	1.52	1.45
21	B	525	CLA	MG-NC	3.79	2.15	2.06
21	B	513	CLA	C4C-C3C	3.79	1.51	1.45
25	B	527	BCR	C26-C25	3.78	1.41	1.34
21	C	477	CLA	C1C-C2C	3.77	1.51	1.44
21	B	522	CLA	C4C-C3C	3.77	1.51	1.45
30	C	475	SQD	O3-C3	3.76	1.51	1.43
21	C	484	CLA	MG-NC	3.76	2.15	2.06
21	B	516	CLA	C5-C3	3.75	1.59	1.51
21	C	488	CLA	CHC-C1C	3.74	1.44	1.35
21	B	512	CLA	C4C-C3C	3.74	1.51	1.45
21	C	485	CLA	MG-NC	3.74	2.15	2.06
21	B	524	CLA	C5-C3	3.74	1.59	1.51
21	C	481	CLA	C1D-C2D	3.74	1.52	1.45
28	A	375	DGD	O6E-C5E	3.74	1.53	1.44
21	C	484	CLA	C4C-C3C	3.72	1.51	1.45
21	C	486	CLA	O1D-CGD	3.72	1.30	1.21
21	B	521	CLA	O1D-CGD	3.71	1.30	1.21
25	C	489	BCR	C2-C1	3.71	1.62	1.54
21	A	362	CLA	C1C-C2C	3.70	1.51	1.44
21	C	484	CLA	C1D-C2D	3.70	1.52	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	511	CLA	O1D-CGD	3.69	1.30	1.21
25	A	369	BCR	C5-C6	3.69	1.40	1.34
30	C	475	SQD	O48-C23	3.69	1.44	1.33
21	B	525	CLA	C4C-C3C	3.67	1.51	1.45
30	C	475	SQD	O6-C1	3.66	1.46	1.40
21	B	511	CLA	CMC-C2C	3.66	1.58	1.50
21	C	478	CLA	C1D-C2D	3.65	1.52	1.45
21	C	482	CLA	O1D-CGD	3.65	1.30	1.21
30	C	475	SQD	O7-S	3.64	1.55	1.45
28	D	362	DGD	C2A-C1A	3.64	1.61	1.50
25	X	107	BCR	C29-C30	3.64	1.62	1.54
21	B	511	CLA	C1C-C2C	3.63	1.51	1.44
21	B	521	CLA	C5-C3	3.63	1.58	1.51
33	F	85	HEM	CBC-CAC	3.63	1.53	1.29
21	B	521	CLA	MG-NC	3.62	2.14	2.06
21	C	488	CLA	O1D-CGD	3.62	1.30	1.21
33	V	164	HEM	CBC-CAC	3.61	1.53	1.29
21	C	488	CLA	C1D-C2D	3.61	1.52	1.45
21	D	356	CLA	MG-NC	3.61	2.14	2.06
25	B	529	BCR	C2-C1	3.61	1.62	1.54
25	C	490	BCR	C2-C1	3.59	1.62	1.54
21	B	526	CLA	MG-NC	3.58	2.14	2.06
21	A	364	CLA	C4B-NB	3.58	1.38	1.35
21	D	356	CLA	C1D-C2D	3.57	1.52	1.45
26	A	371	LHG	O8-C23	3.57	1.43	1.33
21	B	514	CLA	C1D-C2D	3.56	1.52	1.45
21	C	480	CLA	CMC-C2C	3.55	1.58	1.50
21	B	516	CLA	C4B-NB	3.55	1.38	1.35
29	B	535	LMT	O5'-C1'	3.55	1.50	1.41
25	J	112	BCR	C1-C6	3.53	1.58	1.53
21	B	523	CLA	MG-NC	3.52	2.14	2.06
21	D	356	CLA	C4B-NB	3.52	1.38	1.35
29	D	536	LMT	O5B-C1B	3.52	1.50	1.41
25	J	112	BCR	C2-C1	3.51	1.62	1.54
33	F	85	HEM	O2D-CGD	3.51	1.42	1.30
29	D	363	LMT	O5'-C1'	3.50	1.50	1.41
29	I	274	LMT	O5B-C1B	3.50	1.50	1.41
21	B	517	CLA	C5-C3	3.49	1.58	1.51
28	D	362	DGD	O2G-C1B	3.49	1.44	1.34
21	C	480	CLA	C1D-C2D	3.48	1.52	1.45
21	C	487	CLA	CMC-C2C	3.48	1.58	1.50
25	J	115	BCR	C1-C6	3.47	1.58	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	C	487	CLA	CAA-C2A	3.46	1.60	1.54
30	D	361	SQD	O8-S	3.46	1.59	1.47
28	A	375	DGD	O6E-C1E	3.45	1.50	1.41
25	A	369	BCR	C2-C1	3.45	1.62	1.54
21	C	482	CLA	CBA-CGA	3.44	1.60	1.50
32	D	357	PL9	C6-C5	3.43	1.53	1.35
29	A	376	LMT	O1B-C1B	3.43	1.51	1.41
29	O	274	LMT	O1B-C4'	3.42	1.52	1.43
21	A	362	CLA	C1D-C2D	3.42	1.52	1.45
21	B	518	CLA	MG-NC	3.42	2.14	2.06
21	B	514	CLA	MG-NC	3.42	2.14	2.06
25	J	112	BCR	C29-C30	3.42	1.62	1.54
21	B	526	CLA	O1D-CGD	3.41	1.29	1.21
29	T	226	LMT	O5'-C1'	3.41	1.50	1.41
28	C	493	DGD	O5D-C6D	-3.41	1.37	1.43
21	B	515	CLA	C1D-C2D	3.40	1.52	1.45
25	J	115	BCR	C14-C13	3.40	1.40	1.35
25	Z	116	BCR	C5-C6	3.39	1.40	1.34
29	B	535	LMT	O1B-C1B	3.38	1.51	1.41
26	C	476	LHG	O7-C7	3.38	1.43	1.34
21	B	523	CLA	C1D-C2D	3.38	1.52	1.45
21	B	515	CLA	CHC-C1C	3.38	1.43	1.35
21	A	366	CLA	O1D-CGD	3.38	1.29	1.21
25	B	527	BCR	C5-C6	3.37	1.40	1.34
32	D	357	PL9	C12-C13	-3.37	1.39	1.50
21	C	483	CLA	CMC-C2C	3.37	1.57	1.50
25	Z	116	BCR	C29-C30	3.36	1.61	1.54
21	A	362	CLA	C4B-NB	3.36	1.38	1.35
21	C	481	CLA	CMC-C2C	3.36	1.57	1.50
21	D	354	CLA	MG-ND	-3.34	1.99	2.05
21	B	523	CLA	CHC-C1C	3.34	1.43	1.35
21	B	513	CLA	MG-NC	3.34	2.14	2.06
32	D	357	PL9	C32-C33	-3.33	1.39	1.50
21	B	526	CLA	C1C-C2C	3.32	1.51	1.44
21	C	482	CLA	CMC-C2C	3.32	1.57	1.50
25	A	369	BCR	C29-C30	3.32	1.61	1.54
29	B	535	LMT	O1'-C1'	3.32	1.45	1.40
25	Z	116	BCR	C2-C1	3.32	1.61	1.54
21	C	487	CLA	O1D-CGD	3.32	1.29	1.21
21	B	515	CLA	CMC-C2C	3.31	1.57	1.50
32	D	357	PL9	C37-C38	-3.31	1.39	1.50
21	A	366	CLA	CHC-C1C	3.31	1.43	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	V	164	HEM	O2A-CGA	-3.31	1.19	1.30
21	C	485	CLA	CMC-C2C	3.29	1.57	1.50
30	D	361	SQD	O48-C23	3.29	1.42	1.33
29	O	274	LMT	O5'-C1'	3.29	1.50	1.41
25	B	527	BCR	C2-C1	3.29	1.61	1.54
28	D	362	DGD	O1G-C1G	3.27	1.52	1.45
21	C	482	CLA	CAC-C3C	3.27	1.59	1.51
32	D	357	PL9	C27-C28	-3.27	1.39	1.50
21	B	512	CLA	C1D-C2D	3.26	1.51	1.45
21	A	362	CLA	CHC-C1C	3.26	1.43	1.35
21	B	519	CLA	CMC-C2C	3.26	1.57	1.50
21	D	356	CLA	CMC-C2C	3.26	1.57	1.50
21	C	486	CLA	CHD-C4C	3.26	1.46	1.39
21	B	511	CLA	CBA-CGA	3.26	1.60	1.50
28	D	362	DGD	O6E-C1E	3.25	1.50	1.41
21	A	363	CLA	CMC-C2C	3.25	1.57	1.50
21	B	515	CLA	MG-NC	3.25	2.14	2.06
21	B	525	CLA	C5-C3	3.25	1.58	1.51
32	D	357	PL9	C2-C1	3.24	1.53	1.44
25	B	527	BCR	C29-C30	3.24	1.61	1.54
21	C	477	CLA	MG-NC	3.24	2.14	2.06
30	F	224	SQD	C1-C2	3.24	1.61	1.52
21	C	483	CLA	CHC-C1C	3.23	1.43	1.35
21	C	477	CLA	C1D-C2D	3.23	1.51	1.45
21	C	478	CLA	CMC-C2C	3.22	1.57	1.50
25	C	489	BCR	C29-C30	3.21	1.61	1.54
29	O	274	LMT	O1B-C1B	3.21	1.50	1.41
30	L	213	SQD	O5-C1	3.21	1.50	1.41
21	A	362	CLA	O1D-CGD	3.21	1.29	1.21
21	B	520	CLA	CMC-C2C	3.21	1.57	1.50
28	C	493	DGD	O5D-C1E	3.21	1.45	1.40
30	F	224	SQD	C8-C7	3.21	1.60	1.50
21	B	515	CLA	C5-C3	3.20	1.57	1.51
21	B	519	CLA	MG-NC	3.20	2.13	2.06
29	A	376	LMT	O1B-C4'	3.20	1.52	1.43
28	D	362	DGD	C1G-C2G	3.19	1.60	1.50
33	F	85	HEM	O2A-CGA	-3.18	1.20	1.30
21	A	364	CLA	MG-NA	3.18	2.13	2.06
30	L	213	SQD	O8-S	3.18	1.58	1.47
25	D	358	BCR	C2-C1	3.18	1.61	1.54
25	X	107	BCR	C2-C1	3.18	1.61	1.54
30	F	224	SQD	O3-C3	3.18	1.50	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	517	CLA	O1D-CGD	3.17	1.29	1.21
25	C	490	BCR	C29-C30	3.17	1.61	1.54
21	C	485	CLA	CHC-C1C	3.17	1.43	1.35
21	B	512	CLA	O1D-CGD	3.16	1.29	1.21
25	X	107	BCR	C1-C6	3.16	1.58	1.53
25	Z	116	BCR	C38-C26	3.16	1.56	1.50
29	I	274	LMT	C3'-C4'	3.14	1.60	1.52
25	J	115	BCR	C2-C1	3.13	1.61	1.54
25	C	490	BCR	C14-C13	3.13	1.39	1.35
30	F	224	SQD	O5-C1	3.13	1.49	1.41
21	B	516	CLA	CMC-C2C	3.12	1.57	1.50
21	C	477	CLA	C4B-NB	3.11	1.38	1.35
21	D	354	CLA	CHC-C1C	3.11	1.42	1.35
29	T	226	LMT	O1'-C1'	3.10	1.45	1.40
29	A	376	LMT	C4'-C5'	3.10	1.61	1.52
21	B	513	CLA	C1D-C2D	3.10	1.51	1.45
21	B	520	CLA	C1D-C2D	3.10	1.51	1.45
21	B	513	CLA	CHC-C1C	3.09	1.42	1.35
21	B	523	CLA	C4B-NB	3.09	1.38	1.35
21	A	366	CLA	C1D-C2D	3.08	1.51	1.45
21	C	478	CLA	O1D-CGD	3.08	1.29	1.21
21	B	515	CLA	C4C-C3C	3.08	1.50	1.45
21	B	525	CLA	O1D-CGD	3.07	1.28	1.21
21	A	363	CLA	C1D-C2D	3.07	1.51	1.45
21	C	484	CLA	O1D-CGD	3.07	1.28	1.21
21	C	483	CLA	C5-C3	3.07	1.57	1.51
29	I	274	LMT	C4'-C5'	3.07	1.61	1.52
30	D	361	SQD	O3-C3	3.06	1.50	1.43
21	B	513	CLA	O1D-CGD	3.06	1.28	1.21
21	B	524	CLA	CHC-C1C	3.05	1.42	1.35
28	A	375	DGD	O1G-C1G	3.04	1.52	1.45
21	B	519	CLA	C4B-NB	3.04	1.37	1.35
27	C	494	LMG	O6-C1	3.04	1.49	1.41
21	K	483	CLA	C4B-NB	3.04	1.37	1.35
30	D	361	SQD	O6-C1	3.03	1.45	1.40
30	F	224	SQD	O8-S	3.03	1.58	1.47
28	C	493	DGD	C5B-C4B	-3.03	1.34	1.51
21	D	356	CLA	MG-NA	3.03	2.13	2.06
21	K	483	CLA	CMC-C2C	3.03	1.57	1.50
21	A	363	CLA	CBA-CGA	3.03	1.59	1.50
21	B	514	CLA	MG-ND	-3.03	1.99	2.05
30	F	224	SQD	C24-C23	3.02	1.59	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	F	85	HEM	CAA-C2A	3.01	1.56	1.52
21	C	479	CLA	O1D-CGD	3.01	1.28	1.21
21	A	362	CLA	O2A-CGA	3.01	1.42	1.33
21	C	477	CLA	O1D-CGD	3.01	1.28	1.21
21	B	518	CLA	O1D-CGD	3.01	1.28	1.21
21	C	478	CLA	C4B-NB	3.00	1.37	1.35
21	C	481	CLA	O1D-CGD	3.00	1.28	1.21
28	B	533	DGD	O2G-C1B	3.00	1.42	1.34
25	B	530	BCR	C14-C13	3.00	1.39	1.35
21	C	487	CLA	CBA-CGA	2.99	1.59	1.50
21	A	363	CLA	O1D-CGD	2.99	1.28	1.21
21	C	479	CLA	CMC-C2C	2.99	1.57	1.50
21	B	524	CLA	C4B-NB	2.99	1.37	1.35
21	B	516	CLA	C1D-C2D	2.98	1.51	1.45
21	C	486	CLA	CHD-C1D	2.97	1.44	1.38
28	D	362	DGD	O1G-C1A	2.97	1.42	1.33
28	C	474	DGD	C4E-C3E	2.97	1.59	1.52
21	A	366	CLA	CMC-C2C	2.96	1.57	1.50
21	D	356	CLA	CHC-C1C	2.96	1.42	1.35
21	C	477	CLA	CMC-C2C	2.96	1.57	1.50
21	A	363	CLA	CHC-C1C	2.96	1.42	1.35
29	O	274	LMT	O1'-C1'	2.95	1.45	1.40
21	C	481	CLA	CAA-C2A	-2.95	1.48	1.54
21	B	514	CLA	CBA-CGA	2.95	1.59	1.50
21	D	354	CLA	CMC-C2C	2.94	1.57	1.50
21	C	482	CLA	MG-NA	2.94	2.13	2.06
21	A	364	CLA	CMC-C2C	2.94	1.57	1.50
28	C	491	DGD	O2E-C2E	-2.93	1.36	1.43
21	B	513	CLA	CMC-C2C	2.93	1.57	1.50
21	B	516	CLA	O1D-CGD	2.93	1.28	1.21
21	C	478	CLA	MG-NC	2.93	2.13	2.06
21	B	522	CLA	MG-NC	2.92	2.13	2.06
29	A	376	LMT	O5'-C1'	2.92	1.49	1.41
21	B	520	CLA	O1D-CGD	2.92	1.28	1.21
21	B	526	CLA	CHC-C1C	2.92	1.42	1.35
21	C	479	CLA	MG-NA	2.91	2.13	2.06
21	C	480	CLA	CHC-C1C	2.90	1.42	1.35
21	B	524	CLA	O1D-CGD	2.90	1.28	1.21
21	B	523	CLA	MG-ND	-2.90	2.00	2.05
21	D	354	CLA	C1D-ND	-2.90	1.34	1.37
21	B	517	CLA	CMC-C2C	2.90	1.56	1.50
33	F	85	HEM	FE-NB	2.90	2.11	1.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	O	274	LMT	C4'-C5'	2.90	1.60	1.52
21	B	512	CLA	MG-NC	2.89	2.13	2.06
21	C	483	CLA	O1D-CGD	2.88	1.28	1.21
21	B	523	CLA	O1D-CGD	2.87	1.28	1.21
32	D	357	PL9	C33-C34	2.86	1.39	1.33
30	C	475	SQD	C20-C19	-2.86	1.35	1.51
27	I	220	LMG	O6-C1	2.86	1.49	1.41
21	C	480	CLA	MG-NC	2.84	2.13	2.06
21	A	364	CLA	O1D-CGD	2.83	1.28	1.21
21	B	525	CLA	C1D-C2D	2.83	1.50	1.45
28	C	491	DGD	C5B-C4B	-2.83	1.35	1.51
21	C	487	CLA	C1D-C2D	2.83	1.50	1.45
21	A	363	CLA	CAA-C2A	2.83	1.59	1.54
29	T	226	LMT	C1B-C2B	2.82	1.60	1.52
21	B	515	CLA	C4B-NB	2.81	1.37	1.35
21	C	482	CLA	CHC-C1C	2.81	1.42	1.35
25	C	489	BCR	C5-C6	2.81	1.39	1.34
21	A	363	CLA	C1D-ND	-2.81	1.34	1.37
21	B	522	CLA	CAC-C3C	2.81	1.58	1.51
21	B	514	CLA	C4B-NB	2.81	1.37	1.35
21	B	516	CLA	MG-ND	-2.80	2.00	2.05
33	V	164	HEM	C1D-C2D	2.79	1.50	1.44
21	B	521	CLA	C4B-NB	2.79	1.37	1.35
29	D	363	LMT	O5B-C1B	2.79	1.48	1.41
21	K	483	CLA	C1D-C2D	2.78	1.50	1.45
25	B	529	BCR	C14-C13	2.78	1.39	1.35
21	A	364	CLA	MG-NC	2.77	2.12	2.06
27	M	217	LMG	O7-C8	2.77	1.53	1.46
29	D	363	LMT	C4'-C5'	2.77	1.60	1.52
30	C	475	SQD	C19-C18	-2.77	1.36	1.51
30	C	475	SQD	C33-C32	-2.77	1.36	1.51
27	C	494	LMG	O7-C8	2.76	1.53	1.46
21	B	519	CLA	O1D-CGD	2.76	1.28	1.21
21	B	524	CLA	CMC-C2C	2.76	1.56	1.50
33	V	164	HEM	C3B-C4B	2.76	1.50	1.44
21	B	514	CLA	CMC-C2C	2.75	1.56	1.50
28	C	493	DGD	C3G-C2G	2.75	1.59	1.50
32	D	357	PL9	C8-C9	2.75	1.39	1.33
21	B	512	CLA	C4B-NB	2.75	1.37	1.35
30	C	475	SQD	C8-C7	2.75	1.58	1.50
25	D	358	BCR	C5-C6	2.75	1.39	1.34
29	B	535	LMT	O1B-C4'	2.75	1.51	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	M	217	LMG	O6-C1	2.75	1.48	1.41
27	J	492	LMG	O6-C1	2.74	1.48	1.41
21	C	479	CLA	C5-C3	2.74	1.57	1.51
21	C	479	CLA	CHC-C1C	2.74	1.42	1.35
30	C	475	SQD	O8-S	2.74	1.57	1.47
21	B	522	CLA	CHC-C1C	2.73	1.42	1.35
25	C	489	BCR	C26-C25	2.73	1.39	1.34
27	M	217	LMG	O7-C10	2.72	1.42	1.34
21	A	362	CLA	MG-NC	2.71	2.12	2.06
32	D	357	PL9	C18-C19	2.71	1.39	1.33
29	A	376	LMT	O1'-C1'	2.71	1.44	1.40
30	C	475	SQD	O5-C1	2.71	1.48	1.41
28	C	492	DGD	O2G-C1B	2.71	1.41	1.34
25	J	112	BCR	C26-C25	2.71	1.39	1.34
30	F	224	SQD	O6-C1	2.70	1.44	1.40
32	D	357	PL9	C38-C39	2.70	1.39	1.33
32	D	357	PL9	C43-C44	2.70	1.39	1.33
27	I	220	LMG	C4-C5	2.70	1.58	1.53
21	B	513	CLA	CBA-CGA	2.69	1.58	1.50
28	D	362	DGD	C3D-C2D	2.69	1.59	1.52
21	B	522	CLA	CMC-C2C	2.69	1.56	1.50
21	D	356	CLA	CBA-CGA	2.69	1.58	1.50
28	B	533	DGD	C4E-C3E	2.68	1.59	1.52
30	F	224	SQD	C14-C13	-2.68	1.36	1.51
30	D	361	SQD	C15-C14	-2.68	1.36	1.51
25	C	489	BCR	C19-C18	-2.68	1.40	1.45
29	T	226	LMT	O5B-C1B	2.67	1.48	1.41
21	C	480	CLA	O1D-CGD	2.67	1.27	1.21
21	D	356	CLA	O1D-CGD	2.67	1.27	1.21
21	B	524	CLA	MG-NA	2.67	2.12	2.06
30	L	213	SQD	C12-C11	-2.67	1.36	1.51
30	C	475	SQD	C17-C16	-2.67	1.36	1.51
21	B	518	CLA	CBA-CGA	2.67	1.58	1.50
30	D	361	SQD	C14-C13	-2.66	1.36	1.51
21	B	525	CLA	CHC-C1C	2.66	1.41	1.35
30	F	224	SQD	C13-C12	-2.66	1.36	1.51
21	A	364	CLA	CBA-CGA	2.65	1.58	1.50
30	C	475	SQD	C12-C11	-2.65	1.36	1.51
25	X	107	BCR	C5-C6	2.65	1.39	1.34
22	D	355	PHO	CMC-C2C	2.65	1.57	1.51
27	J	492	LMG	O7-C10	2.65	1.41	1.34
28	A	375	DGD	C2A-C1A	2.65	1.58	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	C	492	DGD	O5D-C6D	-2.65	1.38	1.43
27	I	220	LMG	O8-C28	2.65	1.41	1.33
30	D	361	SQD	C16-C15	-2.64	1.36	1.51
25	J	112	BCR	C14-C13	2.64	1.39	1.35
33	F	85	HEM	C4D-C3D	2.64	1.49	1.45
33	V	164	HEM	C1B-C2B	-2.64	1.39	1.44
30	D	361	SQD	C12-C11	-2.64	1.36	1.51
30	D	361	SQD	C13-C12	-2.63	1.36	1.51
29	I	274	LMT	O1'-C1'	2.63	1.44	1.40
21	B	524	CLA	CBA-CGA	2.63	1.58	1.50
28	D	362	DGD	C1E-C2E	2.63	1.60	1.52
30	F	224	SQD	C17-C16	-2.62	1.36	1.51
30	L	213	SQD	O3-C3	2.62	1.49	1.43
30	L	213	SQD	C16-C15	-2.62	1.36	1.51
21	B	526	CLA	C5-C3	2.62	1.56	1.51
28	C	491	DGD	O6D-C5D	2.62	1.50	1.44
21	C	484	CLA	CAC-C3C	2.61	1.57	1.51
30	F	224	SQD	C12-C11	-2.61	1.36	1.51
30	L	213	SQD	C17-C16	-2.60	1.37	1.51
21	B	513	CLA	C1B-NB	2.60	1.37	1.35
29	D	536	LMT	O5'-C1'	2.60	1.48	1.41
21	D	354	CLA	O1D-CGD	2.60	1.27	1.21
21	C	487	CLA	CAC-C3C	2.60	1.57	1.51
28	C	492	DGD	O5D-C1E	2.60	1.44	1.40
33	F	85	HEM	C1B-C2B	-2.60	1.39	1.44
21	B	522	CLA	O1D-CGD	2.60	1.27	1.21
21	C	488	CLA	CAC-C3C	2.60	1.57	1.51
21	C	485	CLA	O1D-CGD	2.60	1.27	1.21
21	B	517	CLA	C6-C7	2.59	1.63	1.52
33	V	164	HEM	CMC-C2C	2.59	1.57	1.51
22	A	365	PHO	O1D-CGD	2.59	1.27	1.21
30	F	224	SQD	C15-C14	-2.59	1.37	1.51
30	C	475	SQD	C11-C10	-2.59	1.37	1.51
25	B	529	BCR	C10-C9	2.58	1.39	1.35
25	B	530	BCR	C38-C26	2.58	1.55	1.50
30	D	361	SQD	C11-C10	-2.58	1.37	1.51
21	C	482	CLA	CAA-C2A	2.58	1.58	1.54
29	A	376	LMT	C1B-C2B	2.58	1.59	1.52
27	C	494	LMG	O1-C7	2.58	1.48	1.43
21	D	356	CLA	C5-C3	2.57	1.56	1.51
28	D	362	DGD	O2G-C2G	2.57	1.53	1.46
21	B	517	CLA	CHD-C1D	2.57	1.43	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	C	475	SQD	C32-C31	-2.57	1.37	1.51
21	B	518	CLA	O2A-C1	2.57	1.53	1.46
28	D	362	DGD	O6D-C5D	2.56	1.50	1.44
21	C	488	CLA	CHD-C4C	2.55	1.45	1.39
28	D	362	DGD	C3G-C2G	2.55	1.58	1.50
21	A	364	CLA	MG-ND	-2.55	2.00	2.05
30	C	475	SQD	C18-C17	-2.55	1.37	1.51
27	D	359	LMG	C16-C15	-2.54	1.37	1.51
25	C	489	BCR	C10-C9	2.54	1.39	1.35
30	L	213	SQD	C11-C10	-2.54	1.37	1.51
28	A	375	DGD	C5B-C4B	-2.54	1.37	1.51
21	B	515	CLA	CBA-CGA	2.53	1.58	1.50
21	B	524	CLA	MG-NC	2.53	2.12	2.06
30	L	213	SQD	C8-C7	2.53	1.58	1.50
28	C	474	DGD	C3E-C2E	2.53	1.58	1.52
30	D	361	SQD	C8-C7	2.52	1.58	1.50
28	C	493	DGD	O3G-C1D	2.52	1.44	1.40
21	C	483	CLA	CAC-C3C	2.51	1.57	1.51
21	B	517	CLA	O2A-C1	2.51	1.53	1.46
21	C	486	CLA	CBA-CGA	2.51	1.58	1.50
21	B	512	CLA	CHC-C1C	2.51	1.41	1.35
30	C	475	SQD	C16-C15	-2.51	1.37	1.51
21	C	480	CLA	C5-C3	2.51	1.56	1.51
25	B	529	BCR	C38-C26	2.50	1.55	1.50
21	B	523	CLA	CMC-C2C	2.50	1.56	1.50
21	C	488	CLA	CMC-C2C	2.50	1.56	1.50
32	D	357	PL9	C48-C49	2.50	1.39	1.32
25	D	358	BCR	C19-C18	-2.50	1.40	1.45
25	C	490	BCR	C26-C25	2.50	1.38	1.34
21	B	525	CLA	CMC-C2C	2.49	1.56	1.50
21	D	354	CLA	C1D-C2D	2.49	1.50	1.45
21	B	513	CLA	C1D-ND	-2.49	1.34	1.37
29	O	274	LMT	O5B-C5B	2.49	1.50	1.44
33	V	164	HEM	C4D-C3D	2.47	1.49	1.45
21	B	518	CLA	C5-C3	2.47	1.56	1.51
30	F	224	SQD	C16-C15	-2.47	1.37	1.51
21	A	366	CLA	MG-ND	-2.47	2.00	2.05
21	B	518	CLA	CHC-C1C	2.47	1.41	1.35
21	B	518	CLA	CMC-C2C	2.46	1.56	1.50
21	A	364	CLA	C1D-ND	-2.45	1.34	1.37
28	C	474	DGD	C5B-C4B	-2.45	1.37	1.51
21	C	487	CLA	C2A-C1A	2.45	1.57	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	C	482	CLA	CMD-C2D	2.45	1.56	1.50
21	B	514	CLA	O1D-CGD	2.45	1.27	1.21
28	C	491	DGD	C3G-C2G	2.45	1.58	1.50
29	D	363	LMT	O5'-C5'	2.44	1.50	1.44
21	A	362	CLA	CMC-C2C	2.44	1.56	1.50
30	L	213	SQD	C13-C12	-2.44	1.37	1.51
29	I	274	LMT	C1B-C2B	2.44	1.59	1.52
27	I	220	LMG	O6-C5	2.44	1.50	1.44
29	I	274	LMT	C3B-C2B	2.44	1.58	1.52
21	B	516	CLA	O2A-C1	2.44	1.53	1.46
21	C	487	CLA	CHC-C1C	2.43	1.41	1.35
30	L	213	SQD	C15-C14	-2.43	1.37	1.51
26	C	476	LHG	C4-C5	2.43	1.58	1.50
21	B	512	CLA	MG-NA	2.42	2.12	2.06
33	F	85	HEM	C1D-C2D	2.42	1.49	1.44
21	B	522	CLA	C1D-C2D	2.42	1.50	1.45
30	L	213	SQD	C20-C19	-2.42	1.38	1.51
28	C	493	DGD	O2E-C2E	-2.42	1.37	1.43
27	D	359	LMG	O6-C1	2.41	1.48	1.41
29	D	536	LMT	C4'-C5'	2.41	1.59	1.52
21	B	519	CLA	CMD-C2D	2.41	1.55	1.50
28	B	533	DGD	C2B-C1B	2.40	1.57	1.50
21	B	511	CLA	CAA-C2A	2.40	1.58	1.54
30	C	475	SQD	C13-C12	-2.40	1.38	1.51
21	B	522	CLA	C1D-ND	-2.40	1.34	1.37
30	L	213	SQD	C14-C13	-2.40	1.38	1.51
21	B	511	CLA	CHD-C1D	2.39	1.43	1.38
27	C	494	LMG	C16-C15	-2.39	1.38	1.51
21	C	479	CLA	CMD-C2D	2.39	1.55	1.50
30	C	475	SQD	C15-C14	-2.39	1.38	1.51
21	B	525	CLA	CBA-CGA	2.38	1.57	1.50
21	C	486	CLA	CMC-C2C	2.38	1.55	1.50
32	D	357	PL9	C23-C24	2.38	1.38	1.33
32	D	357	PL9	C5-C4	2.37	1.55	1.47
21	C	477	CLA	CHC-C1C	2.37	1.41	1.35
28	C	493	DGD	C4E-C3E	2.36	1.58	1.52
27	B	531	LMG	O6-C1	2.36	1.47	1.41
21	D	356	CLA	C1D-ND	-2.36	1.34	1.37
21	B	522	CLA	MG-ND	-2.36	2.01	2.05
29	I	274	LMT	O5'-C1'	2.35	1.47	1.41
29	D	536	LMT	C4B-C5B	2.35	1.58	1.53
30	L	213	SQD	C44-C45	2.35	1.57	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	D	357	PL9	C10-C9	2.34	1.56	1.50
29	O	274	LMT	O5'-C5'	2.34	1.50	1.44
25	Z	116	BCR	C23-C22	-2.33	1.40	1.45
21	B	517	CLA	CHD-C4C	2.33	1.44	1.39
21	B	511	CLA	CAC-C3C	2.32	1.57	1.51
30	L	213	SQD	C19-C18	-2.32	1.38	1.51
21	D	354	CLA	CHD-C1D	2.32	1.42	1.38
25	J	115	BCR	C10-C9	2.32	1.38	1.35
30	D	361	SQD	O5-C1	2.32	1.47	1.41
21	B	524	CLA	CAC-C3C	2.32	1.57	1.51
21	A	364	CLA	C3D-C2D	-2.32	1.32	1.39
21	C	486	CLA	MG-NC	2.32	2.11	2.06
27	I	220	LMG	C16-C15	-2.32	1.38	1.51
28	C	493	DGD	C4D-C3D	-2.32	1.46	1.52
21	B	521	CLA	CBA-CGA	2.31	1.57	1.50
21	B	511	CLA	C5-C3	2.31	1.56	1.51
25	B	530	BCR	C7-C6	2.31	1.53	1.45
21	B	518	CLA	C4B-NB	2.30	1.37	1.35
30	C	475	SQD	C14-C13	-2.30	1.38	1.51
27	B	531	LMG	C16-C15	-2.30	1.38	1.51
25	B	527	BCR	C38-C26	2.30	1.54	1.50
21	A	364	CLA	CHC-C1C	2.30	1.40	1.35
21	A	362	CLA	CHD-C4C	2.29	1.44	1.39
25	J	115	BCR	C17-C18	2.28	1.38	1.35
21	A	363	CLA	C4B-NB	2.28	1.37	1.35
32	D	357	PL9	C36-C37	-2.28	1.46	1.53
22	D	355	PHO	C1A-C2A	2.28	1.54	1.51
21	B	519	CLA	MG-ND	-2.27	2.01	2.05
21	B	511	CLA	MG-ND	-2.27	2.01	2.05
21	C	478	CLA	CHC-C1C	2.26	1.40	1.35
33	F	85	HEM	CMC-C2C	2.26	1.57	1.51
27	M	217	LMG	C16-C15	-2.25	1.38	1.51
21	B	516	CLA	CHC-C1C	2.25	1.40	1.35
25	C	490	BCR	C10-C9	2.25	1.38	1.35
21	C	484	CLA	OBD-CAD	2.25	1.26	1.22
25	B	530	BCR	C10-C9	2.25	1.38	1.35
21	A	363	CLA	C4C-C3C	2.25	1.48	1.45
29	T	226	LMT	C4B-C5B	2.25	1.57	1.53
28	C	474	DGD	C2A-C1A	2.25	1.57	1.50
21	B	521	CLA	CMD-C2D	2.24	1.55	1.50
33	F	85	HEM	CHA-C4D	2.24	1.40	1.35
21	C	478	CLA	CAC-C3C	2.24	1.56	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	C	486	CLA	C5-C3	2.23	1.55	1.51
21	B	524	CLA	CMD-C2D	2.23	1.55	1.50
27	J	492	LMG	C4-C5	2.23	1.57	1.53
33	V	164	HEM	CAB-C3B	-2.23	1.41	1.47
30	F	224	SQD	C11-C10	-2.23	1.39	1.51
21	C	481	CLA	CHD-C4C	2.23	1.44	1.39
21	B	511	CLA	CBD-CHA	2.22	1.62	1.52
21	C	478	CLA	C5-C3	2.22	1.55	1.51
29	I	274	LMT	O5'-C5'	2.22	1.49	1.44
28	B	528	DGD	O5D-C1E	2.22	1.44	1.40
21	C	483	CLA	MG-ND	-2.21	2.01	2.05
21	A	366	CLA	MG-NA	2.21	2.11	2.06
21	C	488	CLA	CMD-C2D	2.21	1.55	1.50
21	B	520	CLA	CAC-C3C	2.21	1.56	1.51
27	I	220	LMG	O8-C9	2.21	1.50	1.45
29	B	535	LMT	C1B-C2B	2.20	1.58	1.52
21	B	515	CLA	O1D-CGD	2.20	1.26	1.21
27	J	492	LMG	C11-C10	2.20	1.57	1.50
27	D	360	LMG	O1-C1	2.20	1.43	1.40
22	A	365	PHO	CMC-C2C	2.20	1.56	1.51
28	C	474	DGD	C4A-C3A	-2.20	1.39	1.51
21	K	483	CLA	MG-ND	-2.20	2.01	2.05
22	D	355	PHO	O1D-CGD	2.20	1.26	1.21
28	C	492	DGD	C9A-C8A	-2.20	1.39	1.51
28	C	492	DGD	C4A-C3A	-2.20	1.39	1.51
28	B	528	DGD	O3G-C1D	2.20	1.43	1.40
27	I	220	LMG	C7-C8	2.19	1.57	1.50
30	L	213	SQD	C24-C23	2.19	1.57	1.50
28	B	533	DGD	C4A-C3A	-2.19	1.39	1.51
25	J	115	BCR	C24-C23	2.19	1.39	1.33
21	B	520	CLA	MG-ND	-2.19	2.01	2.05
21	A	362	CLA	C1D-ND	-2.18	1.35	1.37
21	C	479	CLA	CBA-CGA	2.18	1.57	1.50
21	B	521	CLA	CMC-C2C	2.18	1.55	1.50
27	B	531	LMG	C39-C38	-2.18	1.39	1.51
29	B	535	LMT	C10-C9	-2.18	1.39	1.51
27	I	220	LMG	O1-C7	2.18	1.47	1.43
27	C	494	LMG	C34-C33	-2.18	1.39	1.51
28	C	493	DGD	C4A-C3A	-2.18	1.39	1.51
27	A	373	LMG	O1-C1	2.18	1.43	1.40
21	B	520	CLA	C4B-NB	2.18	1.37	1.35
28	B	533	DGD	CEB-CDB	-2.18	1.39	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	C	493	DGD	O6E-C5E	-2.17	1.39	1.44
29	D	536	LMT	C10-C9	-2.17	1.39	1.51
28	C	493	DGD	CFB-CEB	-2.17	1.39	1.51
21	C	483	CLA	CBA-CGA	2.17	1.57	1.50
27	D	359	LMG	C34-C33	-2.17	1.39	1.51
28	C	493	DGD	CEB-CDB	-2.17	1.39	1.51
25	B	530	BCR	C24-C23	2.17	1.39	1.33
28	C	492	DGD	CFB-CEB	-2.17	1.39	1.51
29	T	226	LMT	C10-C9	-2.17	1.39	1.51
30	D	361	SQD	C6-S	2.17	1.85	1.77
29	I	274	LMT	C10-C9	-2.16	1.39	1.51
27	C	494	LMG	C7-C8	2.16	1.57	1.50
29	D	536	LMT	C5-C4	-2.16	1.39	1.51
28	C	493	DGD	C9A-C8A	-2.16	1.39	1.51
27	I	220	LMG	C34-C33	-2.16	1.39	1.51
28	C	491	DGD	C4A-C3A	-2.16	1.39	1.51
25	J	115	BCR	C21-C22	2.15	1.38	1.35
21	K	483	CLA	CHC-C1C	2.15	1.40	1.35
21	B	523	CLA	C5-C3	2.15	1.55	1.51
28	C	493	DGD	C9B-C8B	-2.15	1.39	1.51
29	O	274	LMT	C10-C9	-2.15	1.39	1.51
28	C	493	DGD	CDA-CCA	-2.15	1.39	1.51
29	B	535	LMT	C5-C4	-2.15	1.39	1.51
27	D	359	LMG	C39-C38	-2.15	1.39	1.51
28	B	533	DGD	C5B-C4B	-2.15	1.39	1.51
28	B	533	DGD	CDA-CCA	-2.15	1.39	1.51
27	B	531	LMG	C20-C19	-2.15	1.39	1.51
30	L	213	SQD	C18-C17	-2.15	1.39	1.51
27	J	492	LMG	C34-C33	-2.15	1.39	1.51
28	B	533	DGD	C9A-C8A	-2.15	1.39	1.51
21	C	477	CLA	CBA-CGA	2.15	1.57	1.50
29	O	274	LMT	C5-C4	-2.15	1.39	1.51
27	B	531	LMG	C34-C33	-2.14	1.39	1.51
28	B	533	DGD	CFB-CEB	-2.14	1.39	1.51
30	C	475	SQD	C21-C20	-2.14	1.36	1.51
21	B	511	CLA	CHD-C4C	2.14	1.44	1.39
28	D	362	DGD	CEB-CDB	-2.14	1.39	1.51
21	B	520	CLA	C1D-ND	-2.14	1.35	1.37
28	A	375	DGD	C4A-C3A	-2.14	1.39	1.51
28	C	492	DGD	CEB-CDB	-2.14	1.39	1.51
29	T	226	LMT	O5B-C5B	2.14	1.49	1.44
30	F	224	SQD	C44-C45	2.14	1.57	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	D	362	DGD	CFB-CEB	-2.14	1.39	1.51
29	A	376	LMT	C10-C9	-2.14	1.39	1.51
29	A	376	LMT	C5-C4	-2.14	1.39	1.51
30	L	213	SQD	C6-S	2.14	1.85	1.77
28	D	362	DGD	CDA-CCA	-2.14	1.39	1.51
27	M	217	LMG	C34-C33	-2.14	1.39	1.51
21	C	482	CLA	CHD-C4C	2.14	1.44	1.39
27	J	492	LMG	C39-C38	-2.13	1.39	1.51
28	C	474	DGD	C9B-C8B	-2.13	1.39	1.51
29	I	274	LMT	C5-C4	-2.13	1.39	1.51
27	C	494	LMG	C20-C19	-2.13	1.39	1.51
28	C	491	DGD	C9A-C8A	-2.13	1.39	1.51
28	C	474	DGD	C9A-C8A	-2.13	1.39	1.51
27	D	359	LMG	C20-C19	-2.13	1.39	1.51
21	C	485	CLA	MG-ND	-2.13	2.01	2.05
29	T	226	LMT	C5-C4	-2.13	1.39	1.51
28	A	375	DGD	C9B-C8B	-2.13	1.39	1.51
28	C	492	DGD	C9B-C8B	-2.13	1.39	1.51
28	B	533	DGD	C9B-C8B	-2.12	1.39	1.51
21	B	518	CLA	C1D-ND	-2.12	1.35	1.37
21	A	363	CLA	MG-NC	2.12	2.11	2.06
21	B	526	CLA	C4D-ND	2.12	1.40	1.37
29	D	536	LMT	C1B-C2B	2.12	1.58	1.52
27	I	220	LMG	C20-C19	-2.12	1.39	1.51
28	D	362	DGD	C9A-C8A	-2.12	1.39	1.51
30	D	361	SQD	C17-C16	-2.12	1.36	1.51
27	J	492	LMG	C20-C19	-2.11	1.39	1.51
27	M	217	LMG	C20-C19	-2.11	1.39	1.51
29	D	363	LMT	C5-C4	-2.11	1.39	1.51
29	D	536	LMT	C3'-C4'	2.11	1.58	1.52
28	D	362	DGD	C5B-C4B	-2.10	1.39	1.51
28	D	362	DGD	C4A-C3A	-2.10	1.39	1.51
27	M	217	LMG	C11-C10	2.10	1.56	1.50
28	D	362	DGD	C9B-C8B	-2.10	1.39	1.51
28	A	375	DGD	C1G-C2G	2.10	1.57	1.50
21	B	511	CLA	C1B-CHB	2.09	1.46	1.41
21	B	526	CLA	CMC-C2C	2.09	1.55	1.50
21	B	512	CLA	CMC-C2C	2.09	1.55	1.50
21	K	483	CLA	O1D-CGD	2.09	1.26	1.21
30	C	475	SQD	C34-C33	-2.08	1.36	1.51
21	B	512	CLA	MG-ND	-2.08	2.01	2.05
21	B	526	CLA	CHD-C4C	2.08	1.44	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	O	274	LMT	C1B-C2B	2.07	1.58	1.52
21	C	481	CLA	CHD-C1D	2.07	1.42	1.38
21	B	511	CLA	C4D-ND	2.07	1.40	1.37
25	J	112	BCR	C19-C18	-2.07	1.41	1.45
25	C	489	BCR	C20-C21	-2.07	1.37	1.43
29	D	536	LMT	O1B-C1B	2.06	1.47	1.41
32	D	357	PL9	C11-C9	2.06	1.55	1.51
21	C	480	CLA	OBD-CAD	2.06	1.26	1.22
33	F	85	HEM	C2A-C3A	2.06	1.43	1.37
28	C	492	DGD	C5B-C4B	-2.06	1.40	1.51
25	X	107	BCR	C14-C13	2.05	1.38	1.35
30	C	475	SQD	C24-C23	2.05	1.56	1.50
28	D	362	DGD	C2B-C1B	2.05	1.56	1.50
27	I	220	LMG	C1-C2	2.05	1.58	1.52
29	I	274	LMT	O5B-C5B	2.03	1.49	1.44
21	C	486	CLA	OBD-CAD	2.03	1.26	1.22
21	C	484	CLA	CMD-C2D	2.03	1.55	1.50
32	D	357	PL9	C7-C3	2.03	1.53	1.51
30	F	224	SQD	C18-C17	-2.03	1.37	1.51
29	A	376	LMT	O5B-C5B	2.02	1.49	1.44
29	B	535	LMT	C3B-C2B	2.02	1.57	1.52
21	C	481	CLA	CBD-CHA	2.01	1.61	1.52
21	A	366	CLA	C5-C3	2.00	1.55	1.51
21	C	480	CLA	CBA-CGA	2.00	1.56	1.50
21	C	485	CLA	CMD-C2D	2.00	1.55	1.50

All (1168) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	C	474	DGD	O1G-C1G-C2G	12.38	144.47	108.43
28	C	493	DGD	O5D-C6D-C5D	10.84	129.11	109.05
25	J	115	BCR	C32-C1-C6	-10.58	93.14	110.30
28	C	492	DGD	O5D-C1E-C2E	10.56	124.80	108.30
28	C	491	DGD	O5D-C1E-C2E	10.32	124.41	108.30
21	B	518	CLA	C4A-NA-C1A	10.31	111.34	106.71
28	C	474	DGD	O5D-C6D-C5D	10.09	127.71	109.05
28	D	362	DGD	O5D-C1E-C2E	9.83	123.66	108.30
21	C	487	CLA	C4A-NA-C1A	9.75	111.09	106.71
28	C	493	DGD	O5D-C1E-C2E	9.73	123.49	108.30
21	B	525	CLA	C4A-NA-C1A	9.65	111.05	106.71
33	F	85	HEM	CMA-C3A-C2A	-9.47	107.09	124.94
27	D	359	LMG	C8-O7-C10	9.42	140.99	117.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	J	115	BCR	C32-C1-C31	-9.35	79.83	108.53
21	C	477	CLA	C4A-NA-C1A	9.30	110.89	106.71
21	B	516	CLA	C4A-NA-C1A	9.25	110.86	106.71
21	D	356	CLA	C4A-NA-C1A	9.23	110.86	106.71
27	C	494	LMG	C8-O7-C10	9.20	140.44	117.79
30	L	213	SQD	O5-C1-O6	9.20	131.75	109.97
21	A	366	CLA	C4A-NA-C1A	9.14	110.82	106.71
32	D	357	PL9	C7-C8-C9	-9.06	111.71	126.79
28	C	474	DGD	O5D-C1E-C2E	9.04	122.41	108.30
21	C	479	CLA	C4A-NA-C1A	8.98	110.74	106.71
21	C	488	CLA	C4A-NA-C1A	8.89	110.70	106.71
21	C	482	CLA	C4A-NA-C1A	8.89	110.70	106.71
30	F	224	SQD	O5-C1-O6	8.87	130.97	109.97
30	D	361	SQD	O7-S-C6	8.82	117.42	106.94
21	B	526	CLA	C4A-NA-C1A	8.74	110.64	106.71
27	B	531	LMG	C8-O7-C10	8.70	139.20	117.79
28	A	375	DGD	C2G-O2G-C1B	8.68	139.15	117.79
21	C	485	CLA	C4A-NA-C1A	8.66	110.60	106.71
21	B	511	CLA	C4A-NA-C1A	8.62	110.58	106.71
21	B	513	CLA	C4A-NA-C1A	8.61	110.58	106.71
33	F	85	HEM	CMA-C3A-C4A	8.56	141.62	128.46
28	C	474	DGD	O6D-C5D-C6D	8.56	123.95	106.67
33	V	164	HEM	CMA-C3A-C2A	-8.54	108.84	124.94
32	D	357	PL9	C7-C3-C4	8.52	123.80	116.88
28	C	491	DGD	C2G-O2G-C1B	8.46	138.62	117.79
21	C	483	CLA	C4A-NA-C1A	8.45	110.50	106.71
21	K	483	CLA	C4A-NA-C1A	8.41	110.49	106.71
28	C	493	DGD	O6D-C5D-C6D	8.41	123.63	106.67
33	V	164	HEM	C4A-C3A-C2A	-8.39	101.16	107.00
30	C	475	SQD	O7-S-C6	8.32	116.83	106.94
21	A	364	CLA	C4A-NA-C1A	8.29	110.44	106.71
30	D	361	SQD	O5-C1-O6	8.26	129.54	109.97
21	A	362	CLA	C4A-NA-C1A	8.25	110.42	106.71
30	C	475	SQD	O5-C1-O6	8.21	129.41	109.97
21	C	480	CLA	C4A-NA-C1A	8.21	110.39	106.71
30	L	213	SQD	O7-S-C6	8.17	116.64	106.94
21	C	484	CLA	C4A-NA-C1A	8.14	110.37	106.71
21	B	520	CLA	C4A-NA-C1A	8.14	110.36	106.71
30	F	224	SQD	O7-S-C6	8.07	116.53	106.94
28	C	491	DGD	O5D-C6D-C5D	8.05	123.95	109.05
27	I	220	LMG	C8-O7-C10	8.05	137.60	117.79
21	B	522	CLA	C4A-NA-C1A	8.04	110.32	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	D	362	DGD	O5D-C6D-C5D	8.04	123.92	109.05
21	C	486	CLA	C4A-NA-C1A	7.83	110.22	106.71
21	C	478	CLA	C4A-NA-C1A	7.80	110.21	106.71
28	D	362	DGD	C3G-O3G-C1D	-7.78	98.55	113.74
21	B	515	CLA	C4A-NA-C1A	7.77	110.20	106.71
21	B	521	CLA	C4A-NA-C1A	7.76	110.20	106.71
28	C	493	DGD	C2G-O2G-C1B	7.67	136.66	117.79
33	F	85	HEM	C4A-C3A-C2A	-7.64	101.68	107.00
33	V	164	HEM	CMA-C3A-C4A	7.64	140.21	128.46
21	B	519	CLA	C4A-NA-C1A	7.58	110.12	106.71
28	C	492	DGD	O5D-C6D-C5D	7.57	123.05	109.05
21	B	512	CLA	C4A-NA-C1A	7.40	110.03	106.71
21	B	523	CLA	C4A-NA-C1A	7.39	110.03	106.71
21	A	363	CLA	C4A-NA-C1A	7.39	110.03	106.71
28	C	491	DGD	O6D-C5D-C6D	7.37	121.54	106.67
21	B	517	CLA	C4A-NA-C1A	7.33	110.00	106.71
30	C	475	SQD	O6-C1-C2	7.12	119.43	108.30
28	C	492	DGD	O6D-C5D-C6D	7.09	120.97	106.67
21	B	524	CLA	C4A-NA-C1A	7.07	109.88	106.71
28	B	533	DGD	O2G-C1B-C2B	7.02	126.63	111.50
28	C	474	DGD	C6D-C5D-C4D	-6.97	97.53	112.09
28	C	493	DGD	C6D-O5D-C1E	-6.94	100.17	113.74
30	D	361	SQD	O6-C1-C2	6.94	119.13	108.30
21	C	481	CLA	C4A-NA-C1A	6.92	109.82	106.71
27	J	492	LMG	O7-C10-C11	6.91	126.39	111.50
28	C	492	DGD	C6D-O5D-C1E	-6.89	100.28	113.74
27	B	531	LMG	C13-C12-C11	-6.79	88.78	113.19
30	L	213	SQD	O6-C1-C2	6.78	118.89	108.30
25	J	115	BCR	C2-C1-C6	6.70	120.79	110.48
25	X	107	BCR	C38-C26-C25	6.69	132.04	124.53
28	C	474	DGD	O2G-C1B-C2B	6.67	125.88	111.50
25	J	115	BCR	C32-C1-C2	-6.65	82.33	108.91
21	D	354	CLA	C4A-NA-C1A	6.61	109.68	106.71
28	C	474	DGD	O1G-C1A-C2A	6.56	132.49	111.91
25	D	358	BCR	C38-C26-C25	6.50	131.82	124.53
32	D	357	PL9	C46-C47-C48	6.40	132.92	111.88
26	C	476	LHG	C25-C24-C23	6.39	136.87	113.62
27	B	531	LMG	C19-C18-C17	-6.34	82.22	114.42
28	C	493	DGD	C6D-C5D-C4D	-6.32	98.89	112.09
25	J	112	BCR	C33-C5-C6	6.32	131.63	124.53
30	F	224	SQD	C10-C9-C8	6.29	135.81	113.19
30	D	361	SQD	C10-C9-C8	6.28	135.77	113.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	M	217	LMG	O7-C10-C11	6.28	125.03	111.50
28	C	493	DGD	C4B-C3B-C2B	-6.26	90.68	113.19
30	C	475	SQD	C10-C9-C8	6.24	135.62	113.19
25	A	369	BCR	C38-C26-C25	6.22	131.52	124.53
27	D	359	LMG	C13-C12-C11	-6.21	90.85	113.19
26	A	371	LHG	C25-C24-C23	6.21	136.21	113.62
25	B	529	BCR	C38-C26-C25	6.20	131.49	124.53
25	J	115	BCR	C38-C26-C25	6.20	131.49	124.53
30	D	361	SQD	C25-C24-C23	6.17	136.06	113.62
28	C	474	DGD	O6D-C1D-O3G	6.17	124.58	109.97
28	C	493	DGD	C3G-O3G-C1D	-6.16	101.70	113.74
21	C	481	CLA	CAA-C2A-C1A	-6.15	91.83	111.97
30	L	213	SQD	C10-C9-C8	6.13	135.21	113.19
28	C	474	DGD	O3G-C1D-C2D	-6.12	98.74	108.30
21	B	514	CLA	C4A-NA-C1A	6.09	109.44	106.71
30	F	224	SQD	O6-C1-C2	6.08	117.79	108.30
25	J	115	BCR	C33-C5-C6	6.08	131.35	124.53
25	B	529	BCR	C33-C5-C6	6.07	131.35	124.53
30	F	224	SQD	C25-C24-C23	6.06	135.67	113.62
22	D	355	PHO	O2D-CGD-CBD	6.06	118.67	111.00
25	B	527	BCR	C38-C26-C25	6.06	131.33	124.53
27	D	359	LMG	C7-O1-C1	-5.97	102.08	113.74
30	L	213	SQD	C25-C24-C23	5.96	135.31	113.62
28	D	362	DGD	O3G-C3G-C2G	5.96	125.28	110.90
22	A	365	PHO	O2D-CGD-CBD	5.95	118.53	111.00
25	B	527	BCR	C33-C5-C6	5.93	131.19	124.53
21	C	481	CLA	CBA-CAA-C2A	5.89	131.24	113.86
28	A	375	DGD	C6D-O5D-C1E	-5.86	102.29	113.74
25	Z	116	BCR	C38-C26-C25	5.85	131.10	124.53
25	D	358	BCR	C33-C5-C6	5.84	131.09	124.53
27	B	531	LMG	C17-C16-C15	-5.79	85.05	114.42
28	D	362	DGD	O6D-C5D-C6D	5.77	118.32	106.67
32	D	357	PL9	C32-C33-C34	-5.75	113.82	127.66
21	C	480	CLA	CBA-CAA-C2A	5.66	130.57	113.86
30	C	475	SQD	C25-C24-C23	5.62	134.07	113.62
28	C	492	DGD	C4A-C3A-C2A	-5.62	92.99	113.19
27	B	531	LMG	C7-O1-C1	-5.62	102.77	113.74
21	A	364	CLA	C4D-C3D-CAD	5.61	114.71	108.10
28	C	474	DGD	C6D-O5D-C1E	-5.61	102.79	113.74
28	C	491	DGD	C4B-C3B-C2B	-5.57	93.17	113.19
28	C	491	DGD	C1G-O1G-C1A	5.57	137.74	117.12
21	C	481	CLA	CAA-CBA-CGA	-5.57	96.99	113.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	C	490	BCR	C33-C5-C6	5.56	130.77	124.53
25	C	489	BCR	C38-C26-C25	5.53	130.74	124.53
28	C	492	DGD	C6A-C5A-C4A	-5.53	86.37	114.42
28	C	492	DGD	O2G-C1B-C2B	5.52	123.39	111.50
28	C	491	DGD	O1G-C1G-C2G	-5.50	92.41	108.43
30	F	224	SQD	O8-S-C6	-5.50	96.97	105.74
25	J	115	BCR	C31-C1-C6	5.44	119.12	110.30
32	D	357	PL9	C11-C9-C8	-5.43	110.12	121.12
33	V	164	HEM	CBA-CAA-C2A	5.41	121.85	112.62
27	I	220	LMG	C13-C12-C11	-5.38	93.84	113.19
25	B	530	BCR	C38-C26-C25	5.38	130.56	124.53
21	B	524	CLA	O2D-CGD-CBD	5.37	120.81	111.27
28	C	474	DGD	C3G-O3G-C1D	5.34	124.17	113.74
28	A	375	DGD	C3G-O3G-C1D	5.34	124.17	113.74
28	D	362	DGD	C6D-O5D-C1E	-5.33	103.33	113.74
28	A	375	DGD	O3G-C1D-C2D	-5.31	100.01	108.30
21	C	482	CLA	C4D-C3D-CAD	5.24	114.27	108.10
33	F	85	HEM	CAD-C3D-C2D	5.23	137.62	127.88
28	C	491	DGD	C6D-C5D-C4D	-5.20	101.24	112.09
30	L	213	SQD	C44-O6-C1	5.18	123.87	113.74
29	D	536	LMT	C1B-O1B-C4'	-5.18	105.14	117.96
21	C	481	CLA	C4D-C3D-CAD	5.18	114.20	108.10
25	X	107	BCR	C15-C14-C13	5.17	134.69	127.31
21	C	480	CLA	CAA-C2A-C1A	-5.17	95.05	111.97
21	B	511	CLA	O2D-CGD-CBD	5.16	120.43	111.27
28	C	492	DGD	C6D-C5D-C4D	-5.15	101.35	112.09
28	A	375	DGD	C6D-C5D-C4D	-5.13	101.39	112.09
25	Z	116	BCR	C33-C5-C6	5.13	130.28	124.53
32	D	357	PL9	C12-C13-C14	-5.12	115.34	127.66
33	V	164	HEM	C1B-NB-C4B	5.11	110.35	105.07
25	B	527	BCR	C8-C7-C6	5.10	141.54	127.20
28	A	375	DGD	C4B-C3B-C2B	-5.10	94.84	113.19
27	D	359	LMG	O1-C7-C8	5.10	123.20	110.90
28	C	474	DGD	C1G-O1G-C1A	-5.09	98.27	117.12
25	A	369	BCR	C24-C23-C22	5.08	133.92	126.23
21	B	518	CLA	CAA-C2A-C1A	-5.04	95.46	111.97
28	C	492	DGD	C3G-O3G-C1D	-5.02	103.94	113.74
25	J	115	BCR	C23-C24-C25	5.00	141.25	127.20
28	A	375	DGD	O5D-C1E-C2E	4.96	116.05	108.30
25	A	369	BCR	C33-C5-C6	4.96	130.09	124.53
25	C	490	BCR	C38-C26-C25	4.93	130.07	124.53
30	L	213	SQD	O8-S-C6	-4.93	97.88	105.74

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	C	479	CLA	O2D-CGD-CBD	4.93	120.03	111.27
22	D	355	PHO	C4A-C3A-C2A	4.90	107.50	102.84
25	B	530	BCR	C33-C5-C6	4.89	130.02	124.53
25	J	112	BCR	C38-C26-C25	4.89	130.02	124.53
28	C	493	DGD	C1D-O6D-C5D	-4.88	104.10	113.69
21	B	517	CLA	C4D-C3D-CAD	4.87	113.84	108.10
21	C	483	CLA	C4D-C3D-CAD	4.87	113.83	108.10
32	D	357	PL9	C22-C23-C24	-4.87	115.94	127.66
21	A	362	CLA	C4D-C3D-CAD	4.83	113.78	108.10
32	D	357	PL9	C42-C43-C44	-4.82	116.05	127.66
21	B	524	CLA	CBA-CAA-C2A	4.82	128.10	113.86
28	C	474	DGD	C1D-O6D-C5D	-4.79	104.28	113.69
28	A	375	DGD	O5D-C6D-C5D	4.77	117.87	109.05
28	C	492	DGD	C1D-O6D-C5D	-4.77	104.33	113.69
21	B	516	CLA	C2A-C1A-CHA	4.75	132.16	123.86
25	X	107	BCR	C33-C5-C6	4.74	129.85	124.53
27	B	531	LMG	O7-C8-C7	4.73	125.52	108.40
28	C	491	DGD	C6D-O5D-C1E	-4.70	104.55	113.74
21	D	354	CLA	C4D-C3D-CAD	4.70	113.64	108.10
22	A	365	PHO	C4A-C3A-C2A	4.70	107.31	102.84
21	B	513	CLA	C4D-C3D-CAD	4.69	113.63	108.10
21	C	488	CLA	C3A-C2A-C1A	4.68	108.35	101.34
21	B	511	CLA	C4D-C3D-CAD	4.68	113.61	108.10
21	K	483	CLA	O2D-CGD-CBD	4.66	119.54	111.27
27	B	531	LMG	C22-C21-C20	-4.65	90.81	114.42
25	B	530	BCR	C7-C8-C9	4.65	133.26	126.23
21	D	356	CLA	C4D-C3D-CAD	4.64	113.57	108.10
28	C	474	DGD	O3G-C3G-C2G	-4.62	99.74	110.90
25	X	107	BCR	C12-C13-C14	-4.62	111.86	118.94
21	B	521	CLA	CBA-CAA-C2A	4.59	127.41	113.86
21	B	525	CLA	C4D-C3D-CAD	4.59	113.50	108.10
21	A	366	CLA	C4D-C3D-CAD	4.58	113.50	108.10
21	B	520	CLA	C4D-C3D-CAD	4.58	113.50	108.10
27	B	531	LMG	C9-C8-C7	-4.58	100.95	111.79
27	C	494	LMG	C9-O8-C28	4.57	134.05	117.12
28	C	492	DGD	C8A-C7A-C6A	-4.57	91.25	114.42
21	A	363	CLA	CBA-CAA-C2A	4.56	127.31	113.86
28	C	491	DGD	C4A-C3A-C2A	-4.54	96.86	113.19
21	K	483	CLA	C4D-C3D-CAD	4.53	113.44	108.10
28	C	493	DGD	O6E-C1E-O5D	4.52	120.67	109.97
25	C	489	BCR	C24-C23-C22	4.51	133.06	126.23
33	V	164	HEM	CHA-C4D-C3D	-4.51	116.86	125.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	J	115	BCR	C38-C26-C27	-4.51	104.96	113.62
21	B	524	CLA	C4D-C3D-CAD	4.50	113.41	108.10
21	B	517	CLA	C11-C10-C8	4.49	130.44	115.92
25	J	115	BCR	C1-C6-C5	-4.49	116.29	122.61
25	J	112	BCR	C2-C1-C6	4.48	117.37	110.48
21	C	487	CLA	C4D-C3D-CAD	4.47	113.37	108.10
21	C	479	CLA	C4D-C3D-CAD	4.47	113.36	108.10
21	B	519	CLA	C4D-C3D-CAD	4.47	113.36	108.10
21	B	518	CLA	CBA-CAA-C2A	4.45	127.00	113.86
27	B	531	LMG	C15-C14-C13	-4.44	91.91	114.42
27	D	359	LMG	C9-C8-C7	4.43	122.27	111.79
21	B	518	CLA	C4D-C3D-CAD	4.43	113.31	108.10
21	B	520	CLA	O2D-CGD-CBD	4.42	119.13	111.27
30	D	361	SQD	O8-S-C6	-4.42	98.69	105.74
28	D	362	DGD	C1G-O1G-C1A	4.42	133.47	117.12
21	C	487	CLA	C2A-C1A-CHA	4.41	131.57	123.86
28	B	533	DGD	O6D-C5D-C6D	4.41	115.56	106.67
33	V	164	HEM	CHA-C4D-ND	4.40	129.82	124.38
25	X	107	BCR	C38-C26-C27	-4.40	105.17	113.62
21	C	477	CLA	C3A-C2A-C1A	4.40	107.93	101.34
28	C	493	DGD	O6D-C5D-C4D	4.40	117.68	109.69
29	D	363	LMT	C1-O1'-C1'	4.39	121.13	113.84
21	C	477	CLA	C4D-C3D-CAD	4.39	113.27	108.10
21	A	363	CLA	C4D-C3D-CAD	4.39	113.27	108.10
28	C	474	DGD	C3G-C2G-C1G	4.37	122.12	111.79
25	B	529	BCR	C33-C5-C4	-4.36	105.23	113.62
25	J	115	BCR	C8-C7-C6	4.36	139.45	127.20
21	A	363	CLA	O2D-CGD-CBD	4.36	119.01	111.27
21	C	480	CLA	C4D-C3D-CAD	4.35	113.22	108.10
27	C	494	LMG	C13-C12-C11	-4.34	97.57	113.19
21	C	480	CLA	O2D-CGD-CBD	4.34	118.98	111.27
32	D	357	PL9	C10-C9-C8	-4.32	112.59	123.68
25	D	358	BCR	C38-C26-C27	-4.31	105.33	113.62
30	C	475	SQD	O8-S-C6	-4.31	98.88	105.74
30	D	361	SQD	C44-O6-C1	4.31	122.15	113.74
21	B	514	CLA	C4D-C3D-CAD	4.30	113.17	108.10
33	F	85	HEM	C4B-C3B-C2B	-4.30	103.70	107.11
25	C	490	BCR	C24-C23-C22	4.29	132.72	126.23
25	J	112	BCR	C11-C10-C9	4.29	133.44	127.31
21	B	513	CLA	C2A-C1A-CHA	4.29	131.35	123.86
28	A	375	DGD	O6D-C1D-O3G	4.26	120.06	109.97
25	X	107	BCR	C29-C30-C25	4.25	117.03	110.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	C	479	CLA	C1-C2-C3	4.24	133.37	126.04
28	B	533	DGD	O5D-C1E-C2E	4.23	114.91	108.30
21	C	488	CLA	C4D-C3D-CAD	4.23	113.08	108.10
27	D	359	LMG	O7-C8-C7	4.23	123.71	108.40
28	C	474	DGD	C3A-C2A-C1A	-4.22	98.26	113.62
21	B	521	CLA	CAA-C2A-C1A	-4.22	98.15	111.97
32	D	357	PL9	C3-C4-C5	4.21	124.08	118.60
33	F	85	HEM	CHA-C4D-ND	4.20	129.58	124.38
21	C	478	CLA	C4D-C3D-CAD	4.20	113.05	108.10
21	B	516	CLA	C4D-C3D-CAD	4.20	113.04	108.10
21	B	521	CLA	C4D-C3D-CAD	4.20	113.04	108.10
25	J	112	BCR	C33-C5-C4	-4.18	105.58	113.62
21	B	517	CLA	O2D-CGD-CBD	4.18	118.69	111.27
29	D	363	LMT	C1B-O1B-C4'	-4.17	107.65	117.96
33	F	85	HEM	CHA-C4D-C3D	-4.17	117.50	125.33
27	B	531	LMG	C18-C17-C16	4.17	135.58	114.42
27	D	359	LMG	O8-C9-C8	-4.17	96.31	108.43
32	D	357	PL9	C20-C19-C21	4.16	122.28	115.27
25	J	112	BCR	C7-C8-C9	4.16	132.52	126.23
30	F	224	SQD	C11-C10-C9	4.15	135.49	114.42
21	C	485	CLA	C4D-C3D-CAD	4.15	112.99	108.10
27	C	494	LMG	O1-C7-C8	-4.14	100.90	110.90
21	D	356	CLA	O2D-CGD-CBD	4.13	118.61	111.27
25	A	369	BCR	C38-C26-C27	-4.13	105.69	113.62
28	B	533	DGD	O6E-C1E-O5D	4.11	119.71	109.97
21	B	512	CLA	C4D-C3D-CAD	4.11	112.94	108.10
25	D	358	BCR	C24-C23-C22	4.10	132.43	126.23
30	C	475	SQD	C44-O6-C1	4.10	121.75	113.74
32	D	357	PL9	C15-C14-C16	4.08	122.13	115.27
25	C	489	BCR	C38-C26-C27	-4.08	105.78	113.62
32	D	357	PL9	C30-C29-C31	4.05	122.08	115.27
27	I	220	LMG	C9-C8-C7	-4.04	102.22	111.79
21	D	354	CLA	O2D-CGD-CBD	4.04	118.45	111.27
25	D	358	BCR	C33-C5-C4	-4.04	105.86	113.62
30	D	361	SQD	O9-S-C6	-4.03	102.15	106.94
21	C	484	CLA	C4D-C3D-CAD	4.03	112.85	108.10
21	C	486	CLA	CBA-CAA-C2A	4.03	125.75	113.86
25	B	529	BCR	C38-C26-C27	-4.02	105.89	113.62
25	X	107	BCR	C30-C25-C26	-4.02	116.95	122.61
21	B	516	CLA	C3A-C2A-C1A	4.02	107.35	101.34
21	B	515	CLA	C4D-C3D-CAD	4.01	112.82	108.10
21	B	525	CLA	C2A-C1A-CHA	4.00	130.86	123.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	C	483	CLA	O2D-CGD-CBD	4.00	118.38	111.27
21	C	487	CLA	C2A-C3A-C4A	4.00	108.33	101.87
21	C	480	CLA	C3A-C2A-C1A	4.00	107.33	101.34
25	J	115	BCR	C33-C5-C4	-4.00	105.94	113.62
33	F	85	HEM	C1B-NB-C4B	3.99	109.20	105.07
25	Z	116	BCR	C29-C30-C25	3.99	116.62	110.48
25	B	530	BCR	C33-C5-C4	-3.97	105.99	113.62
21	B	518	CLA	O2D-CGD-CBD	3.97	118.32	111.27
21	C	485	CLA	C2A-C1A-CHA	3.97	130.80	123.86
21	B	526	CLA	C4D-C3D-CAD	3.96	112.77	108.10
29	A	376	LMT	O1B-C1B-C2B	3.95	118.33	108.10
25	C	490	BCR	C33-C5-C4	-3.95	106.04	113.62
33	V	164	HEM	CAD-C3D-C2D	3.94	135.21	127.88
28	D	362	DGD	C6D-C5D-C4D	-3.94	103.88	112.09
25	C	490	BCR	C29-C30-C25	3.93	116.53	110.48
28	C	493	DGD	C6B-C5B-C4B	-3.93	94.49	114.42
30	F	224	SQD	C44-O6-C1	3.92	121.41	113.74
28	B	533	DGD	C3A-C2A-C1A	-3.92	99.36	113.62
28	B	533	DGD	O1G-C1A-C2A	3.91	124.19	111.91
25	B	527	BCR	C33-C5-C4	-3.91	106.10	113.62
25	X	107	BCR	C8-C7-C6	3.91	138.18	127.20
25	J	112	BCR	C23-C24-C25	3.91	138.17	127.20
32	D	357	PL9	C35-C34-C36	3.90	121.83	115.27
21	B	525	CLA	O2D-CGD-CBD	3.89	118.18	111.27
21	C	481	CLA	C3A-C2A-C1A	3.89	107.17	101.34
30	C	475	SQD	O48-C23-C24	3.88	124.08	111.91
21	A	364	CLA	C2A-C1A-CHA	3.88	130.64	123.86
21	C	482	CLA	CBA-CAA-C2A	3.87	125.28	113.86
25	D	358	BCR	C2-C1-C6	3.86	116.43	110.48
28	C	492	DGD	O2G-C2G-C1G	3.86	122.38	108.40
21	B	522	CLA	C4D-C3D-CAD	3.86	112.64	108.10
21	B	523	CLA	C4D-C3D-CAD	3.86	112.64	108.10
21	B	518	CLA	C3A-C2A-C1A	3.85	107.10	101.34
21	A	366	CLA	O2D-CGD-CBD	3.84	118.10	111.27
30	D	361	SQD	C11-C10-C9	3.84	133.93	114.42
27	M	217	LMG	C9-O8-C28	3.84	131.33	117.12
21	C	486	CLA	C4D-C3D-CAD	3.83	112.61	108.10
27	B	531	LMG	C20-C19-C18	3.83	133.89	114.42
21	A	363	CLA	C1-C2-C3	3.83	132.67	126.04
21	B	515	CLA	CBA-CAA-C2A	3.83	125.16	113.86
21	C	477	CLA	O2D-CGD-CBD	3.82	118.05	111.27
27	I	220	LMG	O7-C8-C7	3.81	122.21	108.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	527	BCR	C38-C26-C27	-3.81	106.30	113.62
21	B	519	CLA	CBA-CAA-C2A	3.81	125.10	113.86
21	C	480	CLA	CAA-CBA-CGA	-3.80	102.15	113.25
22	A	365	PHO	C1A-C2A-C3A	3.80	106.45	102.84
21	A	362	CLA	O2D-CGD-CBD	3.80	118.02	111.27
21	C	486	CLA	C1-C2-C3	3.80	132.61	126.04
30	F	224	SQD	O48-C23-C24	3.80	123.83	111.91
28	C	474	DGD	O6E-C1E-O5D	3.79	118.95	109.97
21	B	526	CLA	C1-C2-C3	3.79	132.60	126.04
21	K	483	CLA	C1-C2-C3	3.79	132.59	126.04
28	C	491	DGD	C3G-O3G-C1D	-3.78	106.35	113.74
21	C	487	CLA	O2D-CGD-CBD	3.78	117.99	111.27
21	B	515	CLA	CAA-C2A-C1A	-3.78	99.59	111.97
27	A	373	LMG	O7-C10-C11	3.78	119.64	111.50
25	B	527	BCR	C29-C30-C25	3.77	116.29	110.48
28	B	528	DGD	O2G-C1B-C2B	3.77	119.63	111.50
30	L	213	SQD	C11-C10-C9	3.77	133.57	114.42
25	B	527	BCR	C16-C17-C18	3.77	132.69	127.31
21	C	478	CLA	O2D-CGD-CBD	3.76	117.96	111.27
28	D	362	DGD	C3G-C2G-C1G	3.76	120.69	111.79
21	A	366	CLA	C2A-C1A-CHA	3.75	130.42	123.86
32	D	357	PL9	C25-C24-C26	3.75	121.58	115.27
21	C	477	CLA	C2A-C1A-CHA	3.74	130.40	123.86
27	D	360	LMG	O7-C10-C11	3.74	119.55	111.50
25	C	489	BCR	C33-C5-C6	3.73	128.72	124.53
25	J	112	BCR	C29-C30-C25	3.73	116.22	110.48
21	B	513	CLA	C2A-C3A-C4A	3.73	107.89	101.87
28	D	362	DGD	O2G-C1B-C2B	3.72	119.53	111.50
29	O	274	LMT	C3B-C4B-C5B	3.72	116.88	110.24
21	C	488	CLA	CAA-CBA-CGA	-3.72	102.38	113.25
33	V	164	HEM	C4C-CHD-C1D	3.72	127.47	122.56
25	D	358	BCR	C1-C6-C5	-3.70	117.39	122.61
21	B	511	CLA	C2A-C3A-C4A	3.70	107.85	101.87
25	Z	116	BCR	C33-C5-C4	-3.70	106.51	113.62
25	C	490	BCR	C38-C26-C27	-3.69	106.52	113.62
28	D	362	DGD	C2G-O2G-C1B	3.69	126.88	117.79
32	D	357	PL9	C7-C3-C2	-3.69	118.45	123.30
30	C	475	SQD	C31-C30-C29	3.68	133.12	114.42
21	B	517	CLA	C3A-C2A-C1A	3.68	106.85	101.34
30	C	475	SQD	C11-C10-C9	3.68	133.11	114.42
27	I	220	LMG	C12-C11-C10	3.68	127.00	113.62
21	B	517	CLA	C1-C2-C3	3.68	132.40	126.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	513	CLA	C3A-C2A-C1A	3.67	106.84	101.34
29	B	535	LMT	C3B-C4B-C5B	3.67	116.79	110.24
29	D	536	LMT	O1'-C1-C2	-3.67	96.70	109.56
21	B	518	CLA	C2A-C3A-C4A	3.66	107.78	101.87
25	B	527	BCR	C2-C1-C6	3.65	116.09	110.48
25	B	530	BCR	C29-C30-C25	3.65	116.09	110.48
29	A	376	LMT	C3B-C4B-C5B	3.64	116.73	110.24
21	B	526	CLA	O2D-CGD-CBD	3.64	117.74	111.27
32	D	357	PL9	C26-C27-C28	3.63	123.82	111.88
29	I	274	LMT	C3B-C4B-C5B	3.63	116.72	110.24
30	L	213	SQD	O9-S-C6	-3.63	102.63	106.94
25	J	112	BCR	C8-C9-C10	-3.62	113.38	118.94
25	X	107	BCR	C2-C1-C6	3.62	116.05	110.48
21	B	519	CLA	C1-C2-C3	3.62	132.30	126.04
25	B	530	BCR	C23-C24-C25	3.61	137.34	127.20
29	B	535	LMT	C1-O1'-C1'	-3.61	107.86	113.84
21	C	487	CLA	C1-C2-C3	3.61	132.28	126.04
32	D	357	PL9	C20-C19-C18	-3.60	114.43	123.68
27	I	220	LMG	C15-C14-C13	-3.60	96.16	114.42
27	B	531	LMG	C38-C37-C36	3.59	132.64	114.42
25	J	115	BCR	C29-C30-C25	3.58	116.00	110.48
21	B	515	CLA	O2D-CGD-CBD	3.58	117.63	111.27
21	C	479	CLA	CBA-CAA-C2A	3.58	124.43	113.86
21	A	364	CLA	CBA-CAA-C2A	3.58	124.42	113.86
25	C	490	BCR	C23-C22-C21	-3.57	113.46	118.94
27	D	359	LMG	C9-O8-C28	3.55	130.28	117.12
25	A	369	BCR	C33-C5-C4	-3.55	106.79	113.62
21	B	522	CLA	C3A-C2A-C1A	3.55	106.65	101.34
27	J	492	LMG	C38-C37-C36	3.55	132.44	114.42
27	D	359	LMG	C12-C11-C10	3.54	126.50	113.62
33	F	85	HEM	CAD-C3D-C4D	-3.54	118.48	124.66
28	C	492	DGD	C3G-C2G-C1G	-3.53	103.43	111.79
21	C	478	CLA	C3A-C2A-C1A	3.53	106.63	101.34
29	D	536	LMT	C3B-C4B-C5B	3.53	116.54	110.24
27	B	531	LMG	C12-C11-C10	3.53	126.46	113.62
28	B	533	DGD	C1D-O6D-C5D	-3.53	106.76	113.69
26	A	371	LHG	O8-C23-C24	3.53	122.97	111.91
28	C	492	DGD	O6D-C5D-C4D	3.53	116.10	109.69
26	C	476	LHG	O7-C7-C8	3.52	119.10	111.50
21	C	488	CLA	C2A-C1A-CHA	3.52	130.02	123.86
21	B	516	CLA	CBA-CAA-C2A	3.52	124.26	113.86
21	B	519	CLA	C3A-C2A-C1A	3.52	106.61	101.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	530	BCR	C38-C26-C27	-3.51	106.86	113.62
25	Z	116	BCR	C38-C26-C27	-3.51	106.87	113.62
21	B	512	CLA	O2D-CGD-CBD	3.51	117.50	111.27
21	B	520	CLA	C2A-C3A-C4A	3.50	107.53	101.87
25	J	112	BCR	C38-C26-C27	-3.50	106.89	113.62
27	C	494	LMG	O7-C8-C7	3.49	121.04	108.40
29	D	363	LMT	C3B-C4B-C5B	3.48	116.45	110.24
21	B	526	CLA	C2A-C1A-CHA	3.48	129.95	123.86
21	A	362	CLA	C2A-C3A-C4A	3.48	107.49	101.87
25	J	112	BCR	C30-C25-C26	-3.47	117.72	122.61
25	Z	116	BCR	C23-C24-C25	3.47	136.96	127.20
21	B	525	CLA	C2A-C3A-C4A	3.47	107.48	101.87
21	C	485	CLA	C3A-C2A-C1A	3.47	106.54	101.34
27	J	492	LMG	C12-C11-C10	-3.47	101.00	113.62
25	B	530	BCR	C2-C1-C6	3.47	115.82	110.48
25	C	489	BCR	C29-C30-C25	3.47	115.82	110.48
21	B	526	CLA	C2A-C3A-C4A	3.47	107.47	101.87
21	C	484	CLA	C3A-C2A-C1A	3.46	106.53	101.34
21	A	366	CLA	C3A-C2A-C1A	3.46	106.53	101.34
21	D	356	CLA	C2A-C3A-C4A	3.46	107.46	101.87
25	X	107	BCR	C33-C5-C4	-3.46	106.97	113.62
21	B	517	CLA	C2A-C1A-CHA	3.46	129.91	123.86
21	C	483	CLA	C2A-C1A-CHA	3.45	129.90	123.86
21	B	526	CLA	C3A-C2A-C1A	3.45	106.51	101.34
21	C	479	CLA	C2A-C3A-C4A	3.45	107.44	101.87
27	C	494	LMG	C38-C37-C36	3.45	131.93	114.42
21	B	513	CLA	O2D-CGD-CBD	3.45	117.39	111.27
27	J	492	LMG	C8-O7-C10	3.44	126.27	117.79
21	K	483	CLA	C3A-C2A-C1A	3.44	106.50	101.34
21	B	524	CLA	CAA-C2A-C1A	-3.43	100.72	111.97
28	A	375	DGD	O6D-C5D-C6D	3.43	113.59	106.67
21	A	363	CLA	CAA-C2A-C1A	-3.43	100.73	111.97
25	D	358	BCR	C29-C30-C25	3.43	115.76	110.48
25	D	358	BCR	C30-C25-C26	-3.43	117.78	122.61
27	B	531	LMG	C16-C15-C14	3.42	131.80	114.42
25	B	529	BCR	C29-C30-C25	3.42	115.75	110.48
25	B	527	BCR	C12-C13-C14	-3.42	113.69	118.94
25	B	530	BCR	C30-C25-C26	-3.42	117.80	122.61
21	B	515	CLA	C3A-C2A-C1A	3.42	106.46	101.34
25	A	369	BCR	C30-C25-C26	-3.42	117.80	122.61
25	J	112	BCR	C1-C6-C5	-3.41	117.81	122.61
30	L	213	SQD	O48-C23-C24	3.41	122.59	111.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	C	486	CLA	CAA-C2A-C1A	-3.39	100.86	111.97
21	C	478	CLA	C2A-C3A-C4A	3.38	107.33	101.87
27	D	360	LMG	C8-O7-C10	-3.38	109.47	117.79
21	C	484	CLA	C1-C2-C3	3.38	131.89	126.04
21	B	521	CLA	O2D-CGD-CBD	3.37	117.27	111.27
21	B	517	CLA	C2A-C3A-C4A	3.37	107.32	101.87
29	O	274	LMT	O1'-C1-C2	-3.37	97.76	109.56
21	D	356	CLA	C2A-C1A-CHA	3.37	129.75	123.86
21	C	484	CLA	CBA-CAA-C2A	3.37	123.80	113.86
28	B	528	DGD	C2G-O2G-C1B	-3.37	109.50	117.79
25	X	107	BCR	C16-C17-C18	3.36	132.11	127.31
27	A	373	LMG	C8-O7-C10	-3.36	109.51	117.79
25	C	490	BCR	C8-C7-C6	3.36	136.63	127.20
21	D	356	CLA	CBA-CAA-C2A	3.36	123.77	113.86
30	D	361	SQD	O48-C23-C24	3.36	122.44	111.91
28	C	492	DGD	O6E-C1E-O5D	3.35	117.92	109.97
21	C	481	CLA	O2D-CGD-CBD	3.35	117.21	111.27
21	A	364	CLA	C3A-C2A-C1A	3.35	106.35	101.34
21	A	364	CLA	C2A-C3A-C4A	3.34	107.27	101.87
21	C	484	CLA	CAA-C2A-C1A	-3.34	101.02	111.97
21	D	354	CLA	C12-C11-C10	-3.34	97.88	113.24
25	X	107	BCR	C35-C13-C12	3.34	123.34	118.08
21	C	477	CLA	CAA-C2A-C1A	-3.34	101.03	111.97
21	C	482	CLA	C2A-C3A-C4A	3.33	107.25	101.87
25	J	115	BCR	C30-C25-C26	-3.33	117.92	122.61
29	T	226	LMT	C3B-C4B-C5B	3.33	116.18	110.24
21	B	518	CLA	CAA-CBA-CGA	-3.32	103.54	113.25
21	B	524	CLA	C2A-C3A-C4A	3.32	107.24	101.87
21	A	362	CLA	C3A-C2A-C1A	3.32	106.31	101.34
21	B	515	CLA	C2A-C3A-C4A	3.32	107.23	101.87
21	K	483	CLA	C2A-C3A-C4A	3.31	107.22	101.87
21	B	525	CLA	C3A-C2A-C1A	3.31	106.30	101.34
25	Z	116	BCR	C8-C7-C6	3.31	136.49	127.20
21	B	516	CLA	C2A-C3A-C4A	3.30	107.20	101.87
21	C	484	CLA	O2D-CGD-CBD	3.30	117.14	111.27
21	B	519	CLA	O2D-CGD-CBD	3.29	117.12	111.27
21	A	363	CLA	C3A-C2A-C1A	3.29	106.27	101.34
27	J	492	LMG	C14-C13-C12	-3.29	97.72	114.42
21	D	354	CLA	C2A-C3A-C4A	3.29	107.19	101.87
21	B	521	CLA	C2A-C3A-C4A	3.29	107.18	101.87
25	Z	116	BCR	C16-C17-C18	3.29	132.00	127.31
28	A	375	DGD	O2G-C2G-C3G	3.29	120.30	108.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	363	CLA	C2A-C3A-C4A	3.28	107.17	101.87
21	C	488	CLA	C1-C2-C3	3.28	131.72	126.04
21	C	477	CLA	C2A-C3A-C4A	3.28	107.17	101.87
27	B	531	LMG	O1-C7-C8	3.28	118.81	110.90
25	A	369	BCR	C29-C30-C25	3.28	115.53	110.48
21	B	519	CLA	C2A-C1A-CHA	3.28	129.59	123.86
21	C	482	CLA	CED-O2D-CGD	3.27	123.33	115.94
25	C	489	BCR	C35-C13-C12	3.27	123.23	118.08
21	B	522	CLA	CED-O2D-CGD	3.26	123.32	115.94
28	A	375	DGD	C3G-C2G-C1G	-3.26	104.07	111.79
21	A	364	CLA	O2D-CGD-CBD	3.26	117.06	111.27
28	C	493	DGD	O1G-C1G-C2G	-3.25	98.97	108.43
21	C	481	CLA	C2A-C3A-C4A	3.24	107.11	101.87
21	B	522	CLA	C2A-C1A-CHA	3.24	129.53	123.86
21	B	514	CLA	C2A-C3A-C4A	3.24	107.10	101.87
28	A	375	DGD	C6B-C5B-C4B	-3.24	97.98	114.42
21	A	366	CLA	C2A-C3A-C4A	3.24	107.10	101.87
21	C	484	CLA	CED-O2D-CGD	3.24	123.26	115.94
25	C	489	BCR	C33-C5-C4	-3.23	107.40	113.62
21	D	356	CLA	C3A-C2A-C1A	3.23	106.18	101.34
28	C	491	DGD	C3B-C2B-C1B	3.23	125.36	113.62
21	B	516	CLA	CED-O2D-CGD	3.21	123.20	115.94
21	B	524	CLA	C1-C2-C3	3.20	131.57	126.04
25	B	530	BCR	C24-C23-C22	3.19	131.06	126.23
28	C	474	DGD	O2G-C2G-C1G	3.19	119.96	108.40
25	X	107	BCR	C1-C6-C5	-3.19	118.12	122.61
27	I	220	LMG	C17-C16-C15	-3.19	98.22	114.42
27	C	494	LMG	C7-O1-C1	3.19	119.97	113.74
21	C	486	CLA	C3A-C2A-C1A	3.18	106.11	101.34
21	C	478	CLA	CBA-CAA-C2A	3.18	123.26	113.86
21	C	483	CLA	C1-C2-C3	3.18	131.55	126.04
21	B	518	CLA	C11-C10-C8	3.18	126.19	115.92
21	B	519	CLA	CAA-CBA-CGA	-3.18	103.97	113.25
21	B	521	CLA	C3A-C2A-C1A	3.18	106.09	101.34
25	C	490	BCR	C2-C1-C6	3.17	115.37	110.48
21	C	485	CLA	C2A-C3A-C4A	3.17	107.00	101.87
21	C	486	CLA	C2A-C3A-C4A	3.17	106.99	101.87
25	D	358	BCR	C23-C24-C25	3.17	136.11	127.20
25	X	107	BCR	C24-C23-C22	3.17	131.03	126.23
29	O	274	LMT	C1-O1'-C1'	3.17	119.09	113.84
21	C	483	CLA	C2A-C3A-C4A	3.17	106.99	101.87
21	B	512	CLA	C2A-C3A-C4A	3.17	106.98	101.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	C	483	CLA	C3A-C2A-C1A	3.16	106.08	101.34
28	C	474	DGD	O1G-C1A-O1A	-3.16	115.62	123.59
30	D	361	SQD	C3-C4-C5	-3.15	104.62	110.24
30	C	475	SQD	C3-C4-C5	-3.15	104.62	110.24
28	C	491	DGD	C6B-C5B-C4B	-3.15	98.44	114.42
25	B	529	BCR	C8-C7-C6	3.14	136.03	127.20
21	B	514	CLA	CBA-CAA-C2A	3.14	123.13	113.86
27	C	494	LMG	C31-C30-C29	-3.13	101.93	113.19
21	C	479	CLA	O1D-CGD-CBD	-3.13	118.09	124.48
26	C	476	LHG	O8-C23-C24	3.12	121.71	111.91
28	D	362	DGD	O6D-C5D-C4D	3.12	115.36	109.69
33	V	164	HEM	CAB-C3B-C2B	-3.12	118.33	128.60
28	A	375	DGD	C3B-C2B-C1B	3.12	124.96	113.62
21	C	482	CLA	C3A-C2A-C1A	3.11	106.00	101.34
29	D	536	LMT	C4-C3-C2	-3.11	98.62	114.42
25	C	490	BCR	C30-C25-C26	-3.11	118.24	122.61
25	X	107	BCR	C23-C24-C25	3.11	135.93	127.20
21	B	520	CLA	C3A-C2A-C1A	3.11	105.99	101.34
27	D	359	LMG	C15-C14-C13	-3.10	98.70	114.42
21	B	519	CLA	C2A-C3A-C4A	3.10	106.87	101.87
25	J	112	BCR	C24-C23-C22	3.09	130.91	126.23
25	B	527	BCR	C35-C13-C12	3.09	122.95	118.08
25	B	529	BCR	C23-C24-C25	3.09	135.88	127.20
21	K	483	CLA	C2A-C1A-CHA	3.09	129.25	123.86
21	C	479	CLA	CAA-C2A-C1A	-3.08	101.88	111.97
28	C	492	DGD	C5A-C4A-C3A	3.08	130.04	114.42
33	V	164	HEM	C4B-CHC-C1C	3.07	126.61	122.56
25	B	530	BCR	C1-C6-C5	-3.07	118.29	122.61
28	A	375	DGD	O6D-C5D-C4D	-3.07	104.12	109.69
22	A	365	PHO	O1D-CGD-CBD	-3.07	119.63	124.74
21	B	523	CLA	O2D-CGD-CBD	3.06	116.71	111.27
25	D	358	BCR	C8-C7-C6	3.06	135.80	127.20
25	B	527	BCR	C30-C25-C26	-3.06	118.30	122.61
21	B	521	CLA	C5-C3-C2	3.06	127.30	121.12
21	B	523	CLA	C3A-C2A-C1A	3.05	105.91	101.34
25	C	489	BCR	C2-C1-C6	3.05	115.18	110.48
32	D	357	PL9	C35-C34-C33	-3.05	115.84	123.68
21	C	485	CLA	CED-O2D-CGD	3.05	122.83	115.94
21	B	512	CLA	C3A-C2A-C1A	3.04	105.90	101.34
28	C	474	DGD	O1A-C1A-C2A	-3.04	111.86	123.73
25	B	529	BCR	C2-C1-C6	3.04	115.16	110.48
25	C	489	BCR	C1-C6-C5	-3.04	118.33	122.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	516	CLA	C1-C2-C3	3.04	131.29	126.04
28	C	493	DGD	O3D-C3D-C2D	3.03	117.35	110.35
27	B	531	LMG	C21-C20-C19	3.03	129.81	114.42
27	I	220	LMG	O8-C28-C29	3.03	121.42	111.91
21	C	484	CLA	C2A-C3A-C4A	3.02	106.75	101.87
21	B	524	CLA	O1D-CGD-CBD	-3.02	118.30	124.48
28	C	491	DGD	O6E-C1E-O5D	3.02	117.12	109.97
21	B	522	CLA	C2A-C3A-C4A	3.01	106.73	101.87
21	B	520	CLA	C1-C2-C3	3.01	131.25	126.04
25	C	490	BCR	C1-C6-C5	-3.01	118.38	122.61
28	C	493	DGD	C3B-C2B-C1B	3.01	124.56	113.62
25	C	489	BCR	C23-C22-C21	-3.01	114.33	118.94
25	B	527	BCR	C1-C6-C5	-3.01	118.38	122.61
25	C	489	BCR	C30-C25-C26	-3.01	118.38	122.61
25	Z	116	BCR	C30-C25-C26	-3.00	118.38	122.61
21	B	514	CLA	O2D-CGD-CBD	3.00	116.61	111.27
29	D	536	LMT	C1-O1'-C1'	3.00	118.82	113.84
30	F	224	SQD	C3-C4-C5	-3.00	104.88	110.24
21	C	482	CLA	O2D-CGD-CBD	3.00	116.60	111.27
28	C	493	DGD	O3G-C3G-C2G	3.00	118.14	110.90
21	C	477	CLA	CED-O2D-CGD	3.00	122.71	115.94
30	F	224	SQD	C45-O47-C7	2.99	125.16	117.79
21	A	363	CLA	C2A-C1A-CHA	2.98	129.07	123.86
32	D	357	PL9	C15-C14-C13	-2.98	116.04	123.68
30	D	361	SQD	C45-O47-C7	2.97	125.11	117.79
27	I	220	LMG	O8-C9-C8	2.97	117.09	108.43
30	C	475	SQD	C32-C31-C30	2.97	129.51	114.42
25	J	112	BCR	C30-C25-C24	2.97	124.18	115.78
21	B	523	CLA	C2A-C1A-CHA	2.97	129.05	123.86
33	F	85	HEM	C4C-CHD-C1D	2.97	126.48	122.56
21	C	486	CLA	CED-O2D-CGD	2.97	122.64	115.94
21	B	521	CLA	CHD-C1D-ND	-2.96	121.73	124.45
32	D	357	PL9	C10-C9-C11	-2.96	110.29	115.27
21	B	523	CLA	C2A-C3A-C4A	2.96	106.64	101.87
21	B	516	CLA	CAA-CBA-CGA	-2.95	104.62	113.25
21	B	523	CLA	C4D-CHA-C1A	2.95	124.84	121.25
25	B	529	BCR	C1-C6-C5	-2.95	118.45	122.61
25	C	489	BCR	C32-C1-C6	2.95	115.08	110.30
28	C	491	DGD	C1D-O6D-C5D	-2.95	107.91	113.69
25	Z	116	BCR	C2-C1-C6	2.93	115.00	110.48
21	B	519	CLA	CED-O2D-CGD	2.93	122.56	115.94
25	B	527	BCR	C19-C18-C17	-2.92	114.45	118.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	519	CLA	CAA-C2A-C1A	-2.92	102.40	111.97
21	C	478	CLA	CAA-C2A-C1A	-2.91	102.42	111.97
25	D	358	BCR	C37-C22-C23	2.91	122.67	118.08
28	C	474	DGD	C4A-C3A-C2A	2.91	123.66	113.19
21	C	480	CLA	C2A-C3A-C4A	2.91	106.57	101.87
25	B	527	BCR	C23-C24-C25	2.91	135.37	127.20
21	C	477	CLA	CAA-CBA-CGA	-2.91	104.75	113.25
27	J	492	LMG	C9-C8-C7	-2.90	104.93	111.79
29	I	274	LMT	O1'-C1-C2	-2.89	99.42	109.56
25	C	490	BCR	C20-C21-C22	2.88	131.42	127.31
21	B	524	CLA	C3A-C2A-C1A	2.87	105.64	101.34
29	I	274	LMT	O1B-C4'-C3'	2.87	114.92	107.28
28	C	491	DGD	O3G-C3G-C2G	2.87	117.81	110.90
30	F	224	SQD	O9-S-C6	-2.87	103.53	106.94
29	A	376	LMT	C7-C6-C5	-2.87	99.88	114.42
25	C	489	BCR	C37-C22-C23	2.86	122.59	118.08
28	C	492	DGD	CBA-CAA-C9A	-2.86	99.90	114.42
25	Z	116	BCR	C32-C1-C6	2.86	114.93	110.30
29	D	363	LMT	O1'-C1-C2	-2.85	99.57	109.56
27	J	492	LMG	O8-C9-C8	2.85	116.73	108.43
21	B	517	CLA	CAA-C2A-C1A	-2.85	102.65	111.97
21	B	523	CLA	C1-C2-C3	2.84	130.96	126.04
21	B	521	CLA	CED-O2D-CGD	2.84	122.36	115.94
30	D	361	SQD	O47-C7-C8	2.84	117.62	111.50
28	C	493	DGD	C8B-C7B-C6B	-2.84	100.02	114.42
25	C	490	BCR	C15-C14-C13	2.84	131.36	127.31
21	B	518	CLA	C5-C3-C2	2.84	126.86	121.12
33	F	85	HEM	CAB-C3B-C2B	-2.84	119.26	128.60
21	C	485	CLA	O2D-CGD-CBD	2.83	116.30	111.27
28	A	375	DGD	O3G-C3G-C2G	-2.83	104.07	110.90
30	L	213	SQD	C3-C4-C5	-2.83	105.20	110.24
21	B	521	CLA	CAA-CBA-CGA	-2.83	104.99	113.25
28	C	493	DGD	C1G-O1G-C1A	2.83	127.59	117.12
33	V	164	HEM	C3D-C4D-ND	2.83	113.31	110.17
21	B	521	CLA	C2A-C1A-CHA	2.83	128.80	123.86
25	B	529	BCR	C21-C20-C19	2.82	132.02	123.22
21	C	488	CLA	O2D-CGD-CBD	2.82	116.28	111.27
25	B	529	BCR	C30-C25-C26	-2.82	118.64	122.61
21	B	513	CLA	CHB-C4A-NA	2.82	128.41	124.51
21	C	488	CLA	C2A-C3A-C4A	2.82	106.42	101.87
25	D	358	BCR	C20-C21-C22	2.82	131.33	127.31
21	B	526	CLA	CED-O2D-CGD	2.82	122.31	115.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	522	CLA	O2D-CGD-CBD	2.81	116.26	111.27
25	C	490	BCR	C35-C13-C12	2.81	122.50	118.08
25	B	527	BCR	C11-C10-C9	2.81	131.32	127.31
25	B	529	BCR	C24-C23-C22	2.79	130.46	126.23
21	B	520	CLA	C2A-C1A-CHA	2.79	128.74	123.86
21	B	525	CLA	C1-C2-C3	2.79	130.87	126.04
21	B	514	CLA	C3A-C2A-C1A	2.78	105.50	101.34
25	D	358	BCR	C23-C22-C21	-2.78	114.68	118.94
29	O	274	LMT	C4-C3-C2	-2.78	100.34	114.42
28	D	362	DGD	O2G-C2G-C1G	2.77	118.44	108.40
28	C	493	DGD	C8A-C7A-C6A	-2.77	100.37	114.42
32	D	357	PL9	O1-C4-C3	-2.77	117.67	120.72
21	A	364	CLA	C1-C2-C3	2.76	130.82	126.04
21	B	518	CLA	C3D-C4D-ND	2.76	114.70	110.24
21	B	515	CLA	C3D-C4D-ND	2.76	114.70	110.24
29	I	274	LMT	C4-C3-C2	-2.75	100.44	114.42
28	B	533	DGD	O1G-C1A-O1A	-2.75	116.65	123.59
21	C	488	CLA	CED-O2D-CGD	2.75	122.15	115.94
21	C	478	CLA	CED-O2D-CGD	2.74	122.13	115.94
21	C	478	CLA	C2A-C1A-CHA	2.74	128.65	123.86
21	B	515	CLA	CED-O2D-CGD	2.74	122.12	115.94
25	B	529	BCR	C11-C10-C9	2.73	131.21	127.31
21	B	511	CLA	C2A-C1A-CHA	2.73	128.64	123.86
33	F	85	HEM	C4B-CHC-C1C	2.73	126.16	122.56
25	A	369	BCR	C37-C22-C23	2.73	122.37	118.08
21	C	479	CLA	C3A-C2A-C1A	2.72	105.41	101.34
28	B	533	DGD	C6D-C5D-C4D	-2.72	106.42	112.09
25	C	490	BCR	C30-C25-C24	2.71	123.46	115.78
27	D	359	LMG	C17-C16-C15	-2.71	100.66	114.42
21	B	511	CLA	C1-C2-C3	2.71	130.73	126.04
21	A	364	CLA	CED-O2D-CGD	2.71	122.07	115.94
27	J	492	LMG	O7-C8-C9	2.71	118.21	108.40
21	B	511	CLA	CED-O2D-CGD	2.71	122.06	115.94
27	D	359	LMG	C38-C37-C36	2.71	128.16	114.42
22	A	365	PHO	CMA-C3A-C4A	-2.70	108.46	114.38
21	C	486	CLA	C2C-C1C-NC	-2.70	107.44	109.97
29	I	274	LMT	C1-O1'-C1'	2.70	118.32	113.84
25	J	112	BCR	C8-C7-C6	2.70	134.78	127.20
21	C	484	CLA	C3D-C4D-ND	2.70	114.60	110.24
33	F	85	HEM	CAB-C3B-C4B	2.70	137.03	124.47
25	C	490	BCR	C37-C22-C23	2.69	122.32	118.08
25	J	112	BCR	C35-C13-C12	2.69	122.32	118.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	L	213	SQD	C15-C14-C13	2.69	128.09	114.42
21	B	523	CLA	CED-O2D-CGD	2.69	122.02	115.94
21	B	517	CLA	CBA-CAA-C2A	2.69	121.79	113.86
29	A	376	LMT	C4-C3-C2	-2.69	100.79	114.42
30	C	475	SQD	O8-S-O9	-2.68	104.72	111.27
25	J	112	BCR	C32-C1-C2	-2.68	98.19	108.91
21	B	521	CLA	C3D-C4D-ND	2.68	114.57	110.24
21	A	362	CLA	C2A-C1A-CHA	2.67	128.53	123.86
33	V	164	HEM	C4B-C3B-C2B	-2.67	104.99	107.11
25	J	112	BCR	C34-C9-C8	2.67	122.28	118.08
21	A	362	CLA	CED-O2D-CGD	2.67	121.97	115.94
21	A	363	CLA	C3D-C4D-ND	2.67	114.56	110.24
21	B	516	CLA	CMB-C2B-C1B	-2.67	124.36	128.46
21	C	483	CLA	CED-O2D-CGD	2.66	121.96	115.94
29	D	536	LMT	O1'-C1'-C2'	-2.66	104.14	108.30
28	C	492	DGD	O2G-C2G-C3G	2.66	118.04	108.40
21	C	478	CLA	O1D-CGD-CBD	-2.66	119.04	124.48
29	I	274	LMT	C7-C6-C5	-2.66	100.94	114.42
21	D	356	CLA	CAA-C2A-C1A	-2.65	103.29	111.97
30	C	475	SQD	O9-S-C6	-2.65	103.79	106.94
25	C	490	BCR	C40-C30-C29	-2.65	98.31	108.91
21	C	477	CLA	CBA-CAA-C2A	2.65	121.68	113.86
21	B	517	CLA	O2A-CGA-CBA	2.65	120.22	111.91
30	L	213	SQD	C31-C30-C29	2.65	133.51	113.42
27	C	494	LMG	C6-C5-C4	-2.65	106.81	113.00
21	B	513	CLA	CMB-C2B-C1B	-2.64	124.40	128.46
21	C	481	CLA	C2C-C1C-NC	-2.64	107.50	109.97
25	B	527	BCR	C36-C18-C19	2.64	122.23	118.08
21	C	487	CLA	CHA-C1A-NA	-2.63	120.36	126.40
28	B	533	DGD	C4A-C3A-C2A	2.63	122.66	113.19
21	C	479	CLA	CHD-C1D-ND	-2.63	122.03	124.45
29	D	536	LMT	C7-C6-C5	-2.63	101.07	114.42
33	V	164	HEM	CAB-C3B-C4B	2.62	136.67	124.47
21	B	513	CLA	CAA-C2A-C3A	-2.62	105.61	112.78
29	O	274	LMT	O1'-C1'-C2'	-2.61	104.22	108.30
27	B	531	LMG	C14-C13-C12	2.61	127.69	114.42
21	B	516	CLA	CAA-C2A-C3A	-2.61	105.63	112.78
26	A	371	LHG	O7-C7-C8	2.61	117.12	111.50
25	D	358	BCR	C35-C13-C12	2.61	122.19	118.08
25	C	489	BCR	C1-C6-C7	2.61	123.15	115.78
21	C	478	CLA	C3D-C4D-ND	2.61	114.45	110.24
27	I	220	LMG	C19-C18-C17	-2.60	101.21	114.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	524	CLA	C3D-C4D-ND	2.60	114.45	110.24
21	C	485	CLA	C1-C2-C3	2.60	130.54	126.04
28	D	362	DGD	O6E-C1E-O5D	2.60	116.13	109.97
29	T	226	LMT	C1-O1'-C1'	-2.59	109.54	113.84
21	B	522	CLA	C1-C2-C3	2.59	130.52	126.04
28	C	493	DGD	O6E-C1E-C2E	2.59	115.83	110.35
27	D	359	LMG	O7-C8-C9	-2.58	99.04	108.40
21	B	513	CLA	CED-O2D-CGD	2.58	121.77	115.94
21	C	482	CLA	C5-C3-C2	2.58	126.33	121.12
21	C	478	CLA	CHD-C1D-ND	-2.57	122.09	124.45
27	C	494	LMG	C9-C8-C7	2.57	117.88	111.79
27	J	492	LMG	C39-C38-C37	2.57	127.48	114.42
21	C	488	CLA	CAA-C2A-C1A	-2.57	103.55	111.97
25	Z	116	BCR	C19-C18-C17	-2.57	115.00	118.94
21	C	480	CLA	C3D-C4D-ND	2.57	114.39	110.24
28	C	474	DGD	C4D-C3D-C2D	2.57	115.31	110.82
21	B	519	CLA	CHD-C1D-ND	-2.57	122.09	124.45
21	C	486	CLA	O2D-CGD-CBD	2.56	115.82	111.27
21	B	518	CLA	C2A-C1A-CHA	2.56	128.34	123.86
21	A	364	CLA	C2D-C1D-ND	-2.56	108.22	110.10
21	C	482	CLA	CAA-C2A-C1A	-2.55	103.62	111.97
25	J	115	BCR	C21-C20-C19	2.55	131.17	123.22
21	B	517	CLA	C3D-C4D-ND	2.55	114.36	110.24
21	B	517	CLA	C11-C12-C13	2.55	124.15	115.92
21	B	514	CLA	C3D-C4D-ND	2.55	114.36	110.24
21	B	519	CLA	C3D-C4D-ND	2.55	114.36	110.24
25	B	529	BCR	C16-C17-C18	2.54	130.94	127.31
21	C	486	CLA	C2A-C1A-CHA	2.54	128.31	123.86
25	B	527	BCR	C24-C23-C22	2.54	130.08	126.23
21	D	356	CLA	C1-C2-C3	2.54	130.44	126.04
21	C	481	CLA	C3D-C4D-ND	2.54	114.35	110.24
32	D	357	PL9	C40-C39-C41	2.54	119.54	115.27
28	C	491	DGD	O6D-C1D-O3G	2.54	115.99	109.97
21	B	522	CLA	O1D-CGD-CBD	-2.54	119.29	124.48
21	C	485	CLA	CHD-C1D-ND	-2.54	122.12	124.45
33	V	164	HEM	C2C-C3C-C4C	-2.53	105.13	106.90
22	D	355	PHO	CMA-C3A-C4A	-2.53	108.83	114.38
30	C	475	SQD	C15-C14-C13	2.53	127.29	114.42
28	C	492	DGD	O6E-C1E-C2E	2.53	115.71	110.35
25	C	489	BCR	C40-C30-C25	2.53	114.40	110.30
32	D	357	PL9	C25-C24-C23	-2.53	117.19	123.68
21	B	511	CLA	CMB-C2B-C1B	-2.53	124.58	128.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	520	CLA	O1D-CGD-CBD	-2.53	119.31	124.48
28	C	493	DGD	CBA-CAA-C9A	-2.53	101.60	114.42
27	J	492	LMG	C34-C33-C32	-2.52	101.63	114.42
30	D	361	SQD	C31-C30-C29	2.52	132.52	113.42
21	B	518	CLA	CHD-C1D-ND	-2.51	122.14	124.45
21	C	488	CLA	CHD-C1D-ND	-2.51	122.15	124.45
28	C	491	DGD	O2G-C2G-C3G	2.51	117.48	108.40
27	J	492	LMG	C13-C12-C11	2.51	122.20	113.19
21	C	481	CLA	C1D-ND-C4D	-2.51	104.56	106.33
25	Z	116	BCR	C15-C14-C13	2.50	130.88	127.31
21	C	479	CLA	C3D-C4D-ND	2.50	114.29	110.24
21	D	354	CLA	C3A-C2A-C1A	2.50	105.09	101.34
21	C	488	CLA	C2C-C1C-NC	-2.49	107.64	109.97
28	B	533	DGD	O2G-C1B-O1B	-2.49	117.68	123.70
29	D	363	LMT	O1'-C1'-C2'	-2.49	104.42	108.30
21	A	364	CLA	CAA-C2A-C1A	-2.49	103.83	111.97
21	A	362	CLA	CHD-C1D-ND	-2.48	122.17	124.45
25	A	369	BCR	C7-C8-C9	2.48	129.98	126.23
21	A	363	CLA	CHD-C1D-ND	-2.48	122.18	124.45
27	D	360	LMG	O8-C28-C29	2.48	119.69	111.91
21	D	354	CLA	CED-O2D-CGD	2.47	121.53	115.94
25	D	358	BCR	C16-C17-C18	2.47	130.84	127.31
27	A	373	LMG	O8-C28-C29	2.47	119.67	111.91
33	F	85	HEM	C3D-C4D-ND	2.47	112.92	110.17
22	D	355	PHO	O1D-CGD-CBD	-2.47	120.62	124.74
21	B	511	CLA	C2D-C1D-ND	-2.46	108.29	110.10
21	A	362	CLA	C3D-C4D-ND	2.46	114.22	110.24
27	M	217	LMG	C12-C11-C10	-2.46	104.68	113.62
28	B	528	DGD	O1G-C1A-C2A	2.46	119.62	111.91
21	A	363	CLA	CMB-C2B-C1B	-2.45	124.69	128.46
28	A	375	DGD	C6E-C5E-C4E	-2.45	107.26	113.00
25	C	490	BCR	C23-C24-C25	2.45	134.09	127.20
21	C	486	CLA	C3B-C4B-NB	-2.45	106.04	109.21
22	A	365	PHO	CED-O2D-CGD	2.45	121.48	115.94
21	C	480	CLA	C2A-C1A-CHA	2.45	128.14	123.86
21	B	511	CLA	C3A-C2A-C1A	2.45	105.00	101.34
27	M	217	LMG	O7-C10-O9	-2.44	117.79	123.70
29	A	376	LMT	C1B-O1B-C4'	-2.44	111.92	117.96
25	B	529	BCR	C40-C30-C25	2.44	114.26	110.30
25	B	530	BCR	C35-C13-C12	2.44	121.92	118.08
30	C	475	SQD	C45-O47-C7	2.44	123.80	117.79
21	D	354	CLA	C2D-C1D-ND	-2.44	108.31	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	C	483	CLA	CMB-C2B-C1B	-2.44	124.72	128.46
21	C	480	CLA	CHD-C1D-ND	-2.44	122.22	124.45
28	C	491	DGD	C3A-C2A-C1A	2.43	122.47	113.62
21	K	483	CLA	CED-O2D-CGD	2.42	121.42	115.94
21	B	513	CLA	O1D-CGD-CBD	-2.42	119.53	124.48
28	B	533	DGD	O3G-C3G-C2G	-2.42	105.06	110.90
28	A	375	DGD	C1D-O6D-C5D	-2.42	108.94	113.69
27	C	494	LMG	O8-C9-C8	-2.42	101.40	108.43
21	B	522	CLA	C3D-C4D-ND	2.42	114.14	110.24
21	A	364	CLA	CMB-C2B-C1B	-2.41	124.75	128.46
25	B	530	BCR	C3-C4-C5	2.41	118.39	114.08
21	A	362	CLA	O2A-C1-C2	-2.41	102.30	108.64
21	C	483	CLA	O1D-CGD-CBD	-2.41	119.55	124.48
28	C	493	DGD	O6E-C5E-C4E	2.41	114.07	109.69
21	B	514	CLA	C2A-C1A-CHA	2.40	128.06	123.86
21	D	354	CLA	C2A-C1A-CHA	2.40	128.06	123.86
25	B	530	BCR	C37-C22-C23	2.40	121.86	118.08
30	F	224	SQD	C15-C14-C13	2.40	126.60	114.42
28	A	375	DGD	O1G-C1A-C2A	2.40	119.43	111.91
21	B	514	CLA	CMB-C2B-C1B	-2.40	124.78	128.46
21	C	484	CLA	C3B-C4B-NB	-2.40	106.11	109.21
25	A	369	BCR	C35-C13-C12	2.39	121.85	118.08
25	B	530	BCR	C34-C9-C8	2.39	121.85	118.08
21	A	363	CLA	O1D-CGD-CBD	-2.39	119.58	124.48
21	D	354	CLA	CMB-C2B-C1B	-2.39	124.78	128.46
28	C	474	DGD	O1B-C1B-C2B	-2.39	114.42	123.73
33	F	85	HEM	CAA-CBA-CGA	2.39	120.45	113.76
21	B	512	CLA	C2A-C1A-CHA	2.38	128.03	123.86
28	C	493	DGD	CFB-CEB-CDB	-2.38	102.33	114.42
29	A	376	LMT	O1'-C1'-C2'	-2.38	104.58	108.30
21	B	512	CLA	C3D-C4D-ND	2.38	114.09	110.24
21	B	516	CLA	C12-C11-C10	-2.38	102.30	113.24
30	L	213	SQD	C45-O47-C7	2.38	123.65	117.79
21	B	521	CLA	C6-C5-C3	2.38	119.69	113.45
25	J	112	BCR	C40-C30-C25	2.38	114.16	110.30
25	X	107	BCR	C37-C22-C23	2.38	121.82	118.08
21	C	481	CLA	CHD-C1D-ND	-2.38	122.27	124.45
25	A	369	BCR	C30-C25-C24	2.37	122.50	115.78
33	V	164	HEM	C4D-C3D-C2D	-2.37	103.44	106.90
21	B	520	CLA	C3D-C4D-ND	2.37	114.08	110.24
25	B	530	BCR	C30-C25-C24	2.37	122.48	115.78
21	B	523	CLA	C3D-C4D-ND	2.37	114.07	110.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	D	357	PL9	C53-C6-C1	2.37	119.84	114.99
21	B	516	CLA	CMB-C2B-C3B	2.37	129.11	124.68
30	L	213	SQD	O47-C7-C8	2.37	116.60	111.50
25	J	112	BCR	C12-C13-C14	-2.37	115.31	118.94
21	B	516	CLA	CAA-C2A-C1A	-2.36	104.24	111.97
30	L	213	SQD	C17-C16-C15	2.36	126.41	114.42
26	A	371	LHG	O8-C6-C5	2.36	115.29	108.43
29	D	536	LMT	O1B-C1B-C2B	2.36	114.20	108.10
28	D	362	DGD	CBA-CAA-C9A	-2.36	102.47	114.42
25	Z	116	BCR	C35-C13-C12	2.35	121.78	118.08
21	C	477	CLA	C3D-C4D-ND	2.35	114.03	110.24
27	C	494	LMG	C19-C18-C17	-2.35	102.52	114.42
21	C	482	CLA	C2A-C1A-CHA	2.34	127.96	123.86
21	B	518	CLA	CED-O2D-CGD	2.34	121.24	115.94
21	B	517	CLA	C3B-C4B-NB	-2.34	106.18	109.21
21	B	518	CLA	O2A-C1-C2	2.34	114.79	108.64
21	C	478	CLA	C1-C2-C3	2.34	130.09	126.04
27	D	359	LMG	C6-C5-C4	-2.34	107.53	113.00
21	C	487	CLA	C3A-C2A-C1A	2.34	104.84	101.34
25	B	530	BCR	C16-C17-C18	2.33	130.64	127.31
22	D	355	PHO	OBD-CAD-CBD	-2.33	122.40	125.82
25	A	369	BCR	C2-C1-C6	2.33	114.06	110.48
28	B	533	DGD	C3G-O3G-C1D	-2.32	109.20	113.74
28	A	375	DGD	C8B-C7B-C6B	-2.32	102.64	114.42
21	C	485	CLA	C3D-C4D-ND	2.32	113.99	110.24
21	A	362	CLA	C7-C6-C5	-2.32	107.06	113.36
25	J	112	BCR	C37-C22-C23	2.32	121.73	118.08
25	X	107	BCR	C19-C18-C17	-2.32	115.39	118.94
21	D	356	CLA	C3D-C4D-ND	2.31	113.98	110.24
21	K	483	CLA	O1D-CGD-CBD	-2.31	119.76	124.48
21	B	525	CLA	CED-O2D-CGD	2.31	121.16	115.94
25	C	490	BCR	C32-C1-C6	2.31	114.04	110.30
21	D	356	CLA	O1D-CGD-CBD	-2.31	119.77	124.48
21	C	485	CLA	O1D-CGD-CBD	-2.30	119.77	124.48
25	B	527	BCR	C32-C1-C6	2.30	114.03	110.30
28	C	491	DGD	C4E-C3E-C2E	-2.30	106.81	110.82
21	B	518	CLA	CMB-C2B-C1B	-2.30	124.93	128.46
25	B	527	BCR	C15-C14-C13	2.30	130.59	127.31
25	J	115	BCR	C40-C30-C25	2.30	114.03	110.30
25	J	112	BCR	C16-C17-C18	2.30	130.59	127.31
21	D	356	CLA	CED-O2D-CGD	2.30	121.13	115.94
25	Z	116	BCR	C36-C18-C19	2.29	121.69	118.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	529	BCR	C16-C15-C14	2.29	128.17	123.47
28	D	362	DGD	C8A-C7A-C6A	-2.29	102.80	114.42
21	C	482	CLA	C3D-C4D-ND	2.29	113.94	110.24
23	A	367	MES	O3S-S-C8	2.28	109.46	105.77
27	J	492	LMG	O7-C10-O9	-2.28	118.19	123.70
25	D	358	BCR	C12-C13-C14	-2.28	115.44	118.94
28	D	362	DGD	O2G-C2G-C3G	-2.28	100.15	108.40
21	B	512	CLA	CMB-C2B-C1B	-2.27	124.97	128.46
25	B	530	BCR	C40-C30-C25	2.27	113.98	110.30
25	B	527	BCR	C34-C9-C8	2.26	121.64	118.08
21	C	477	CLA	CHD-C1D-ND	-2.26	122.38	124.45
25	J	115	BCR	C31-C1-C2	2.26	117.95	108.91
21	B	523	CLA	C3B-C4B-NB	-2.26	106.29	109.21
21	C	483	CLA	C3B-C4B-NB	-2.26	106.29	109.21
21	A	364	CLA	CHD-C1D-ND	-2.26	122.38	124.45
27	M	217	LMG	C14-C13-C12	-2.26	102.95	114.42
21	C	480	CLA	O1D-CGD-CBD	-2.26	119.86	124.48
21	C	481	CLA	CMB-C2B-C1B	-2.26	124.99	128.46
30	C	475	SQD	C17-C16-C15	2.26	125.89	114.42
28	C	491	DGD	O6E-C5E-C4E	2.26	113.79	109.69
21	B	512	CLA	CED-O2D-CGD	2.26	121.04	115.94
21	B	521	CLA	CMB-C2B-C1B	-2.26	125.00	128.46
21	C	488	CLA	C3B-C4B-NB	-2.25	106.30	109.21
21	B	515	CLA	CHD-C1D-ND	-2.25	122.39	124.45
28	C	492	DGD	C7A-C6A-C5A	2.25	125.83	114.42
21	C	484	CLA	CMB-C2B-C1B	-2.25	125.01	128.46
21	C	482	CLA	C3B-C4B-NB	-2.25	106.31	109.21
21	C	488	CLA	CBA-CAA-C2A	2.24	120.49	113.86
21	B	521	CLA	C4-C3-C5	-2.24	111.50	115.27
25	A	369	BCR	C23-C22-C21	-2.24	115.50	118.94
21	B	511	CLA	O2D-CGD-O1D	-2.24	119.46	123.84
26	C	476	LHG	C6-C5-C4	2.24	117.08	111.79
21	K	483	CLA	C12-C11-C10	-2.24	102.97	113.24
21	B	517	CLA	C2D-C1D-ND	-2.23	108.46	110.10
27	I	220	LMG	C14-C13-C12	2.23	125.76	114.42
21	B	519	CLA	CMB-C2B-C1B	-2.23	125.03	128.46
28	B	533	DGD	C7A-C6A-C5A	-2.23	103.10	114.42
30	L	213	SQD	O8-S-O7	2.23	116.72	111.27
21	A	364	CLA	C3D-C4D-ND	2.23	113.84	110.24
27	C	494	LMG	C17-C16-C15	-2.23	103.11	114.42
21	B	524	CLA	CAA-CBA-CGA	-2.22	106.75	113.25
28	C	493	DGD	C6A-C5A-C4A	-2.22	103.15	114.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	366	CLA	CMB-C2B-C1B	-2.22	125.05	128.46
25	D	358	BCR	C40-C30-C25	2.22	113.90	110.30
21	C	482	CLA	CHD-C1D-ND	-2.22	122.42	124.45
21	K	483	CLA	C3D-C4D-ND	2.21	113.82	110.24
21	B	520	CLA	CMB-C2B-C1B	-2.21	125.06	128.46
28	B	533	DGD	C5B-C4B-C3B	-2.21	103.21	114.42
25	Z	116	BCR	C1-C6-C5	-2.21	119.50	122.61
28	C	474	DGD	O6E-C5E-C4E	2.21	113.70	109.69
21	A	363	CLA	CMB-C2B-C3B	2.21	128.81	124.68
21	B	514	CLA	CMB-C2B-C3B	2.21	128.80	124.68
28	A	375	DGD	O6E-C5E-C6E	2.20	111.92	106.44
28	C	493	DGD	CDB-CCB-CBB	-2.20	103.24	114.42
25	B	529	BCR	C32-C1-C6	2.20	113.87	110.30
21	D	354	CLA	C11-C10-C8	2.20	123.04	115.92
25	A	369	BCR	C32-C1-C6	2.20	113.87	110.30
30	F	224	SQD	C32-C31-C30	2.20	130.13	113.42
27	C	494	LMG	C12-C11-C10	2.20	121.62	113.62
27	B	531	LMG	O8-C28-C29	2.20	118.81	111.91
21	C	482	CLA	O1D-CGD-CBD	-2.20	119.99	124.48
30	F	224	SQD	C17-C16-C15	2.20	125.58	114.42
21	B	513	CLA	C3D-C4D-ND	2.20	113.79	110.24
27	D	360	LMG	C7-O1-C1	-2.20	109.45	113.74
25	C	489	BCR	C7-C8-C9	2.20	129.55	126.23
21	B	514	CLA	C5-C3-C2	2.19	125.56	121.12
21	A	364	CLA	CMD-C2D-C1D	2.19	128.58	124.71
28	D	362	DGD	O3D-C3D-C2D	2.19	115.42	110.35
21	B	524	CLA	C1D-ND-C4D	-2.19	104.78	106.33
27	J	492	LMG	O8-C28-C29	2.19	118.77	111.91
25	Z	116	BCR	C12-C13-C14	-2.19	115.58	118.94
21	C	488	CLA	CMB-C2B-C1B	-2.19	125.11	128.46
28	B	533	DGD	C3G-C2G-C1G	-2.18	106.62	111.79
30	D	361	SQD	C15-C14-C13	2.18	125.51	114.42
28	B	528	DGD	C6D-O5D-C1E	-2.18	109.48	113.74
21	C	479	CLA	C2A-C1A-CHA	2.18	127.67	123.86
21	B	524	CLA	CHD-C1D-ND	-2.18	122.45	124.45
25	B	529	BCR	C7-C8-C9	2.18	129.52	126.23
27	M	217	LMG	C7-O1-C1	-2.18	109.49	113.74
21	C	481	CLA	CED-O2D-CGD	2.18	120.86	115.94
27	I	220	LMG	O6-C1-O1	2.17	115.12	109.97
28	B	528	DGD	C3G-O3G-C1D	-2.17	109.49	113.74
21	B	516	CLA	O2A-C1-C2	2.17	114.35	108.64
29	D	363	LMT	C4-C3-C2	-2.17	103.39	114.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	C	483	CLA	C3D-C4D-ND	2.17	113.75	110.24
21	C	479	CLA	CMB-C2B-C1B	-2.17	125.13	128.46
28	A	375	DGD	C1G-O1G-C1A	2.17	125.14	117.12
21	B	518	CLA	CMB-C2B-C3B	2.17	128.73	124.68
21	B	515	CLA	O1D-CGD-CBD	-2.17	120.05	124.48
21	B	517	CLA	C2C-C1C-NC	-2.16	107.94	109.97
27	A	373	LMG	C7-O1-C1	-2.16	109.51	113.74
25	B	530	BCR	C32-C1-C6	2.16	113.81	110.30
21	C	484	CLA	CHD-C1D-ND	-2.16	122.47	124.45
25	X	107	BCR	C36-C18-C19	2.16	121.48	118.08
27	C	494	LMG	O1-C1-C2	-2.16	104.93	108.30
25	B	530	BCR	C12-C13-C14	-2.16	115.62	118.94
22	D	355	PHO	C1-C2-C3	2.16	129.78	126.04
29	A	376	LMT	C9-C8-C7	-2.16	103.46	114.42
27	D	359	LMG	O7-C10-C11	-2.16	106.85	111.50
28	B	533	DGD	CDA-CCA-CBA	-2.16	103.47	114.42
21	B	525	CLA	CMB-C2B-C1B	-2.16	125.15	128.46
28	D	362	DGD	C4A-C3A-C2A	-2.16	105.44	113.19
25	X	107	BCR	C1-C6-C7	2.16	121.88	115.78
28	C	491	DGD	C5A-C4A-C3A	2.15	125.36	114.42
25	C	490	BCR	C12-C13-C14	-2.15	115.64	118.94
25	B	530	BCR	C28-C27-C26	2.15	117.91	114.08
25	J	112	BCR	C36-C18-C19	2.15	121.46	118.08
23	A	367	MES	O2S-S-C8	2.15	109.50	106.92
21	B	517	CLA	CHD-C1D-ND	-2.14	122.48	124.45
21	B	522	CLA	C3B-C4B-NB	-2.14	106.44	109.21
30	C	475	SQD	O47-C7-C8	2.14	116.12	111.50
21	B	511	CLA	CHA-C1A-NA	-2.14	121.49	126.40
21	B	517	CLA	C12-C11-C10	-2.14	103.41	113.24
21	B	511	CLA	O1D-CGD-CBD	-2.14	120.11	124.48
25	A	369	BCR	C40-C30-C25	2.14	113.77	110.30
27	D	360	LMG	C1-O6-C5	-2.14	109.49	113.69
25	Z	116	BCR	C1-C6-C7	2.13	121.81	115.78
27	A	373	LMG	C1-O6-C5	-2.13	109.50	113.69
27	J	492	LMG	O9-C10-C11	-2.13	115.42	123.73
21	A	363	CLA	CHD-C4C-NC	2.13	127.56	124.20
28	B	533	DGD	C4B-C3B-C2B	2.13	120.85	113.19
21	A	366	CLA	CED-O2D-CGD	2.13	120.75	115.94
28	B	528	DGD	C1D-O6D-C5D	-2.13	109.51	113.69
30	F	224	SQD	O8-S-O7	2.13	116.47	111.27
23	A	367	MES	O1S-S-C8	2.13	109.48	106.92
21	B	526	CLA	C3D-C4D-ND	2.13	113.68	110.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	D	357	PL9	C3-C2-C1	-2.13	118.52	122.52
28	B	528	DGD	C1E-O6E-C5E	-2.12	109.52	113.69
21	B	514	CLA	CAA-C2A-C1A	-2.12	105.02	111.97
21	C	484	CLA	C12-C11-C10	-2.12	103.50	113.24
27	C	494	LMG	C30-C29-C28	2.12	121.33	113.62
28	C	493	DGD	C4D-C3D-C2D	2.12	114.52	110.82
21	B	517	CLA	CMB-C2B-C1B	-2.12	125.21	128.46
21	C	477	CLA	C1-C2-C3	2.12	129.70	126.04
21	B	519	CLA	O1D-CGD-CBD	-2.11	120.16	124.48
25	A	369	BCR	C12-C13-C14	-2.11	115.70	118.94
25	Z	116	BCR	C40-C30-C25	2.11	113.73	110.30
21	A	362	CLA	CMB-C2B-C1B	-2.11	125.22	128.46
21	C	477	CLA	CHC-C1C-NC	2.11	127.41	124.20
21	B	526	CLA	CBA-CAA-C2A	2.11	120.10	113.86
21	C	483	CLA	CHD-C1D-ND	-2.11	122.51	124.45
29	I	274	LMT	O1'-C1'-C2'	-2.11	105.01	108.30
21	A	362	CLA	C2D-C1D-ND	-2.11	108.55	110.10
25	B	530	BCR	C1-C6-C7	2.11	121.74	115.78
21	C	484	CLA	C2C-C1C-NC	-2.11	108.00	109.97
21	B	514	CLA	C2D-C1D-ND	-2.11	108.55	110.10
21	C	486	CLA	C12-C11-C10	-2.11	103.57	113.24
28	C	493	DGD	C5B-C4B-C3B	2.10	125.11	114.42
25	X	107	BCR	C23-C22-C21	-2.10	115.72	118.94
21	C	478	CLA	C1D-ND-C4D	-2.10	104.84	106.33
21	B	516	CLA	O2D-CGD-CBD	2.09	114.99	111.27
21	B	513	CLA	C3B-C4B-NB	-2.09	106.50	109.21
21	C	479	CLA	C2D-C1D-ND	-2.09	108.56	110.10
21	C	488	CLA	C3D-C4D-ND	2.09	113.62	110.24
21	C	480	CLA	CHC-C1C-NC	2.09	127.38	124.20
21	C	486	CLA	C3D-C4D-ND	2.09	113.62	110.24
21	B	521	CLA	C11-C12-C13	2.09	122.66	115.92
25	A	369	BCR	C21-C20-C19	2.09	129.73	123.22
25	J	112	BCR	C40-C30-C29	-2.09	100.56	108.91
21	B	523	CLA	C2D-C1D-ND	-2.08	108.57	110.10
21	C	482	CLA	CMB-C2B-C1B	-2.08	125.27	128.46
21	C	486	CLA	C3C-C4C-NC	-2.08	108.24	110.57
28	C	491	DGD	O3G-C1D-C2D	-2.08	105.06	108.30
27	J	492	LMG	C9-O8-C28	2.08	124.81	117.12
21	B	511	CLA	C3D-C4D-ND	2.08	113.60	110.24
27	M	217	LMG	O8-C9-C8	-2.08	102.39	108.43
21	D	354	CLA	O1D-CGD-CBD	-2.07	120.24	124.48
21	B	517	CLA	C9-C8-C7	-2.07	103.78	111.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	J	492	LMG	C35-C34-C33	2.07	124.95	114.42
30	F	224	SQD	O48-C23-O10	-2.07	118.36	123.59
21	B	518	CLA	C4-C3-C5	-2.07	111.79	115.27
21	B	514	CLA	CED-O2D-CGD	2.07	120.62	115.94
21	B	516	CLA	C3D-C4D-ND	2.07	113.58	110.24
21	B	513	CLA	CAA-C2A-C1A	-2.07	105.19	111.97
28	B	528	DGD	C1G-O1G-C1A	-2.07	109.47	117.12
21	C	482	CLA	CMD-C2D-C1D	2.07	128.36	124.71
21	B	517	CLA	O1D-CGD-CBD	-2.07	120.26	124.48
27	D	359	LMG	C32-C31-C30	-2.06	103.95	114.42
21	C	487	CLA	O1D-CGD-CBD	-2.06	120.26	124.48
30	F	224	SQD	O47-C7-C8	2.06	115.94	111.50
25	B	529	BCR	C28-C27-C26	2.06	117.76	114.08
21	B	515	CLA	C1D-ND-C4D	-2.06	104.87	106.33
28	B	533	DGD	O1B-C1B-C2B	-2.06	115.69	123.73
21	B	523	CLA	O1D-CGD-CBD	-2.06	120.27	124.48
21	B	524	CLA	C3B-C4B-NB	-2.06	106.55	109.21
25	B	530	BCR	C36-C18-C19	2.06	121.32	118.08
21	C	487	CLA	CMB-C2B-C1B	-2.06	125.30	128.46
27	D	360	LMG	C9-O8-C28	-2.06	109.50	117.12
27	I	220	LMG	C16-C15-C14	2.06	124.87	114.42
33	F	85	HEM	C4D-C3D-C2D	-2.05	103.91	106.90
21	C	484	CLA	O1D-CGD-CBD	-2.05	120.29	124.48
21	B	520	CLA	C2D-C1D-ND	-2.05	108.59	110.10
25	C	490	BCR	C28-C27-C26	2.05	117.74	114.08
27	A	373	LMG	C9-O8-C28	-2.05	109.53	117.12
29	O	274	LMT	O5B-C5B-C6B	2.05	111.53	106.44
27	I	220	LMG	O1-C7-C8	-2.05	105.95	110.90
21	B	518	CLA	C16-C15-C13	2.05	122.53	115.92
30	L	213	SQD	C13-C12-C11	2.04	124.80	114.42
28	D	362	DGD	C3A-C2A-C1A	2.04	121.05	113.62
21	C	481	CLA	C3B-C4B-NB	-2.04	106.57	109.21
30	L	213	SQD	C19-C18-C17	2.04	124.78	114.42
21	B	518	CLA	C11-C12-C13	2.04	122.51	115.92
21	C	486	CLA	CHD-C1D-ND	-2.04	122.58	124.45
21	B	525	CLA	C3B-C4B-NB	-2.04	106.58	109.21
28	D	362	DGD	C5A-C4A-C3A	2.04	124.77	114.42
21	B	521	CLA	CMD-C2D-C1D	2.04	128.30	124.71
21	C	485	CLA	C4D-CHA-C1A	2.04	123.73	121.25
25	A	369	BCR	C8-C7-C6	2.04	132.92	127.20
21	A	366	CLA	C1-C2-C3	2.03	129.56	126.04
21	A	366	CLA	C3D-C4D-ND	2.03	113.53	110.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	525	CLA	CHA-C1A-NA	-2.03	121.74	126.40
21	B	526	CLA	CHD-C1D-ND	-2.03	122.59	124.45
21	B	523	CLA	CHD-C1D-ND	-2.03	122.59	124.45
21	C	482	CLA	C4-C3-C5	-2.03	111.86	115.27
28	C	493	DGD	O2G-C2G-C3G	2.02	115.72	108.40
25	B	527	BCR	C37-C22-C23	2.02	121.26	118.08
21	D	356	CLA	CMB-C2B-C1B	-2.02	125.36	128.46
21	A	366	CLA	C3B-C4B-NB	-2.02	106.60	109.21
29	O	274	LMT	C7-C6-C5	-2.02	104.19	114.42
28	C	492	DGD	O3D-C3D-C2D	2.01	115.00	110.35
25	D	358	BCR	C11-C10-C9	2.01	130.18	127.31
27	D	359	LMG	C34-C33-C32	-2.01	104.22	114.42
21	B	521	CLA	C1-C2-C3	2.01	129.51	126.04
21	B	524	CLA	C2A-C1A-CHA	2.01	127.37	123.86
25	D	358	BCR	C36-C18-C19	2.00	121.24	118.08
21	B	523	CLA	CMB-C2B-C1B	-2.00	125.38	128.46
30	F	224	SQD	C31-C30-C29	2.00	133.91	115.30
27	J	492	LMG	C32-C31-C30	-2.00	104.25	114.42
29	A	376	LMT	C1'-O5'-C5'	-2.00	109.76	113.69
21	B	511	CLA	CHC-C1C-NC	2.00	127.24	124.20
21	B	517	CLA	C9-C8-C10	-2.00	104.05	111.29

All (74) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
21	A	362	CLA	ND
21	A	362	CLA	C8
21	A	363	CLA	ND
21	A	363	CLA	C8
21	A	366	CLA	ND
21	A	366	CLA	C8
21	A	364	CLA	ND
21	A	364	CLA	C8
21	B	511	CLA	ND
21	B	511	CLA	C8
21	B	512	CLA	ND
21	B	512	CLA	C8
21	B	513	CLA	ND
21	B	513	CLA	C8
21	B	514	CLA	ND
21	B	514	CLA	C8
21	B	515	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
21	B	515	CLA	C8
21	B	516	CLA	ND
21	B	516	CLA	C8
21	B	517	CLA	ND
21	B	517	CLA	C8
21	B	518	CLA	ND
21	B	518	CLA	C8
21	B	519	CLA	ND
21	B	519	CLA	C8
21	B	520	CLA	ND
21	B	520	CLA	C8
21	B	521	CLA	ND
21	B	521	CLA	C8
21	B	522	CLA	ND
21	B	522	CLA	C8
21	B	523	CLA	ND
21	B	523	CLA	C8
21	B	524	CLA	ND
21	B	524	CLA	C8
21	B	525	CLA	ND
21	B	525	CLA	C8
21	B	526	CLA	ND
21	B	526	CLA	C8
21	C	477	CLA	ND
21	C	477	CLA	C8
21	C	478	CLA	ND
21	C	478	CLA	C8
21	C	479	CLA	ND
21	C	479	CLA	C8
21	C	480	CLA	ND
21	C	480	CLA	C8
21	C	481	CLA	ND
21	C	481	CLA	C8
21	C	482	CLA	ND
21	C	482	CLA	C8
21	C	483	CLA	ND
21	C	483	CLA	C8
21	C	484	CLA	ND
21	C	484	CLA	C8
21	C	485	CLA	ND
21	C	485	CLA	C8
21	C	486	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
21	C	486	CLA	C8
21	C	487	CLA	ND
21	C	487	CLA	C8
21	C	488	CLA	ND
21	C	488	CLA	C8
21	D	354	CLA	ND
21	D	354	CLA	C8
21	D	356	CLA	ND
21	D	356	CLA	C8
21	K	483	CLA	ND
21	K	483	CLA	C8
22	A	365	PHO	C8
22	D	355	PHO	C8
28	C	492	DGD	C1E
28	C	493	DGD	C1E

All (716) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	B	511	CLA	C11-C12-C13-C14
21	B	515	CLA	C2-C3-C5-C6
21	B	515	CLA	C4-C3-C5-C6
21	B	516	CLA	C2-C3-C5-C6
21	B	516	CLA	C4-C3-C5-C6
21	B	517	CLA	C2-C3-C5-C6
21	B	517	CLA	C4-C3-C5-C6
21	B	520	CLA	C2A-CAA-CBA-CGA
21	B	522	CLA	C2A-CAA-CBA-CGA
21	B	524	CLA	CHA-CBD-CGD-O1D
21	B	524	CLA	CHA-CBD-CGD-O2D
21	B	525	CLA	C2-C3-C5-C6
21	B	525	CLA	C4-C3-C5-C6
21	C	477	CLA	CAD-CBD-CGD-O1D
21	C	480	CLA	CHA-CBD-CGD-O2D
21	C	483	CLA	C2-C3-C5-C6
21	C	483	CLA	C4-C3-C5-C6
21	C	484	CLA	C2-C3-C5-C6
21	C	484	CLA	C4-C3-C5-C6
21	C	486	CLA	CHA-CBD-CGD-O1D
21	C	486	CLA	CHA-CBD-CGD-O2D
22	A	365	PHO	O2A-C1-C2-C3
23	A	367	MES	C7-C8-S-O2S

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	A	367	MES	C7-C8-S-O3S
25	A	369	BCR	C6-C7-C8-C9
25	A	369	BCR	C23-C24-C25-C30
25	B	527	BCR	C1-C6-C7-C8
25	B	527	BCR	C5-C6-C7-C8
25	B	527	BCR	C6-C7-C8-C9
25	C	489	BCR	C6-C7-C8-C9
25	C	490	BCR	C6-C7-C8-C9
25	C	490	BCR	C23-C24-C25-C26
25	C	490	BCR	C23-C24-C25-C30
25	D	358	BCR	C1-C6-C7-C8
25	D	358	BCR	C5-C6-C7-C8
25	D	358	BCR	C6-C7-C8-C9
25	J	115	BCR	C6-C7-C8-C9
25	J	112	BCR	C6-C7-C8-C9
25	X	107	BCR	C1-C6-C7-C8
25	X	107	BCR	C5-C6-C7-C8
25	Z	116	BCR	C1-C6-C7-C8
25	Z	116	BCR	C5-C6-C7-C8
26	C	476	LHG	O1-C1-C2-C3
26	C	476	LHG	C8-C7-O7-C5
27	B	531	LMG	C7-C8-O7-C10
27	D	360	LMG	C11-C10-O7-C8
27	J	492	LMG	O7-C8-C9-O8
28	C	474	DGD	O6E-C1E-O5D-C6D
28	C	491	DGD	O6E-C1E-O5D-C6D
28	C	492	DGD	O6E-C1E-O5D-C6D
28	C	493	DGD	O2G-C2G-C3G-O3G
28	C	493	DGD	O6E-C1E-O5D-C6D
28	D	362	DGD	O1G-C1G-C2G-O2G
28	D	362	DGD	O6E-C1E-O5D-C6D
29	I	274	LMT	C3'-C4'-O1B-C1B
30	C	475	SQD	C8-C7-O47-C45
30	D	361	SQD	O49-C7-O47-C45
30	D	361	SQD	C8-C7-O47-C45
30	D	361	SQD	C5-C6-S-O7
30	D	361	SQD	C5-C6-S-O8
30	D	361	SQD	C5-C6-S-O9
30	F	224	SQD	O5-C1-O6-C44
30	F	224	SQD	O5-C5-C6-S
30	F	224	SQD	C5-C6-S-O8
30	L	213	SQD	C2-C1-O6-C44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	L	213	SQD	O49-C7-O47-C45
30	L	213	SQD	C8-C7-O47-C45
32	D	357	PL9	C24-C26-C27-C28
32	D	357	PL9	C26-C27-C28-C29
32	D	357	PL9	C39-C41-C42-C43
32	D	357	PL9	C46-C47-C48-C49
33	F	85	HEM	C2B-C3B-CAB-CBB
33	F	85	HEM	C4B-C3B-CAB-CBB
33	V	164	HEM	C1A-C2A-CAA-CBA
33	V	164	HEM	C3A-C2A-CAA-CBA
33	V	164	HEM	C2B-C3B-CAB-CBB
33	V	164	HEM	C4B-C3B-CAB-CBB
21	B	517	CLA	C13-C15-C16-C17
21	B	522	CLA	C10-C11-C12-C13
22	D	355	PHO	CBD-CGD-O2D-CED
30	F	224	SQD	O10-C23-O48-C46
28	B	528	DGD	O6D-C5D-C6D-O5D
28	C	493	DGD	O6D-C5D-C6D-O5D
26	C	476	LHG	O9-C7-O7-C5
27	D	360	LMG	O9-C10-O7-C8
30	C	475	SQD	O49-C7-O47-C45
21	A	362	CLA	C3-C5-C6-C7
21	A	364	CLA	C3-C5-C6-C7
21	B	511	CLA	C3-C5-C6-C7
21	B	514	CLA	C3-C5-C6-C7
21	B	519	CLA	C3-C5-C6-C7
21	C	478	CLA	C3-C5-C6-C7
21	C	484	CLA	C3-C5-C6-C7
21	A	366	CLA	CBA-CGA-O2A-C1
30	F	224	SQD	C24-C23-O48-C46
29	B	535	LMT	C5'-C4'-O1B-C1B
28	B	528	DGD	C4E-C5E-C6E-O5E
28	B	528	DGD	C4D-C5D-C6D-O5D
29	A	376	LMT	C5'-C4'-O1B-C1B
21	B	516	CLA	C2A-CAA-CBA-CGA
21	B	518	CLA	C2A-CAA-CBA-CGA
21	C	477	CLA	C2A-CAA-CBA-CGA
21	C	481	CLA	C2A-CAA-CBA-CGA
27	B	531	LMG	C36-C37-C38-C39
27	C	494	LMG	C18-C19-C20-C21
27	C	494	LMG	C36-C37-C38-C39
27	D	359	LMG	C18-C19-C20-C21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
27	D	359	LMG	C36-C37-C38-C39
27	D	360	LMG	C36-C37-C38-C39
27	I	220	LMG	C18-C19-C20-C21
27	J	492	LMG	C36-C37-C38-C39
27	M	217	LMG	C18-C19-C20-C21
28	B	533	DGD	C7B-C8B-C9B-CAB
28	C	491	DGD	C7A-C8A-C9A-CAA
28	C	492	DGD	C7B-C8B-C9B-CAB
29	D	536	LMT	C3-C4-C5-C6
29	D	363	LMT	C3-C4-C5-C6
29	I	274	LMT	C3-C4-C5-C6
29	T	226	LMT	C3-C4-C5-C6
21	B	517	CLA	C3-C5-C6-C7
21	C	479	CLA	C3-C5-C6-C7
21	C	481	CLA	C3-C5-C6-C7
21	C	485	CLA	C3-C5-C6-C7
21	A	363	CLA	CBA-CGA-O2A-C1
21	B	524	CLA	CBA-CGA-O2A-C1
21	C	483	CLA	CBA-CGA-O2A-C1
27	B	531	LMG	C18-C19-C20-C21
27	J	492	LMG	C18-C19-C20-C21
28	C	474	DGD	C7A-C8A-C9A-CAA
28	C	493	DGD	C7B-C8B-C9B-CAB
28	D	362	DGD	C7A-C8A-C9A-CAA
29	A	376	LMT	C3-C4-C5-C6
32	D	357	PL9	C7-C8-C9-C10
28	B	533	DGD	C7A-C8A-C9A-CAA
28	B	528	DGD	C7B-C8B-C9B-CAB
28	C	474	DGD	C7B-C8B-C9B-CAB
28	D	362	DGD	C7B-C8B-C9B-CAB
29	O	274	LMT	C3-C4-C5-C6
21	A	363	CLA	O1A-CGA-O2A-C1
21	A	366	CLA	O1A-CGA-O2A-C1
21	C	483	CLA	O1A-CGA-O2A-C1
21	D	354	CLA	O1A-CGA-O2A-C1
26	A	371	LHG	O10-C23-O8-C6
28	C	492	DGD	C7A-C8A-C9A-CAA
28	C	493	DGD	C7A-C8A-C9A-CAA
28	A	375	DGD	C7B-C8B-C9B-CAB
21	C	482	CLA	C3-C5-C6-C7
21	B	522	CLA	CBA-CGA-O2A-C1
27	A	373	LMG	C29-C28-O8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	B	511	CLA	C2C-C3C-CAC-CBC
29	B	535	LMT	C3-C4-C5-C6
21	B	524	CLA	O1A-CGA-O2A-C1
22	D	355	PHO	O1D-CGD-O2D-CED
28	B	528	DGD	C7A-C8A-C9A-CAA
27	A	373	LMG	O10-C28-O8-C9
28	B	528	DGD	O6E-C5E-C6E-O5E
26	C	476	LHG	C23-C24-C25-C26
21	A	362	CLA	CBA-CGA-O2A-C1
21	D	354	CLA	CBA-CGA-O2A-C1
26	A	371	LHG	C24-C23-O8-C6
27	A	373	LMG	O6-C5-C6-O5
21	B	523	CLA	C4-C3-C5-C6
21	C	479	CLA	C4-C3-C5-C6
21	B	523	CLA	C2-C3-C5-C6
21	C	479	CLA	C2-C3-C5-C6
21	B	521	CLA	C2A-CAA-CBA-CGA
21	C	488	CLA	C2A-CAA-CBA-CGA
21	A	362	CLA	O1A-CGA-O2A-C1
21	B	522	CLA	O1A-CGA-O2A-C1
28	B	533	DGD	O6E-C1E-O5D-C6D
21	C	485	CLA	CBA-CGA-O2A-C1
30	D	361	SQD	C24-C23-O48-C46
27	A	373	LMG	C4-C5-C6-O5
30	D	361	SQD	O10-C23-O48-C46
21	C	480	CLA	C3-C5-C6-C7
21	B	518	CLA	CBA-CGA-O2A-C1
21	C	478	CLA	CBA-CGA-O2A-C1
21	C	488	CLA	CBA-CGA-O2A-C1
27	D	360	LMG	C29-C28-O8-C9
22	A	365	PHO	C13-C15-C16-C17
30	D	361	SQD	C2-C1-O6-C44
28	C	474	DGD	O2G-C2G-C3G-O3G
21	B	518	CLA	C11-C12-C13-C14
21	B	520	CLA	C14-C13-C15-C16
21	B	523	CLA	C11-C12-C13-C14
21	C	477	CLA	C6-C7-C8-C9
21	C	480	CLA	C11-C12-C13-C14
21	C	481	CLA	C6-C7-C8-C9
21	C	482	CLA	C6-C7-C8-C9
21	C	486	CLA	C11-C12-C13-C14
22	D	355	PHO	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	D	355	PHO	C14-C13-C15-C16
21	A	363	CLA	C10-C11-C12-C13
22	A	365	PHO	C15-C16-C17-C18
21	C	488	CLA	O1A-CGA-O2A-C1
27	D	360	LMG	O10-C28-O8-C9
21	A	362	CLA	C13-C15-C16-C17
21	B	513	CLA	C10-C11-C12-C13
21	C	480	CLA	C13-C15-C16-C17
22	D	355	PHO	C13-C15-C16-C17
29	O	274	LMT	C5'-C4'-O1B-C1B
21	B	512	CLA	C10-C11-C12-C13
21	B	516	CLA	C13-C15-C16-C17
21	B	525	CLA	C13-C15-C16-C17
27	A	373	LMG	C10-C11-C12-C13
30	C	475	SQD	C23-C24-C25-C26
21	C	480	CLA	C10-C11-C12-C13
21	B	514	CLA	CBA-CGA-O2A-C1
21	B	511	CLA	C4C-C3C-CAC-CBC
21	A	366	CLA	C13-C15-C16-C17
21	C	479	CLA	C13-C15-C16-C17
26	A	371	LHG	C23-C24-C25-C26
27	D	360	LMG	C10-C11-C12-C13
21	B	515	CLA	C11-C12-C13-C15
21	B	516	CLA	C11-C12-C13-C15
21	B	518	CLA	C12-C13-C15-C16
21	B	520	CLA	C12-C13-C15-C16
21	C	482	CLA	C6-C7-C8-C10
21	C	483	CLA	C11-C12-C13-C15
21	C	484	CLA	C12-C13-C15-C16
21	C	488	CLA	C11-C12-C13-C15
21	B	523	CLA	C3-C5-C6-C7
21	B	518	CLA	O1A-CGA-O2A-C1
21	C	478	CLA	O1A-CGA-O2A-C1
21	B	511	CLA	C13-C15-C16-C17
21	C	486	CLA	C13-C15-C16-C17
32	D	357	PL9	C34-C36-C37-C38
28	D	362	DGD	CFB-CGB-CHB-CIB
21	A	362	CLA	C10-C11-C12-C13
21	B	513	CLA	O1A-CGA-O2A-C1
21	C	485	CLA	O1A-CGA-O2A-C1
28	B	528	DGD	C1B-C2B-C3B-C4B
21	C	482	CLA	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	C	492	DGD	CFB-CGB-CHB-CIB
21	B	514	CLA	O1A-CGA-O2A-C1
28	B	533	DGD	CFB-CGB-CHB-CIB
28	C	493	DGD	CFB-CGB-CHB-CIB
21	B	513	CLA	CBA-CGA-O2A-C1
21	C	487	CLA	CBA-CGA-O2A-C1
32	D	357	PL9	C35-C34-C36-C37
21	D	356	CLA	C13-C15-C16-C17
21	B	511	CLA	O1A-CGA-O2A-C1
21	B	526	CLA	C3-C5-C6-C7
21	B	511	CLA	CBA-CGA-O2A-C1
21	B	512	CLA	CBA-CGA-O2A-C1
21	C	479	CLA	CBA-CGA-O2A-C1
21	C	482	CLA	CBA-CGA-O2A-C1
27	A	373	LMG	C30-C31-C32-C33
30	F	224	SQD	C10-C11-C12-C13
28	B	528	DGD	C1G-C2G-O2G-C1B
21	B	514	CLA	C10-C11-C12-C13
27	A	373	LMG	C28-C29-C30-C31
27	D	360	LMG	C13-C14-C15-C16
21	A	363	CLA	C3-C5-C6-C7
27	D	360	LMG	C2-C1-O1-C7
30	C	475	SQD	C2-C1-O6-C44
30	F	224	SQD	C11-C12-C13-C14
21	C	482	CLA	C4-C3-C5-C6
30	C	475	SQD	C17-C18-C19-C20
30	F	224	SQD	C12-C13-C14-C15
21	B	522	CLA	C14-C13-C15-C16
27	D	360	LMG	C11-C12-C13-C14
30	F	224	SQD	C25-C26-C27-C28
21	C	487	CLA	C2A-CAA-CBA-CGA
28	B	528	DGD	C2B-C1B-O2G-C2G
26	A	371	LHG	C11-C10-C9-C8
27	D	360	LMG	O6-C1-O1-C7
26	A	371	LHG	C28-C29-C30-C31
30	F	224	SQD	C27-C28-C29-C30
30	L	213	SQD	C27-C28-C29-C30
21	C	482	CLA	O1A-CGA-O2A-C1
21	C	487	CLA	O1A-CGA-O2A-C1
27	A	373	LMG	C15-C16-C17-C18
30	C	475	SQD	C24-C23-O48-C46
28	C	492	DGD	O6D-C5D-C6D-O5D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	D	355	PHO	C5-C6-C7-C8
26	C	476	LHG	C13-C14-C15-C16
27	A	373	LMG	C36-C37-C38-C39
28	B	528	DGD	O1B-C1B-O2G-C2G
21	C	487	CLA	C10-C11-C12-C13
21	B	520	CLA	C2-C3-C5-C6
21	A	363	CLA	C2A-CAA-CBA-CGA
26	C	476	LHG	O1-C1-C2-O2
21	C	483	CLA	C13-C15-C16-C17
21	B	516	CLA	C2-C1-O2A-CGA
21	B	522	CLA	C2-C1-O2A-CGA
30	L	213	SQD	C25-C26-C27-C28
21	B	524	CLA	C13-C15-C16-C17
21	B	512	CLA	O1A-CGA-O2A-C1
21	C	479	CLA	O1A-CGA-O2A-C1
26	A	371	LHG	C24-C25-C26-C27
26	A	371	LHG	C26-C27-C28-C29
21	C	488	CLA	C3-C5-C6-C7
25	A	369	BCR	C1-C6-C7-C8
25	A	369	BCR	C5-C6-C7-C8
25	A	369	BCR	C23-C24-C25-C26
25	B	530	BCR	C1-C6-C7-C8
25	B	530	BCR	C5-C6-C7-C8
25	B	530	BCR	C23-C24-C25-C26
25	B	530	BCR	C23-C24-C25-C30
25	C	489	BCR	C1-C6-C7-C8
25	C	489	BCR	C5-C6-C7-C8
25	C	489	BCR	C23-C24-C25-C26
25	C	489	BCR	C23-C24-C25-C30
21	A	363	CLA	C13-C15-C16-C17
30	C	475	SQD	O10-C23-O48-C46
27	A	373	LMG	C11-C12-C13-C14
21	B	520	CLA	C4-C3-C5-C6
21	A	364	CLA	C11-C12-C13-C15
21	B	512	CLA	C12-C13-C15-C16
21	B	513	CLA	C12-C13-C15-C16
21	B	519	CLA	C12-C13-C15-C16
21	B	522	CLA	C12-C13-C15-C16
21	B	523	CLA	C11-C12-C13-C15
21	C	481	CLA	C6-C7-C8-C10
21	C	482	CLA	C2-C3-C5-C6
21	C	486	CLA	C11-C12-C13-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	O	274	LMT	C3'-C4'-O1B-C1B
30	F	224	SQD	C15-C16-C17-C18
26	C	476	LHG	C12-C13-C14-C15
30	F	224	SQD	C11-C10-C9-C8
28	B	528	DGD	C1A-C2A-C3A-C4A
27	D	360	LMG	C12-C13-C14-C15
30	D	361	SQD	C10-C11-C12-C13
25	B	527	BCR	C22-C23-C24-C25
30	D	361	SQD	O5-C1-O6-C44
21	B	516	CLA	C10-C11-C12-C13
21	C	486	CLA	C10-C11-C12-C13
30	C	475	SQD	C10-C11-C12-C13
27	D	359	LMG	O1-C7-C8-O7
27	M	217	LMG	O1-C7-C8-O7
28	A	375	DGD	O1G-C1G-C2G-O2G
21	B	518	CLA	C13-C15-C16-C17
32	D	357	PL9	C4-C3-C7-C8
21	A	364	CLA	C11-C12-C13-C14
21	A	364	CLA	C14-C13-C15-C16
21	B	512	CLA	C14-C13-C15-C16
21	B	513	CLA	C14-C13-C15-C16
21	B	515	CLA	C11-C12-C13-C14
21	B	516	CLA	C11-C12-C13-C14
21	B	519	CLA	C14-C13-C15-C16
21	B	525	CLA	C6-C7-C8-C9
21	C	483	CLA	C11-C12-C13-C14
21	C	484	CLA	C14-C13-C15-C16
21	C	485	CLA	C6-C7-C8-C9
21	D	354	CLA	C11-C12-C13-C14
21	D	356	CLA	C3-C5-C6-C7
21	D	356	CLA	C2A-CAA-CBA-CGA
30	C	475	SQD	C24-C25-C26-C27
30	C	475	SQD	C29-C30-C31-C32
27	A	373	LMG	C37-C38-C39-C40
26	C	476	LHG	C11-C12-C13-C14
21	D	354	CLA	C10-C11-C12-C13
21	B	525	CLA	CBA-CGA-O2A-C1
27	D	360	LMG	C16-C17-C18-C19
30	C	475	SQD	C25-C26-C27-C28
30	C	475	SQD	C11-C12-C13-C14
27	A	373	LMG	C16-C17-C18-C19
30	L	213	SQD	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	A	371	LHG	C4-C5-C6-O8
27	A	373	LMG	C7-C8-C9-O8
27	D	359	LMG	O1-C7-C8-C9
27	I	220	LMG	O1-C7-C8-C9
27	M	217	LMG	O1-C7-C8-C9
28	A	375	DGD	C1G-C2G-C3G-O3G
28	D	362	DGD	O1G-C1G-C2G-C3G
30	F	224	SQD	C29-C30-C31-C32
30	L	213	SQD	C19-C20-C21-C22
27	A	373	LMG	C14-C15-C16-C17
21	K	483	CLA	C4-C3-C5-C6
22	D	355	PHO	C4-C3-C5-C6
21	B	525	CLA	O1A-CGA-O2A-C1
21	K	483	CLA	C2-C3-C5-C6
27	C	494	LMG	C7-C8-O7-C10
27	D	359	LMG	C7-C8-O7-C10
27	D	360	LMG	C7-C8-O7-C10
27	J	492	LMG	C9-C8-O7-C10
21	B	521	CLA	C13-C15-C16-C17
28	D	362	DGD	O6D-C5D-C6D-O5D
21	C	480	CLA	O1A-CGA-O2A-C1
30	F	224	SQD	C24-C25-C26-C27
27	A	373	LMG	O7-C8-C9-O8
30	C	475	SQD	O6-C44-C45-O47
30	D	361	SQD	O6-C44-C45-O47
21	C	477	CLA	O1A-CGA-O2A-C1
27	A	373	LMG	C12-C13-C14-C15
21	B	522	CLA	C11-C12-C13-C15
21	B	523	CLA	C6-C7-C8-C10
21	B	525	CLA	C6-C7-C8-C10
21	B	525	CLA	C12-C13-C15-C16
21	C	477	CLA	C6-C7-C8-C10
21	C	477	CLA	C12-C13-C15-C16
21	C	479	CLA	C11-C12-C13-C15
21	C	480	CLA	C11-C12-C13-C15
21	C	480	CLA	C12-C13-C15-C16
21	C	485	CLA	C6-C7-C8-C10
21	D	354	CLA	C11-C12-C13-C15
22	D	355	PHO	C6-C7-C8-C10
21	A	362	CLA	C6-C7-C8-C9
21	A	362	CLA	C14-C13-C15-C16
21	A	363	CLA	C14-C13-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	B	522	CLA	C6-C7-C8-C9
21	B	522	CLA	C11-C12-C13-C14
21	B	523	CLA	C14-C13-C15-C16
21	B	524	CLA	C6-C7-C8-C9
21	B	525	CLA	C14-C13-C15-C16
21	C	477	CLA	C14-C13-C15-C16
21	C	480	CLA	C14-C13-C15-C16
21	C	483	CLA	C14-C13-C15-C16
21	C	477	CLA	CBA-CGA-O2A-C1
26	A	371	LHG	C9-C10-C11-C12
27	A	373	LMG	C29-C30-C31-C32
21	B	521	CLA	CBA-CGA-O2A-C1
21	C	480	CLA	CBA-CGA-O2A-C1
30	L	213	SQD	C17-C18-C19-C20
28	B	528	DGD	O6E-C1E-O5D-C6D
21	B	524	CLA	C4-C3-C5-C6
32	D	357	PL9	C12-C11-C9-C10
32	D	357	PL9	C45-C44-C46-C47
22	D	355	PHO	C2-C3-C5-C6
22	D	355	PHO	C3-C5-C6-C7
21	B	524	CLA	C2C-C3C-CAC-CBC
28	B	528	DGD	C2B-C3B-C4B-C5B
21	D	356	CLA	CBA-CGA-O2A-C1
28	A	375	DGD	O1G-C1G-C2G-C3G
28	B	533	DGD	O1G-C1G-C2G-C3G
28	B	528	DGD	C1G-C2G-C3G-O3G
28	C	491	DGD	C1G-C2G-C3G-O3G
28	C	492	DGD	C1G-C2G-C3G-O3G
30	D	361	SQD	O6-C44-C45-C46
21	B	521	CLA	O1A-CGA-O2A-C1
21	B	515	CLA	CBA-CGA-O2A-C1
26	A	371	LHG	O2-C2-C3-O3
21	C	485	CLA	C10-C11-C12-C13
30	D	361	SQD	C12-C13-C14-C15
26	C	476	LHG	O7-C5-C6-O8
27	B	531	LMG	O7-C8-C9-O8
27	D	360	LMG	O7-C8-C9-O8
28	B	533	DGD	O2G-C2G-C3G-O3G
28	C	491	DGD	O2G-C2G-C3G-O3G
26	C	476	LHG	C9-C10-C11-C12
30	C	475	SQD	O5-C1-O6-C44
21	C	482	CLA	C2-C1-O2A-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	A	366	CLA	C11-C12-C13-C14
21	A	364	CLA	C6-C7-C8-C9
21	B	514	CLA	C11-C12-C13-C14
21	B	520	CLA	C11-C12-C13-C14
21	B	521	CLA	C6-C7-C8-C9
27	D	360	LMG	C15-C16-C17-C18
21	B	517	CLA	C2A-CAA-CBA-CGA
25	J	115	BCR	C5-C6-C7-C8
21	B	517	CLA	C10-C11-C12-C13
29	A	376	LMT	C3'-C4'-O1B-C1B
21	A	362	CLA	C6-C7-C8-C10
21	A	362	CLA	C12-C13-C15-C16
21	A	363	CLA	C12-C13-C15-C16
21	A	366	CLA	C12-C13-C15-C16
21	A	364	CLA	C12-C13-C15-C16
21	B	511	CLA	C11-C12-C13-C15
21	B	511	CLA	C12-C13-C15-C16
21	B	514	CLA	C11-C12-C13-C15
21	B	518	CLA	C11-C12-C13-C15
21	B	520	CLA	C11-C12-C13-C15
21	B	523	CLA	C12-C13-C15-C16
21	B	524	CLA	C6-C7-C8-C10
21	C	478	CLA	C12-C13-C15-C16
21	C	481	CLA	C11-C12-C13-C15
21	C	486	CLA	C12-C13-C15-C16
22	D	355	PHO	C12-C13-C15-C16
32	D	357	PL9	C43-C44-C46-C47
21	A	364	CLA	CBA-CGA-O2A-C1
21	C	479	CLA	C10-C11-C12-C13
21	B	513	CLA	CAA-CBA-CGA-O2A
28	B	528	DGD	C4B-C5B-C6B-C7B
21	B	512	CLA	CAD-CBD-CGD-O2D
21	B	520	CLA	CAD-CBD-CGD-O2D
21	C	478	CLA	CAD-CBD-CGD-O2D
21	C	483	CLA	CAD-CBD-CGD-O2D
27	I	220	LMG	C7-C8-O7-C10
28	A	375	DGD	C3G-C2G-O2G-C1B
28	C	491	DGD	C3G-C2G-O2G-C1B
28	C	492	DGD	C1G-C2G-O2G-C1B
28	C	493	DGD	C3G-C2G-O2G-C1B
25	J	115	BCR	C22-C23-C24-C25
26	C	476	LHG	C4-C5-C6-O8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
27	D	360	LMG	C7-C8-C9-O8
27	J	492	LMG	C7-C8-C9-O8
28	B	533	DGD	C1G-C2G-C3G-O3G
28	C	493	DGD	C1G-C2G-C3G-O3G
28	D	362	DGD	C1G-C2G-C3G-O3G
21	B	519	CLA	C13-C15-C16-C17
30	L	213	SQD	C16-C17-C18-C19
21	A	366	CLA	CHA-CBD-CGD-O1D
21	A	366	CLA	CHA-CBD-CGD-O2D
21	B	522	CLA	CHA-CBD-CGD-O1D
21	B	522	CLA	CHA-CBD-CGD-O2D
21	C	480	CLA	CHA-CBD-CGD-O1D
21	C	485	CLA	CHA-CBD-CGD-O1D
21	C	485	CLA	CHA-CBD-CGD-O2D
21	C	487	CLA	CHA-CBD-CGD-O1D
21	C	487	CLA	CHA-CBD-CGD-O2D
21	K	483	CLA	CHA-CBD-CGD-O1D
21	K	483	CLA	CHA-CBD-CGD-O2D
22	A	365	PHO	C3-C5-C6-C7
21	A	364	CLA	O1A-CGA-O2A-C1
21	B	515	CLA	O1A-CGA-O2A-C1
28	B	528	DGD	O2G-C2G-C3G-O3G
26	A	371	LHG	C25-C26-C27-C28
21	D	356	CLA	O1A-CGA-O2A-C1
21	B	511	CLA	C4-C3-C5-C6
21	A	366	CLA	C14-C13-C15-C16
21	D	354	CLA	C2A-CAA-CBA-CGA
21	C	478	CLA	C10-C11-C12-C13
21	B	526	CLA	CBA-CGA-O2A-C1
26	C	476	LHG	C26-C27-C28-C29
26	A	371	LHG	C2-C3-O3-P
21	B	511	CLA	C2-C3-C5-C6
28	B	528	DGD	C2A-C3A-C4A-C5A
21	B	526	CLA	O1A-CGA-O2A-C1
26	C	476	LHG	C4-O6-P-O4
21	B	519	CLA	C10-C11-C12-C13
21	B	511	CLA	C2A-CAA-CBA-CGA
21	B	513	CLA	C2A-CAA-CBA-CGA
30	L	213	SQD	C14-C15-C16-C17
21	B	522	CLA	CAD-CBD-CGD-O1D
21	B	524	CLA	CAD-CBD-CGD-O1D
21	C	485	CLA	CAD-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	C	487	CLA	CAD-CBD-CGD-O1D
23	A	367	MES	C7-C8-S-O1S
30	C	475	SQD	C5-C6-S-O9
21	B	514	CLA	C12-C13-C15-C16
22	A	365	PHO	C12-C13-C15-C16
30	C	475	SQD	C9-C10-C11-C12
30	C	475	SQD	C12-C13-C14-C15
21	B	524	CLA	C4C-C3C-CAC-CBC
27	I	220	LMG	O1-C7-C8-O7
28	A	375	DGD	O2G-C2G-C3G-O3G
28	B	533	DGD	O1G-C1G-C2G-O2G
28	C	474	DGD	O1G-C1G-C2G-O2G
28	D	362	DGD	O2G-C2G-C3G-O3G
30	L	213	SQD	O6-C44-C45-O47
27	D	360	LMG	C30-C31-C32-C33
21	B	518	CLA	C14-C13-C15-C16
21	B	523	CLA	C6-C7-C8-C9
21	C	478	CLA	C14-C13-C15-C16
21	C	481	CLA	C11-C12-C13-C14
21	C	488	CLA	C11-C12-C13-C14
27	A	373	LMG	C35-C36-C37-C38
21	C	481	CLA	CBA-CGA-O2A-C1
28	C	474	DGD	C1G-C2G-O2G-C1B
28	D	362	DGD	C1G-C2G-O2G-C1B
21	B	523	CLA	C2-C1-O2A-CGA
21	B	524	CLA	C2-C1-O2A-CGA
21	C	479	CLA	C2-C1-O2A-CGA
21	C	484	CLA	C2-C1-O2A-CGA
27	A	373	LMG	C18-C19-C20-C21
21	B	524	CLA	C2-C3-C5-C6
26	A	371	LHG	O7-C5-C6-O8
28	C	493	DGD	O1G-C1G-C2G-O2G
26	A	371	LHG	C3-O3-P-O6
26	C	476	LHG	C3-O3-P-O6
27	D	360	LMG	C19-C20-C21-C22
28	C	492	DGD	O1G-C1G-C2G-C3G
30	L	213	SQD	O6-C44-C45-C46
21	B	512	CLA	C6-C7-C8-C10
29	B	535	LMT	C3'-C4'-O1B-C1B
21	B	511	CLA	C14-C13-C15-C16
21	B	514	CLA	C14-C13-C15-C16
21	C	479	CLA	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	C	486	CLA	C14-C13-C15-C16
22	D	355	PHO	C6-C7-C8-C9
26	A	371	LHG	C1-C2-C3-O3
21	C	485	CLA	C4-C3-C5-C6
21	B	517	CLA	CBA-CGA-O2A-C1
30	L	213	SQD	C13-C14-C15-C16
27	D	360	LMG	C18-C19-C20-C21
21	B	517	CLA	O1A-CGA-O2A-C1
21	A	366	CLA	C3-C5-C6-C7
21	B	520	CLA	O1A-CGA-O2A-C1
21	B	520	CLA	C13-C15-C16-C17
26	C	476	LHG	C11-C10-C9-C8
26	C	476	LHG	C10-C11-C12-C13
21	B	521	CLA	C2-C1-O2A-CGA
33	F	85	HEM	CAA-CBA-CGA-O1A
21	B	513	CLA	C11-C12-C13-C14
21	B	520	CLA	C6-C7-C8-C9
21	B	526	CLA	C11-C12-C13-C14
21	C	482	CLA	C11-C12-C13-C14
30	L	213	SQD	C44-C45-C46-O48
21	B	516	CLA	C3-C5-C6-C7
21	C	488	CLA	C2C-C3C-CAC-CBC
21	A	362	CLA	O2A-C1-C2-C3
28	B	528	DGD	O6D-C1D-O3G-C3G
21	B	526	CLA	C13-C15-C16-C17
28	B	533	DGD	C1G-C2G-O2G-C1B
21	B	526	CLA	C6-C7-C8-C10
21	C	482	CLA	C11-C12-C13-C15
21	C	487	CLA	C6-C7-C8-C10
21	A	364	CLA	C13-C15-C16-C17
21	B	522	CLA	C4-C3-C5-C6
30	D	361	SQD	C11-C10-C9-C8
21	B	520	CLA	CBA-CGA-O2A-C1
33	F	85	HEM	CAA-CBA-CGA-O2A
21	B	526	CLA	C2-C1-O2A-CGA
21	D	356	CLA	C2-C1-O2A-CGA
22	D	355	PHO	C2-C1-O2A-CGA
21	C	485	CLA	C2-C3-C5-C6
21	B	525	CLA	C11-C12-C13-C14
32	D	357	PL9	C2-C3-C7-C8
21	C	482	CLA	CAA-CBA-CGA-O2A
21	C	484	CLA	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	C	475	SQD	O6-C44-C45-C46
21	B	519	CLA	C4-C3-C5-C6
21	C	481	CLA	C4-C3-C5-C6
32	D	357	PL9	C15-C14-C16-C17
32	D	357	PL9	C30-C29-C31-C32
21	B	518	CLA	CAA-CBA-CGA-O2A
33	F	85	HEM	CAD-CBD-CGD-O1D
33	F	85	HEM	CAD-CBD-CGD-O2D
33	V	164	HEM	CAD-CBD-CGD-O1D
30	C	475	SQD	C11-C10-C9-C8
21	B	526	CLA	C4-C3-C5-C6
21	A	366	CLA	C11-C12-C13-C15
21	B	522	CLA	C2-C3-C5-C6
21	B	522	CLA	C6-C7-C8-C10
21	B	526	CLA	C11-C12-C13-C15
21	B	521	CLA	C10-C11-C12-C13
21	C	480	CLA	CAA-CBA-CGA-O2A
33	V	164	HEM	CAD-CBD-CGD-O2D
21	B	513	CLA	CAA-CBA-CGA-O1A
21	C	483	CLA	CAA-CBA-CGA-O2A
21	A	364	CLA	C4-C3-C5-C6
27	A	373	LMG	C32-C33-C34-C35
21	B	512	CLA	C6-C7-C8-C9
21	D	356	CLA	C6-C7-C8-C9
22	A	365	PHO	C14-C13-C15-C16
22	D	355	PHO	CAA-CBA-CGA-O2A
21	B	519	CLA	CAD-CBD-CGD-O2D
21	B	521	CLA	CAD-CBD-CGD-O2D
21	B	525	CLA	CAD-CBD-CGD-O2D
21	C	488	CLA	CAD-CBD-CGD-O2D
22	A	365	PHO	CAD-CBD-CGD-O2D
22	D	355	PHO	CAD-CBD-CGD-O2D
33	V	164	HEM	CAA-CBA-CGA-O2A
21	B	520	CLA	CAA-CBA-CGA-O2A
21	B	515	CLA	CAA-CBA-CGA-O2A
30	F	224	SQD	O6-C44-C45-C46
21	C	487	CLA	C2C-C3C-CAC-CBC
21	B	511	CLA	O2A-C1-C2-C3
21	B	512	CLA	O2A-C1-C2-C3
21	A	364	CLA	CHA-CBD-CGD-O1D
21	A	364	CLA	CHA-CBD-CGD-O2D
21	B	513	CLA	CHA-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	B	515	CLA	CHA-CBD-CGD-O2D
21	C	484	CLA	CHA-CBD-CGD-O1D
21	C	488	CLA	CHA-CBD-CGD-O1D
33	V	164	HEM	CAA-CBA-CGA-O1A
30	C	475	SQD	O47-C7-C8-C9
30	C	475	SQD	C15-C16-C17-C18
21	B	519	CLA	C2-C3-C5-C6
28	B	528	DGD	C2D-C1D-O3G-C3G
21	B	511	CLA	CAA-CBA-CGA-O2A
30	F	224	SQD	O47-C45-C46-O48
21	B	521	CLA	CAA-CBA-CGA-O2A
21	K	483	CLA	CAA-CBA-CGA-O2A
21	B	526	CLA	C2-C3-C5-C6
21	C	484	CLA	C11-C12-C13-C15
21	D	354	CLA	C6-C7-C8-C10
21	B	526	CLA	C6-C7-C8-C9
21	K	483	CLA	C14-C13-C15-C16
21	C	479	CLA	CAA-CBA-CGA-O2A
21	D	354	CLA	CAA-CBA-CGA-O2A
30	L	213	SQD	C4-C5-C6-S
30	F	224	SQD	C7-C8-C9-C10
32	D	357	PL9	C21-C22-C23-C24
21	C	480	CLA	CAA-CBA-CGA-O1A
26	C	476	LHG	C25-C26-C27-C28
30	D	361	SQD	C11-C12-C13-C14
22	A	365	PHO	C2-C3-C5-C6
21	C	483	CLA	CAA-CBA-CGA-O1A
22	D	355	PHO	C15-C16-C17-C18
22	D	355	PHO	CAA-CBA-CGA-O1A
30	C	475	SQD	O49-C7-C8-C9
28	C	474	DGD	O1G-C1G-C2G-C3G
25	X	107	BCR	C6-C7-C8-C9
21	B	521	CLA	CAA-CBA-CGA-O1A
25	J	115	BCR	C1-C6-C7-C8
21	B	511	CLA	CAA-CBA-CGA-O1A
21	B	520	CLA	CAA-CBA-CGA-O1A
30	L	213	SQD	O47-C7-C8-C9
21	A	364	CLA	C2C-C3C-CAC-CBC
32	D	357	PL9	C11-C12-C13-C14
32	D	357	PL9	C41-C42-C43-C44
21	B	513	CLA	CAD-CBD-CGD-O1D
21	B	518	CLA	CAD-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	F	224	SQD	C5-C6-S-O7
21	B	514	CLA	C13-C15-C16-C17
21	B	524	CLA	C14-C13-C15-C16
21	C	484	CLA	C11-C12-C13-C14
21	D	354	CLA	C6-C7-C8-C9
26	A	371	LHG	O7-C7-C8-C9
21	C	481	CLA	O1A-CGA-O2A-C1
21	B	519	CLA	CAA-CBA-CGA-O2A
26	C	476	LHG	O8-C23-C24-C25
21	A	364	CLA	C6-C7-C8-C10
21	B	513	CLA	C11-C12-C13-C15
21	B	521	CLA	C6-C7-C8-C10
21	C	481	CLA	C12-C13-C15-C16
21	D	356	CLA	C6-C7-C8-C10
21	K	483	CLA	CAA-CBA-CGA-O1A
30	F	224	SQD	C23-C24-C25-C26
26	A	371	LHG	O8-C23-C24-C25
21	B	514	CLA	CAA-CBA-CGA-O2A
21	D	354	CLA	CAA-CBA-CGA-O1A
21	C	484	CLA	C13-C15-C16-C17
30	L	213	SQD	C23-C24-C25-C26

There are no ring outliers.

76 monomers are involved in 704 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	C	483	CLA	13	0
21	A	363	CLA	14	0
30	D	361	SQD	9	0
21	C	477	CLA	12	0
21	B	518	CLA	15	0
25	Z	116	BCR	4	0
30	L	213	SQD	2	0
29	D	536	LMT	1	0
29	T	226	LMT	1	0
23	A	367	MES	13	0
33	V	164	HEM	5	0
21	D	356	CLA	5	0
21	A	366	CLA	10	0
21	B	520	CLA	7	0
21	B	512	CLA	9	0
25	D	358	BCR	8	0

Continued on next page...

Continued from previous page...

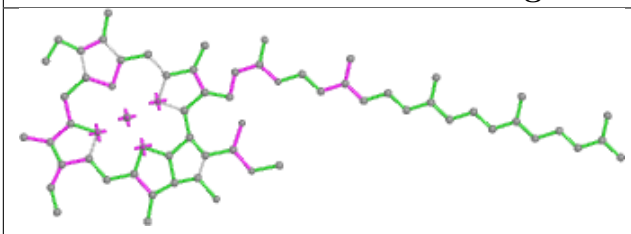
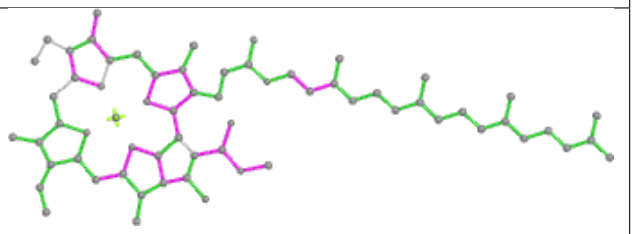
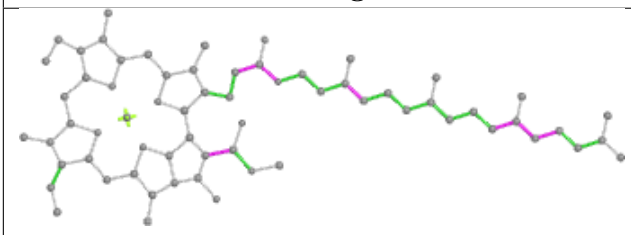
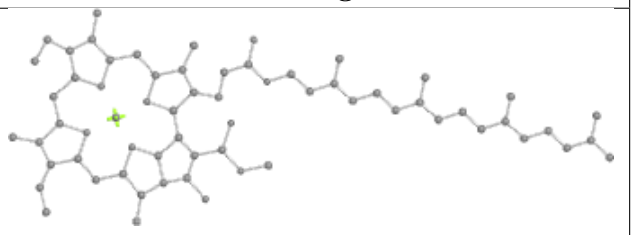
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	365	PHO	8	0
25	X	107	BCR	6	0
21	C	487	CLA	15	0
21	B	522	CLA	13	0
28	C	492	DGD	14	0
21	B	526	CLA	6	0
21	B	521	CLA	12	0
21	B	523	CLA	7	0
21	B	524	CLA	5	0
21	C	479	CLA	18	0
21	C	484	CLA	15	0
22	D	355	PHO	12	0
21	C	480	CLA	11	0
21	C	482	CLA	6	0
27	M	217	LMG	3	0
28	C	491	DGD	17	0
21	C	488	CLA	7	0
28	A	375	DGD	1	0
33	F	85	HEM	6	0
25	C	489	BCR	18	0
25	B	530	BCR	2	0
26	A	371	LHG	7	0
25	J	112	BCR	12	0
21	B	516	CLA	6	0
21	C	485	CLA	5	0
21	B	515	CLA	10	0
29	I	274	LMT	2	0
29	B	535	LMT	2	0
21	C	486	CLA	24	0
28	C	493	DGD	39	0
27	B	531	LMG	6	0
27	J	492	LMG	4	0
27	D	359	LMG	6	0
25	J	115	BCR	7	0
21	A	362	CLA	20	0
27	C	494	LMG	6	0
28	B	533	DGD	19	0
21	B	511	CLA	6	0
21	D	354	CLA	15	0
25	B	529	BCR	5	0
28	C	474	DGD	8	0
21	C	481	CLA	17	0

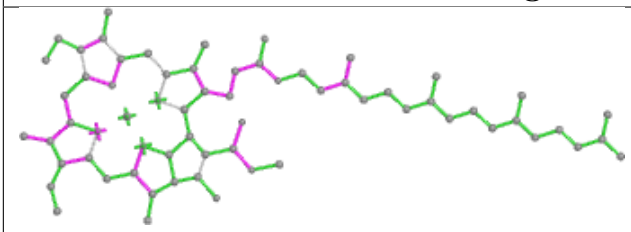
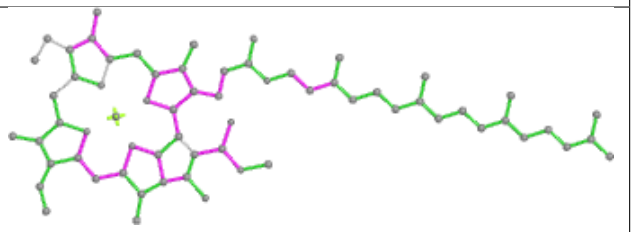
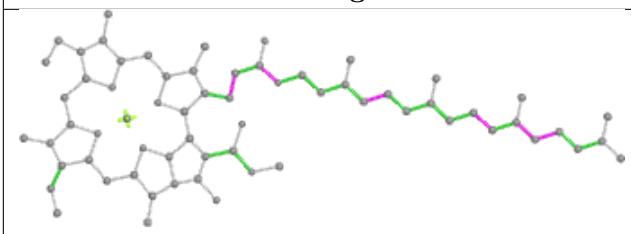
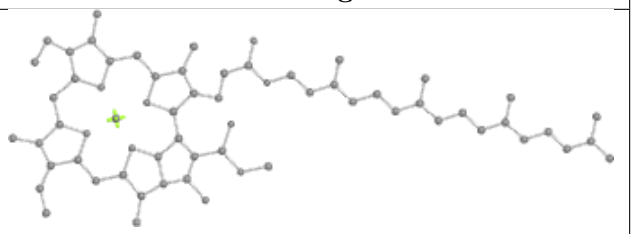
Continued on next page...

Continued from previous page...

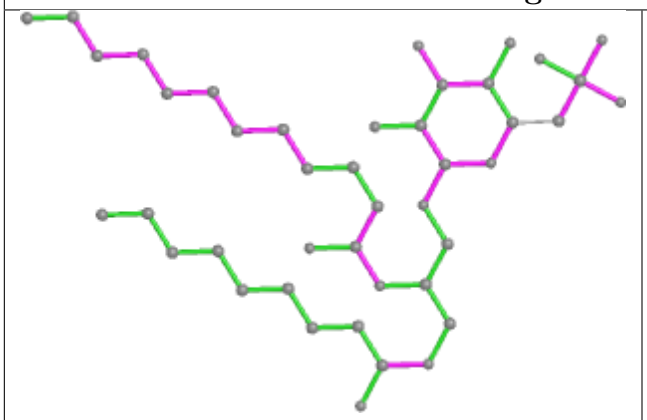
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	B	513	CLA	24	0
25	A	369	BCR	8	0
28	B	528	DGD	23	0
29	D	363	LMT	2	0
26	C	476	LHG	5	0
21	B	517	CLA	20	0
25	C	490	BCR	8	0
30	C	475	SQD	5	0
21	K	483	CLA	15	0
27	A	373	LMG	40	0
27	D	360	LMG	30	0
32	D	357	PL9	31	0
29	O	274	LMT	1	0
21	B	514	CLA	10	0
21	A	364	CLA	6	0
21	C	478	CLA	16	0
21	B	525	CLA	7	0
21	B	519	CLA	8	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.

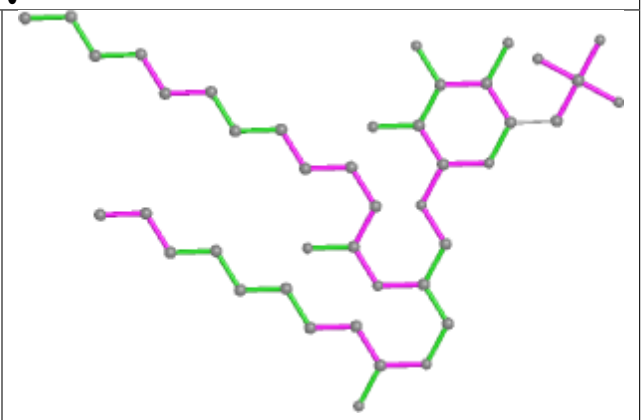
Ligand CLA C 483	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 363	
 Bond lengths	 Bond angles
 Torsions	 Rings

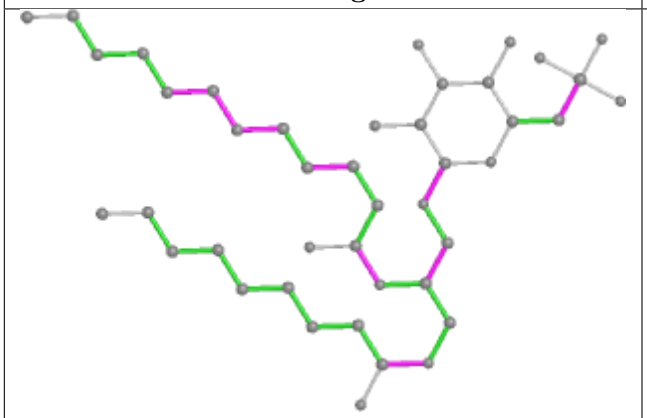
Ligand SQD D 361



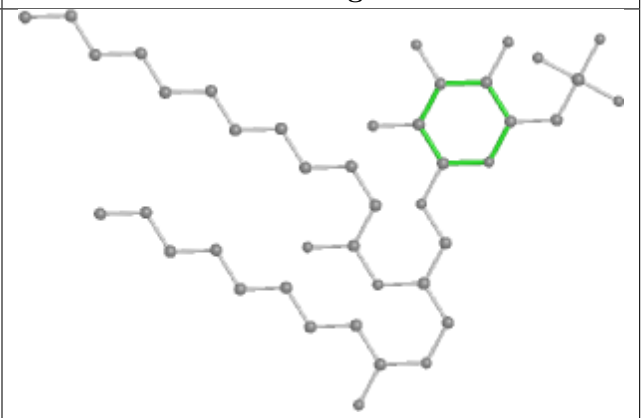
Bond lengths



Bond angles

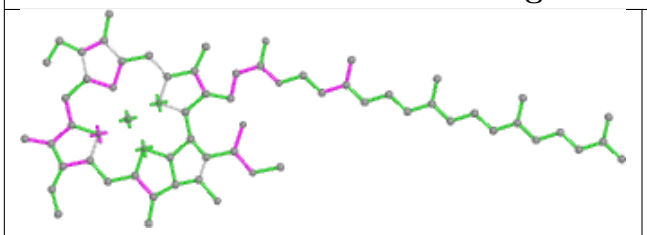


Torsions

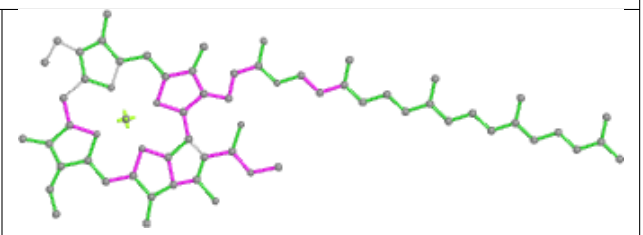


Rings

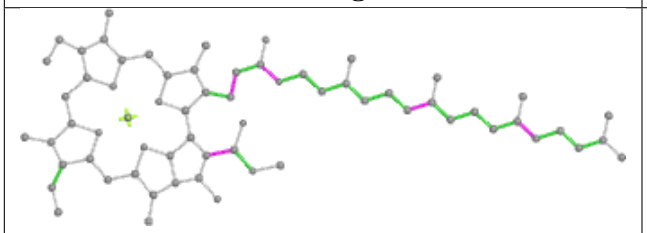
Ligand CLA C 477



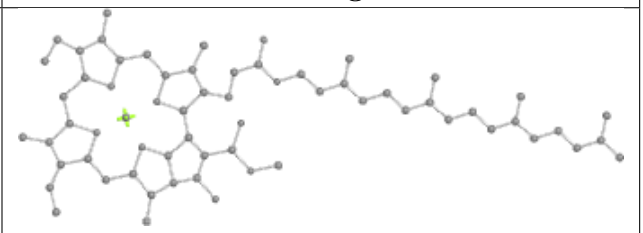
Bond lengths



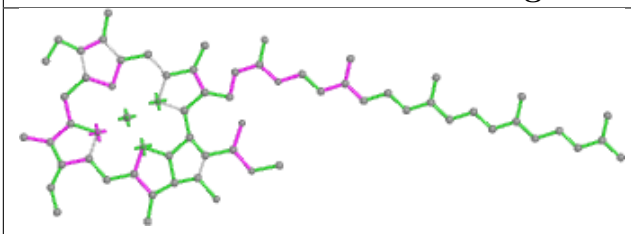
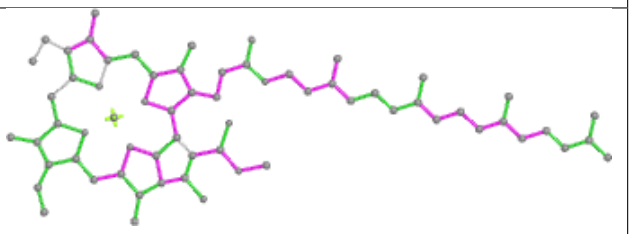
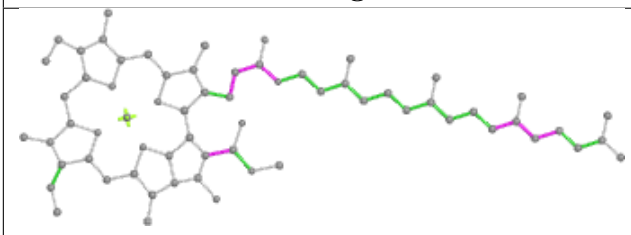
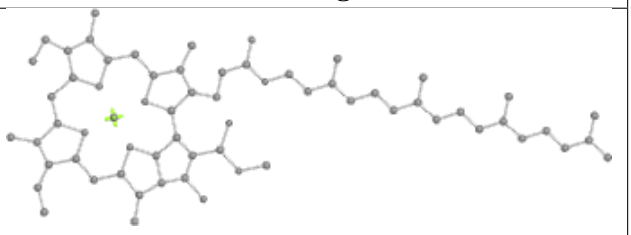
Bond angles

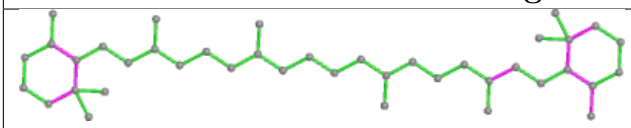
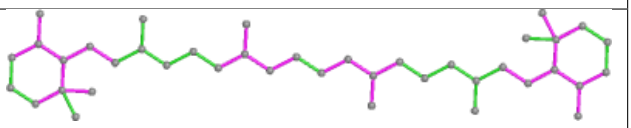
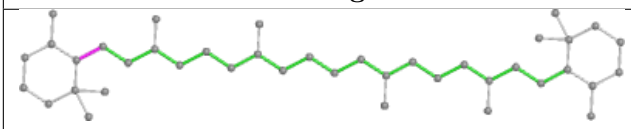


Torsions

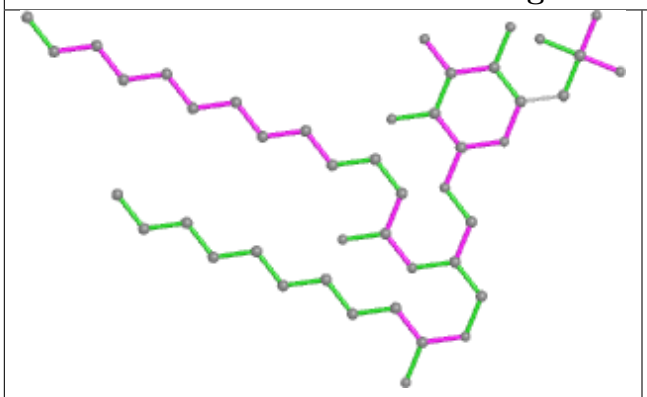


Rings

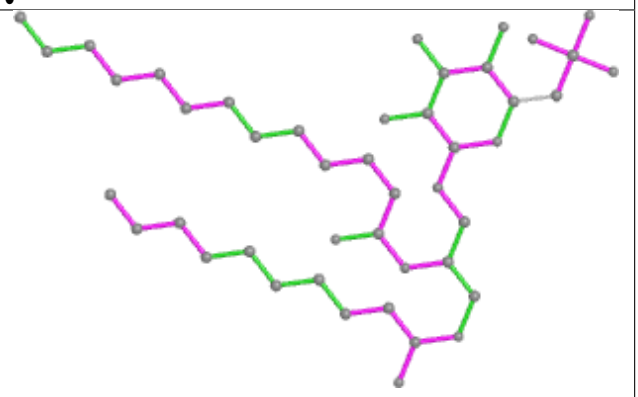
Ligand CLA B 518	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR Z 116	
 Bond lengths	 Bond angles
 Torsions	Rings

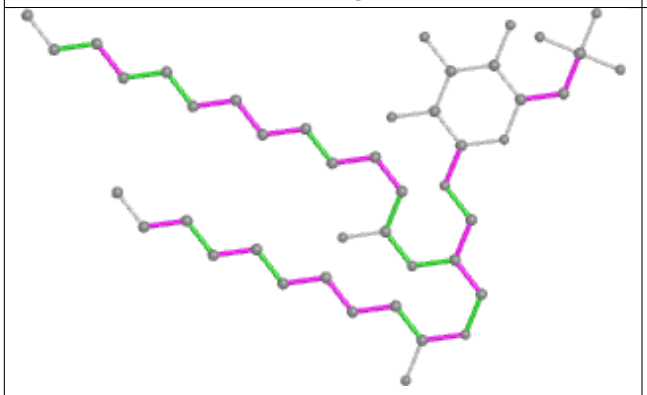
Ligand SQD F 224



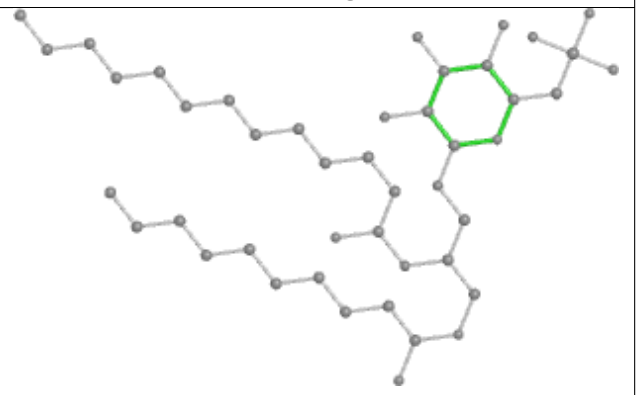
Bond lengths



Bond angles

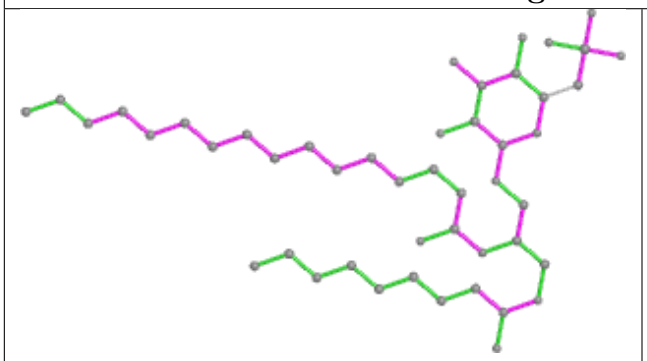


Torsions

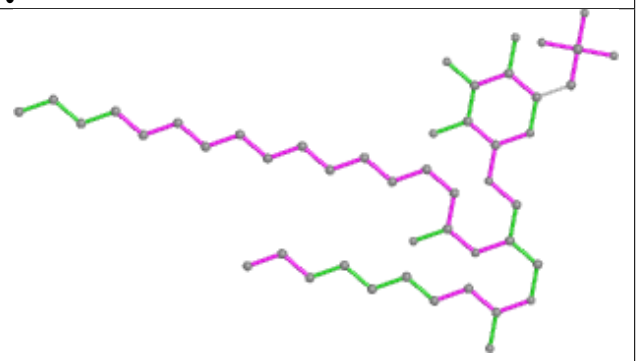


Rings

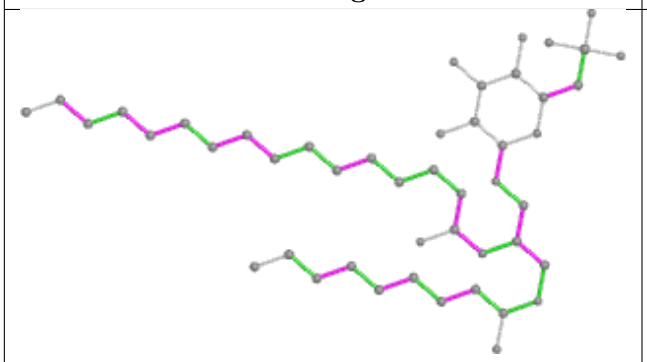
Ligand SQD L 213



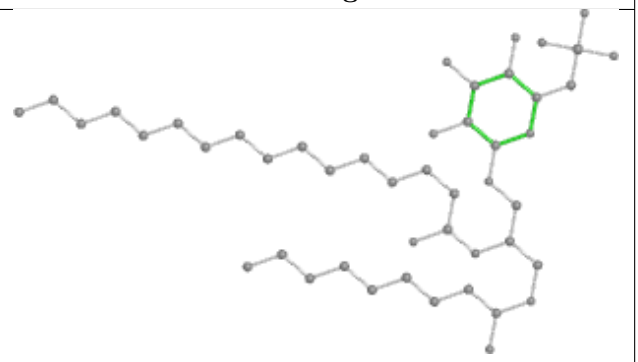
Bond lengths



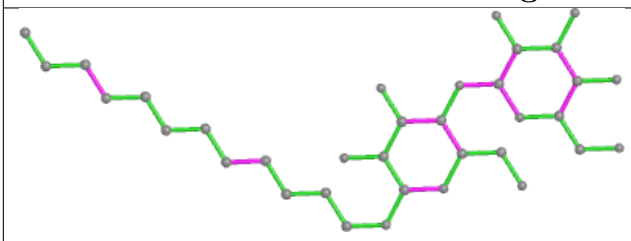
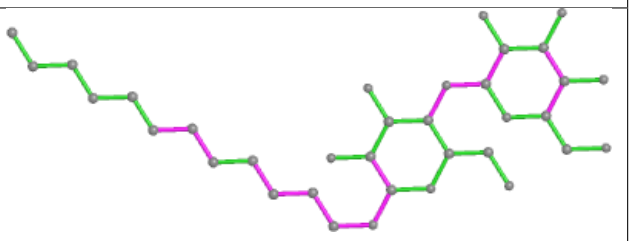
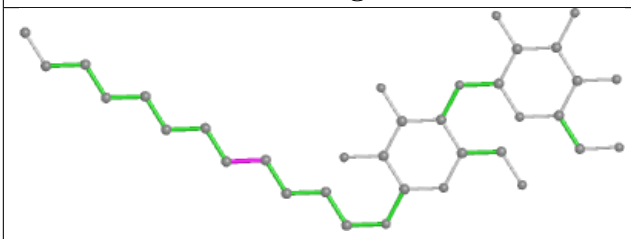
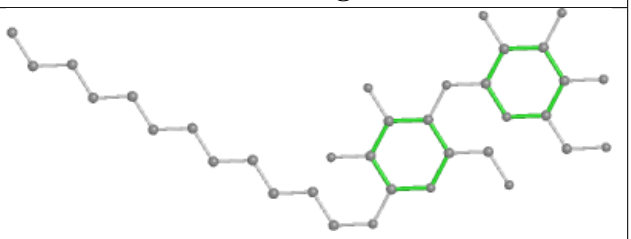
Bond angles

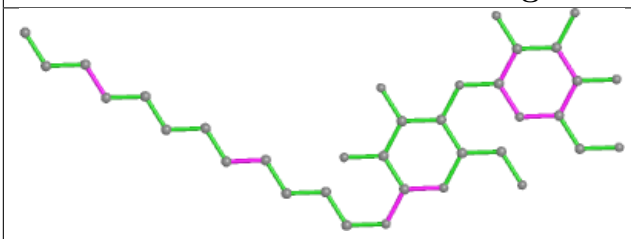
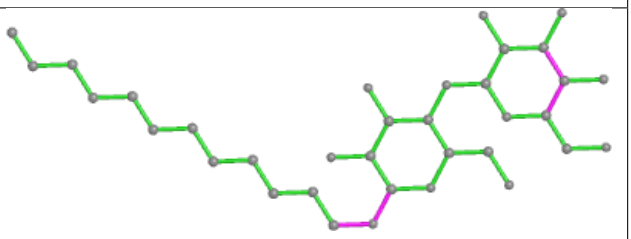
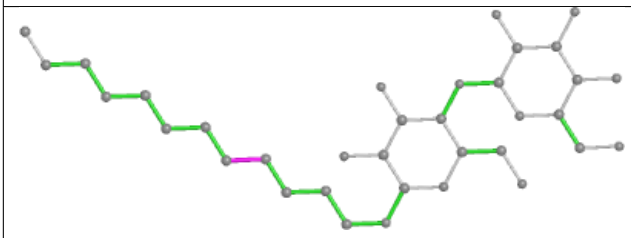
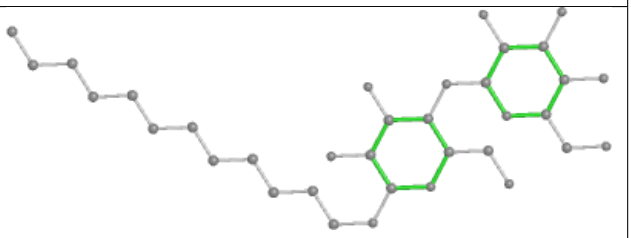


Torsions

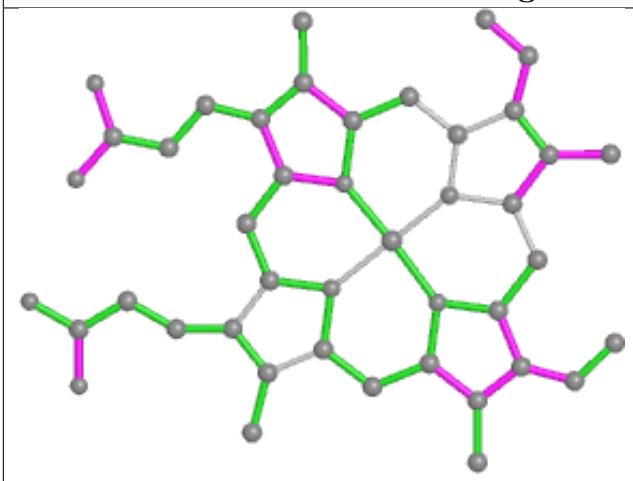


Rings

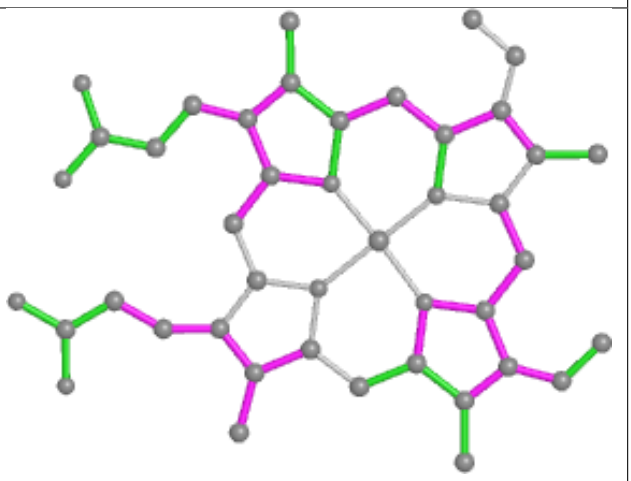
Ligand LMT D 536	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMT T 226	
 Bond lengths	 Bond angles
 Torsions	 Rings

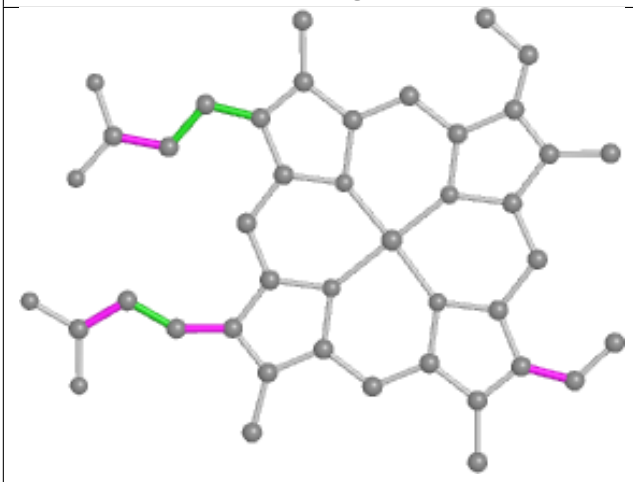
Ligand HEM V 164



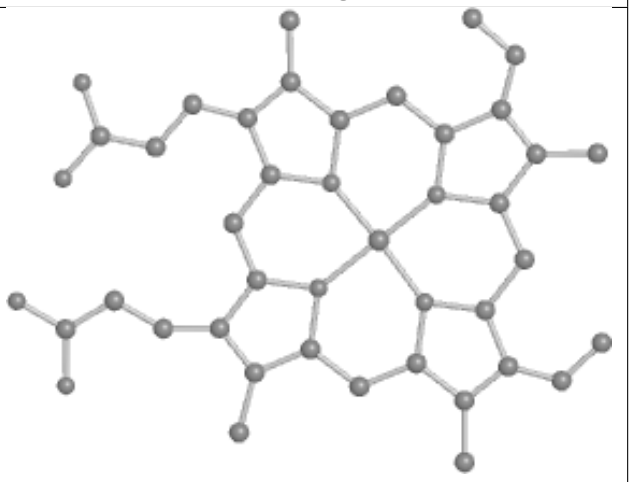
Bond lengths



Bond angles

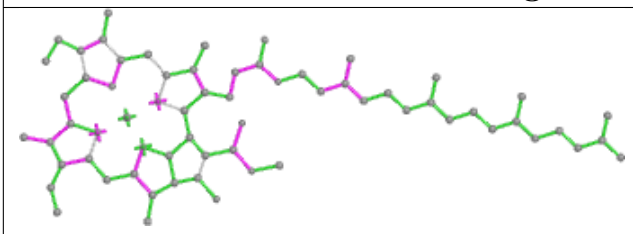


Torsions

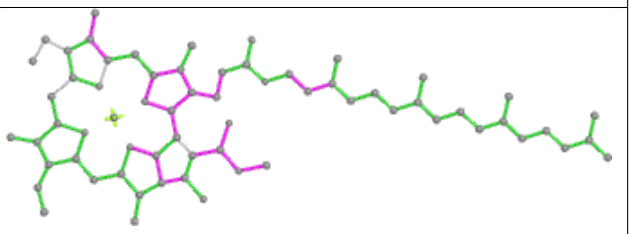


Rings

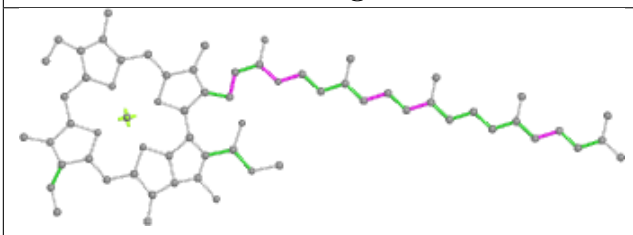
Ligand CLA D 356



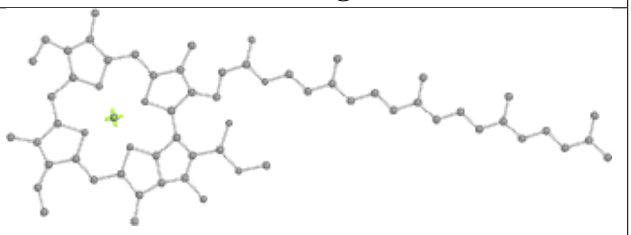
Bond lengths



Bond angles

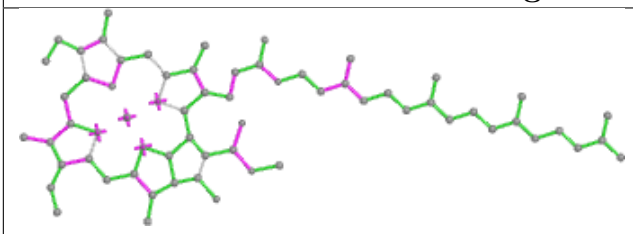


Torsions

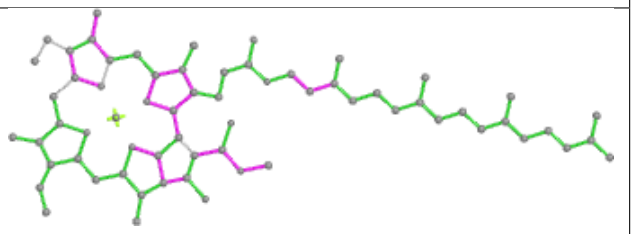


Rings

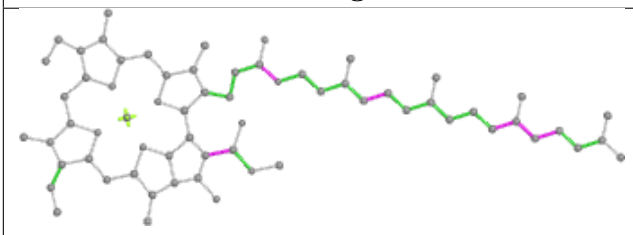
Ligand CLA A 366



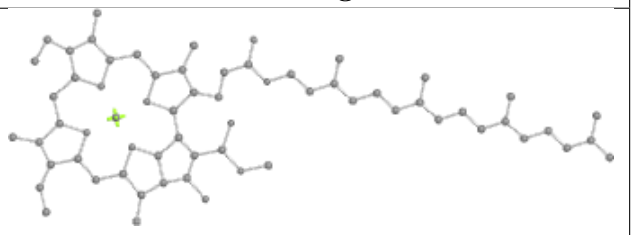
Bond lengths



Bond angles

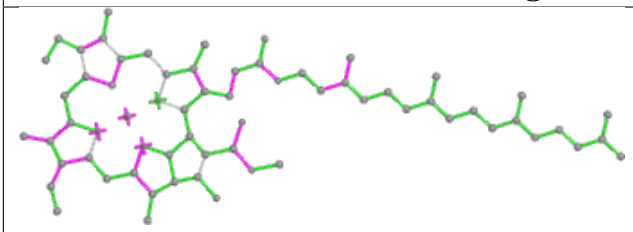


Torsions

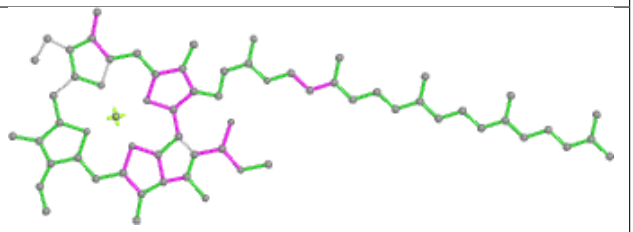


Rings

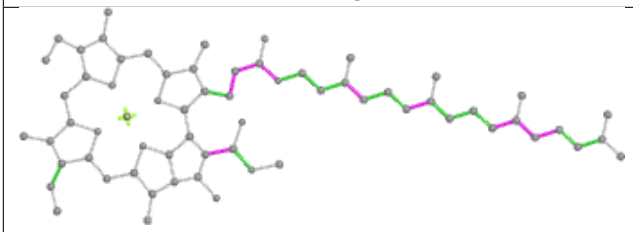
Ligand CLA B 520



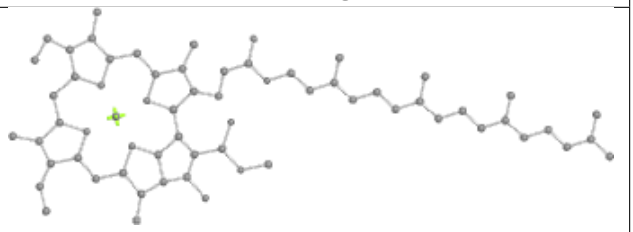
Bond lengths



Bond angles

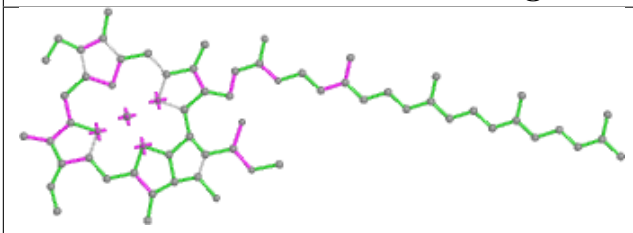


Torsions

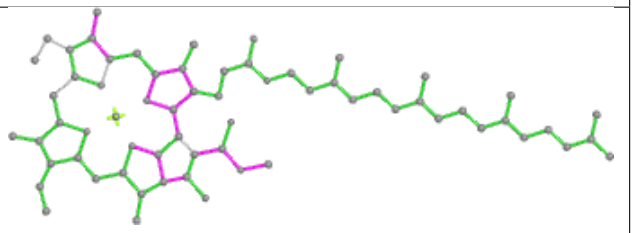


Rings

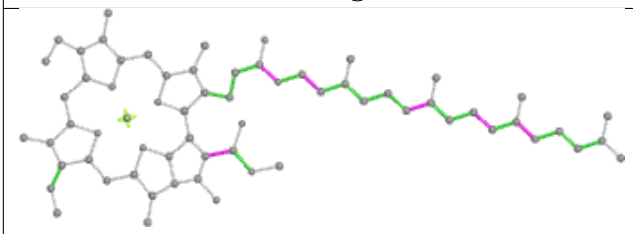
Ligand CLA B 512



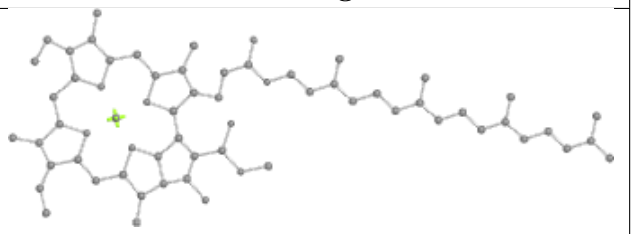
Bond lengths



Bond angles

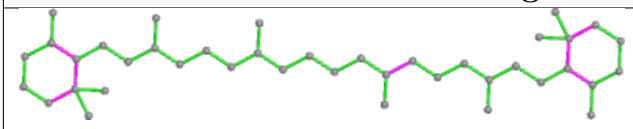


Torsions

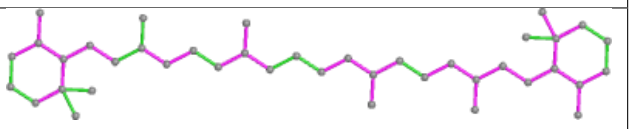


Rings

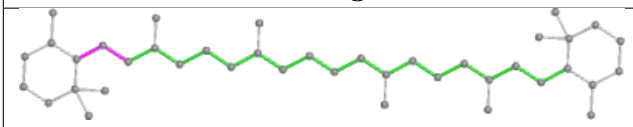
Ligand BCR D 358



Bond lengths



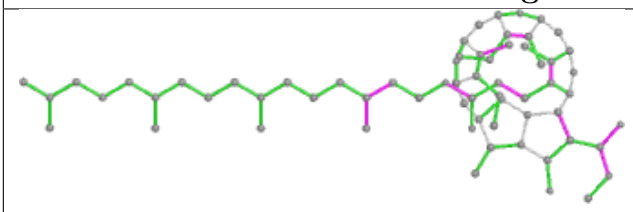
Bond angles



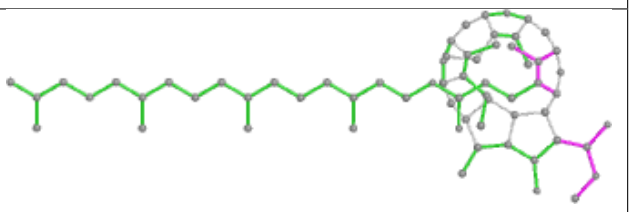
Torsions

Rings

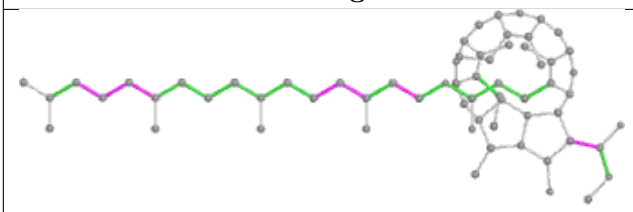
Ligand PHO A 365



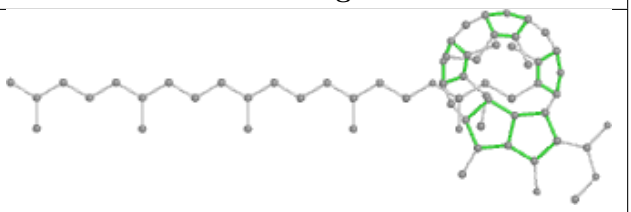
Bond lengths



Bond angles

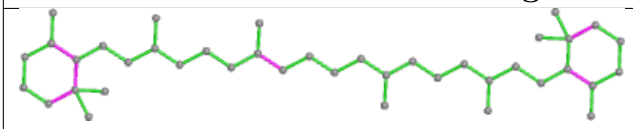


Torsions

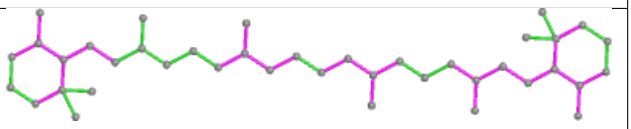


Rings

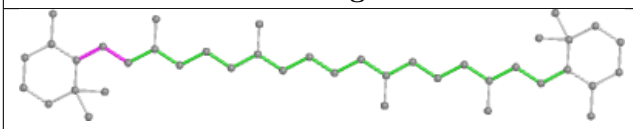
Ligand BCR X 107



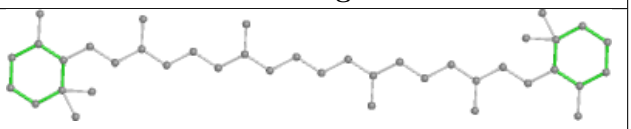
Bond lengths



Bond angles

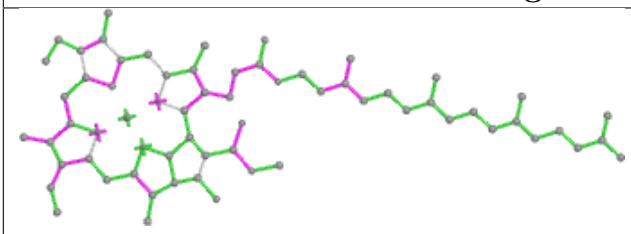


Torsions

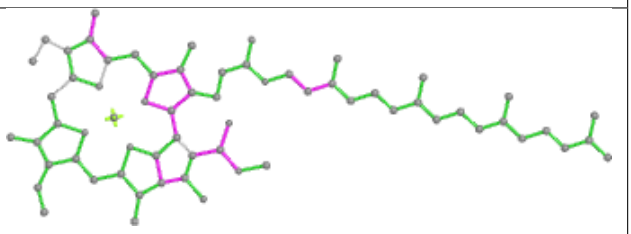


Rings

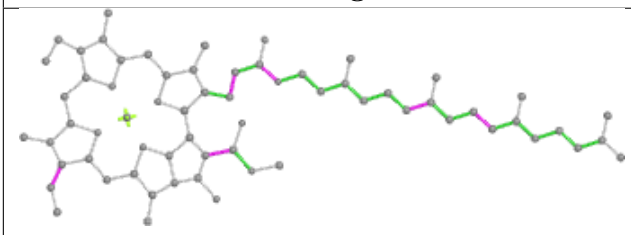
Ligand CLA C 487



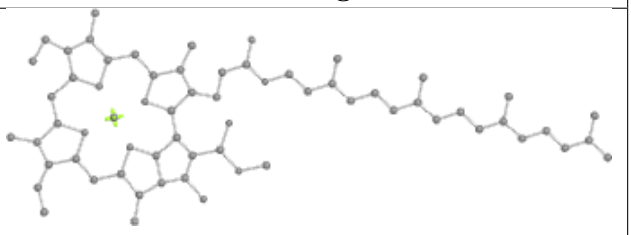
Bond lengths



Bond angles

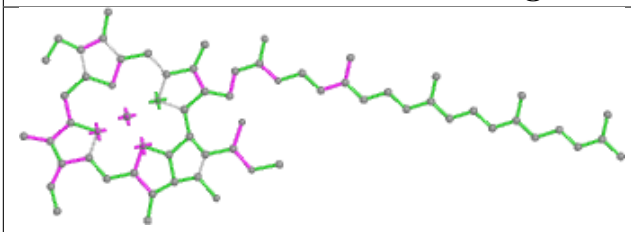


Torsions

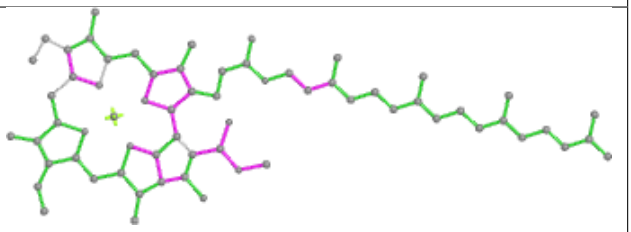


Rings

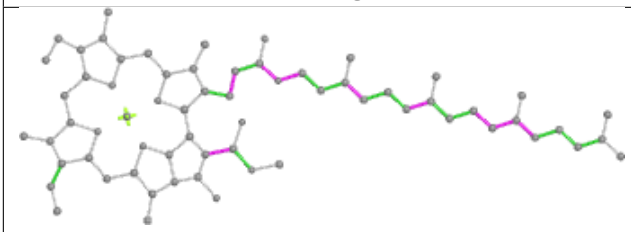
Ligand CLA B 522



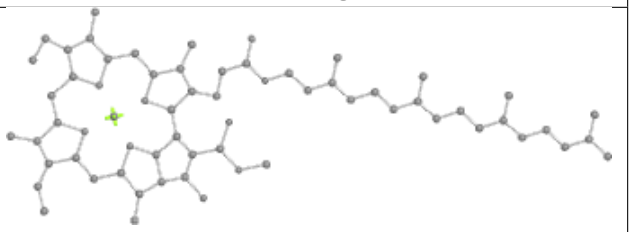
Bond lengths



Bond angles

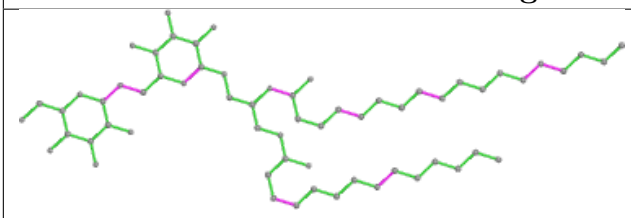


Torsions

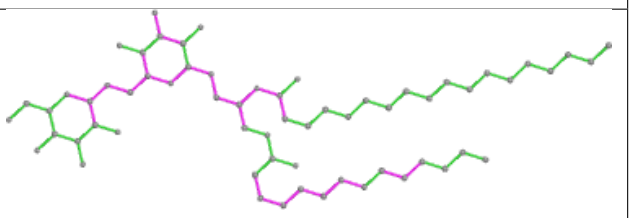


Rings

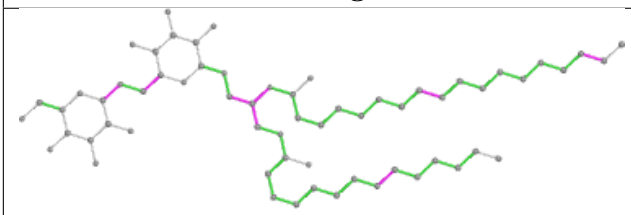
Ligand DGD C 492



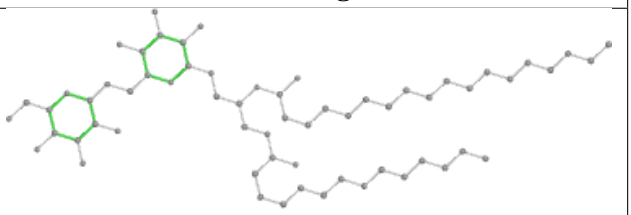
Bond lengths



Bond angles

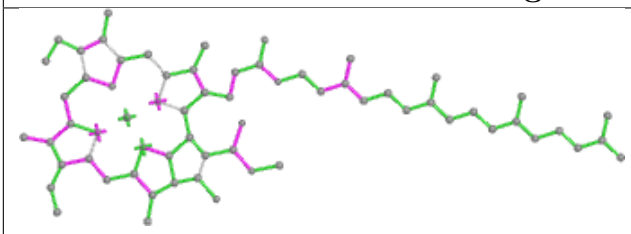


Torsions

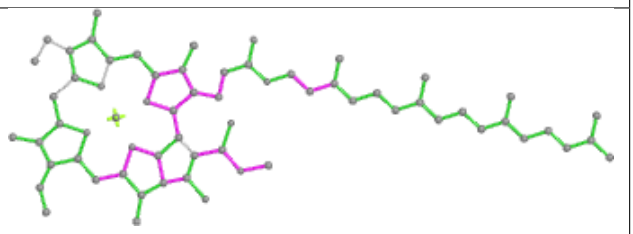


Rings

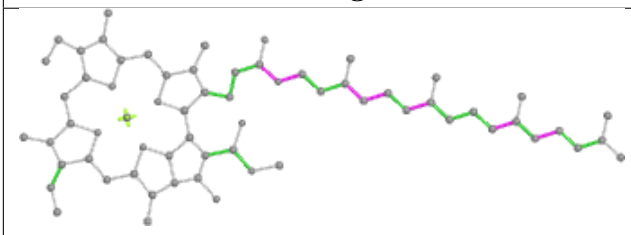
Ligand CLA B 526



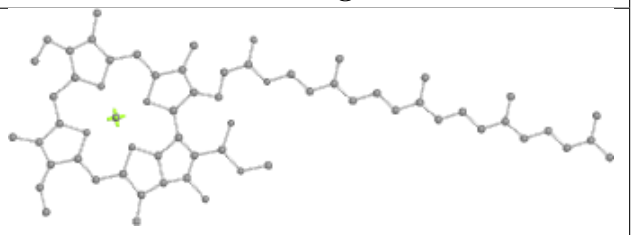
Bond lengths



Bond angles

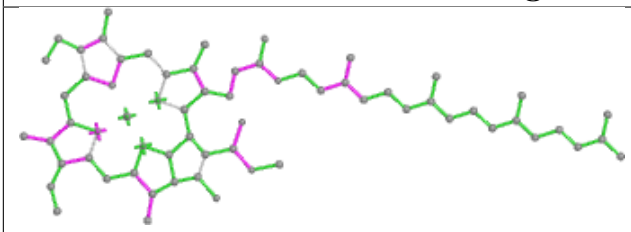


Torsions

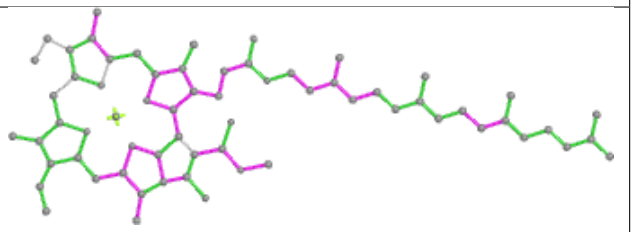


Rings

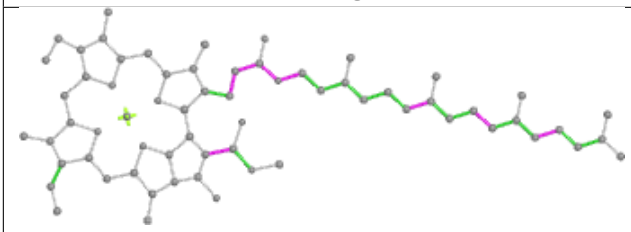
Ligand CLA B 521



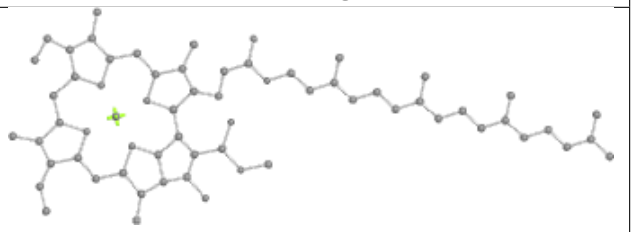
Bond lengths



Bond angles

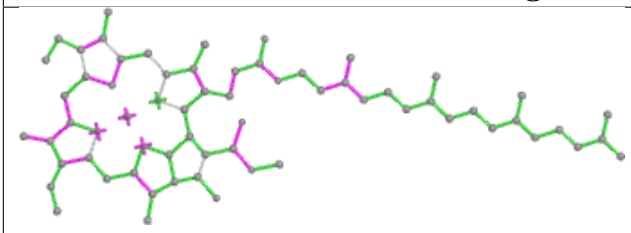


Torsions

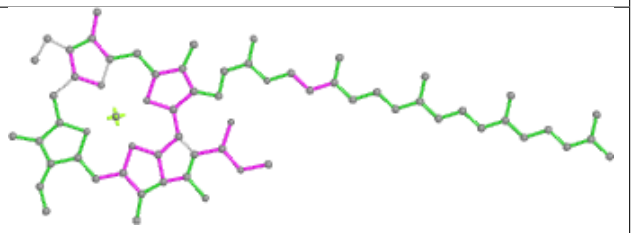


Rings

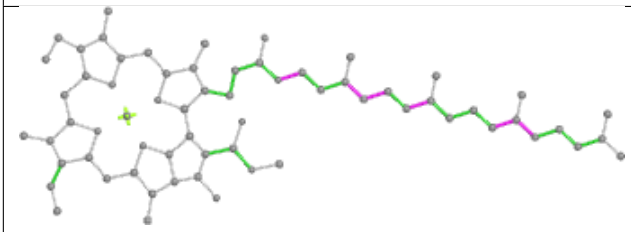
Ligand CLA B 523



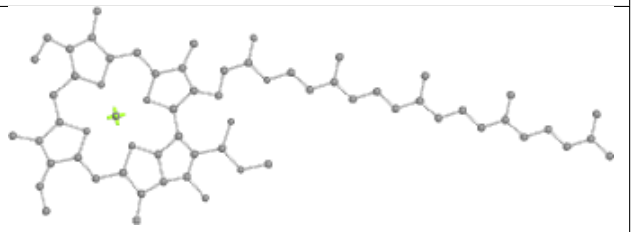
Bond lengths



Bond angles

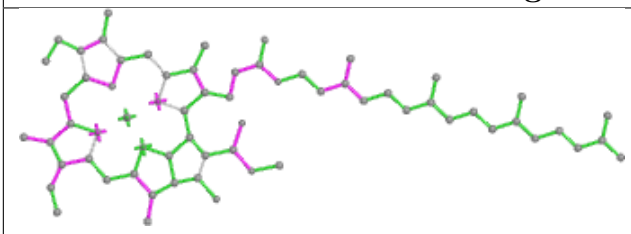


Torsions

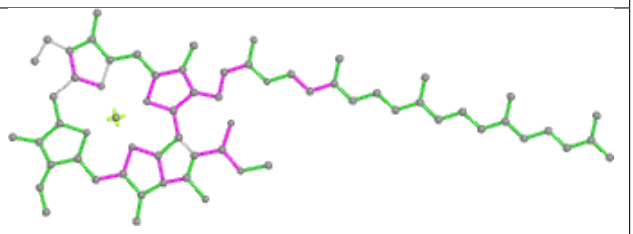


Rings

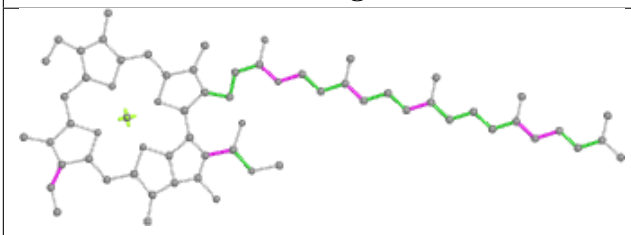
Ligand CLA B 524



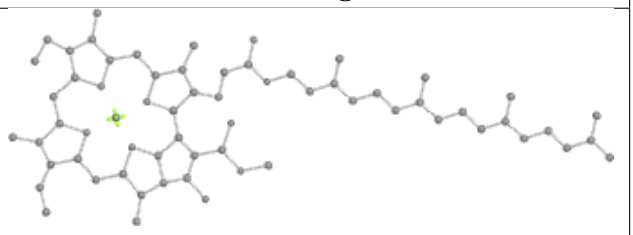
Bond lengths



Bond angles

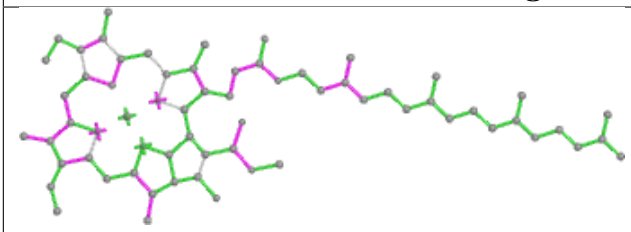


Torsions

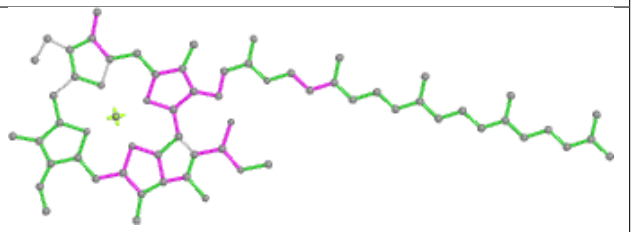


Rings

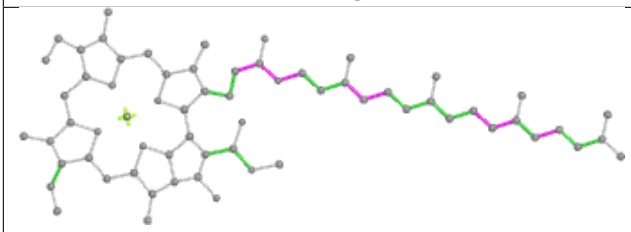
Ligand CLA C 479



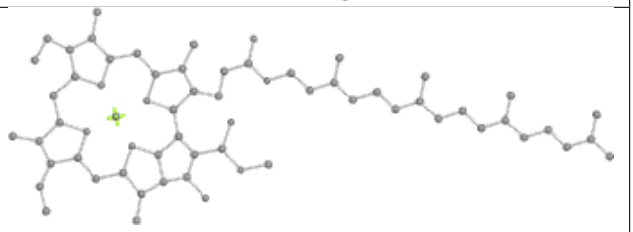
Bond lengths



Bond angles

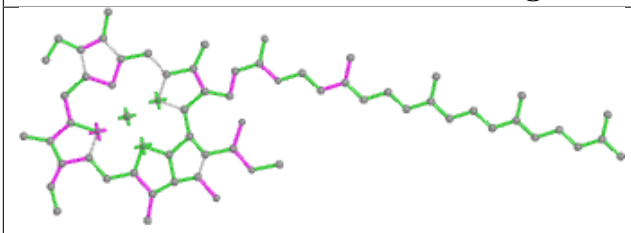


Torsions

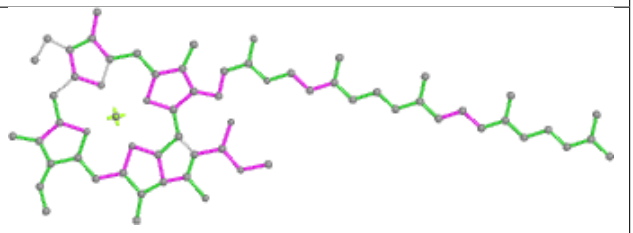


Rings

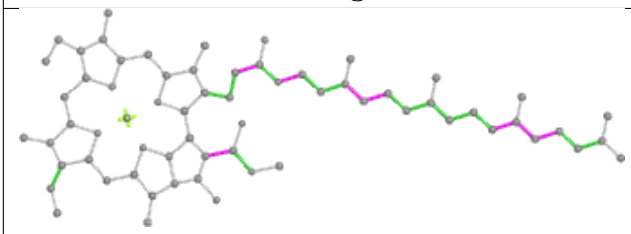
Ligand CLA C 484



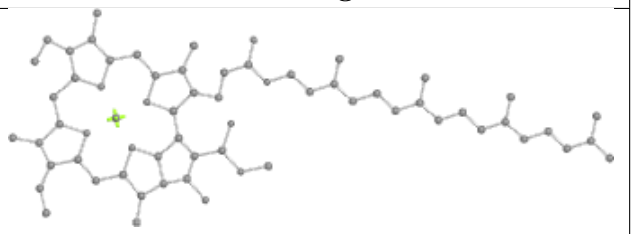
Bond lengths



Bond angles

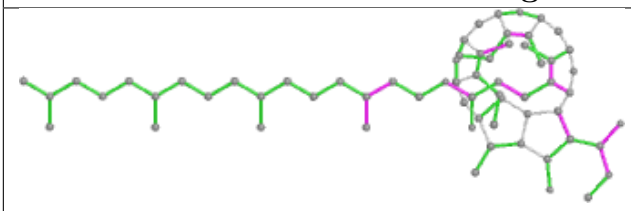


Torsions

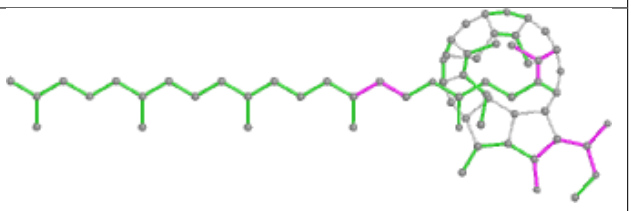


Rings

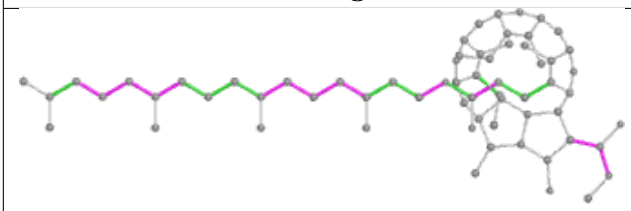
Ligand PHO D 355



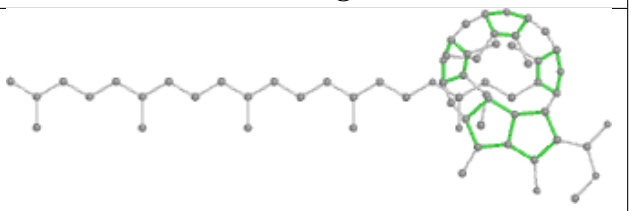
Bond lengths



Bond angles

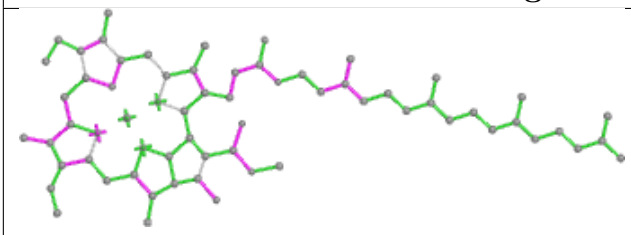


Torsions

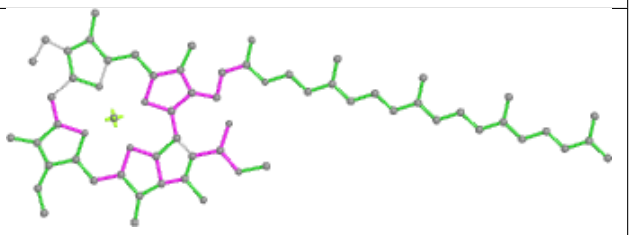


Rings

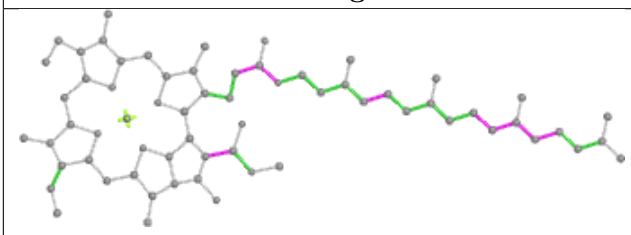
Ligand CLA C 480



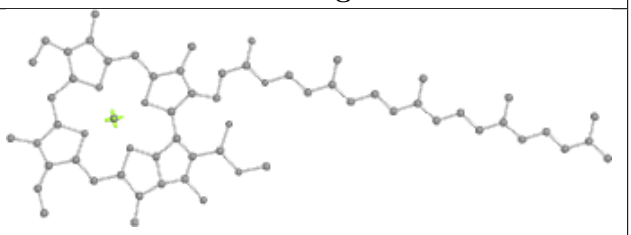
Bond lengths



Bond angles

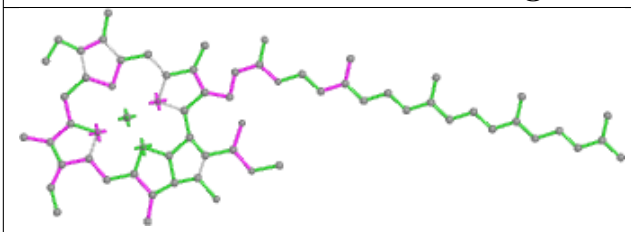


Torsions

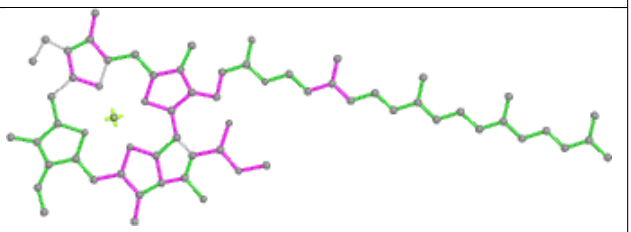


Rings

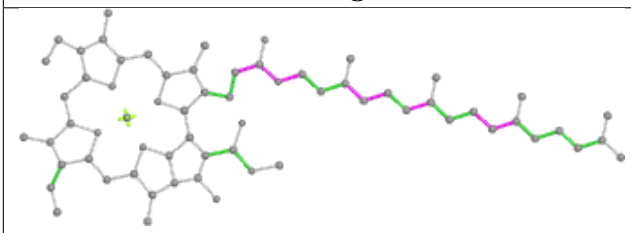
Ligand CLA C 482



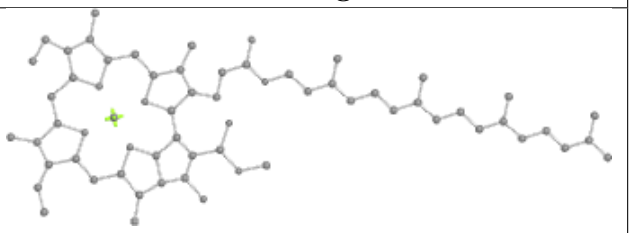
Bond lengths



Bond angles

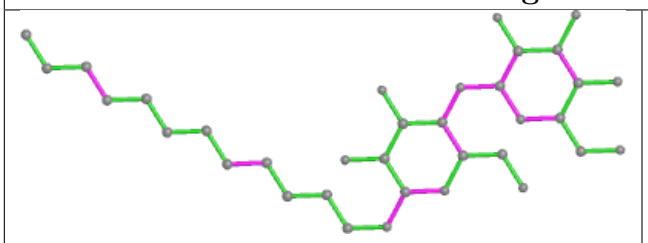


Torsions

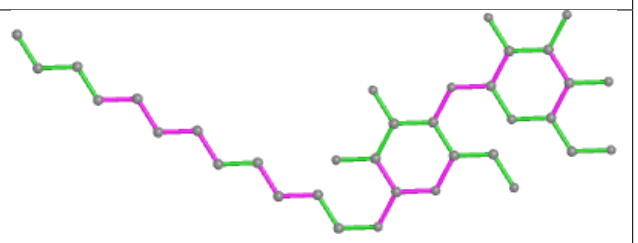


Rings

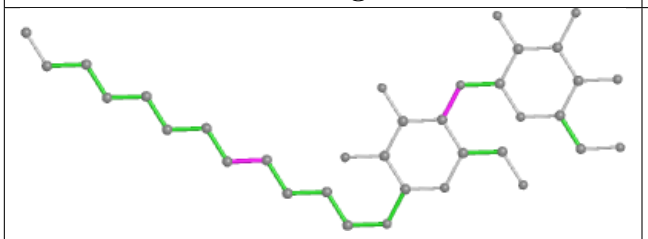
Ligand LMT A 376



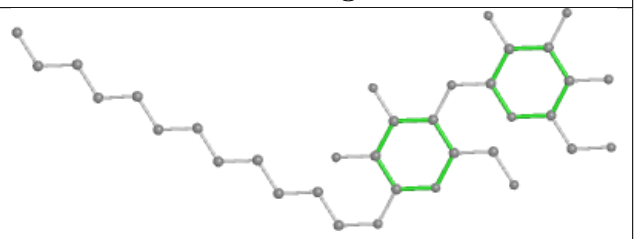
Bond lengths



Bond angles

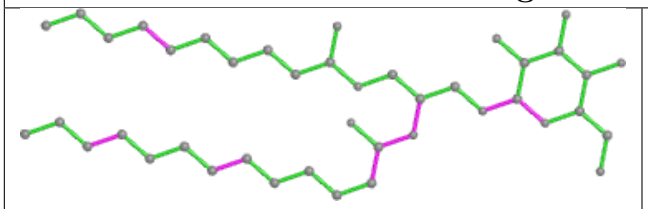


Torsions

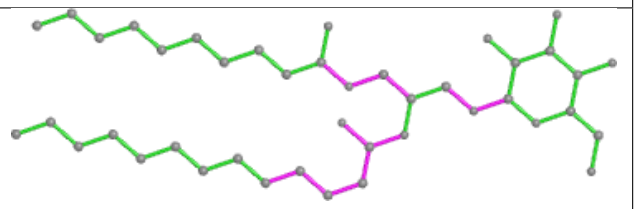


Rings

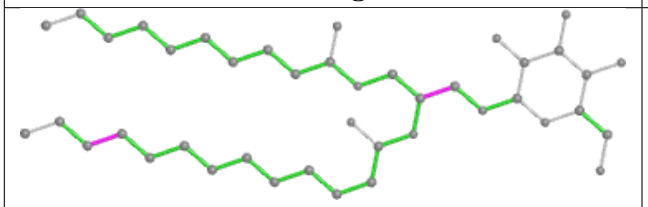
Ligand LMG M 217



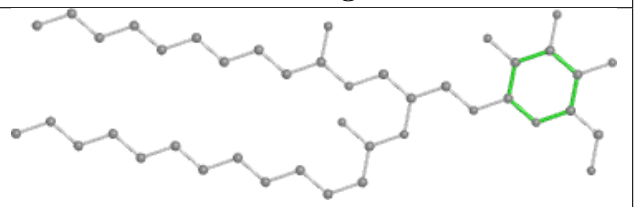
Bond lengths



Bond angles

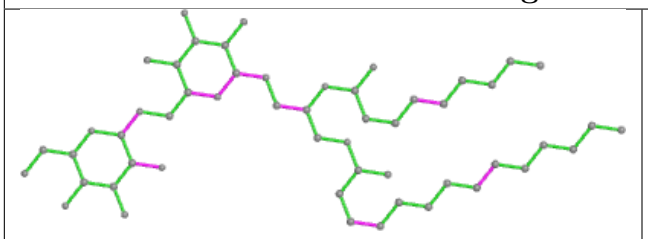


Torsions

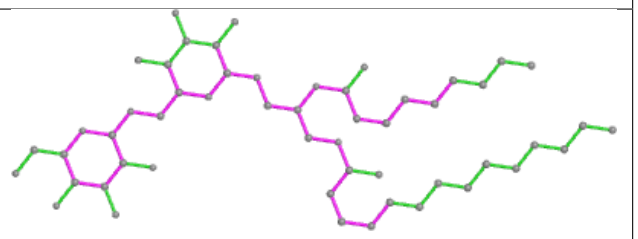


Rings

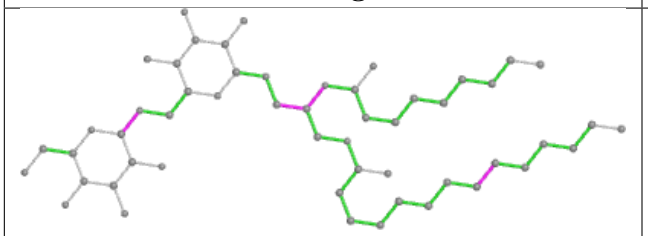
Ligand DGD C 491



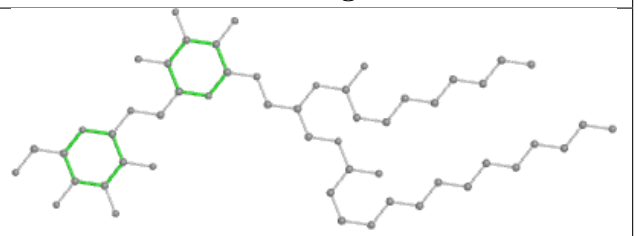
Bond lengths



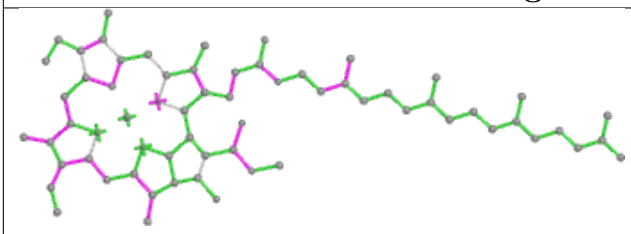
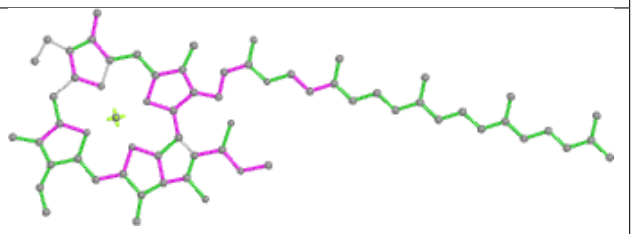
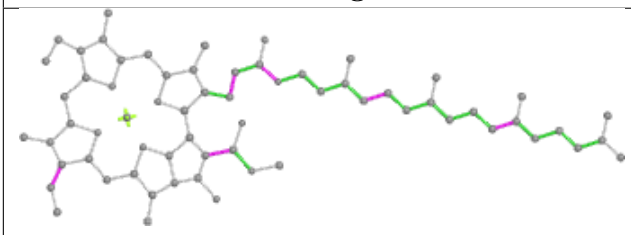
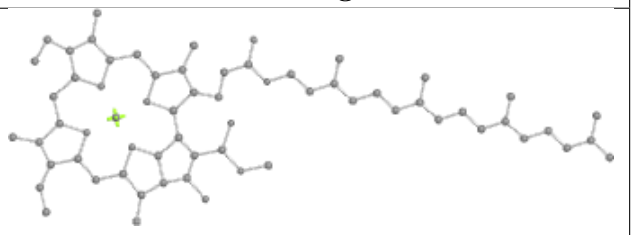
Bond angles

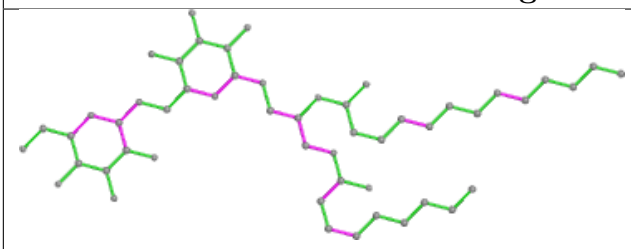
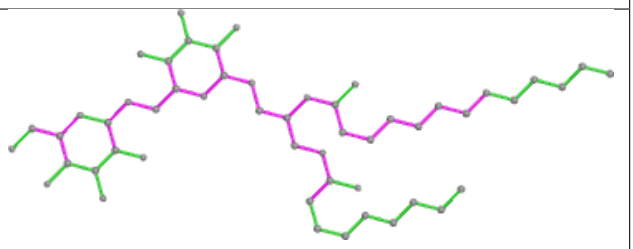
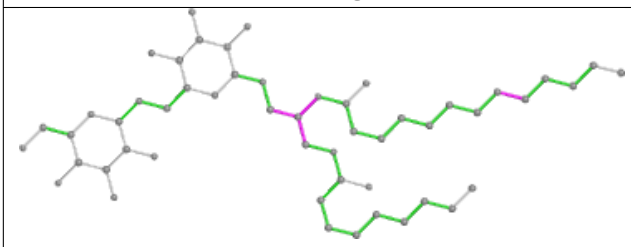
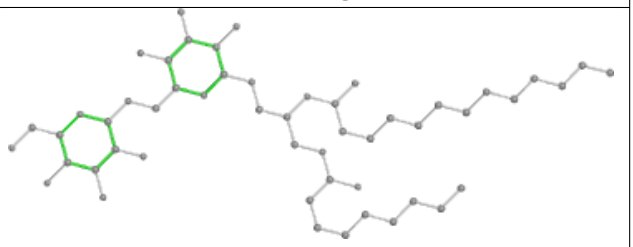


Torsions

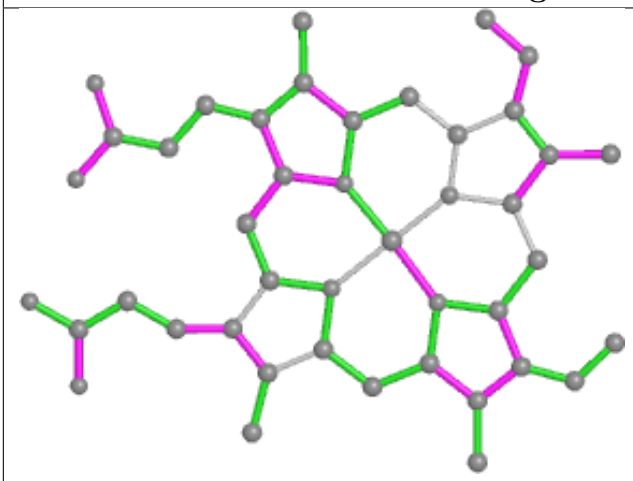


Rings

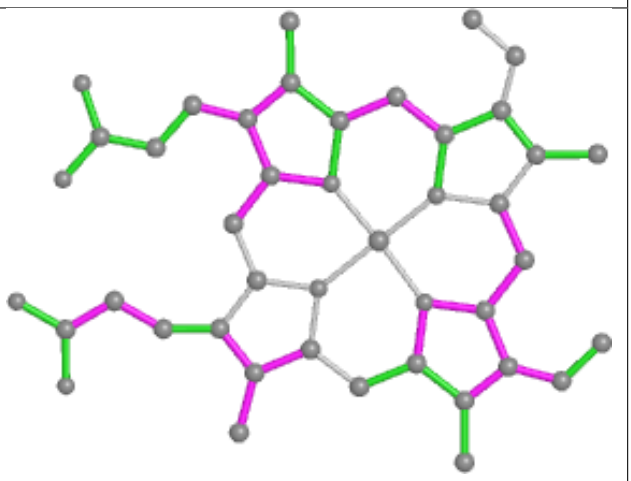
Ligand CLA C 488	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand DGD A 375	
 Bond lengths	 Bond angles
 Torsions	 Rings

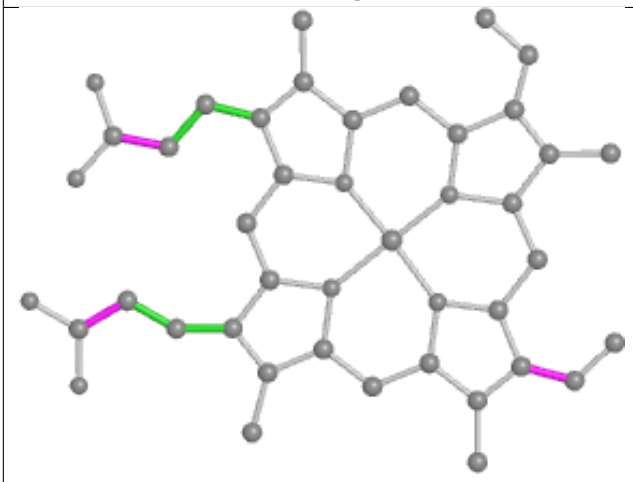
Ligand HEM F 85



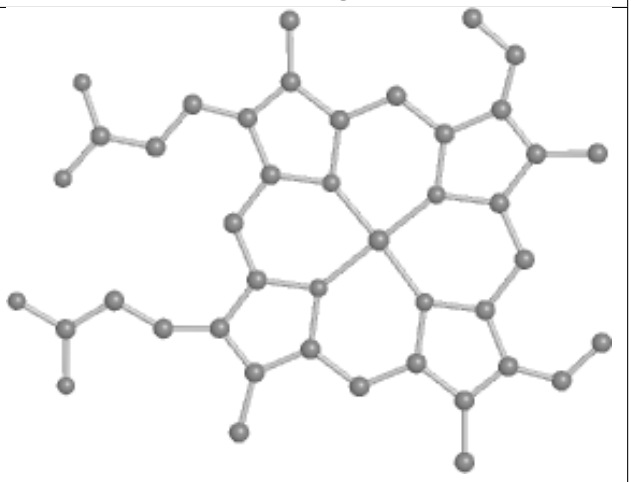
Bond lengths



Bond angles

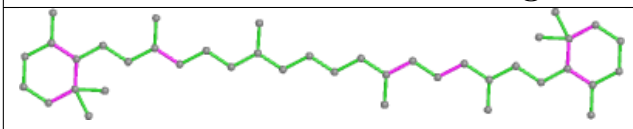


Torsions

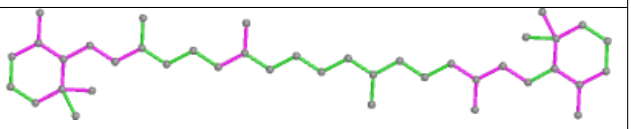


Rings

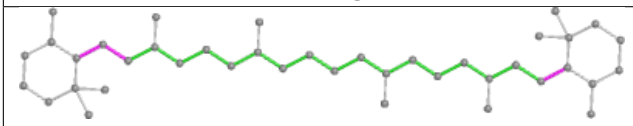
Ligand BCR C 489



Bond lengths



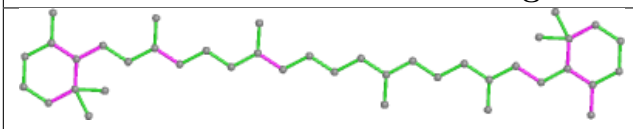
Bond angles



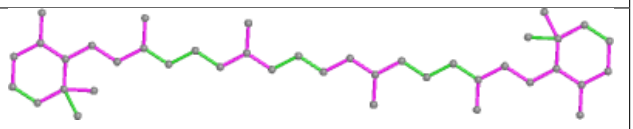
Torsions

Rings

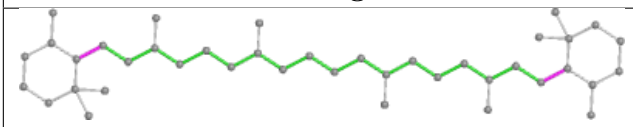
Ligand BCR B 530



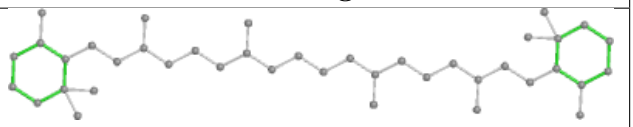
Bond lengths



Bond angles

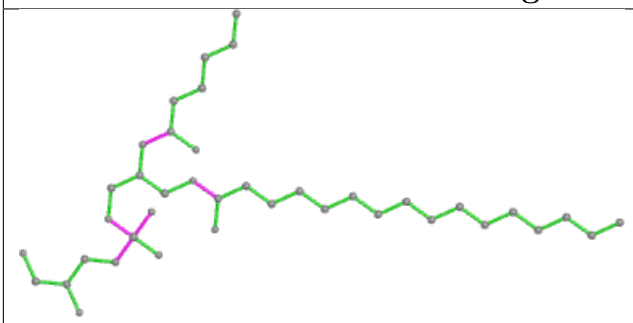


Torsions

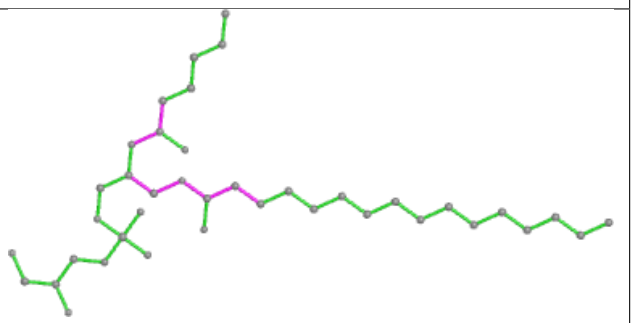


Rings

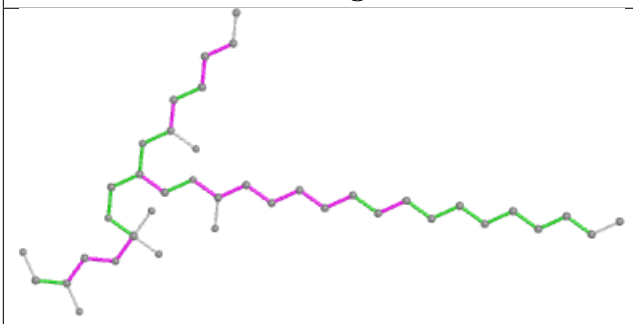
Ligand LHG A 371



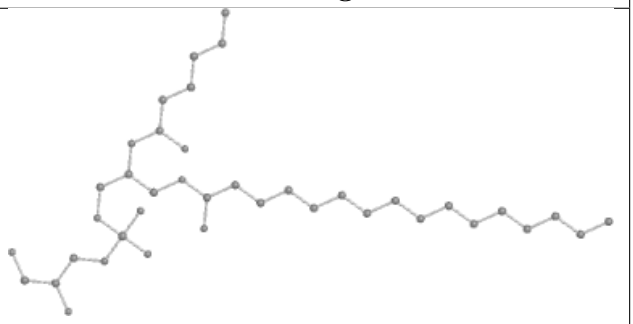
Bond lengths



Bond angles

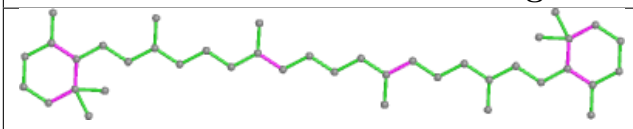


Torsions

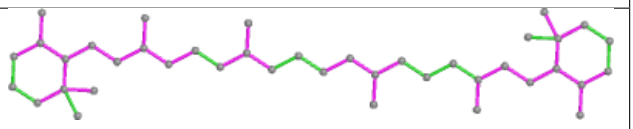


Rings

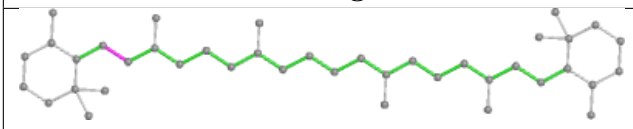
Ligand BCR J 112



Bond lengths



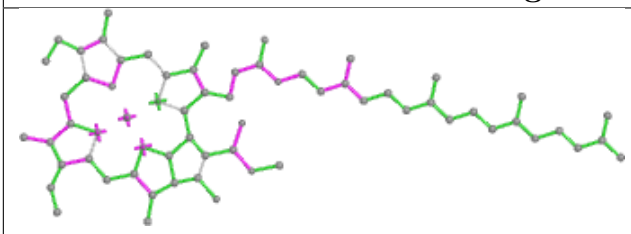
Bond angles



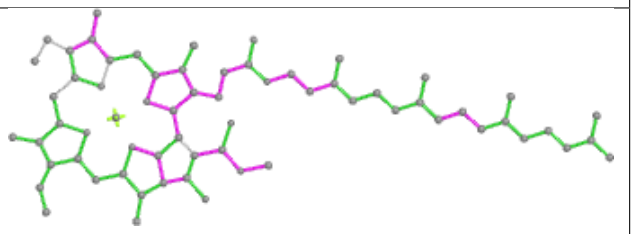
Torsions

Rings

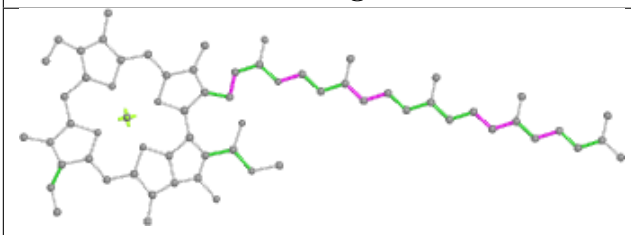
Ligand CLA B 516



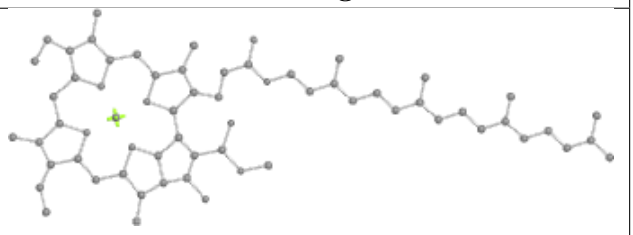
Bond lengths



Bond angles

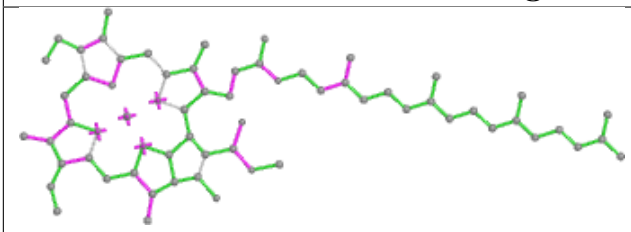


Torsions

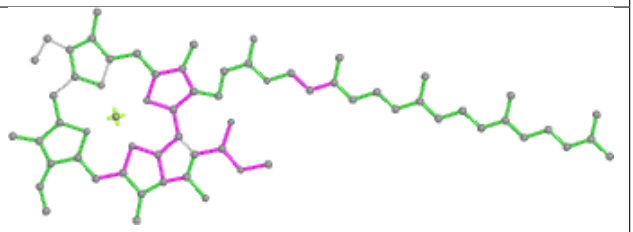


Rings

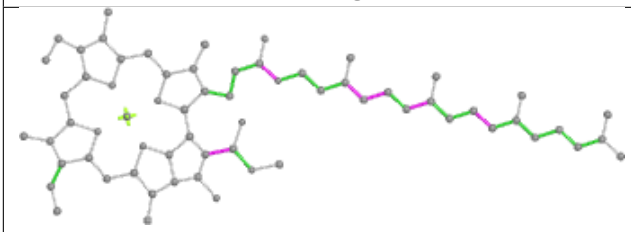
Ligand CLA C 485



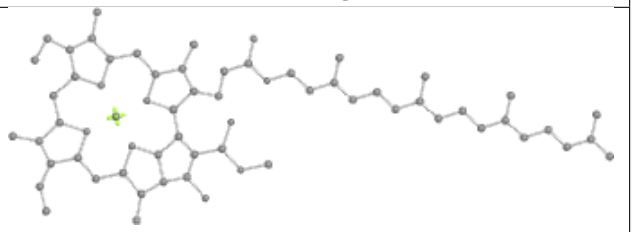
Bond lengths



Bond angles

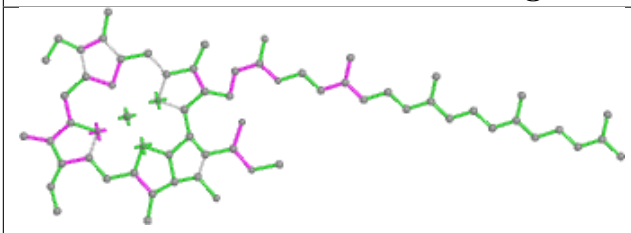


Torsions

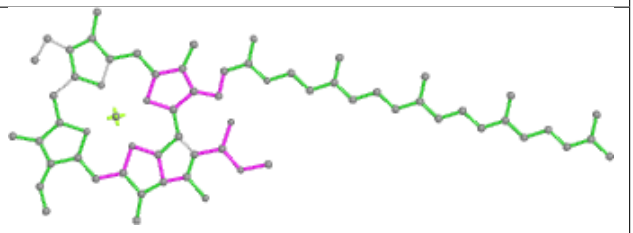


Rings

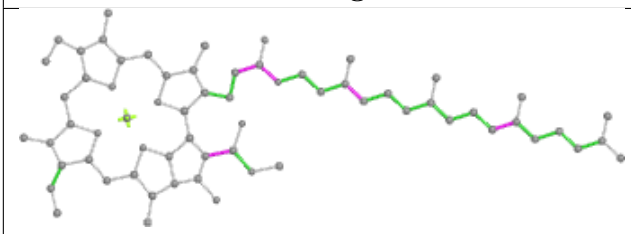
Ligand CLA B 515



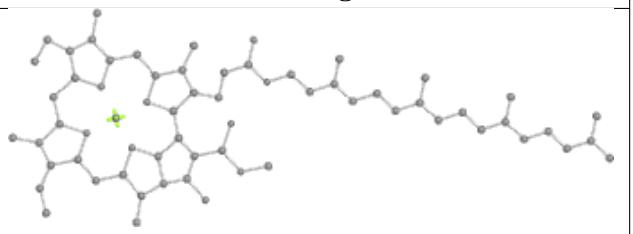
Bond lengths



Bond angles

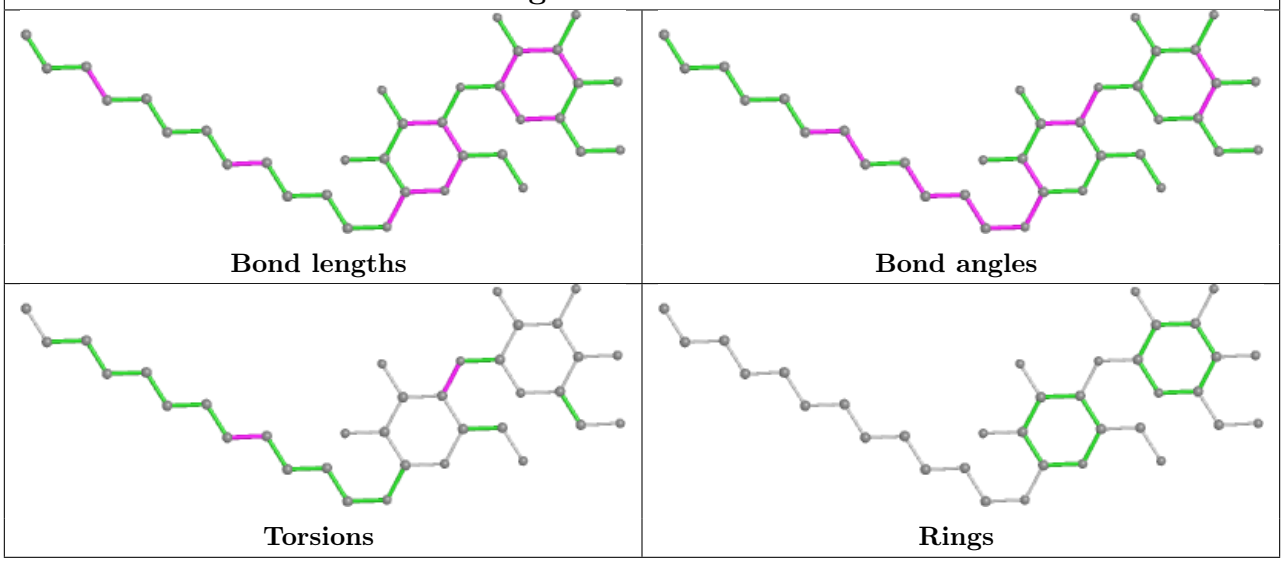


Torsions

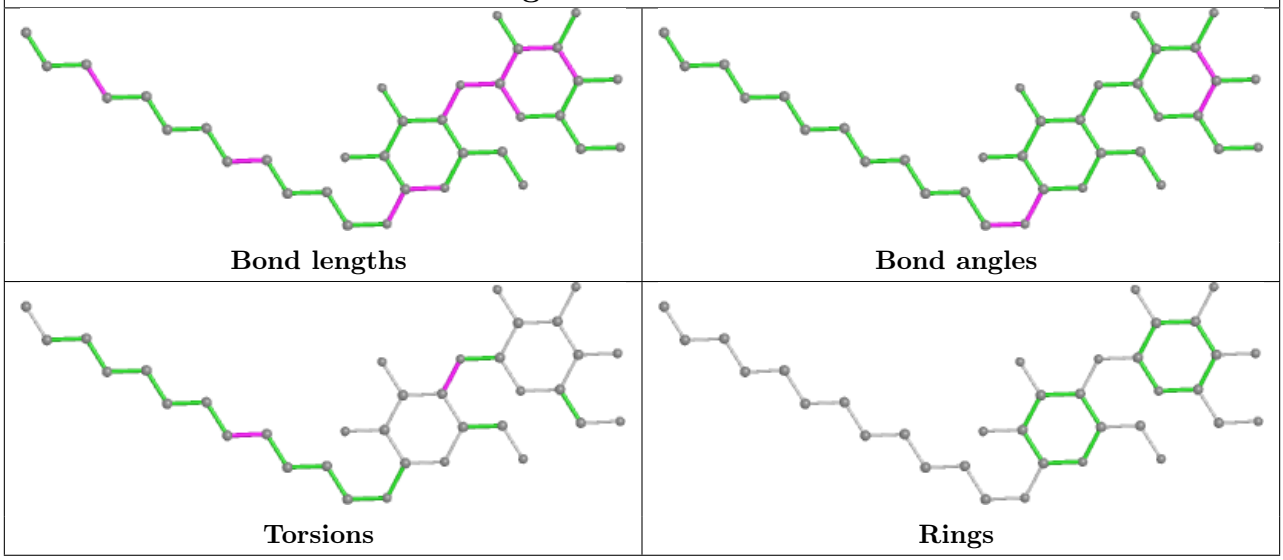


Rings

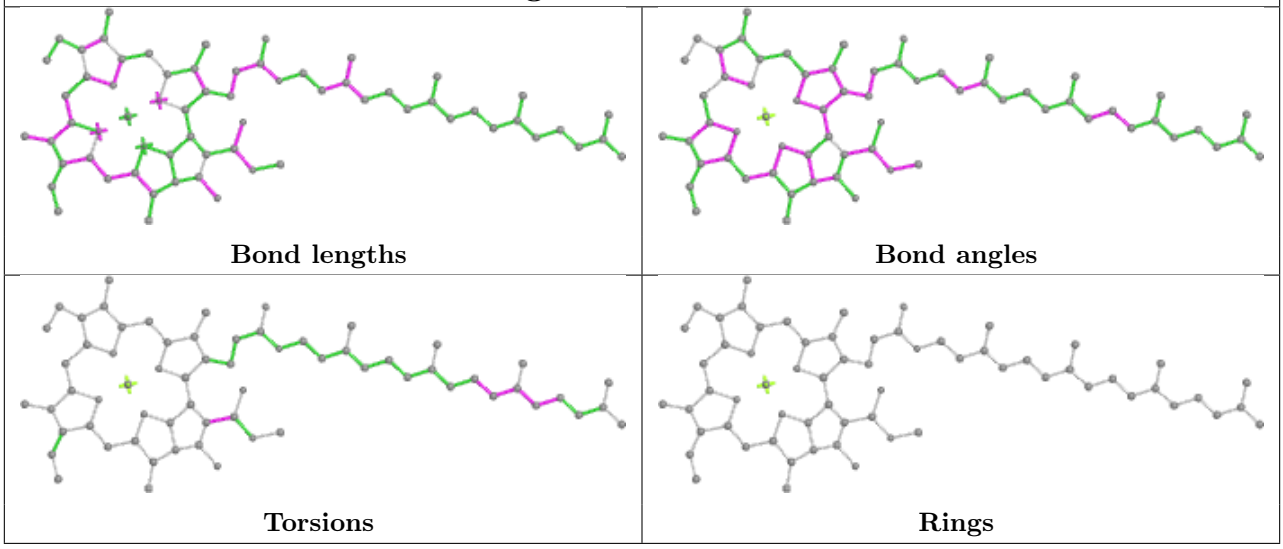
Ligand LMT I 274



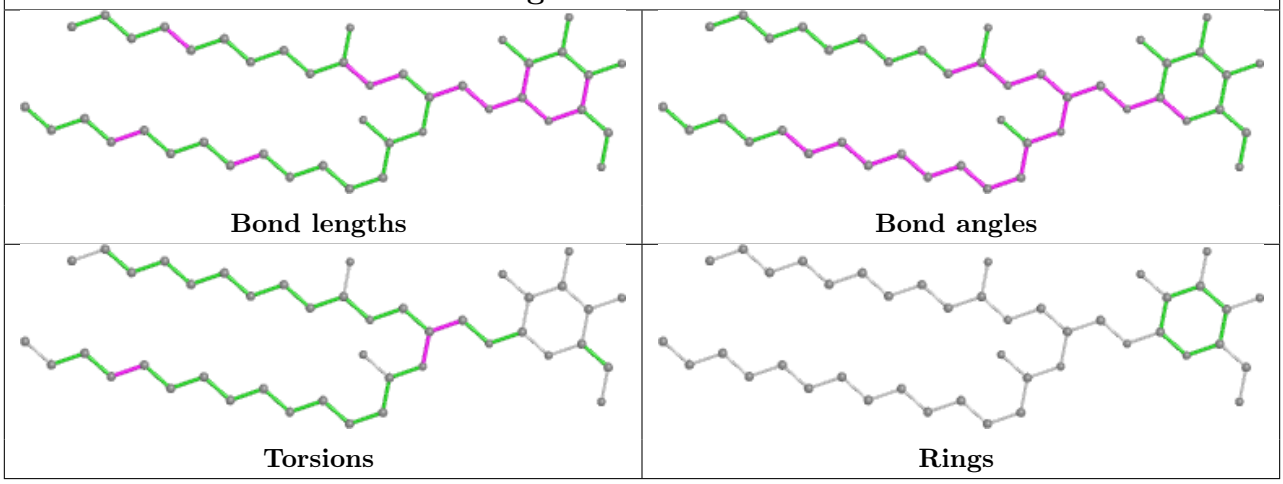
Ligand LMT B 535



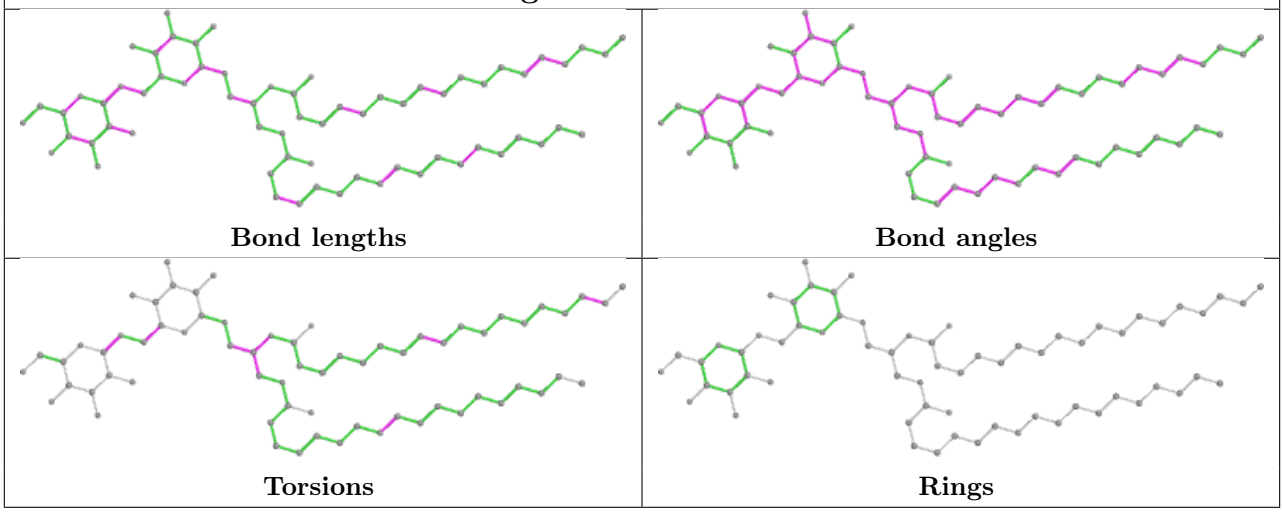
Ligand CLA C 486



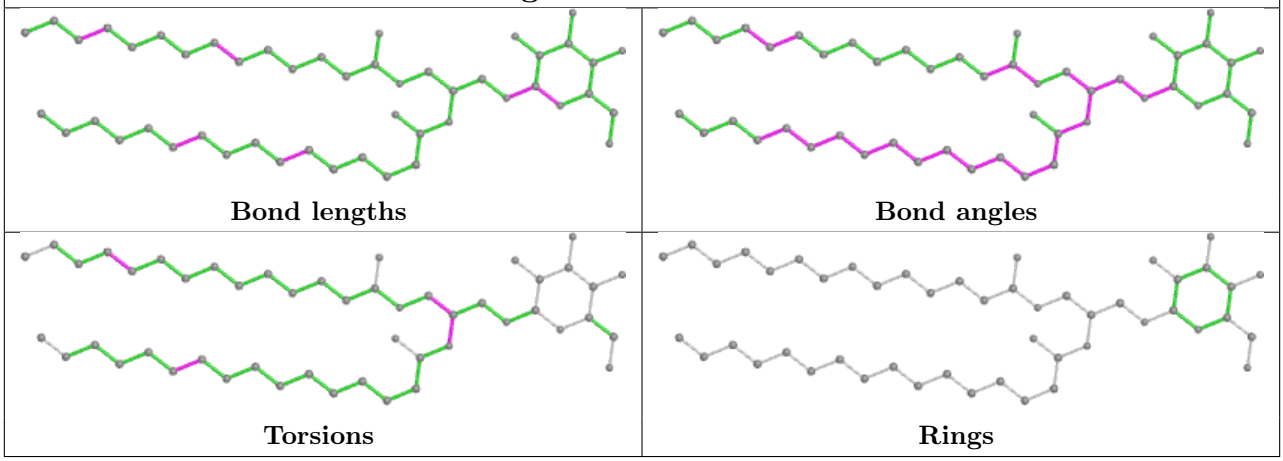
Ligand LMG I 220



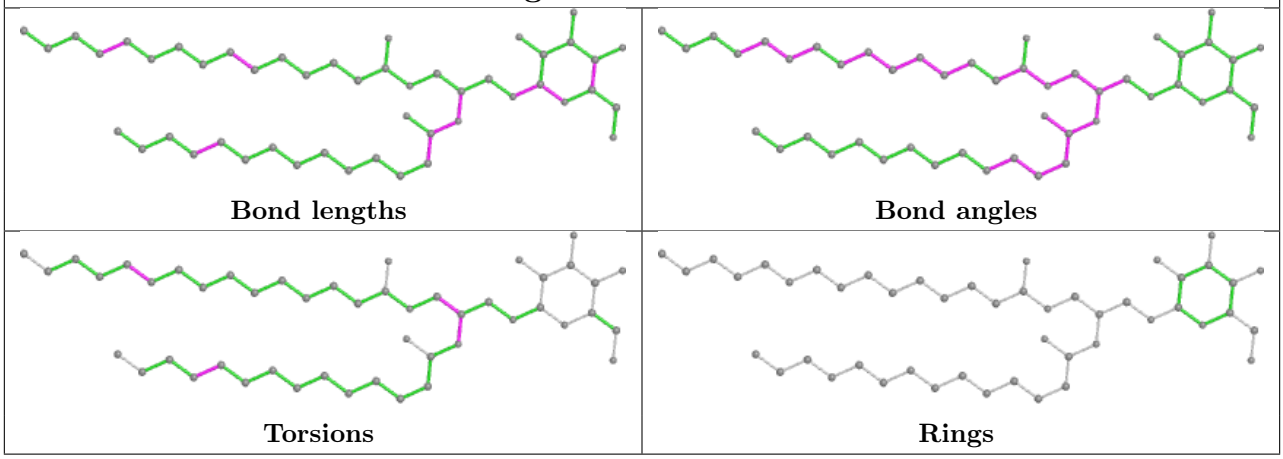
Ligand DGD C 493



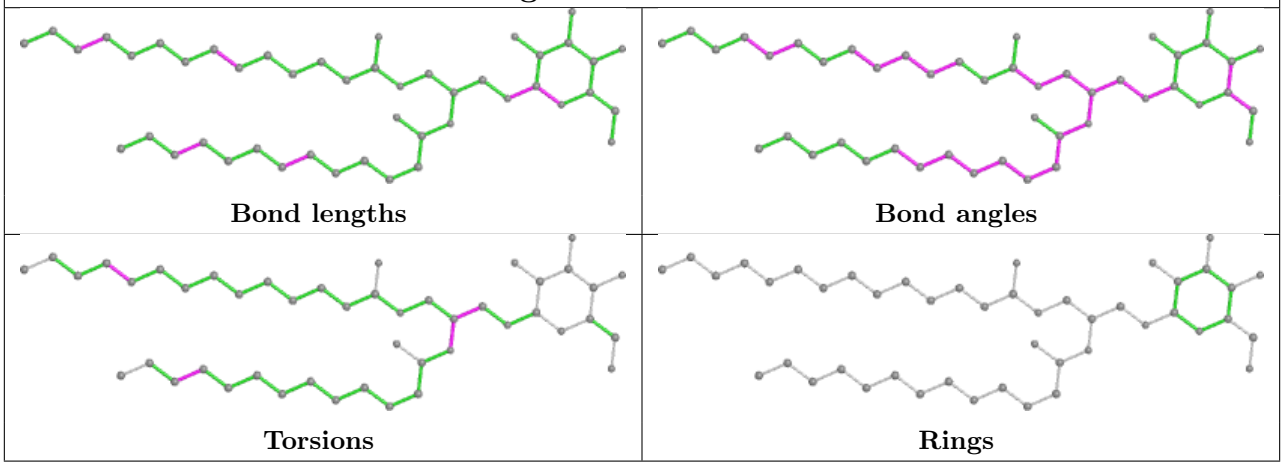
Ligand LMG B 531



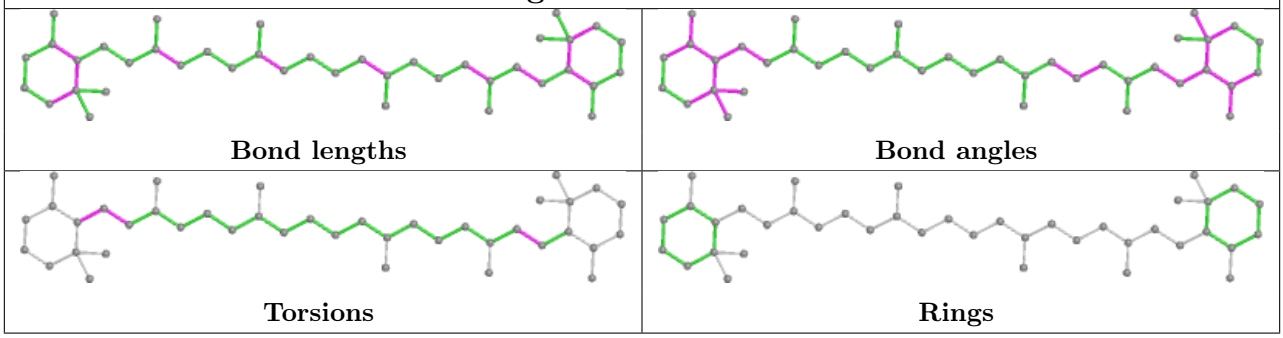
Ligand LMG J 492



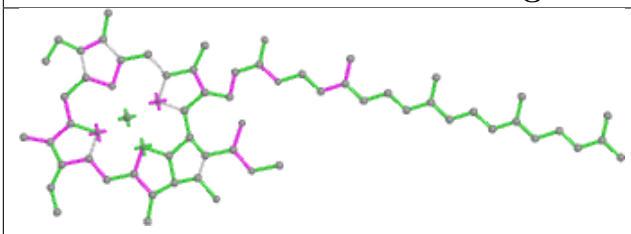
Ligand LMG D 359



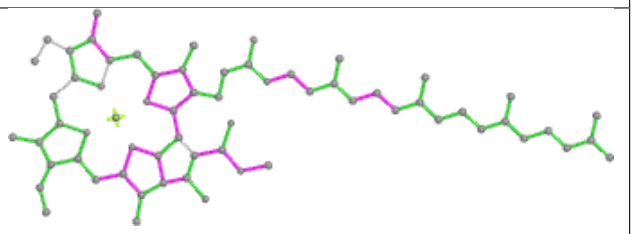
Ligand BCR J 115



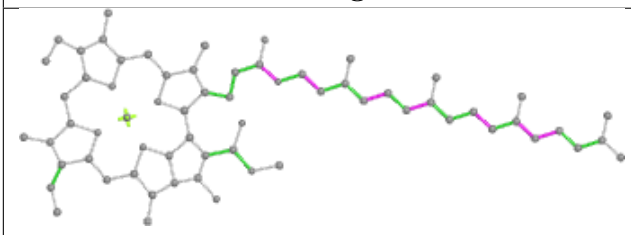
Ligand CLA A 362



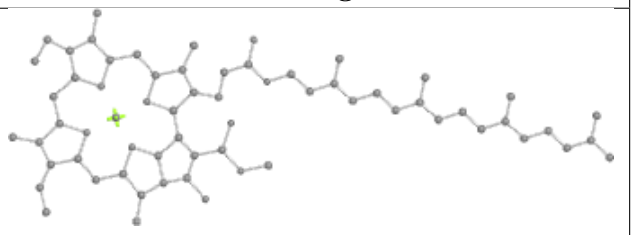
Bond lengths



Bond angles

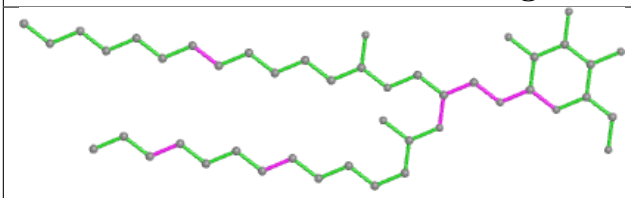


Torsions

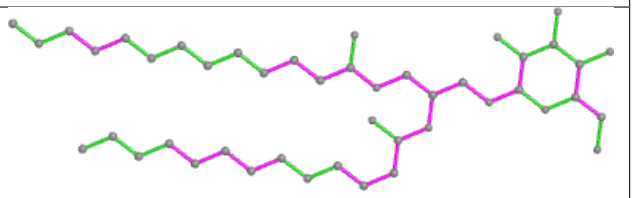


Rings

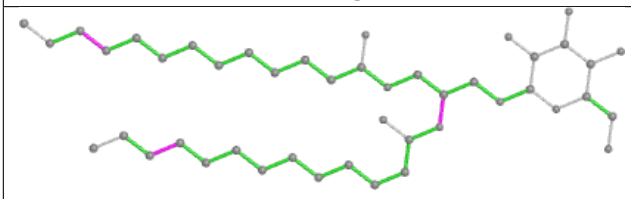
Ligand LMG C 494



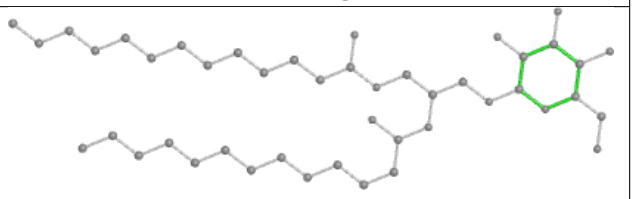
Bond lengths



Bond angles

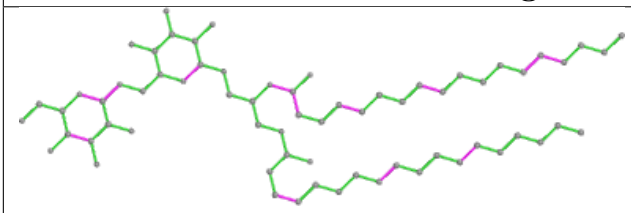


Torsions

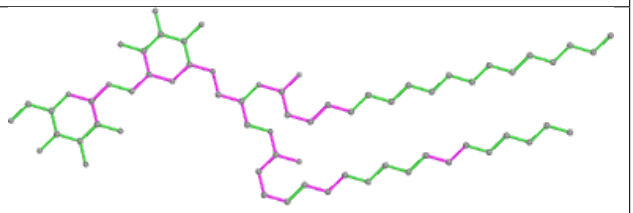


Rings

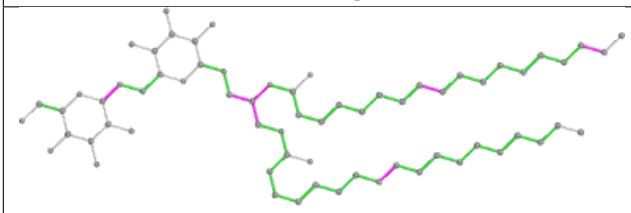
Ligand DGD B 533



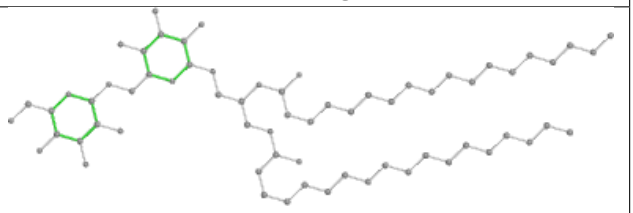
Bond lengths



Bond angles

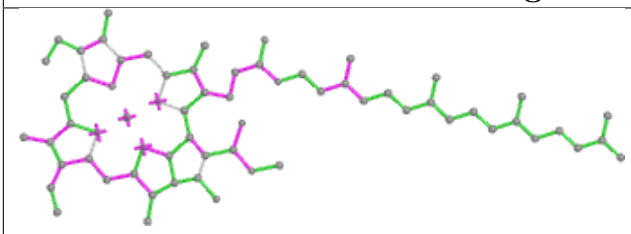


Torsions

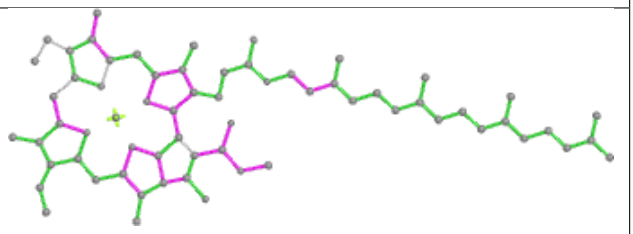


Rings

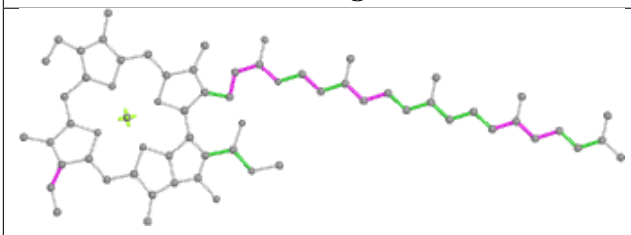
Ligand CLA B 511



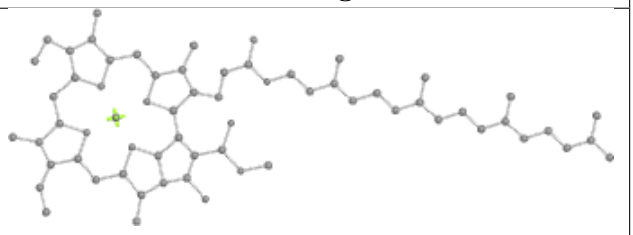
Bond lengths



Bond angles

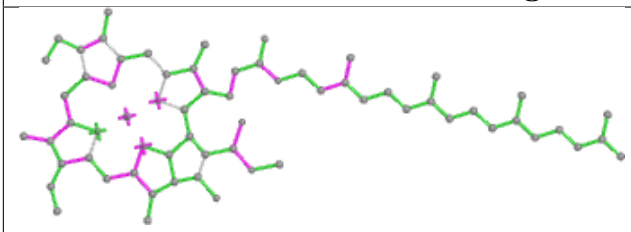


Torsions

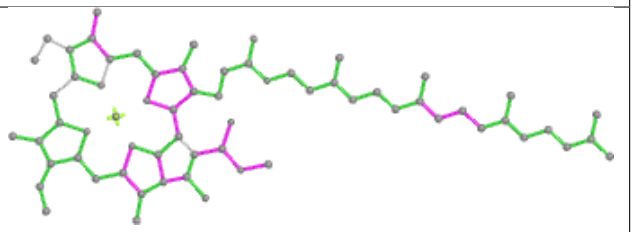


Rings

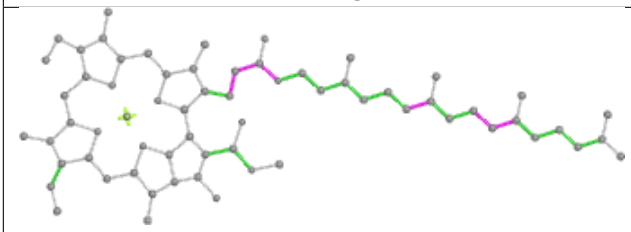
Ligand CLA D 354



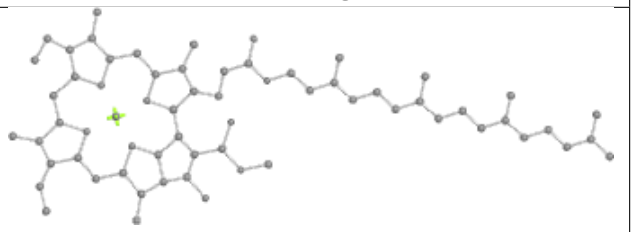
Bond lengths



Bond angles

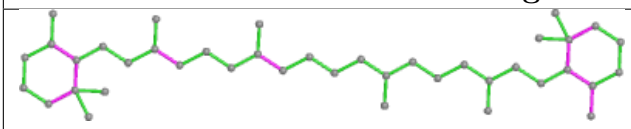


Torsions

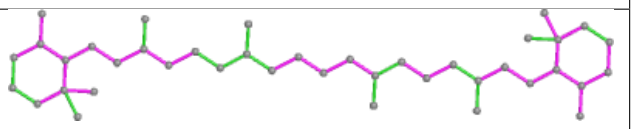


Rings

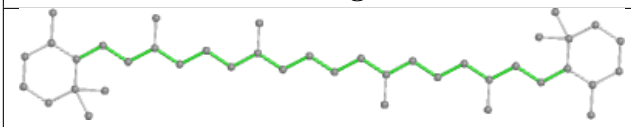
Ligand BCR B 529



Bond lengths



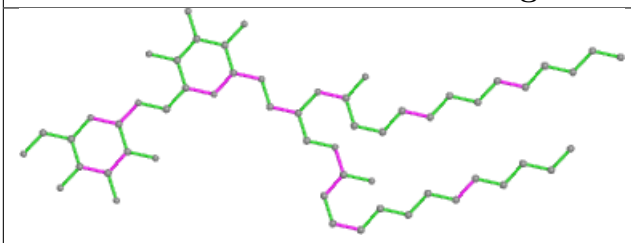
Bond angles



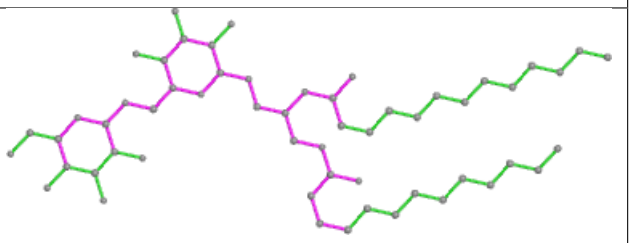
Torsions

Rings

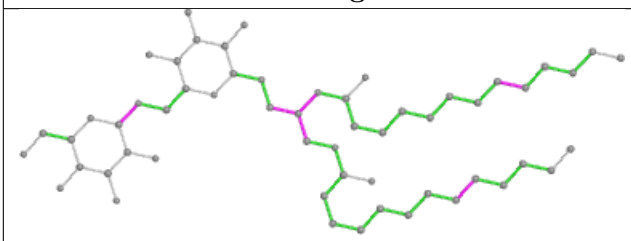
Ligand DGD C 474



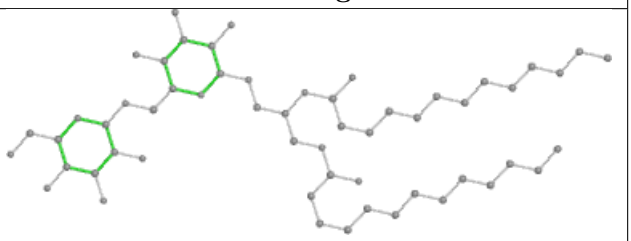
Bond lengths



Bond angles

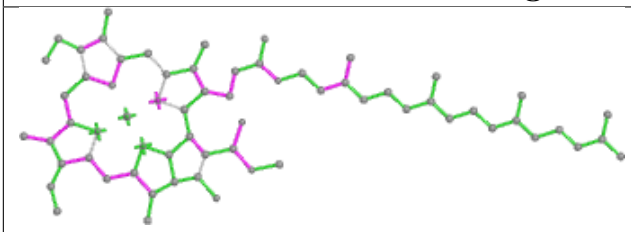


Torsions

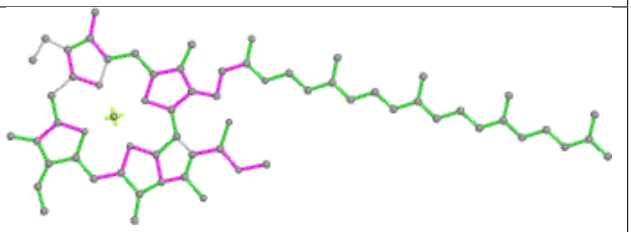


Rings

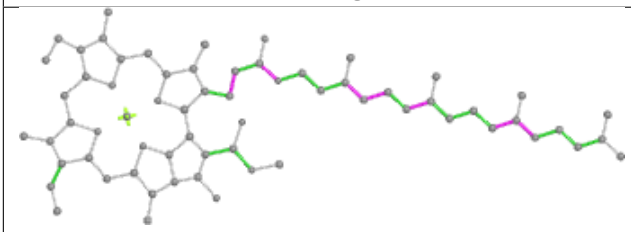
Ligand CLA C 481



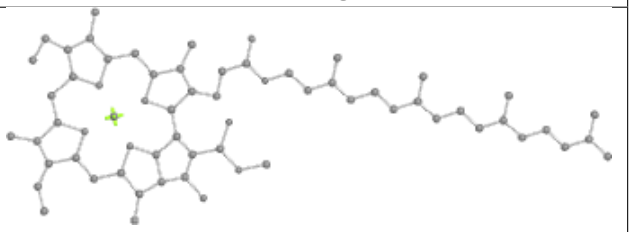
Bond lengths



Bond angles

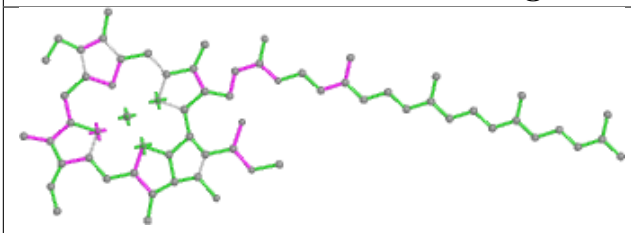


Torsions

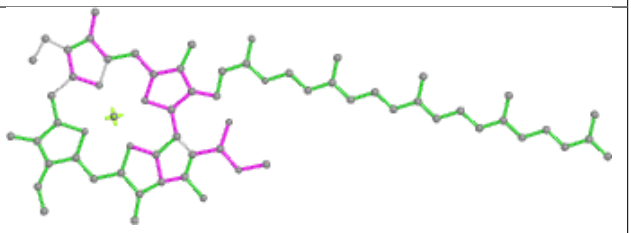


Rings

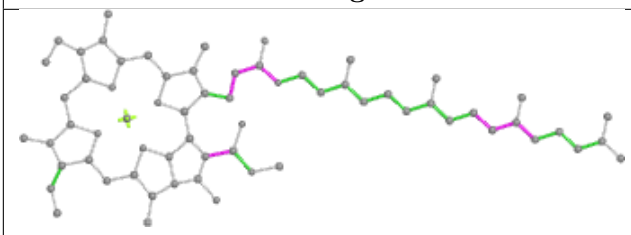
Ligand CLA B 513



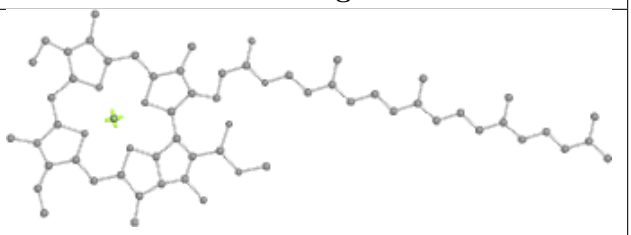
Bond lengths



Bond angles

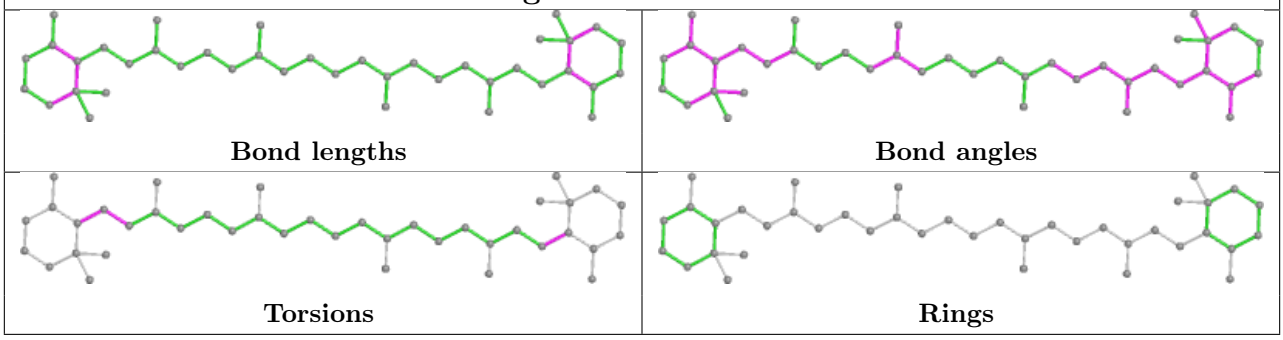


Torsions

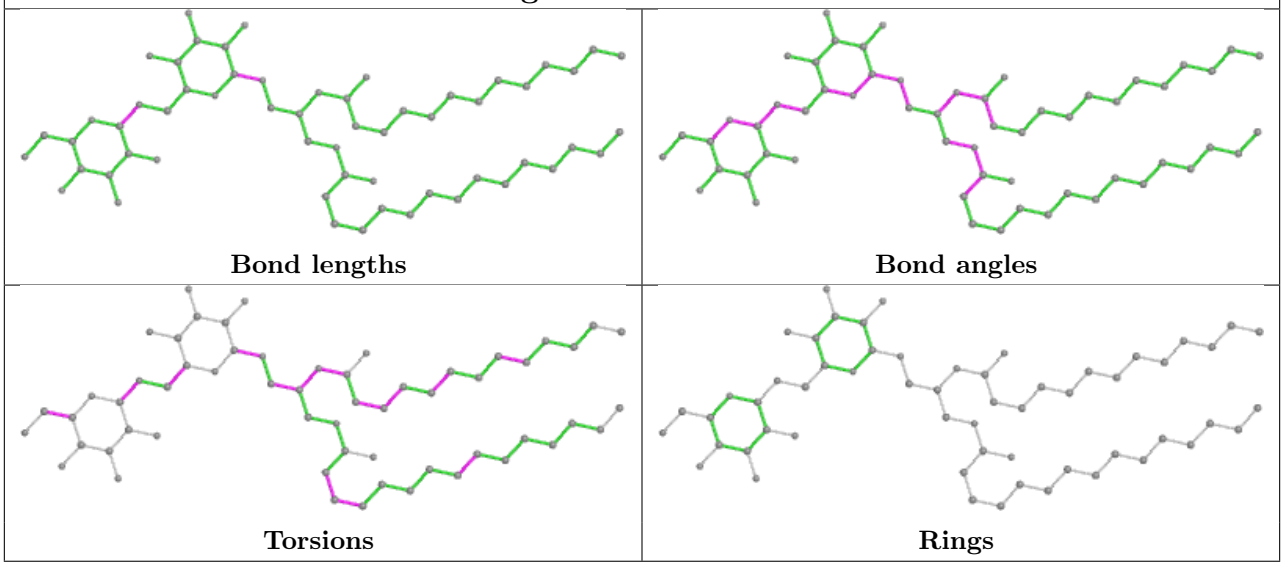


Rings

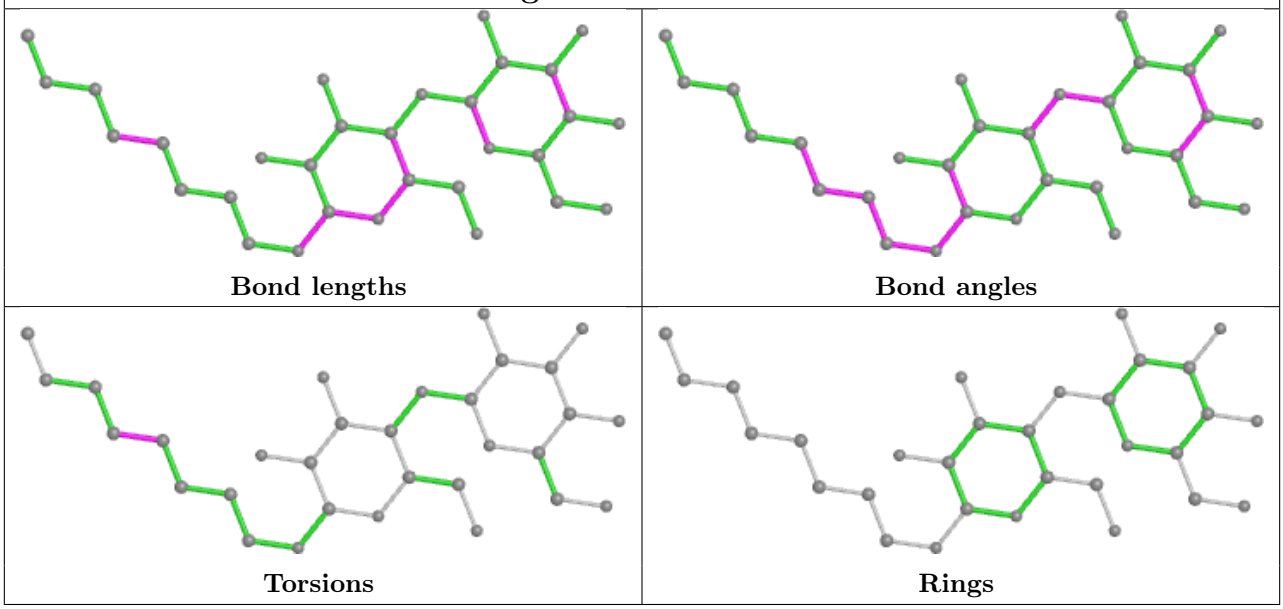
Ligand BCR A 369



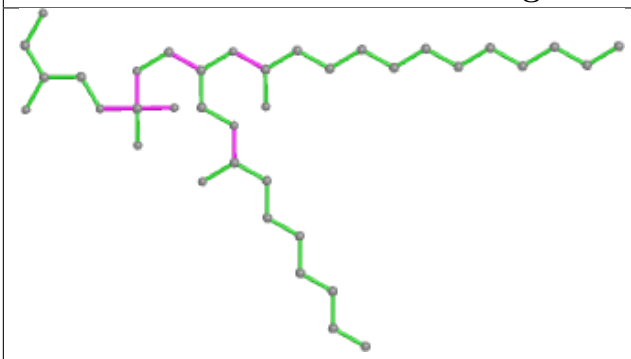
Ligand DGD B 528



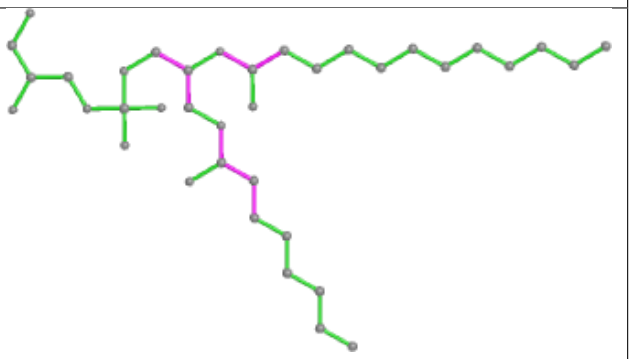
Ligand LMT D 363



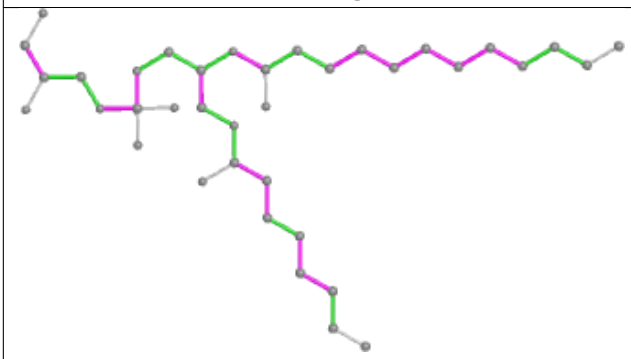
Ligand LHG C 476



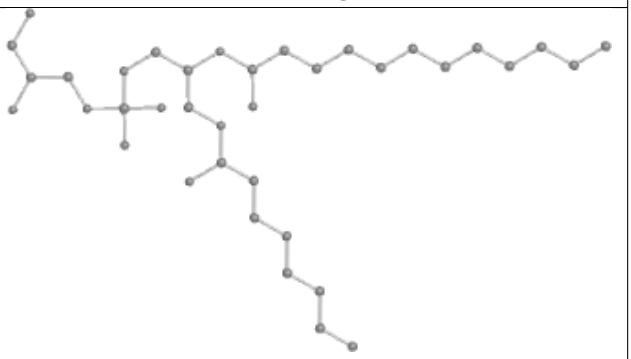
Bond lengths



Bond angles

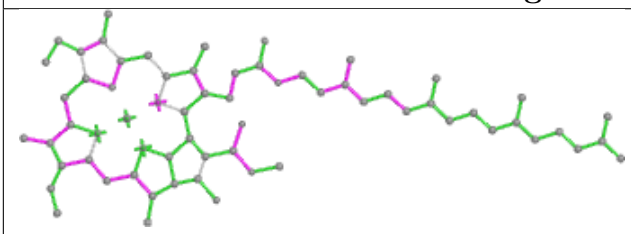


Torsions

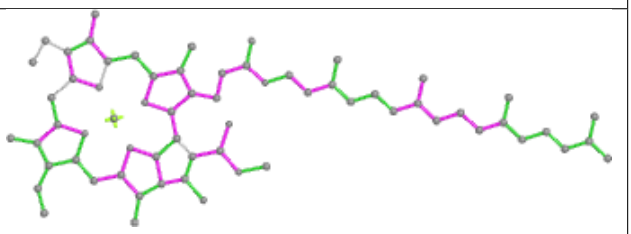


Rings

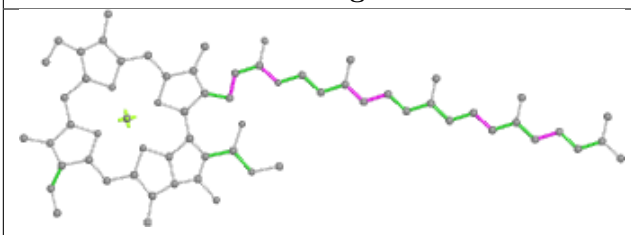
Ligand CLA B 517



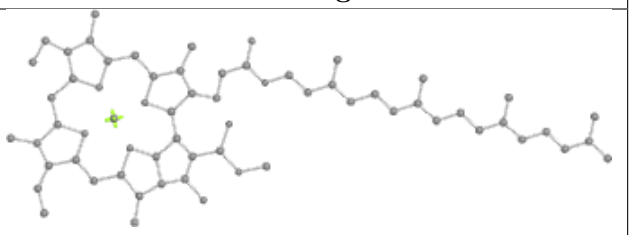
Bond lengths



Bond angles

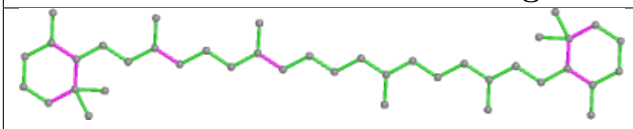


Torsions

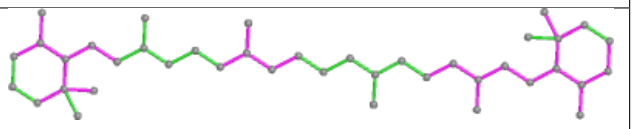


Rings

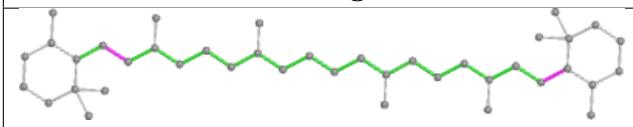
Ligand BCR C 490



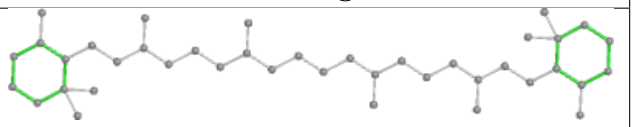
Bond lengths



Bond angles

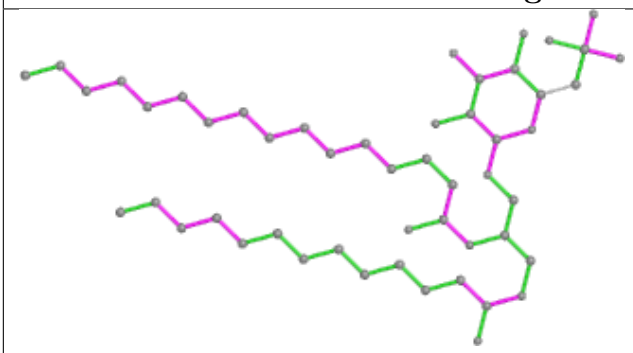


Torsions

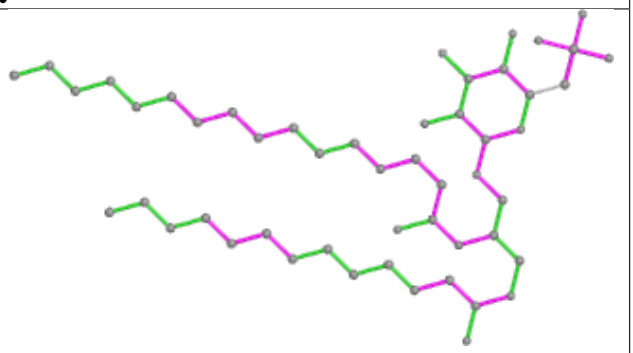


Rings

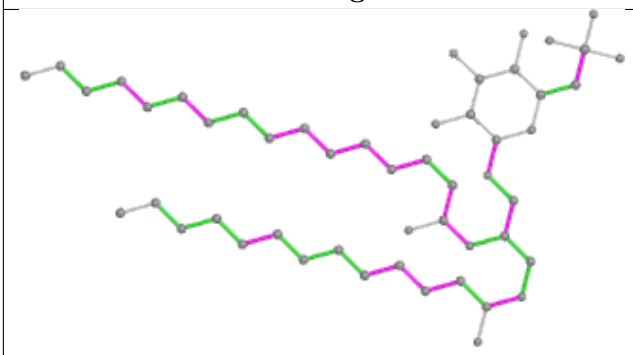
Ligand SQD C 475



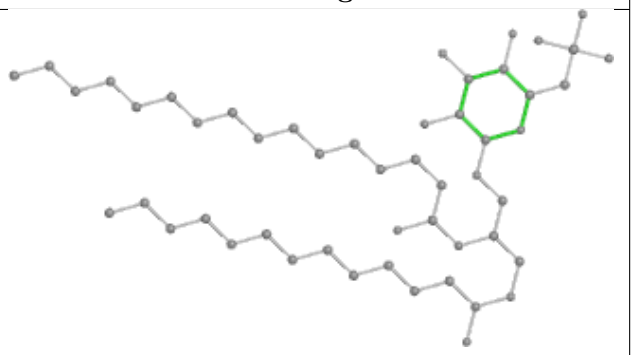
Bond lengths



Bond angles

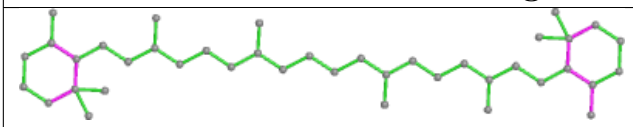


Torsions

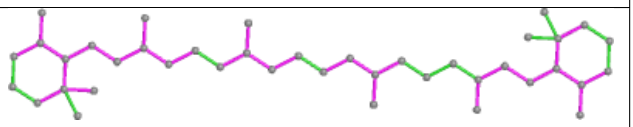


Rings

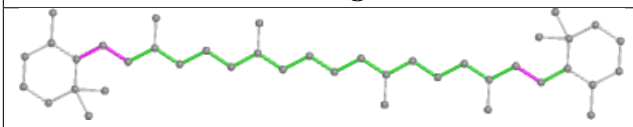
Ligand BCR B 527



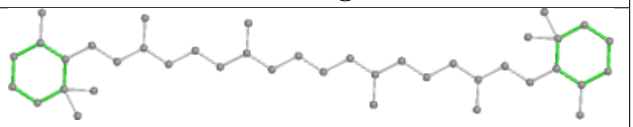
Bond lengths



Bond angles

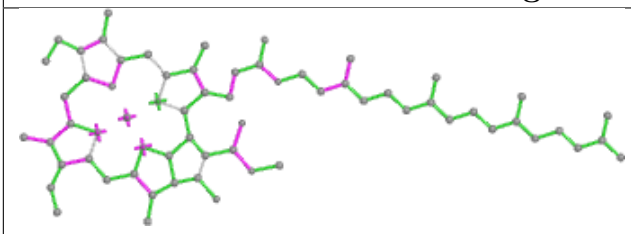


Torsions

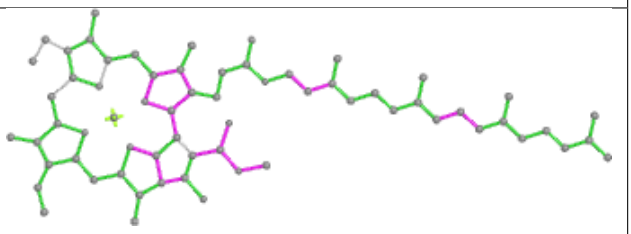


Rings

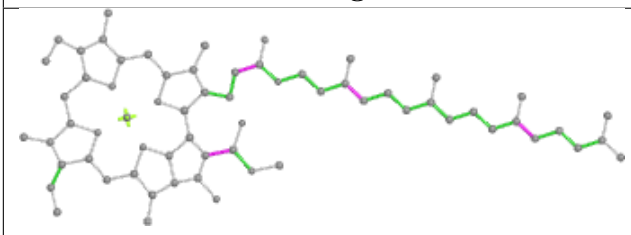
Ligand CLA K 483



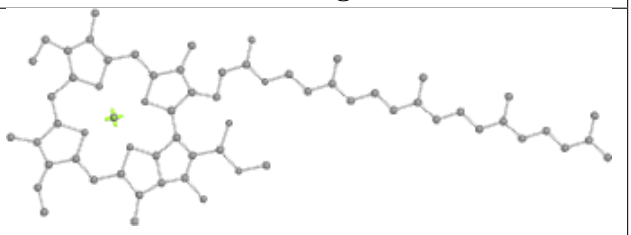
Bond lengths



Bond angles

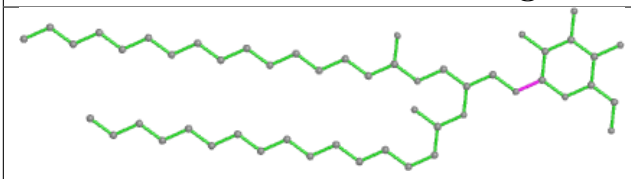


Torsions

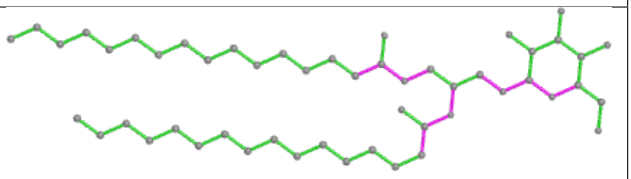


Rings

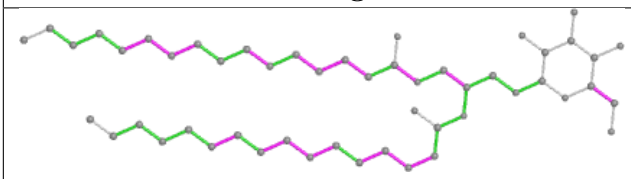
Ligand LMG A 373



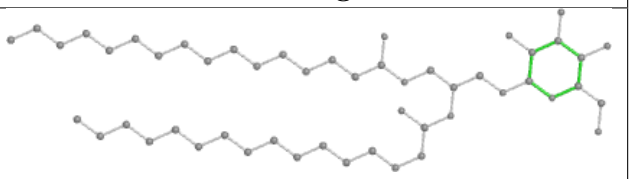
Bond lengths



Bond angles

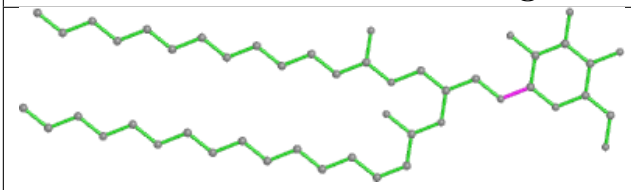


Torsions

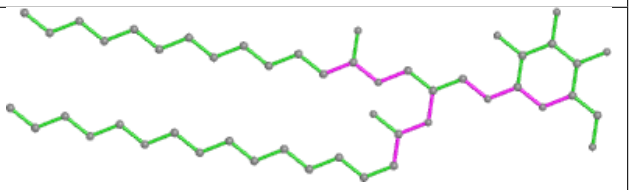


Rings

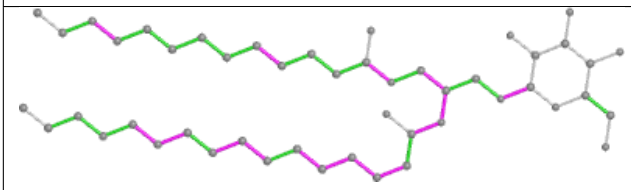
Ligand LMG D 360



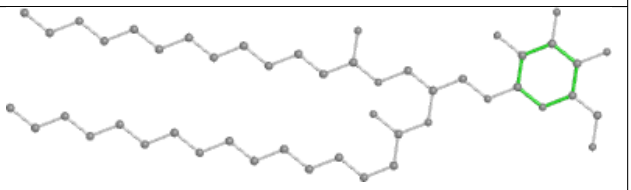
Bond lengths



Bond angles

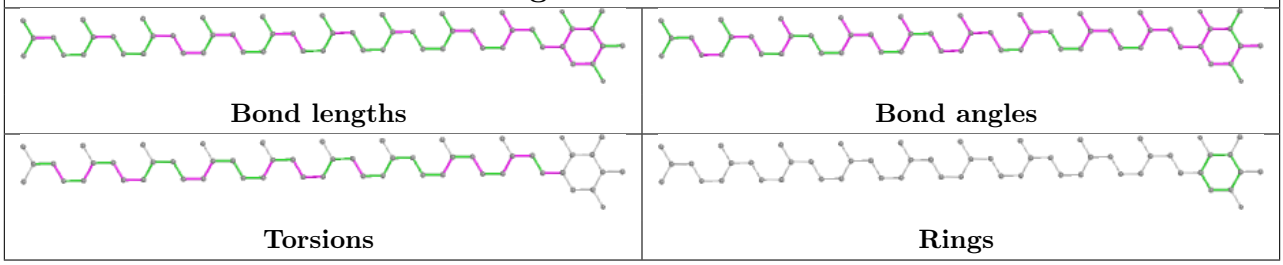


Torsions

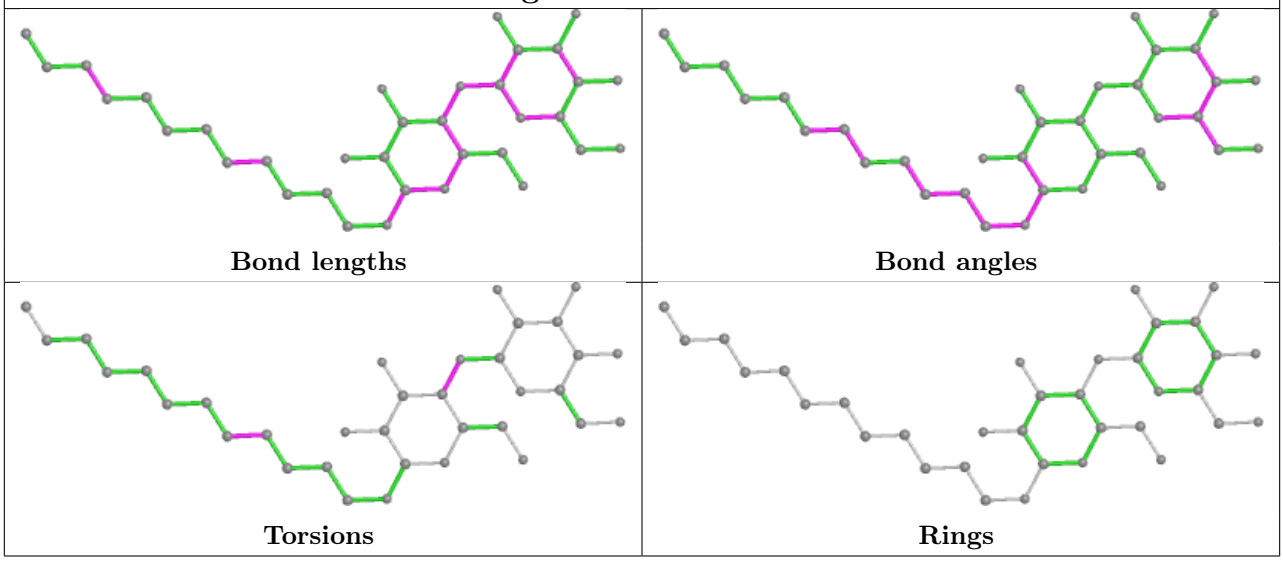


Rings

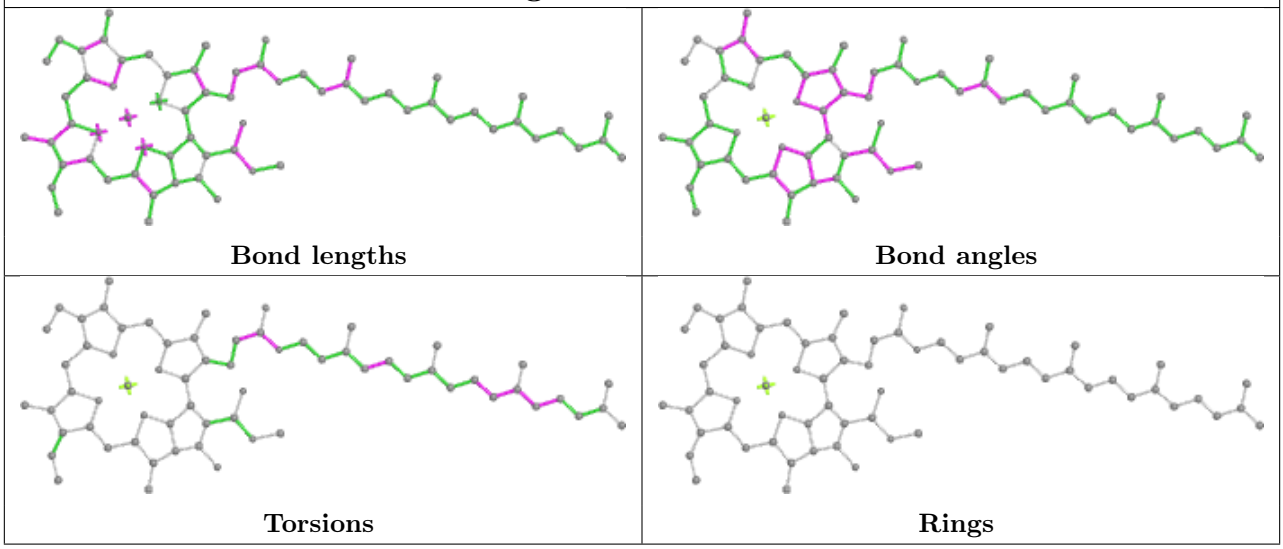
Ligand PL9 D 357



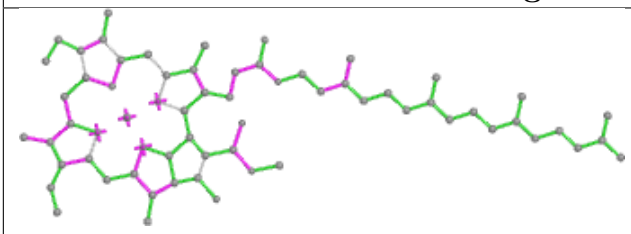
Ligand LMT O 274



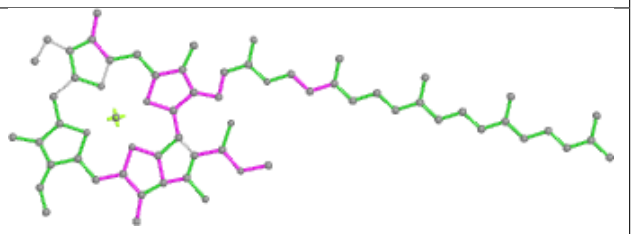
Ligand CLA B 514



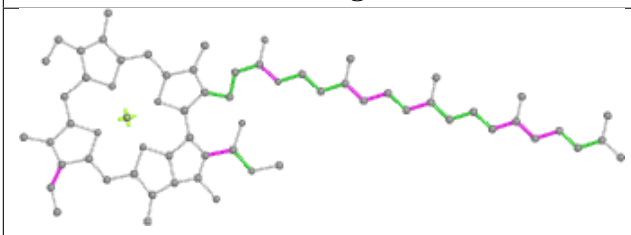
Ligand CLA A 364



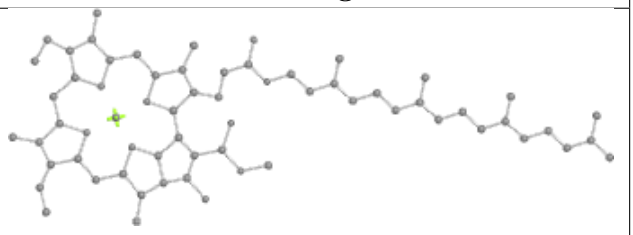
Bond lengths



Bond angles

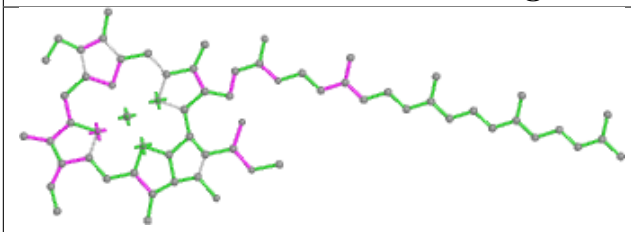


Torsions

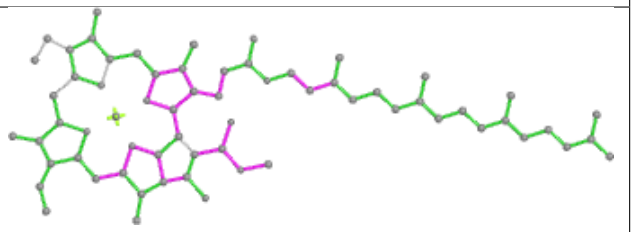


Rings

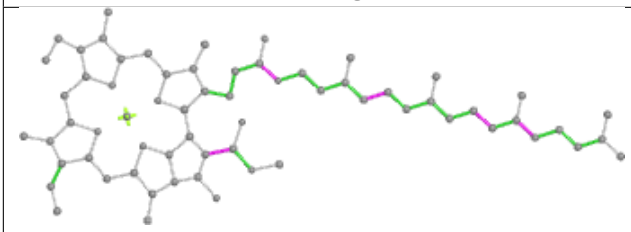
Ligand CLA C 478



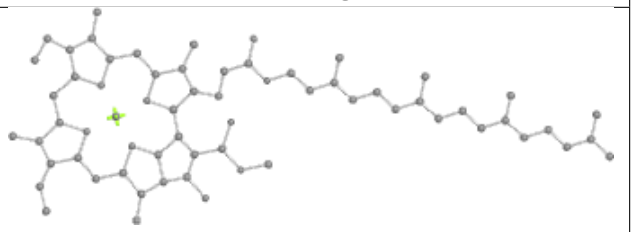
Bond lengths



Bond angles

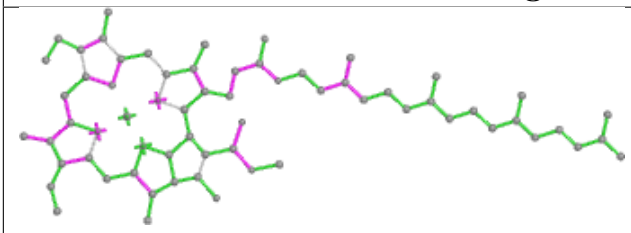


Torsions

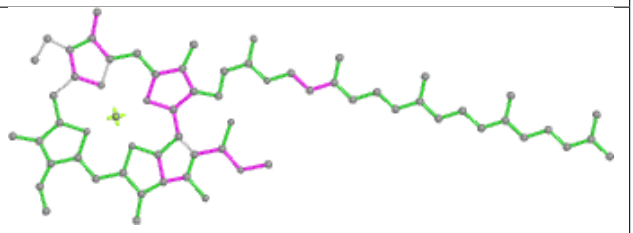


Rings

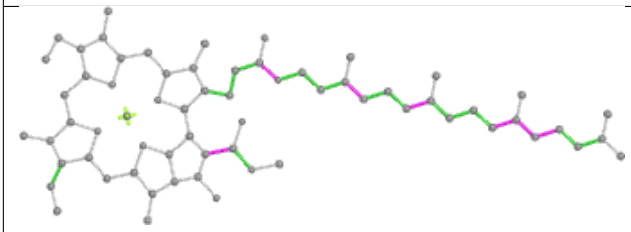
Ligand CLA B 525



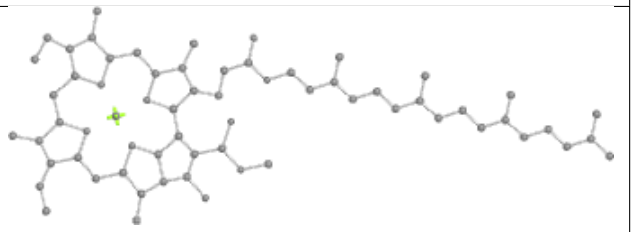
Bond lengths



Bond angles

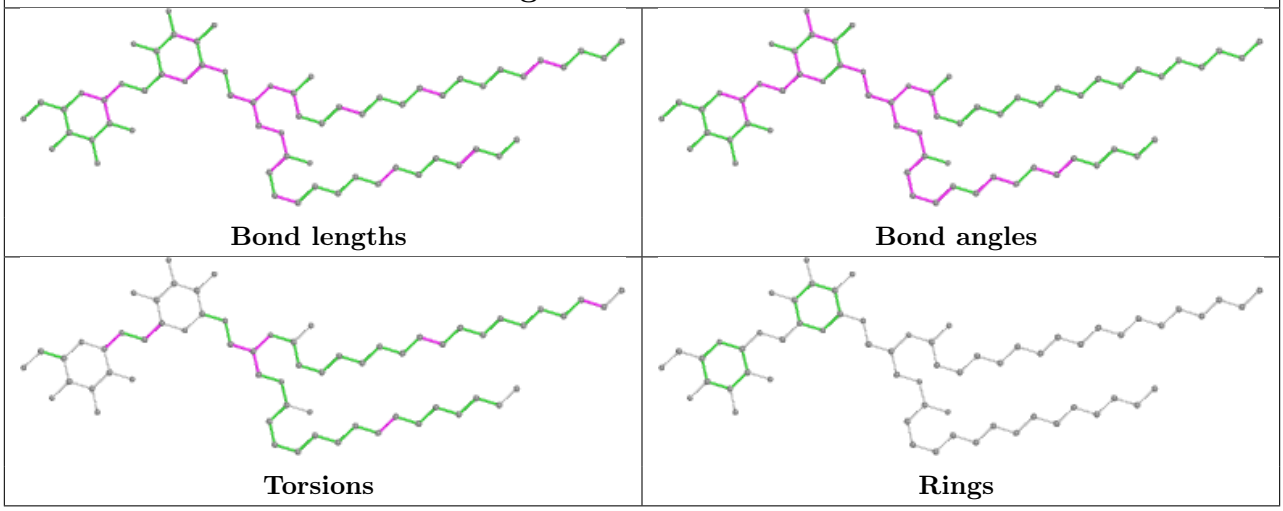


Torsions

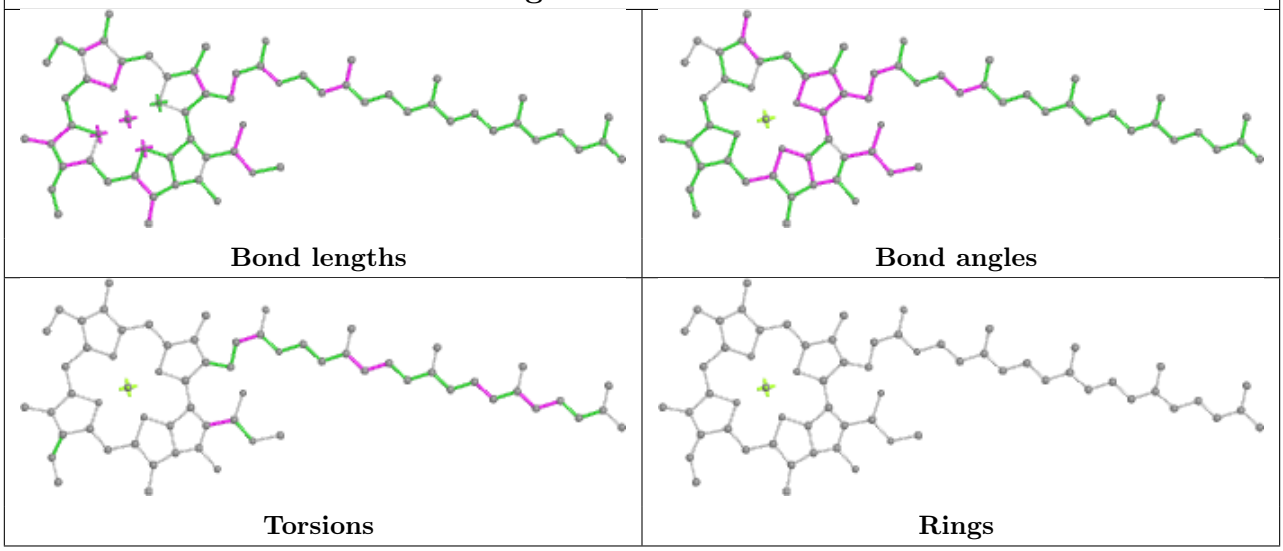


Rings

Ligand DGD D 362



Ligand CLA B 519



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 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	335/344 (97%)	0.08	18 (5%)	25	16	134, 163, 180, 180	0
2	B	485/510 (95%)	-0.04	16 (3%)	46	31	129, 158, 178, 180	0
3	C	448/461 (97%)	0.05	21 (4%)	31	19	136, 168, 180, 180	0
4	D	340/352 (96%)	0.21	25 (7%)	14	9	126, 154, 179, 180	0
5	E	77/83 (92%)	0.13	2 (2%)	56	40	138, 157, 179, 180	0
6	F	38/44 (86%)	0.16	5 (13%)	3	2	138, 157, 169, 177	0
7	H	65/65 (100%)	0.04	2 (3%)	49	33	139, 164, 177, 180	0
8	I	35/38 (92%)	0.26	4 (11%)	5	3	163, 172, 180, 180	0
9	J	34/40 (85%)	-0.43	0	100	100	141, 155, 169, 171	0
10	K	37/37 (100%)	-0.11	1 (2%)	54	38	156, 166, 179, 180	0
11	L	37/37 (100%)	0.23	3 (8%)	12	7	152, 168, 180, 180	0
12	M	34/36 (94%)	0.75	8 (23%)	0	0	153, 165, 180, 180	0
13	O	243/246 (98%)	0.37	20 (8%)	11	7	143, 174, 180, 180	0
14	T	30/32 (93%)	0.09	2 (6%)	17	10	152, 169, 180, 180	0
15	U	97/104 (93%)	0.16	4 (4%)	37	24	141, 160, 171, 179	0
16	V	137/137 (100%)	0.09	6 (4%)	34	21	136, 160, 171, 174	0
17	y	28/46 (60%)	-0.05	2 (7%)	16	9	158, 175, 180, 180	0
18	X	35/40 (87%)	-0.12	4 (11%)	5	3	144, 156, 174, 178	0
19	Z	62/62 (100%)	0.09	5 (8%)	12	7	166, 178, 180, 180	0
All	All	2597/2714 (95%)	0.10	148 (5%)	23	14	126, 164, 180, 180	0

All (148) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
12	M	1	MET	7.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
10	K	46	ARG	5.5
12	M	2	GLU	5.1
4	D	241	GLU	5.0
2	B	85	GLY	5.0
1	A	18	CYS	4.9
1	A	230	THR	4.7
8	I	26	GLY	4.5
7	H	2	ALA	4.5
13	O	113	VAL	4.4
1	A	231	GLU	4.4
3	C	27	ASP	4.3
3	C	135	ARG	4.3
4	D	227	GLU	4.2
13	O	167	ASP	4.2
12	M	33	GLN	4.1
3	C	460	ASP	4.0
13	O	234	THR	4.0
11	L	2	GLU	4.0
1	A	12	ASN	4.0
13	O	51	THR	4.0
3	C	473	ASP	4.0
16	V	125	ASP	3.8
2	B	485	GLU	3.8
4	D	65	SER	3.8
5	E	17	VAL	3.8
12	M	32	GLN	3.7
1	A	11	ALA	3.6
19	Z	62	VAL	3.6
12	M	31	SER	3.5
5	E	84	LYS	3.5
4	D	76	VAL	3.5
4	D	239	GLN	3.5
1	A	266	ASN	3.4
16	V	113	GLU	3.4
3	C	101	PRO	3.4
3	C	260	ALA	3.4
12	M	30	GLU	3.4
13	O	30	THR	3.3
4	D	13	GLY	3.3
3	C	142	GLU	3.3
4	D	79	SER	3.3
18	X	45	LYS	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
13	O	54	GLY	3.2
3	C	30	SER	3.2
3	C	28	GLN	3.2
18	X	42	GLN	3.1
3	C	461	ARG	3.1
6	F	12	SER	3.1
4	D	71	CYS	3.1
19	Z	27	TYR	3.1
6	F	14	PRO	3.1
8	I	34	ARG	3.0
2	B	322	GLY	3.0
4	D	240	ALA	3.0
7	H	24	GLY	3.0
13	O	271	PRO	3.0
3	C	204	LEU	3.0
1	A	232	SER	3.0
2	B	84	THR	3.0
3	C	463	SER	2.9
1	A	228	THR	2.9
3	C	147	PHE	2.9
11	L	11	GLU	2.9
1	A	15	GLU	2.8
3	C	203	THR	2.8
12	M	3	VAL	2.8
4	D	226	GLY	2.8
4	D	233	ARG	2.7
2	B	2	GLY	2.7
14	T	22	PHE	2.7
15	U	39	LEU	2.7
4	D	234	ALA	2.7
17	y	42	ARG	2.7
16	V	103	LYS	2.6
13	O	112	LYS	2.6
1	A	14	TRP	2.6
2	B	180	PRO	2.6
12	M	34	LYS	2.6
4	D	263	ASN	2.6
13	O	84	ASN	2.6
8	I	33	LYS	2.5
4	D	246	MET	2.5
13	O	114	ASN	2.5
6	F	13	TYR	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	338	GLN	2.5
2	B	3	LEU	2.5
4	D	172	SER	2.5
4	D	295	SER	2.5
16	V	135	GLU	2.5
13	O	236	GLU	2.4
13	O	155	THR	2.4
1	A	253	GLY	2.4
13	O	47	THR	2.4
15	U	38	GLU	2.4
4	D	80	THR	2.4
3	C	375	LEU	2.4
4	D	232	PHE	2.4
6	F	42	PHE	2.4
4	D	235	PHE	2.4
3	C	228	ASN	2.3
11	L	3	PRO	2.3
16	V	104	ASN	2.3
2	B	350	GLU	2.3
2	B	336	ILE	2.3
4	D	174	GLY	2.3
13	O	62	GLN	2.3
3	C	352	GLY	2.3
4	D	237	PRO	2.3
19	Z	29	SER	2.3
2	B	76	SER	2.3
4	D	225	ASP	2.3
18	X	38	ILE	2.3
3	C	195	ASP	2.3
3	C	78	GLU	2.3
3	C	41	ARG	2.2
1	A	227	THR	2.2
4	D	17	ILE	2.2
8	I	25	SER	2.2
17	y	45	ASN	2.2
18	X	44	ASP	2.2
2	B	218	LEU	2.2
4	D	165	SER	2.2
13	O	173	ASN	2.2
4	D	238	THR	2.2
13	O	32	THR	2.2
15	U	54	LYS	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	484	PRO	2.2
3	C	100	GLY	2.2
14	T	26	PRO	2.2
19	Z	28	ALA	2.2
6	F	15	ILE	2.2
13	O	83	LYS	2.2
1	A	19	ASN	2.2
2	B	116	VAL	2.1
13	O	82	PRO	2.1
1	A	134	SER	2.1
1	A	243	GLU	2.1
1	A	229	GLU	2.1
2	B	78	TRP	2.1
13	O	138	GLY	2.1
1	A	25	ASP	2.1
19	Z	4	LEU	2.1
1	A	250	ALA	2.1
13	O	31	LEU	2.1
16	V	122	ARG	2.0
2	B	480	SER	2.0
15	U	101	GLN	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
34	CA	O	273	1/1	0.17	0.68	180,180,180,180	0
25	BCR	B	530	40/40	0.42	0.86	173,180,180,180	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
26	LHG	C	476	37/49	0.52	0.43	143,176,180,180	0
30	SQD	F	224	45/54	0.53	0.81	152,179,180,180	0
27	LMG	I	220	43/55	0.61	0.86	158,180,180,180	0
29	LMT	T	226	35/35	0.64	0.95	156,180,180,180	0
32	PL9	D	357	55/55	0.65	0.44	146,153,161,162	0
27	LMG	M	217	42/55	0.65	0.72	166,180,180,180	0
25	BCR	J	115	40/40	0.66	0.73	171,180,180,180	0
27	LMG	D	360	48/55	0.66	0.52	140,169,176,177	0
21	CLA	B	526	65/65	0.67	0.50	167,177,180,180	0
29	LMT	D	363	31/35	0.68	0.68	170,180,180,180	0
27	LMG	A	373	51/55	0.70	0.44	169,174,180,180	0
28	DGD	D	362	63/66	0.71	0.55	177,180,180,180	0
27	LMG	C	494	45/55	0.71	0.58	168,180,180,180	0
28	DGD	C	474	56/66	0.71	0.42	158,180,180,180	0
29	LMT	O	274	35/35	0.72	0.39	180,180,180,180	0
27	LMG	J	492	48/55	0.73	0.50	155,175,180,180	0
29	LMT	A	376	35/35	0.73	0.46	162,180,180,180	0
30	SQD	L	213	47/54	0.73	0.58	155,178,180,180	0
21	CLA	C	482	65/65	0.73	0.46	148,179,180,180	0
21	CLA	B	511	65/65	0.73	0.55	148,179,180,180	0
29	LMT	I	274	35/35	0.74	0.62	170,180,180,180	0
30	SQD	C	475	51/54	0.74	0.43	156,172,180,180	0
29	LMT	D	536	35/35	0.74	0.38	168,173,180,180	0
21	CLA	A	366	65/65	0.76	0.40	152,162,164,166	0
25	BCR	B	529	40/40	0.76	0.55	166,169,173,174	0
28	DGD	C	492	62/66	0.77	0.36	153,171,180,180	0
29	LMT	B	535	35/35	0.77	0.72	163,180,180,180	0
25	BCR	C	490	40/40	0.78	0.51	164,169,180,180	0
28	DGD	A	375	52/66	0.78	0.64	164,180,180,180	0
28	DGD	B	533	66/66	0.78	0.35	166,179,180,180	0
21	CLA	A	363	65/65	0.78	0.43	154,161,175,177	0
25	BCR	B	527	40/40	0.78	0.73	161,169,176,178	0
25	BCR	C	489	40/40	0.78	0.32	152,169,171,171	0
25	BCR	Z	116	40/40	0.79	0.43	163,165,170,171	0
21	CLA	C	488	65/65	0.80	0.33	169,176,179,180	0
25	BCR	X	107	40/40	0.80	0.55	154,158,161,163	0
21	CLA	B	524	65/65	0.80	0.52	157,180,180,180	0
28	DGD	C	493	66/66	0.81	0.35	159,174,180,180	0
34	CA	K	56	1/1	0.81	0.42	180,180,180,180	0
27	LMG	B	531	49/55	0.81	0.35	160,167,175,176	0
28	DGD	B	528	58/66	0.82	0.36	126,136,172,173	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
25	BCR	A	369	40/40	0.82	0.41	164,171,178,178	0
21	CLA	B	519	65/65	0.83	0.33	152,157,158,159	0
21	CLA	C	486	65/65	0.83	0.32	143,180,180,180	0
27	LMG	D	359	46/55	0.83	0.33	142,163,180,180	0
21	CLA	B	525	65/65	0.84	0.36	148,167,180,180	0
25	BCR	J	112	40/40	0.84	0.30	157,160,172,173	0
21	CLA	D	356	65/65	0.84	0.34	149,154,162,164	0
21	CLA	C	487	65/65	0.85	0.34	176,180,180,180	0
21	CLA	C	481	65/65	0.86	0.28	152,180,180,180	0
21	CLA	D	354	65/65	0.86	0.37	135,154,164,168	0
21	CLA	C	478	65/65	0.87	0.32	153,155,166,170	0
21	CLA	C	483	65/65	0.87	0.38	164,180,180,180	0
30	SQD	D	361	43/54	0.87	0.29	160,173,180,180	0
21	CLA	B	517	65/65	0.87	0.27	144,160,164,167	0
21	CLA	C	477	65/65	0.88	0.31	163,169,179,180	0
25	BCR	D	358	40/40	0.88	0.29	135,151,162,162	0
21	CLA	A	364	65/65	0.88	0.31	126,141,175,177	0
21	CLA	C	479	65/65	0.88	0.26	162,180,180,180	0
21	CLA	C	484	65/65	0.88	0.28	168,177,180,180	0
21	CLA	C	485	65/65	0.88	0.30	170,176,178,180	0
28	DGD	C	491	53/66	0.88	0.28	155,160,166,168	0
26	LHG	A	371	39/49	0.88	0.30	156,175,179,180	0
21	CLA	B	516	65/65	0.89	0.27	152,155,180,180	0
24	OEC	A	368	5/9	0.89	0.24	118,138,151,154	0
21	CLA	A	362	65/65	0.89	0.28	149,154,159,163	0
21	CLA	B	518	65/65	0.90	0.33	150,164,167,169	0
21	CLA	C	480	65/65	0.90	0.26	151,159,180,180	0
22	PHO	A	365	64/64	0.91	0.30	143,154,162,164	0
34	CA	F	225	1/1	0.91	0.42	142,142,142,142	0
21	CLA	B	514	65/65	0.91	0.30	139,146,168,169	0
21	CLA	K	483	65/65	0.91	0.39	155,160,174,176	0
21	CLA	B	515	65/65	0.92	0.32	142,162,168,170	0
22	PHO	D	355	64/64	0.92	0.40	140,162,169,171	0
23	MES	A	367	12/12	0.92	0.21	136,144,152,153	0
21	CLA	B	522	65/65	0.92	0.29	134,144,163,165	0
21	CLA	B	521	65/65	0.93	0.26	149,169,175,179	0
33	HEM	F	85	43/43	0.93	0.40	154,159,162,163	0
21	CLA	B	512	65/65	0.93	0.24	142,165,172,173	0
21	CLA	B	513	65/65	0.93	0.27	133,170,171,172	0
21	CLA	B	520	65/65	0.93	0.38	150,162,165,167	0
21	CLA	B	523	65/65	0.94	0.23	134,142,169,170	0
33	HEM	V	164	43/43	0.95	0.29	89,102,122,129	0

Continued on next page...

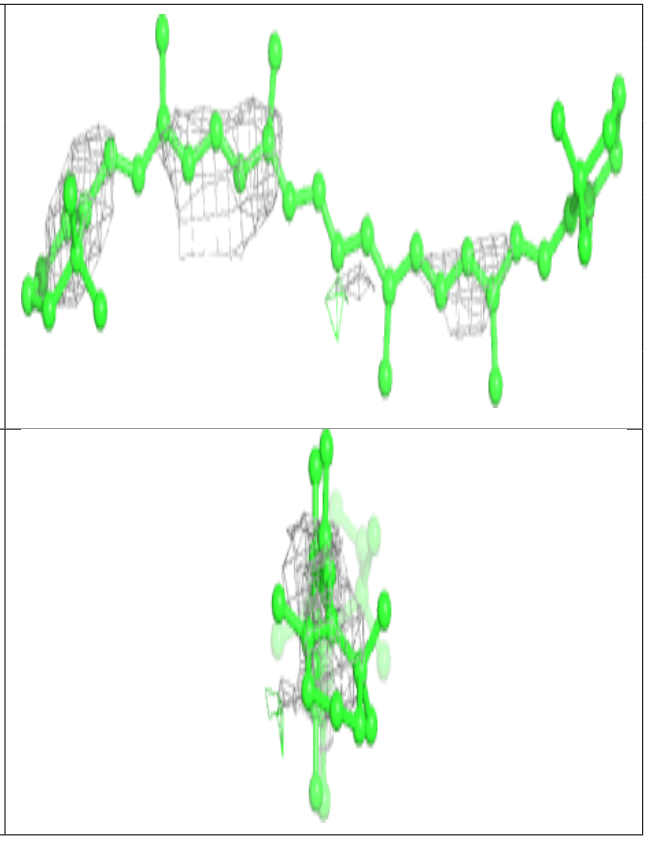
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
20	FE2	A	361	1/1	0.95	0.17	160,160,160,160	0
31	BCT	D	353	4/4	0.97	0.22	169,170,170,171	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

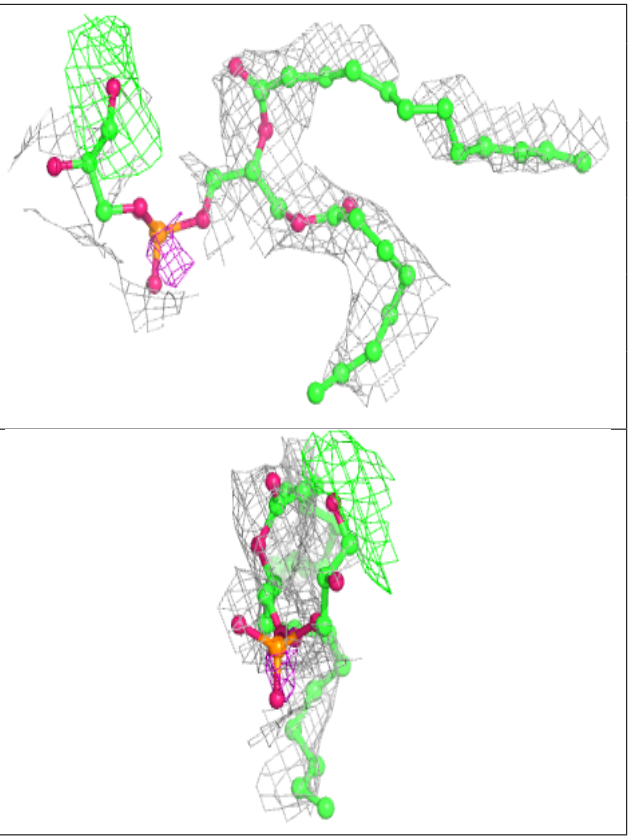
Electron density around BCR B 530:

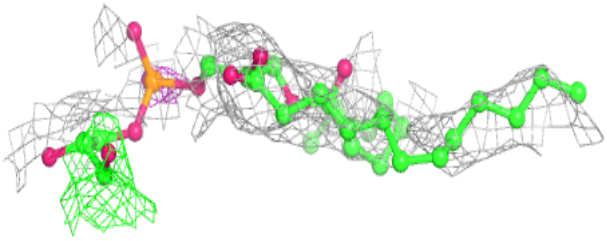
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around LHG C 476:

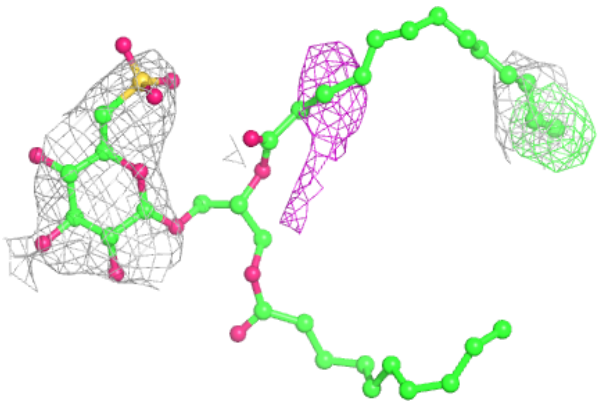
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

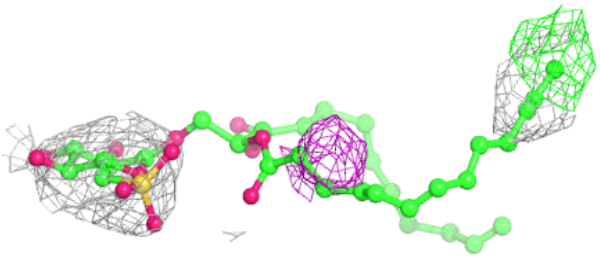


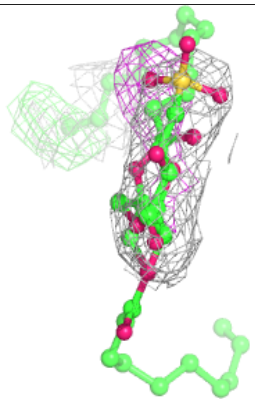


Electron density around SQD F 224:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

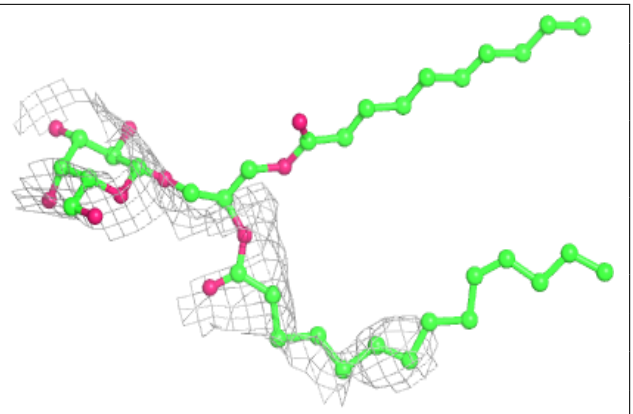


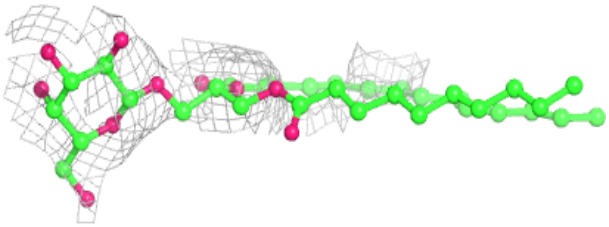


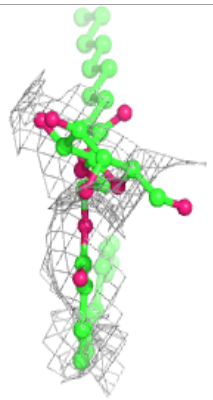


Electron density around LMG I 220:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

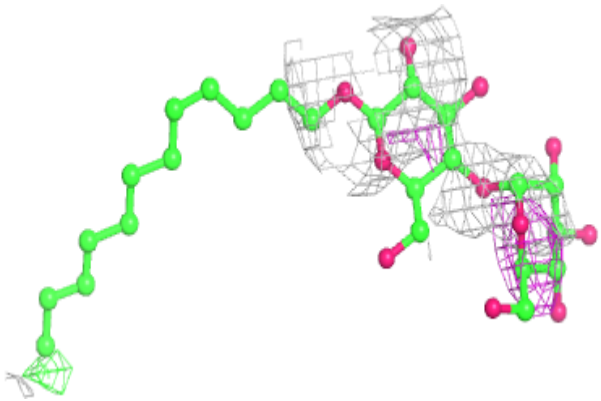


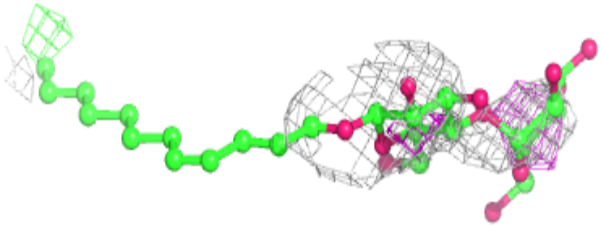


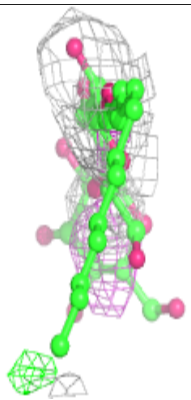


Electron density around LMT T 226:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

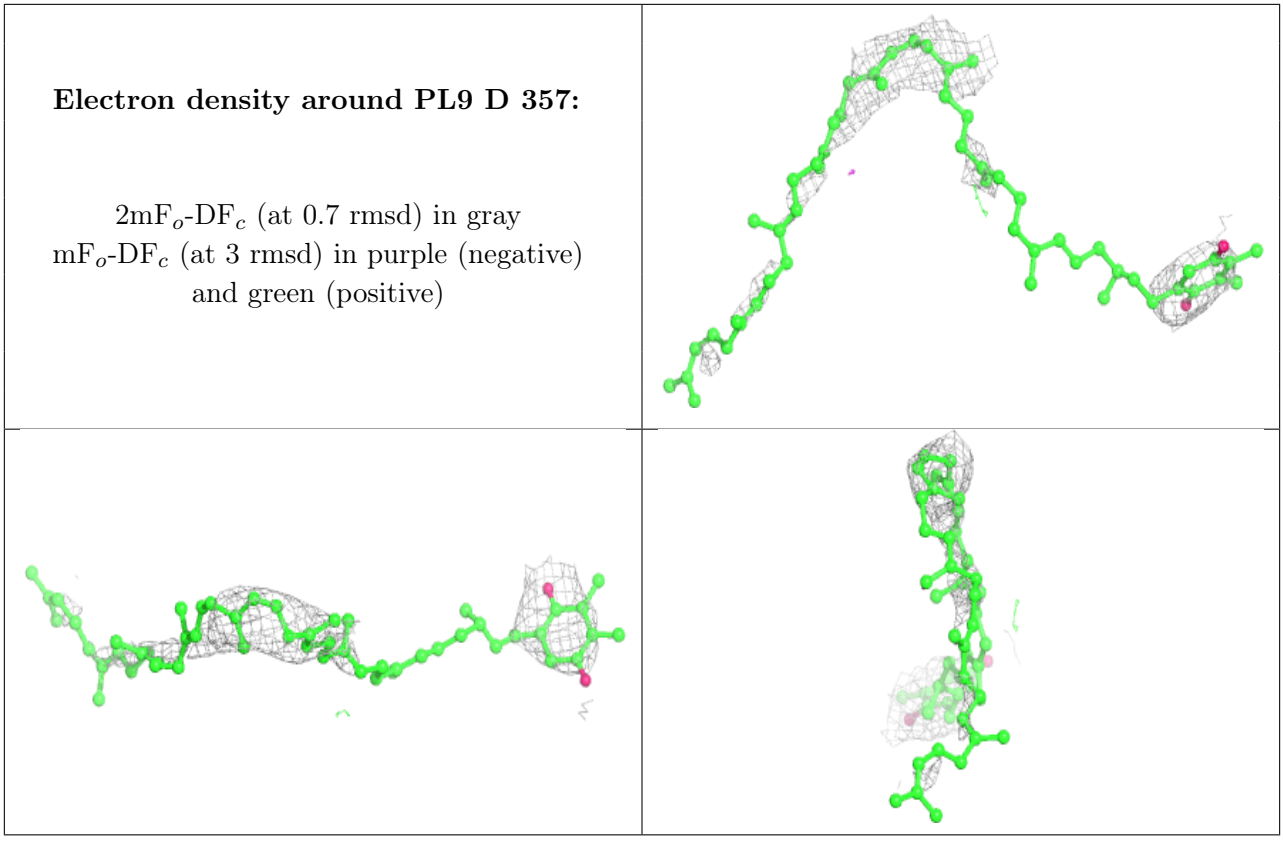






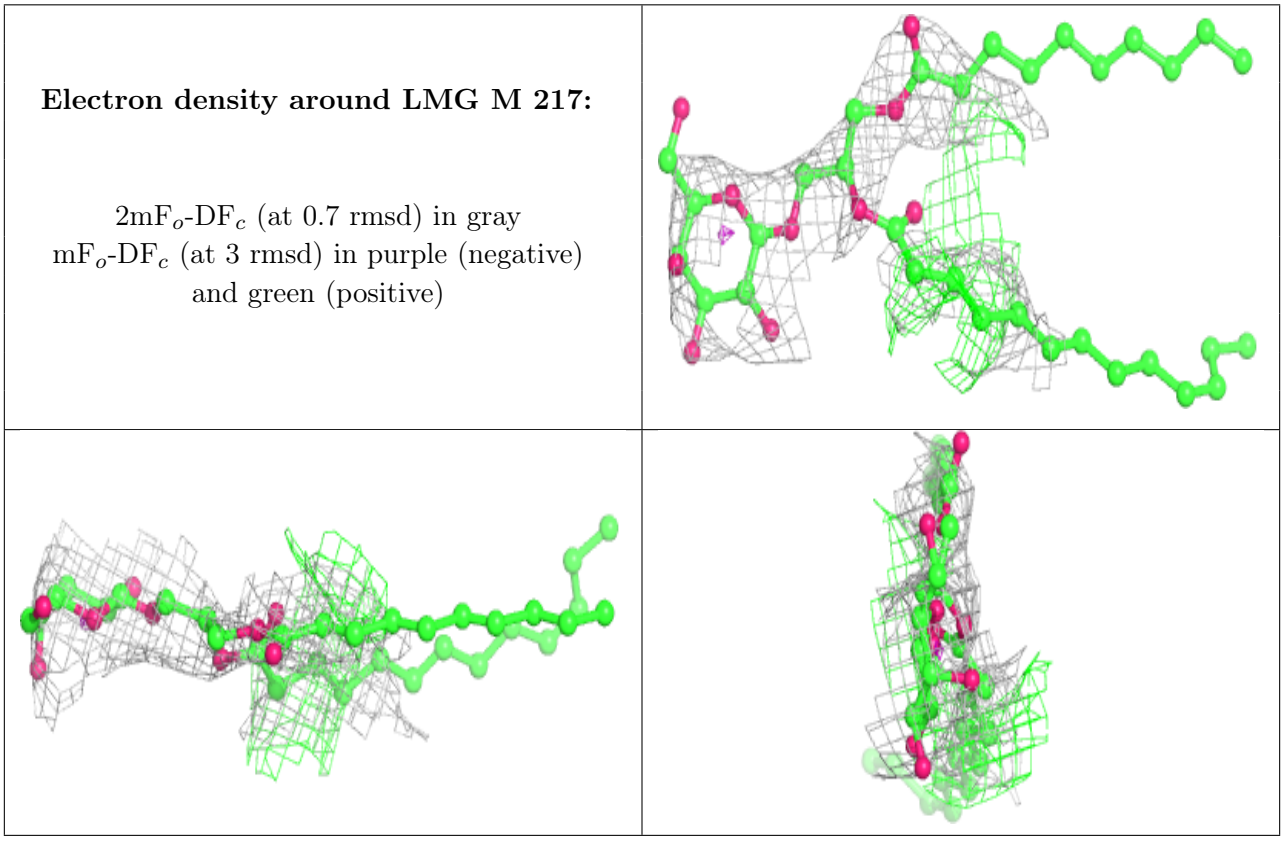
Electron density around PL9 D 357:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



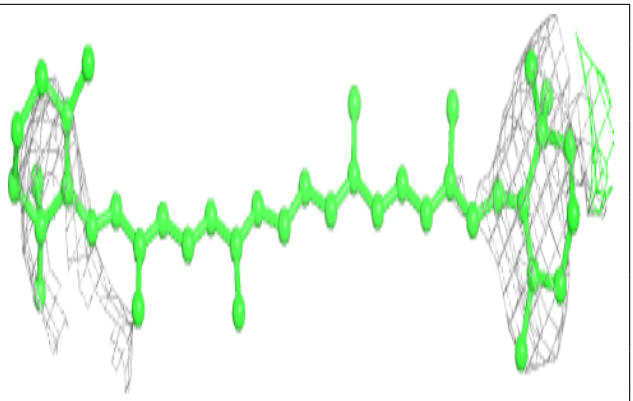
Electron density around LMG M 217:

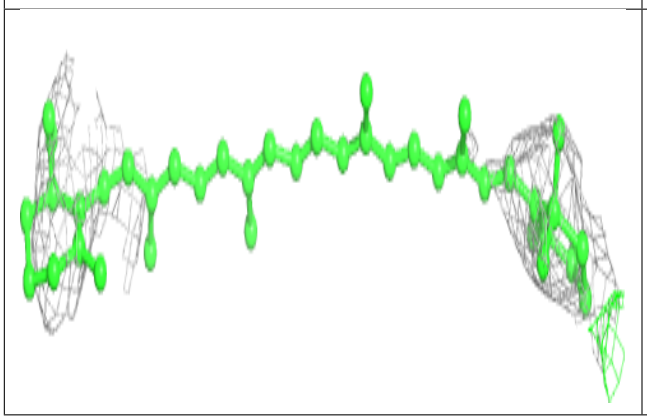
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

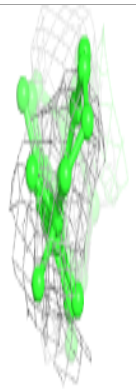


Electron density around BCR J 115:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

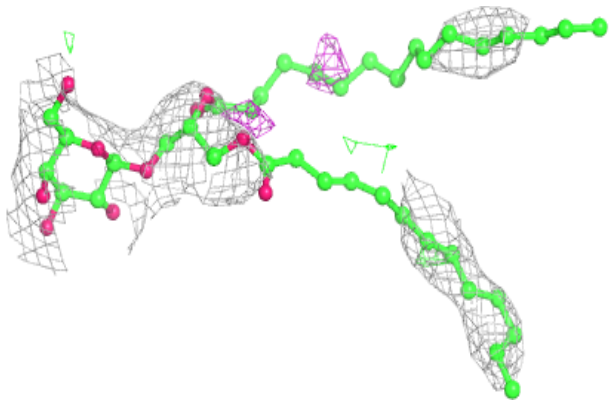


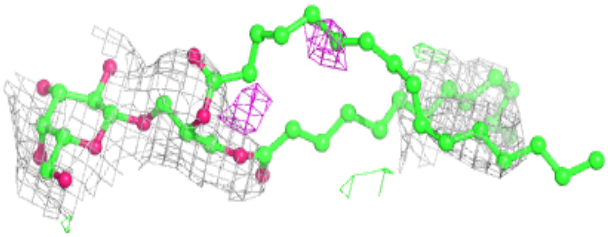


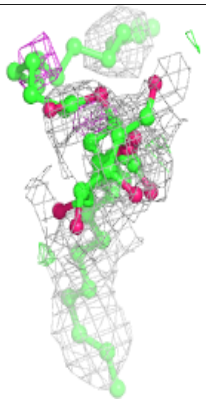


Electron density around LMG D 360:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

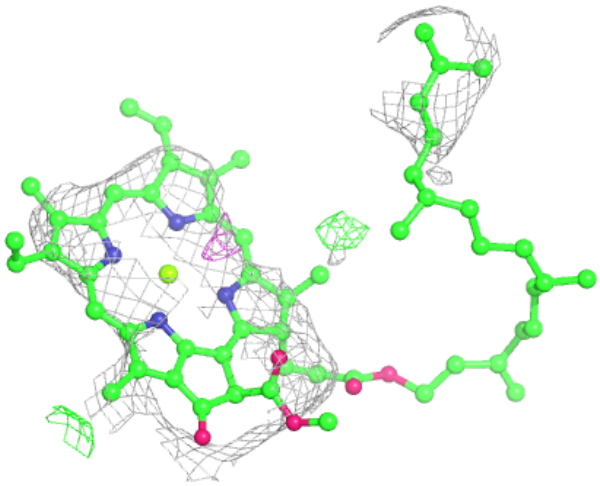


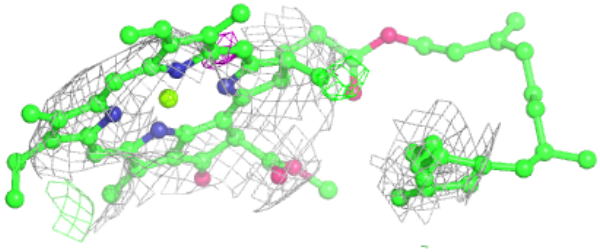


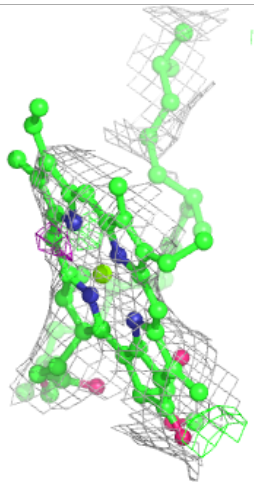


Electron density around CLA B 526:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

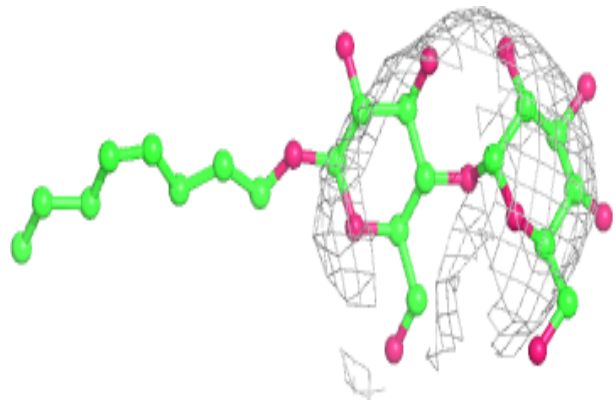


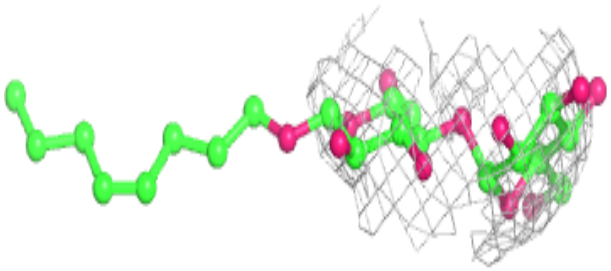


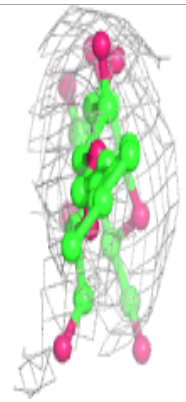


Electron density around LMT D 363:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

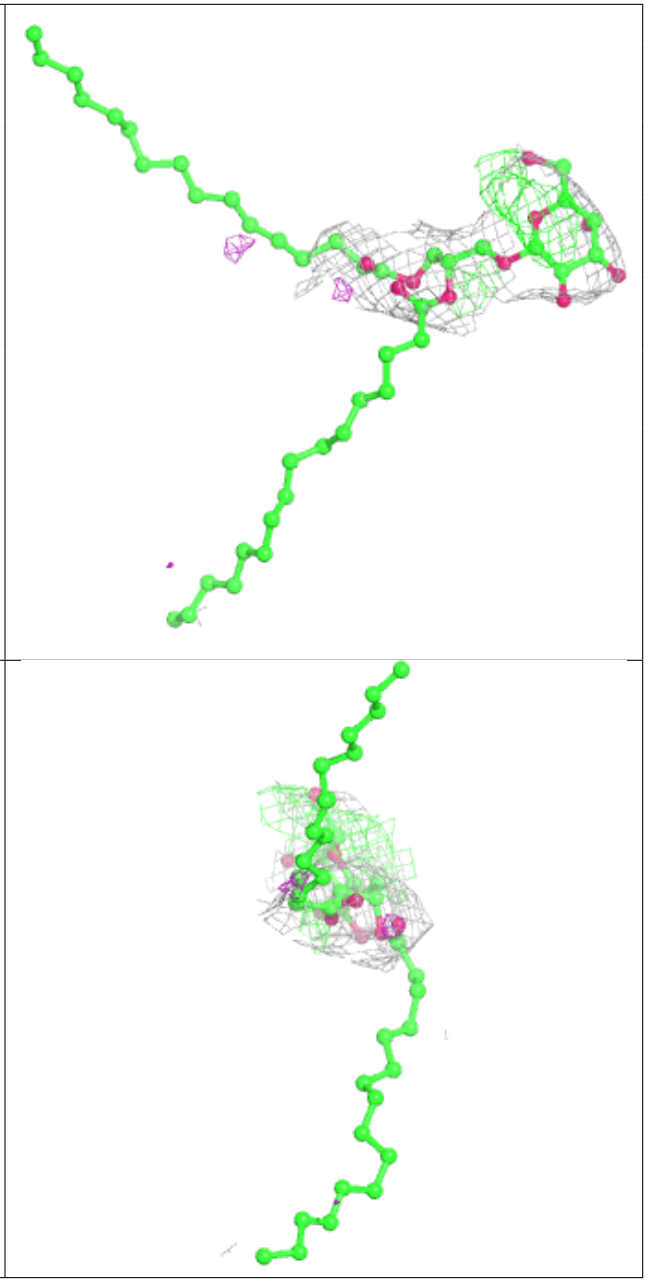






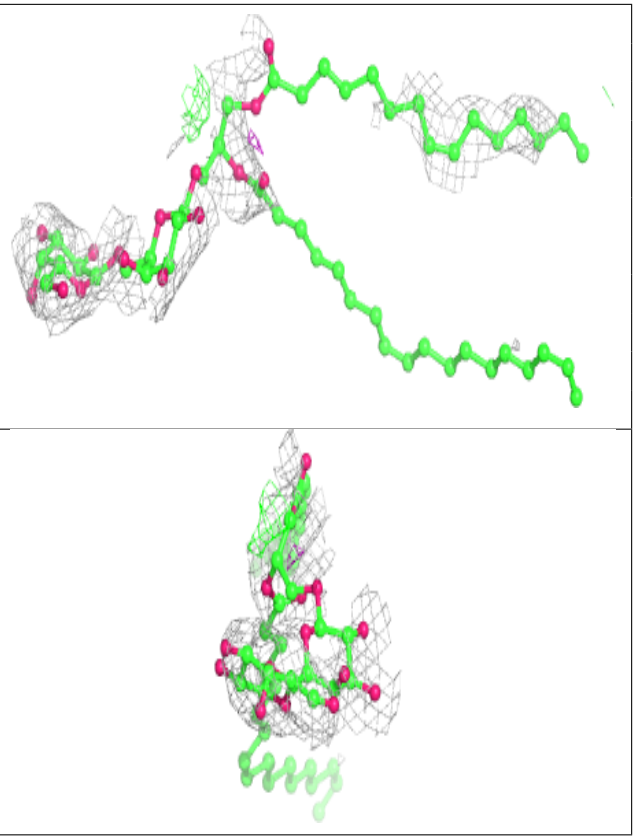
Electron density around LMG A 373:

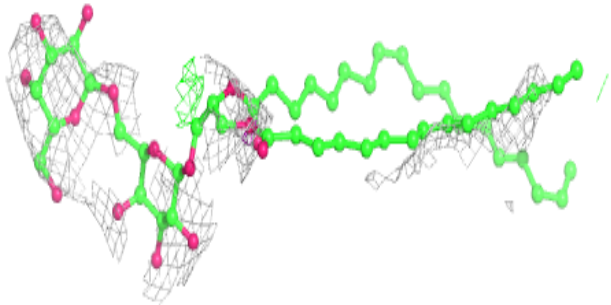
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around DGD D 362:

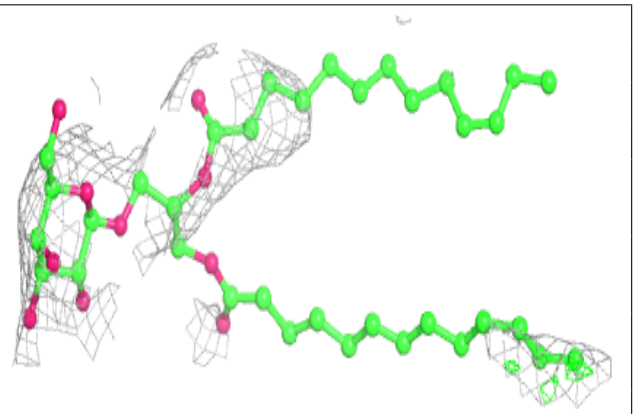
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

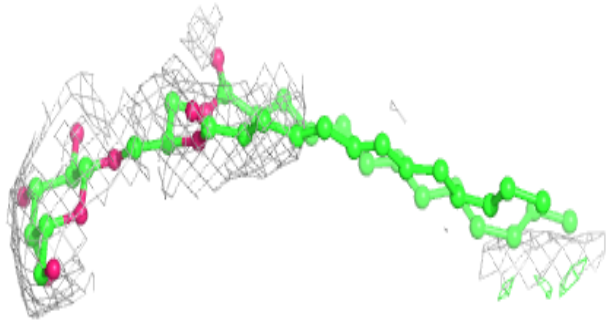


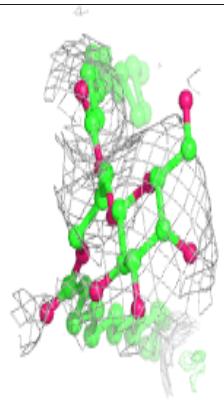


Electron density around LMG C 494:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

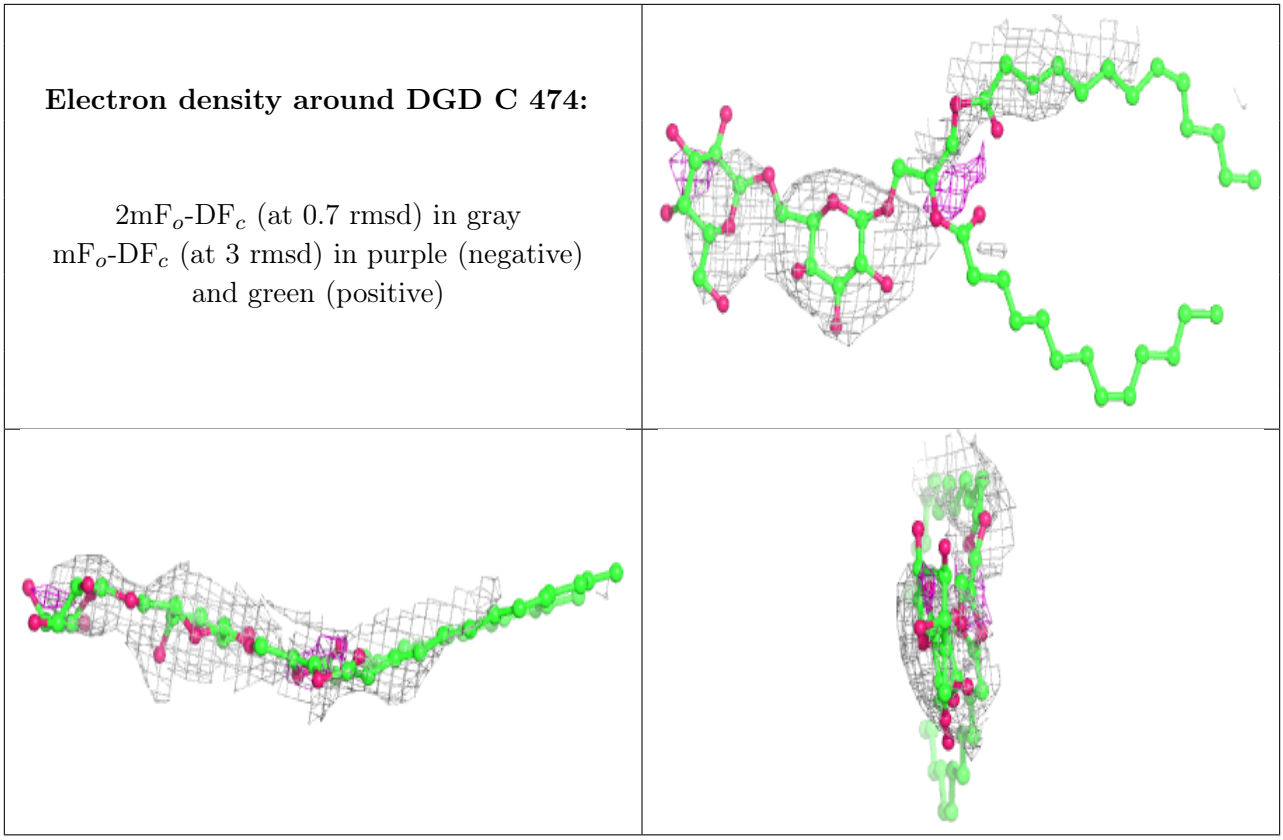






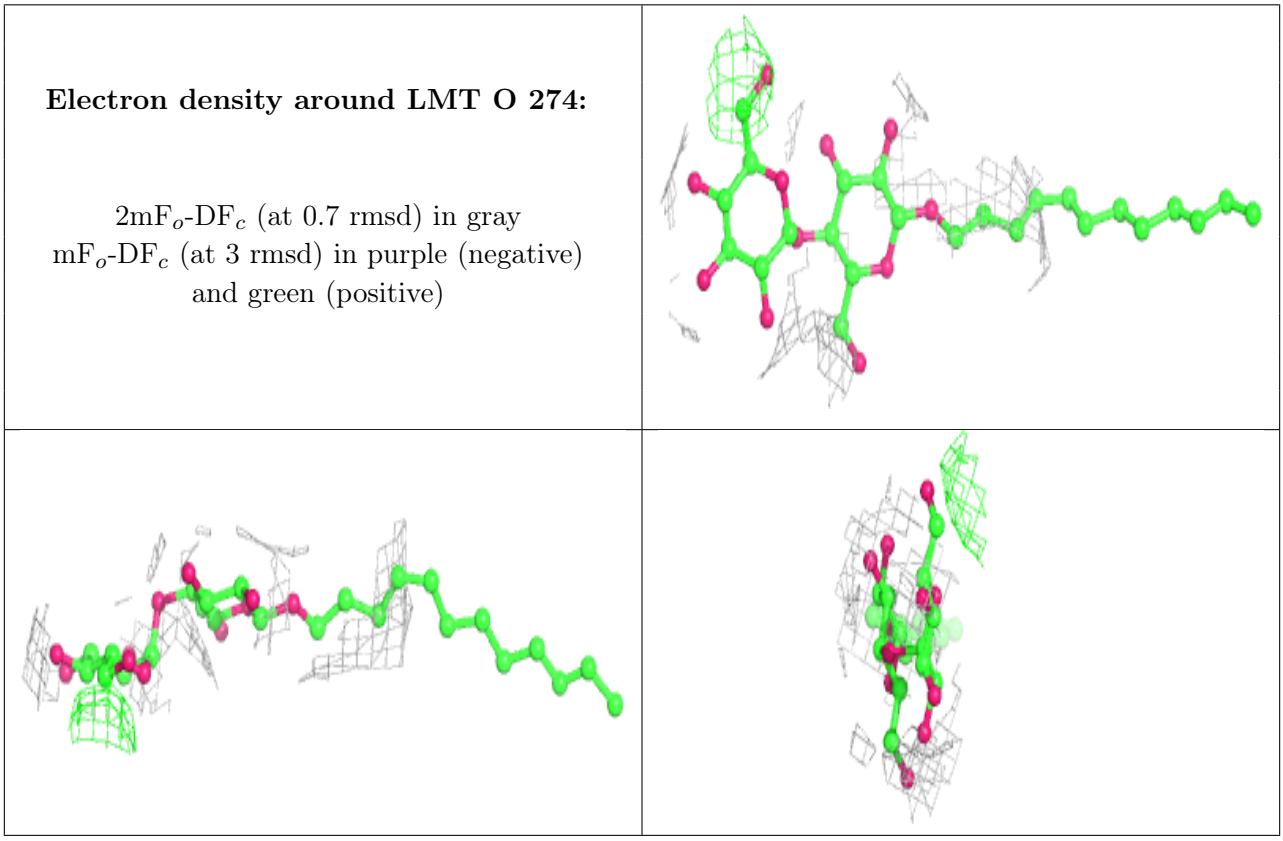
Electron density around DGD C 474:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



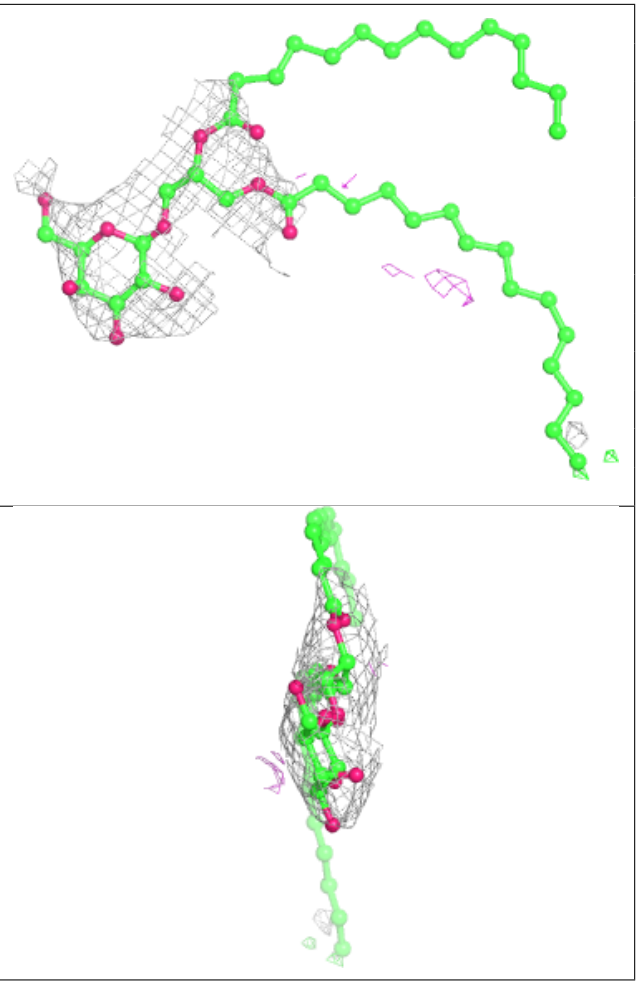
Electron density around LMT O 274:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



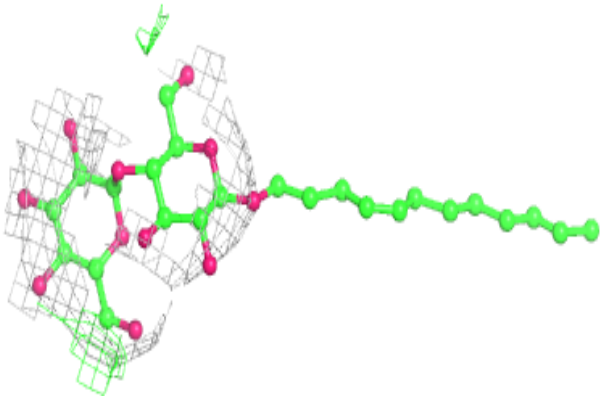
Electron density around LMG J 492:

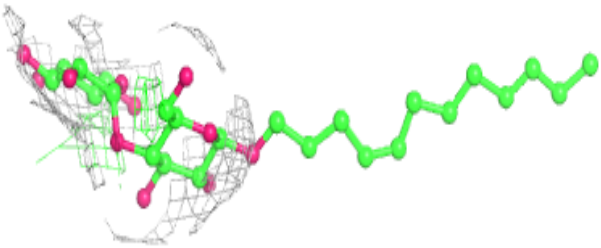
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

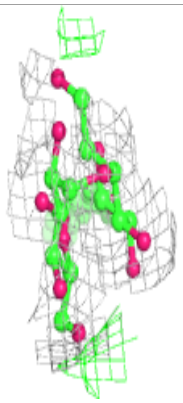


Electron density around LMT A 376:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

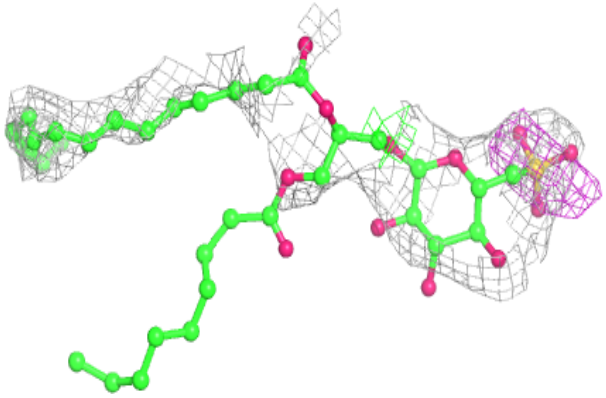


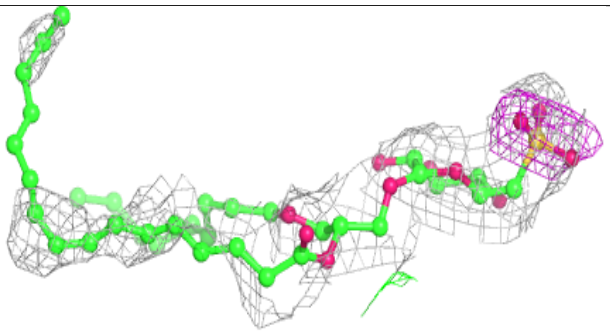


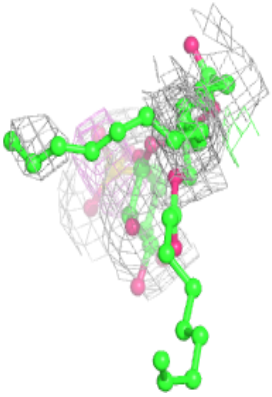


Electron density around SQD L 213:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

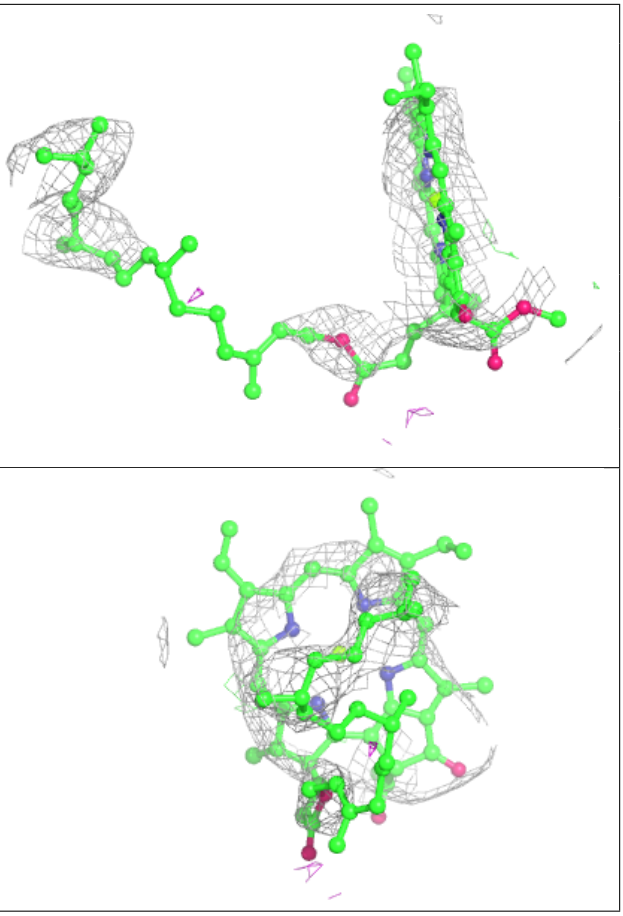


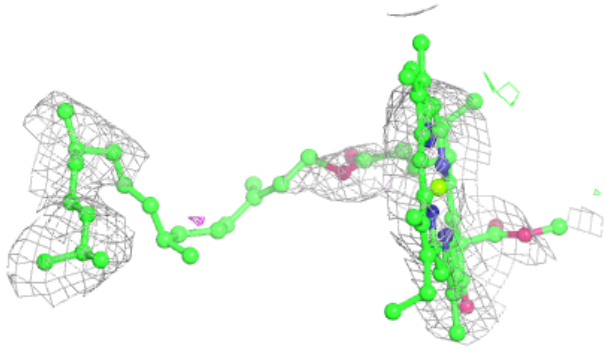




Electron density around CLA C 482:

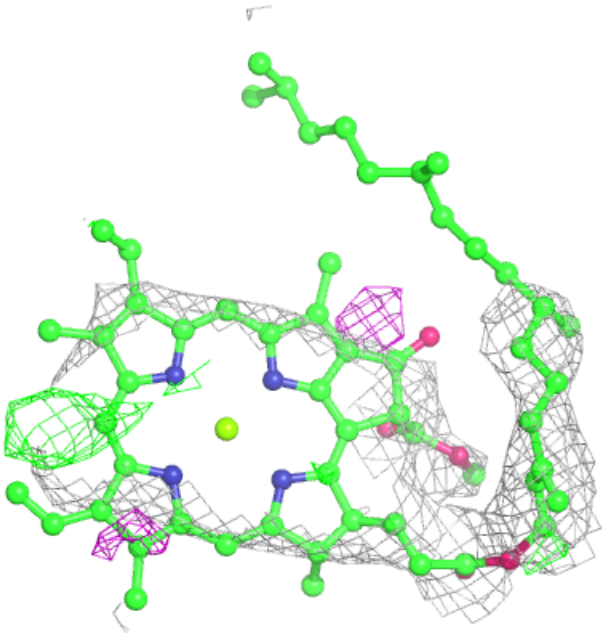
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

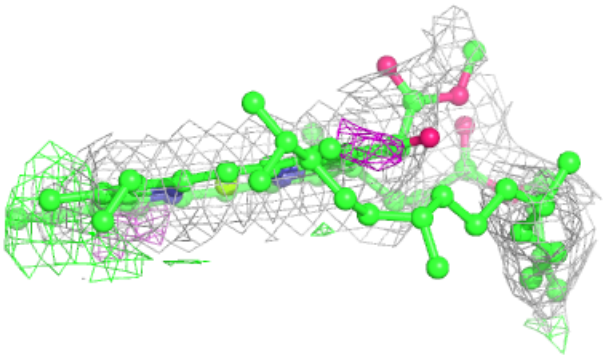


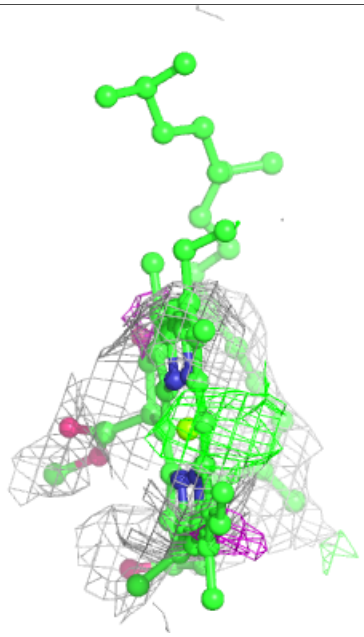


Electron density around CLA B 511:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

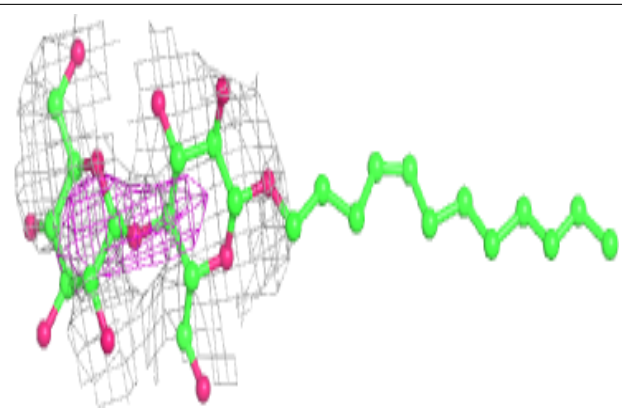


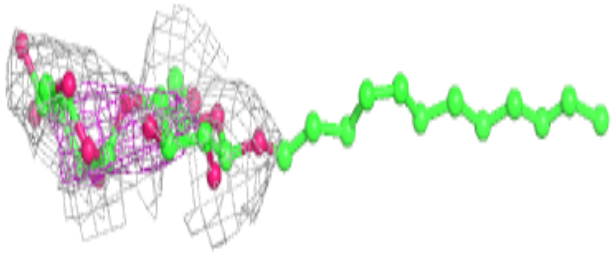


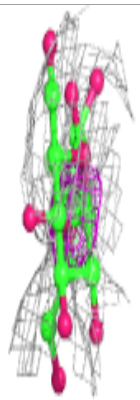


Electron density around LMT I 274:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

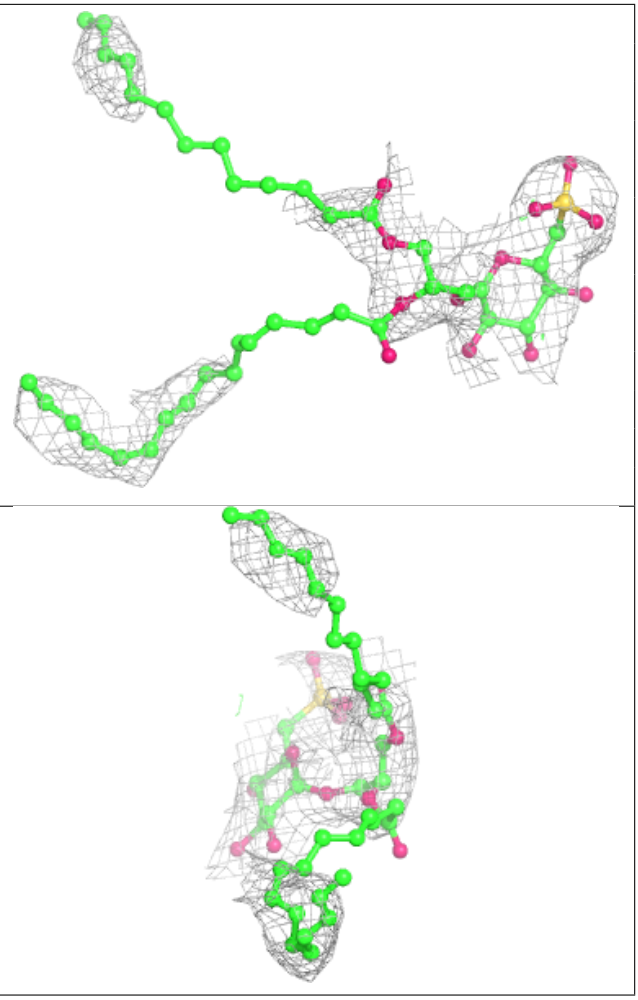






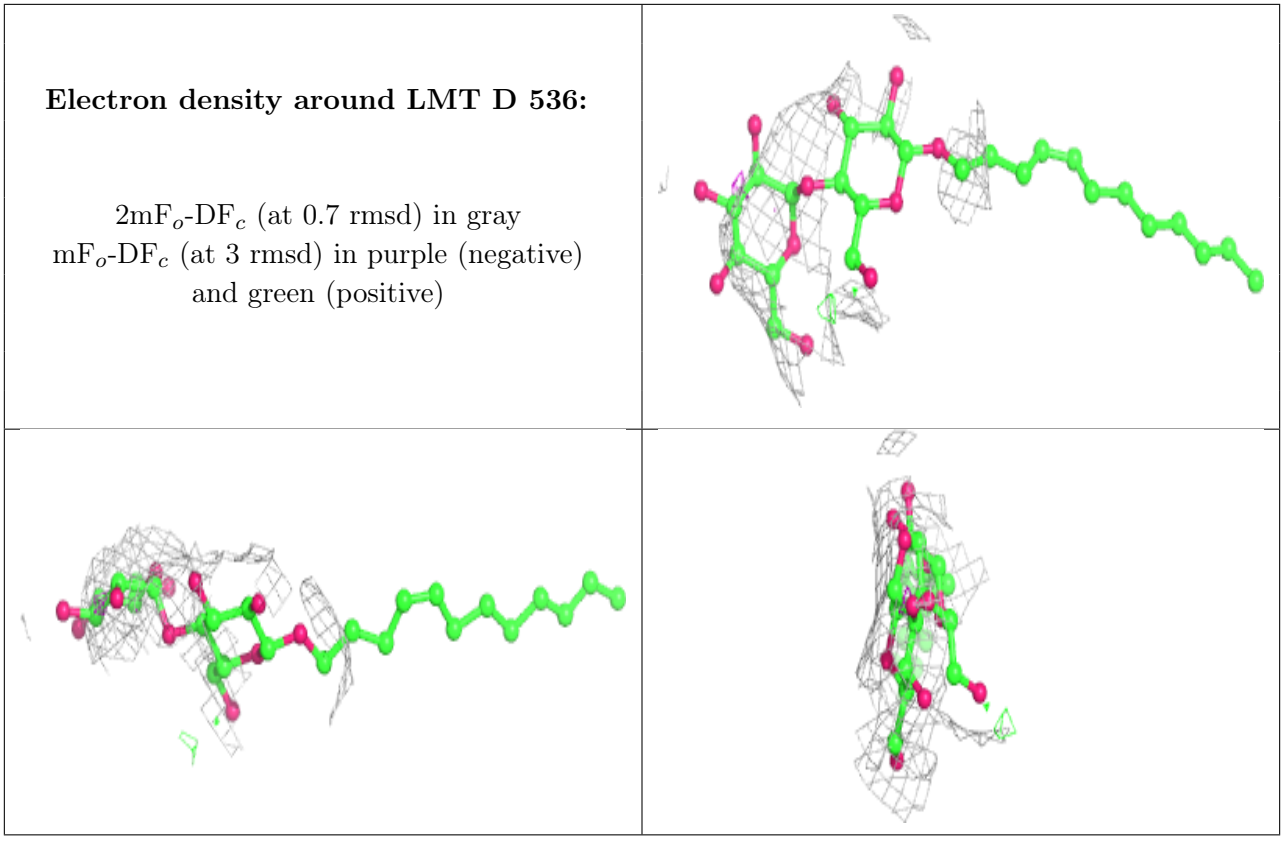
Electron density around SQD C 475:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



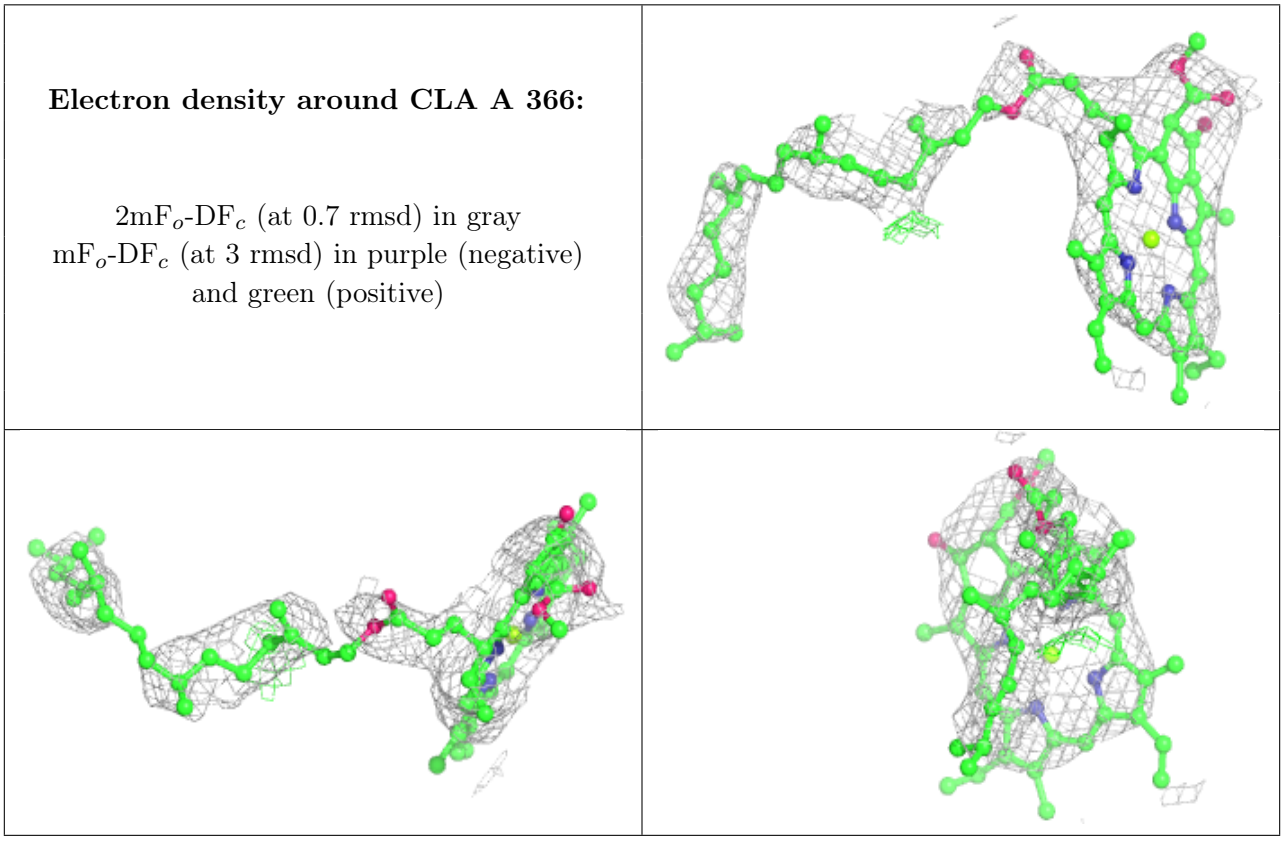
Electron density around LMT D 536:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



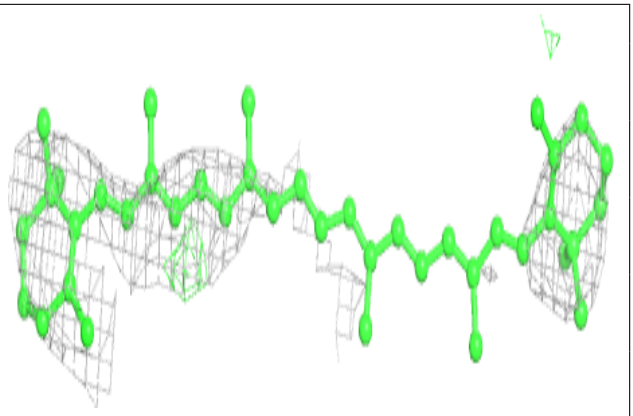
Electron density around CLA A 366:

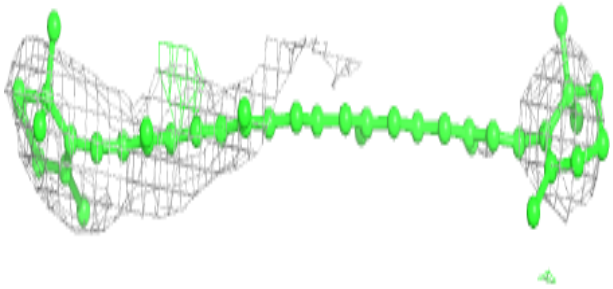
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

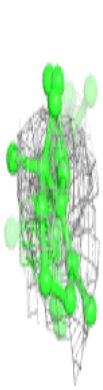


Electron density around BCR B 529:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

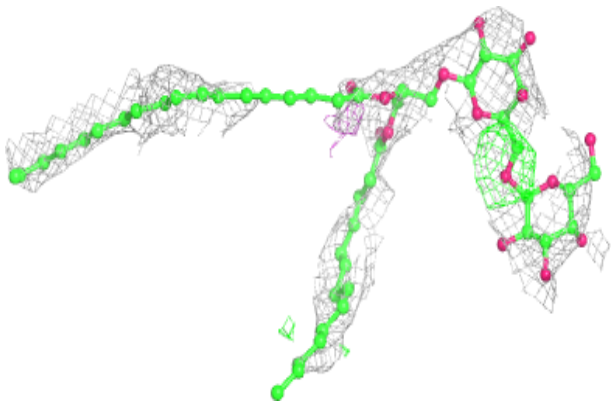


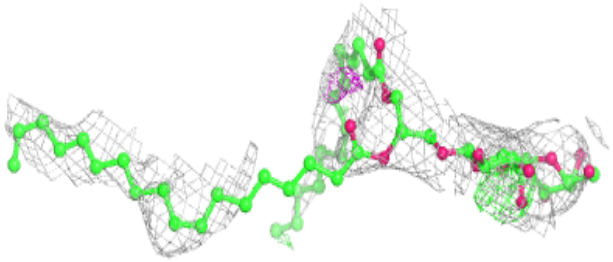


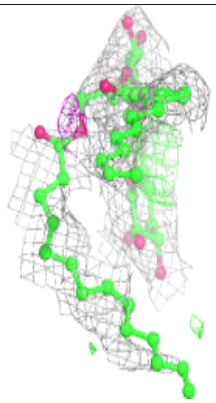


Electron density around DGD C 492:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

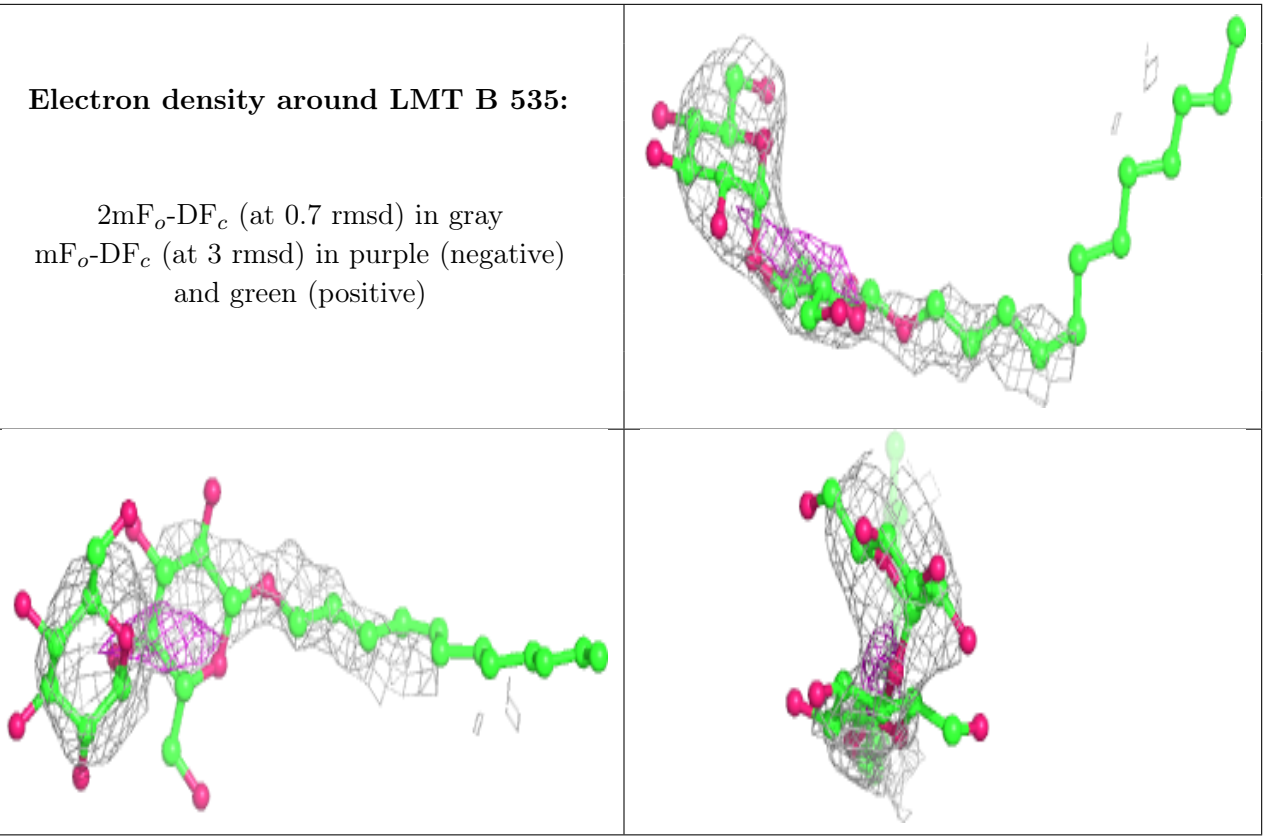






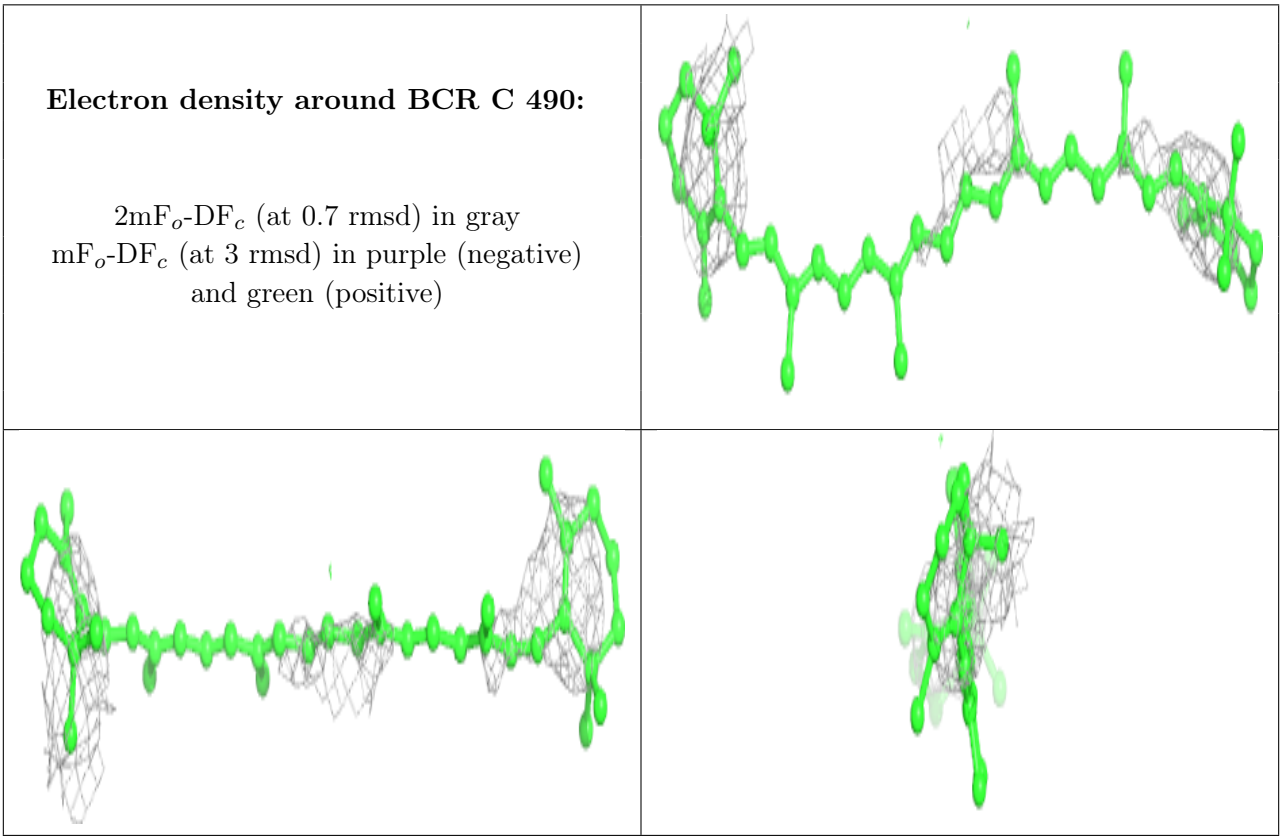
Electron density around LMT B 535:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



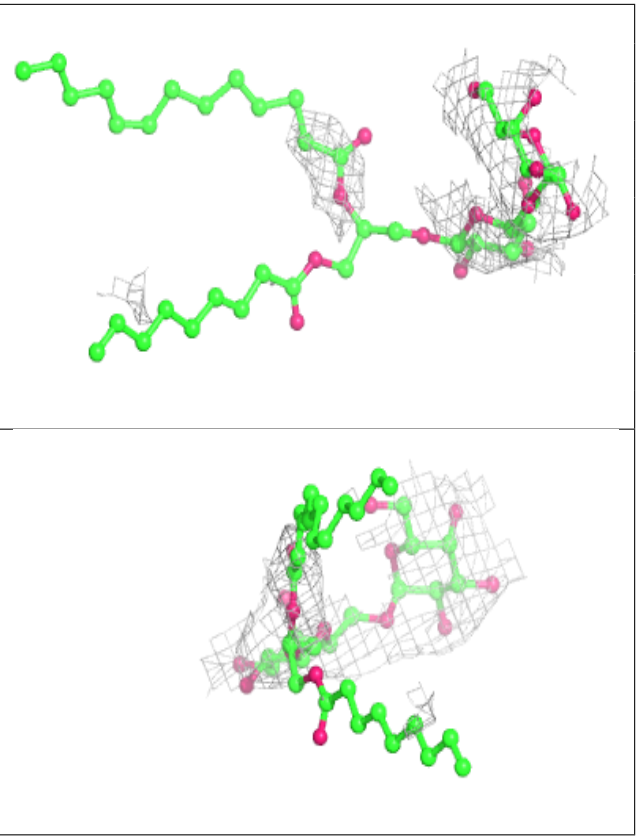
Electron density around BCR C 490:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



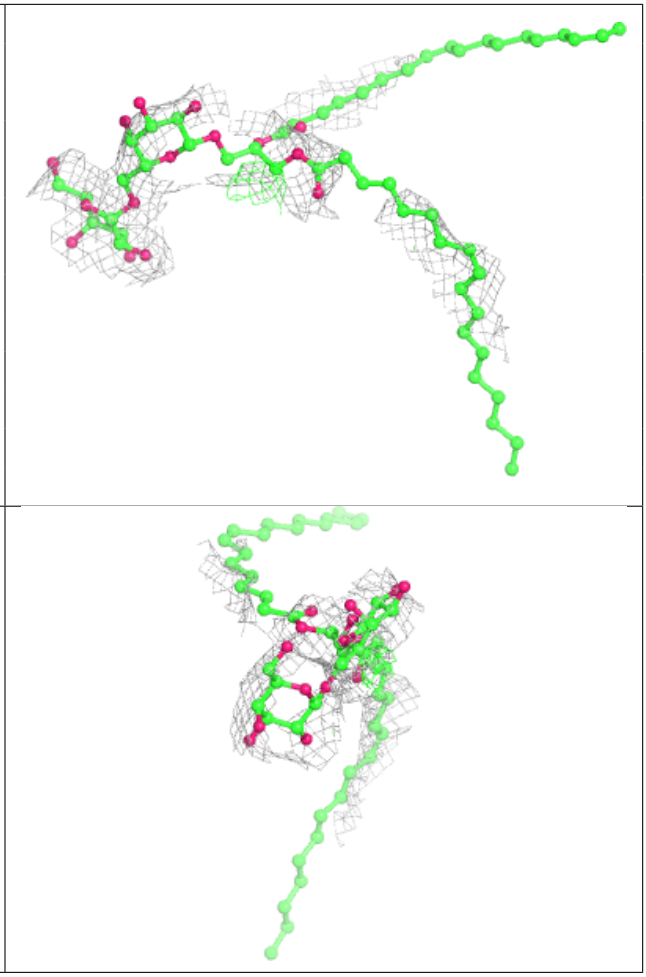
Electron density around DGD A 375:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



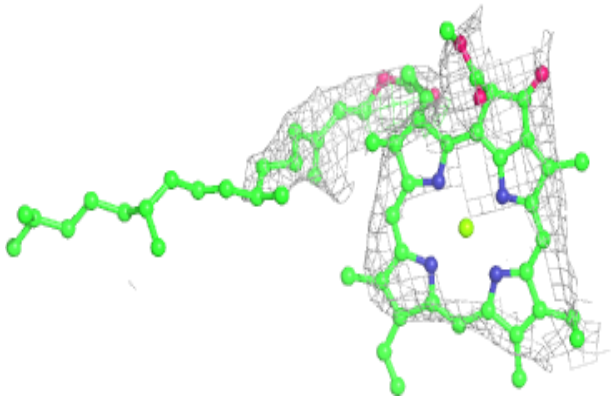
Electron density around DGD B 533:

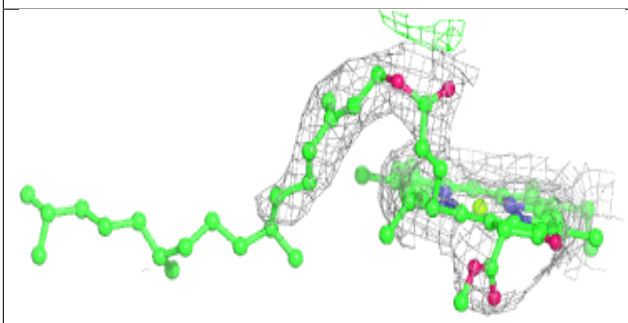
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

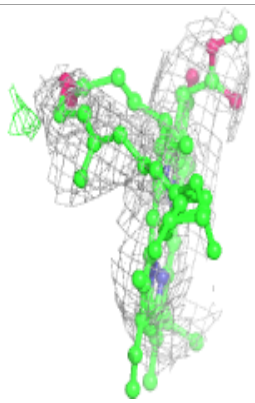


Electron density around CLA A 363:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

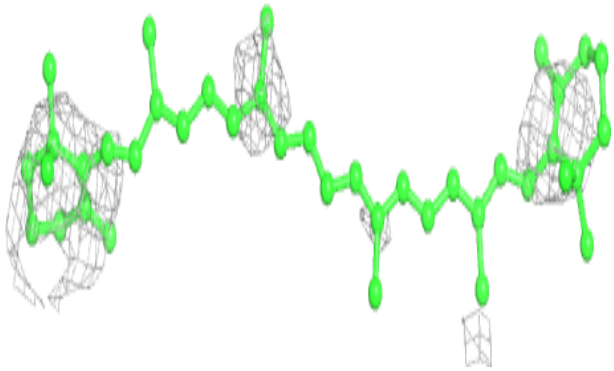


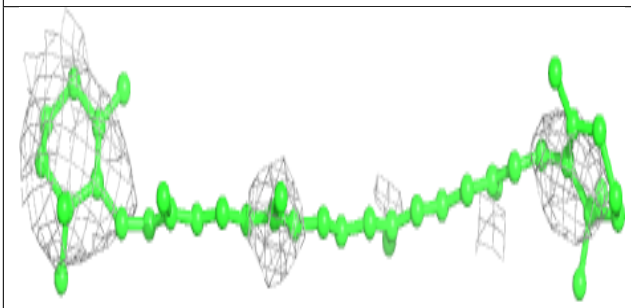


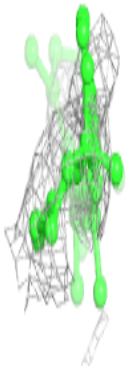


Electron density around BCR B 527:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

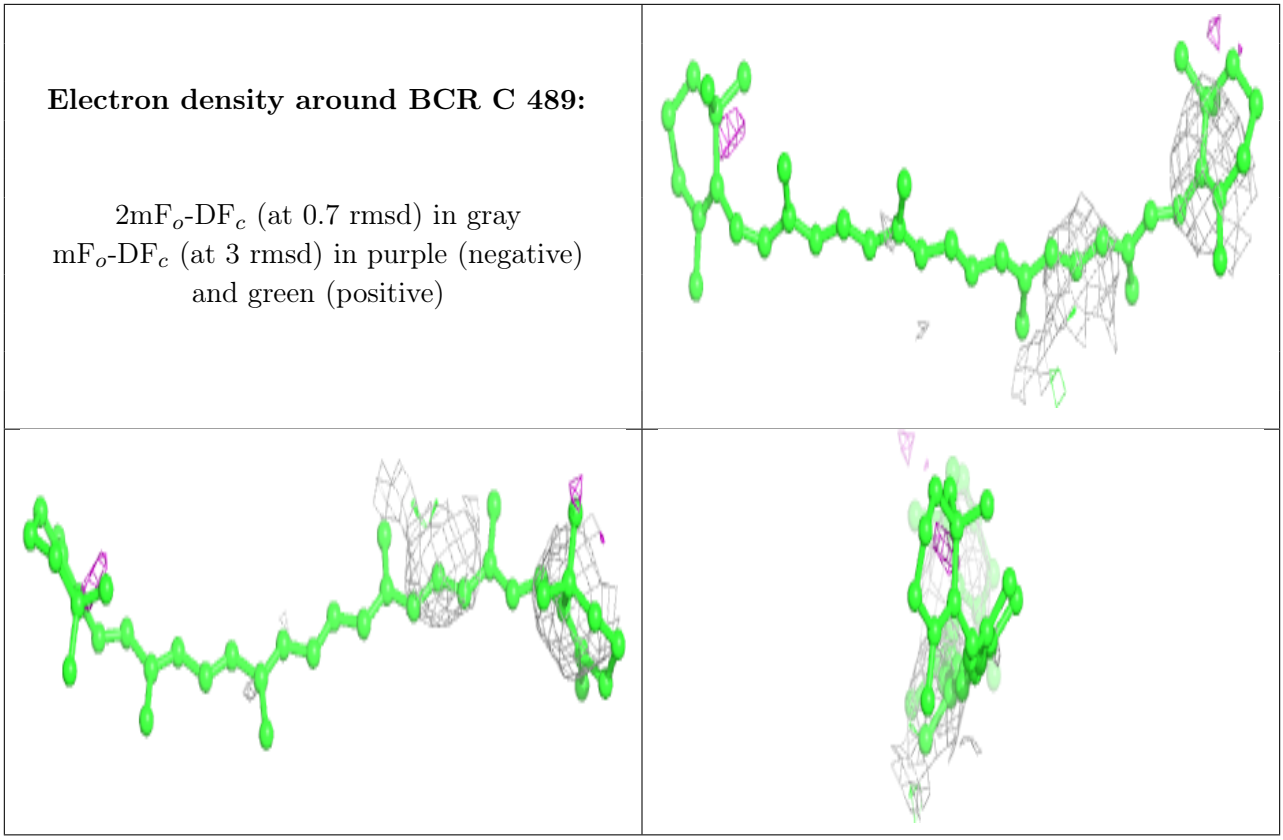






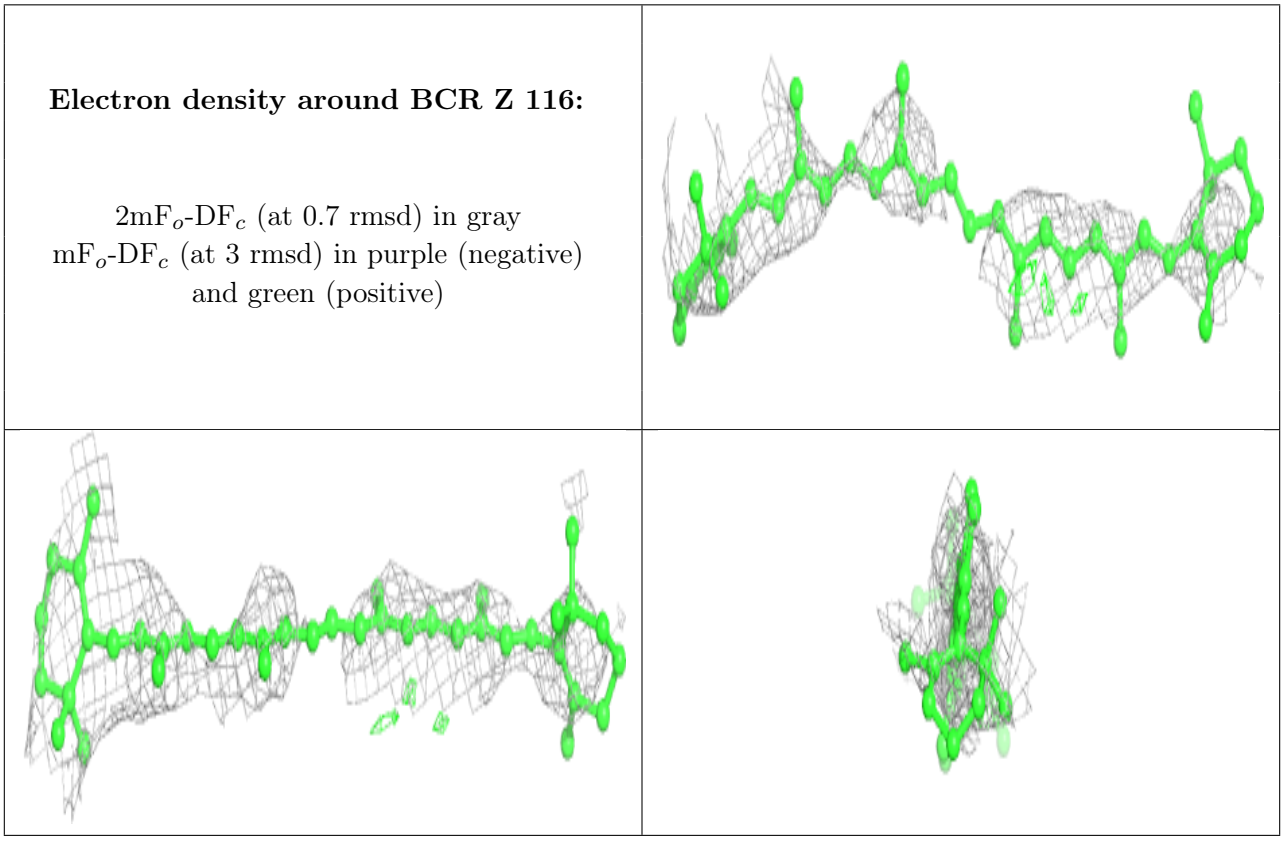
Electron density around BCR C 489:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



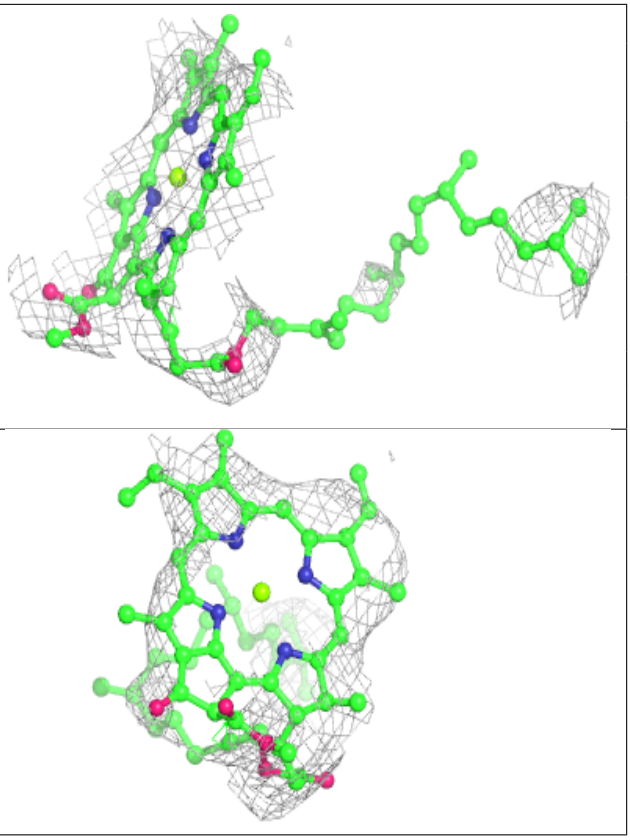
Electron density around BCR Z 116:

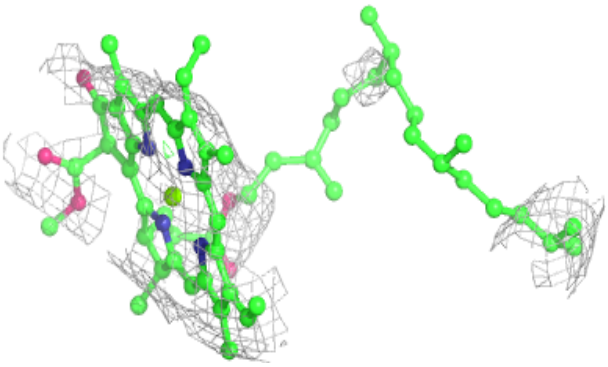
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA C 488:

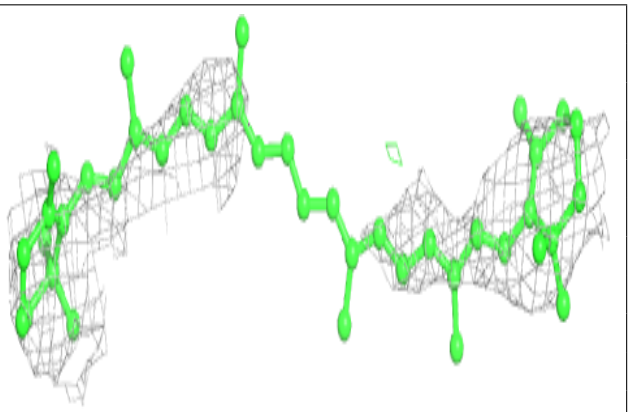
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

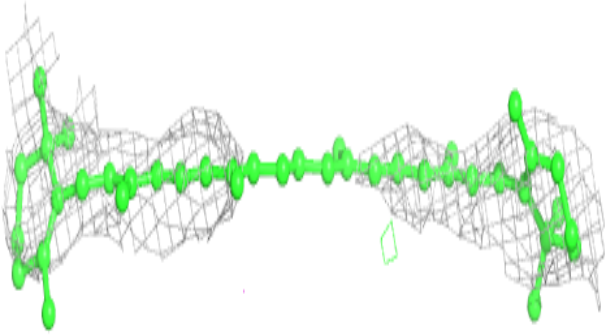


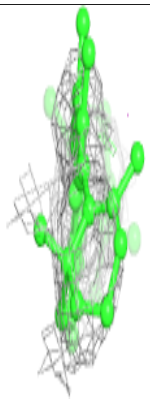


Electron density around BCR X 107:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

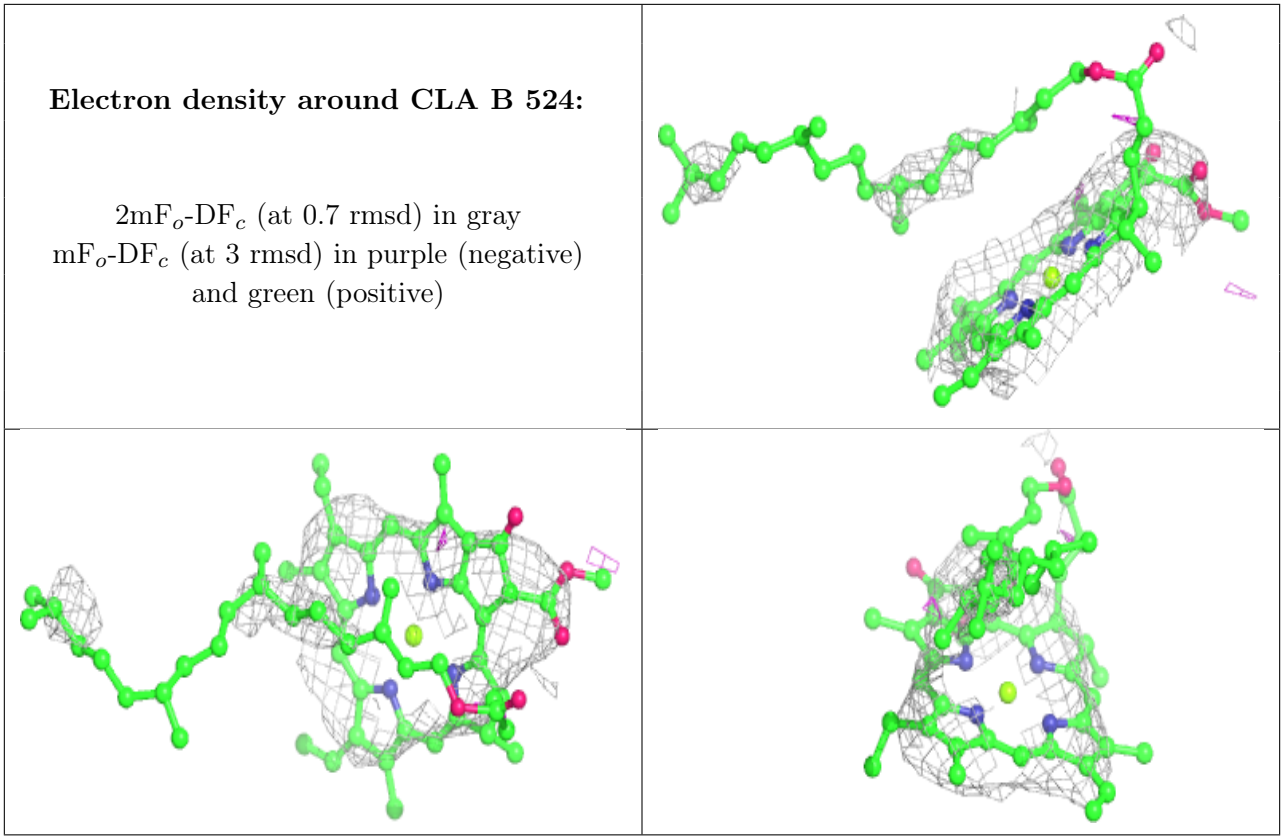






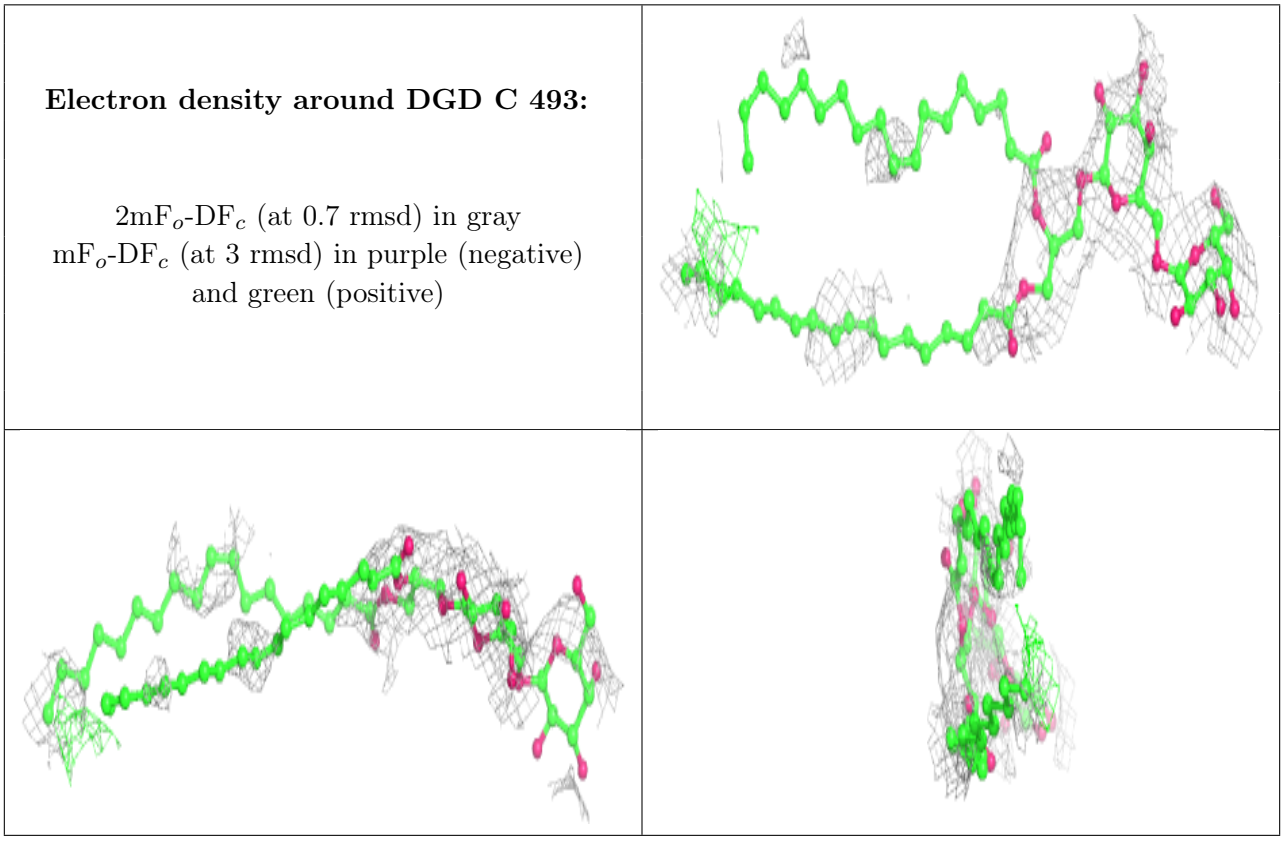
Electron density around CLA B 524:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



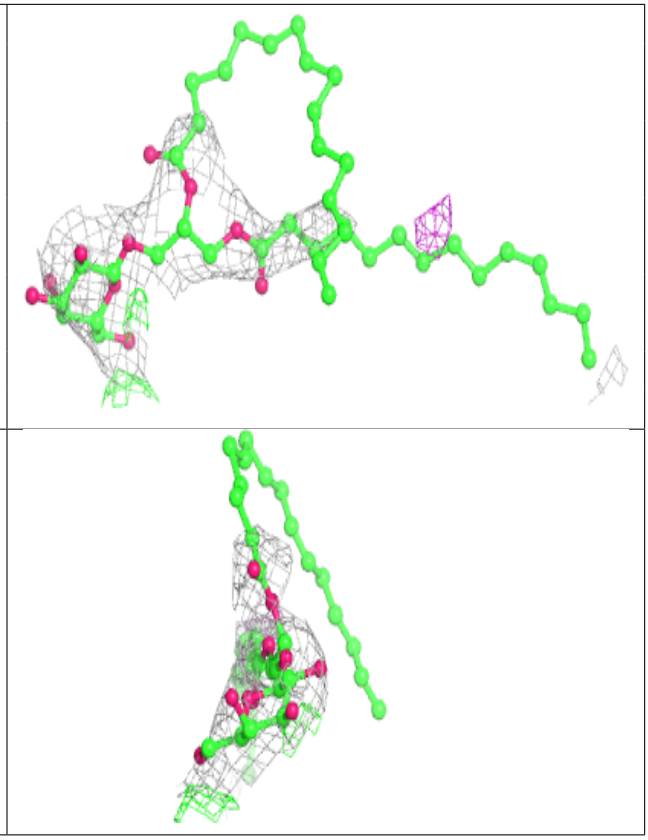
Electron density around DGD C 493:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



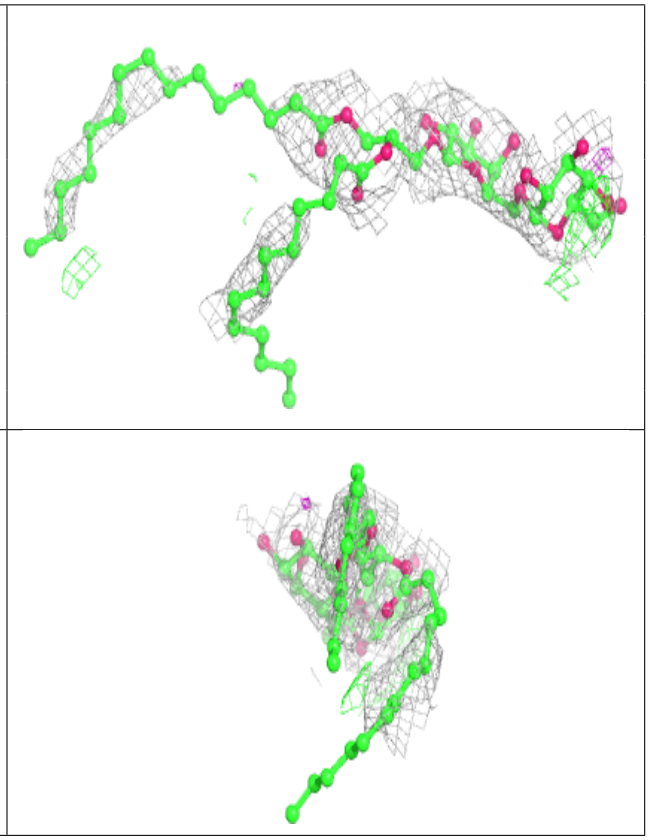
Electron density around LMG B 531:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



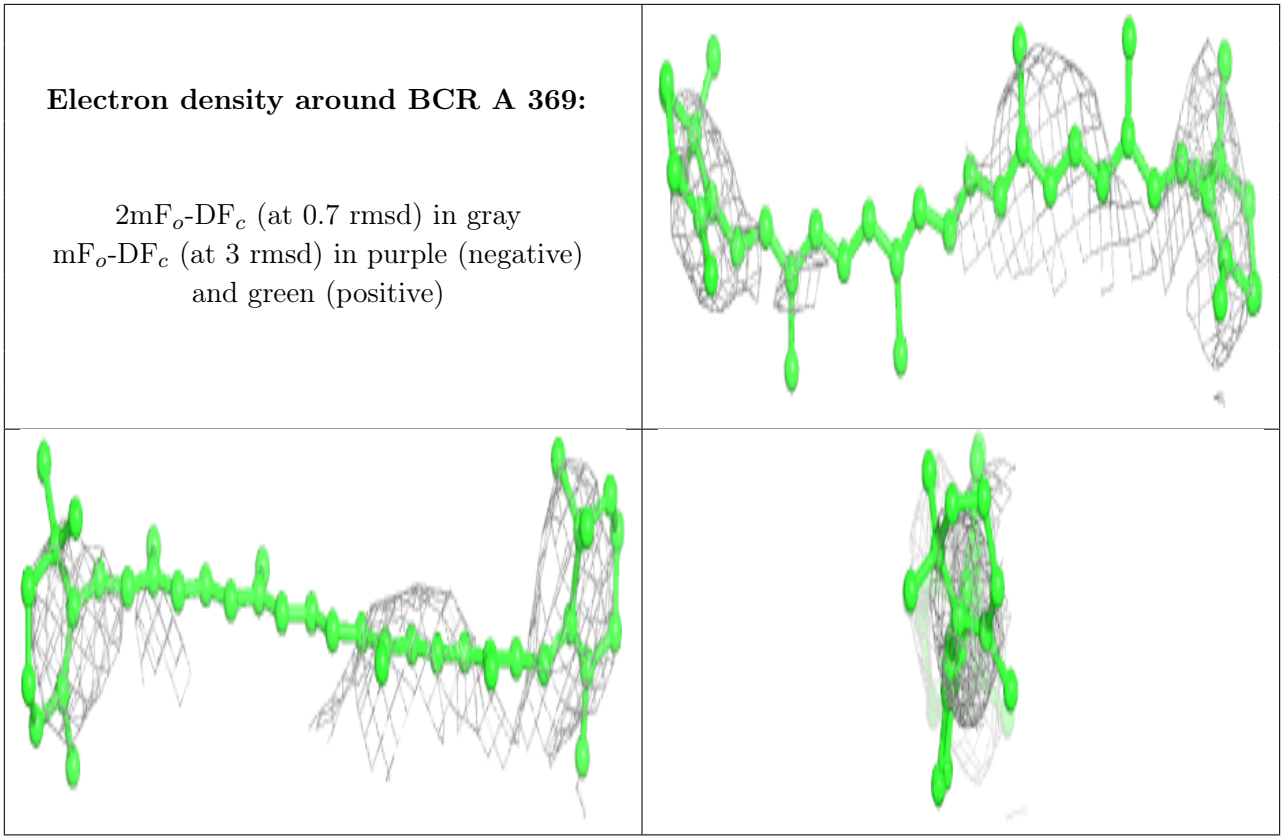
Electron density around DGD B 528:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



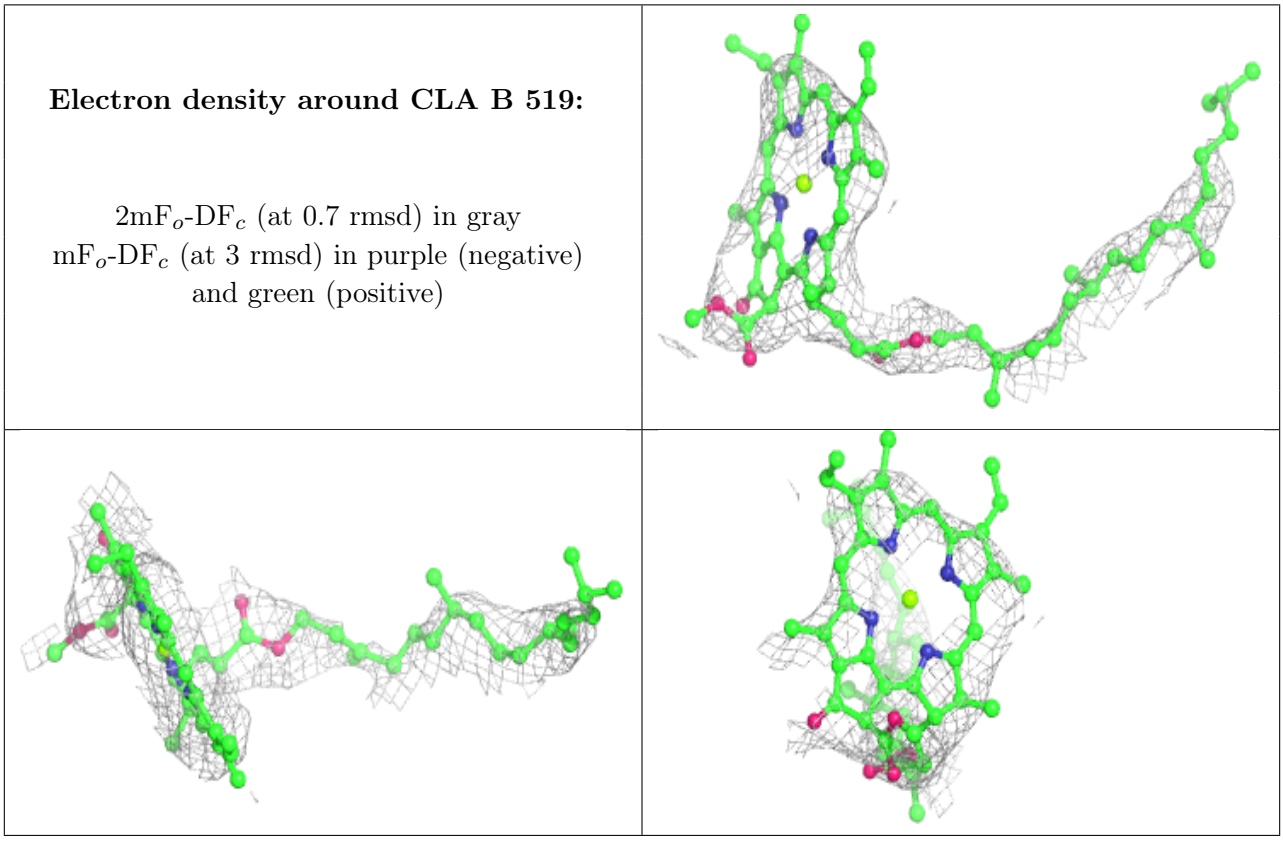
Electron density around BCR A 369:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



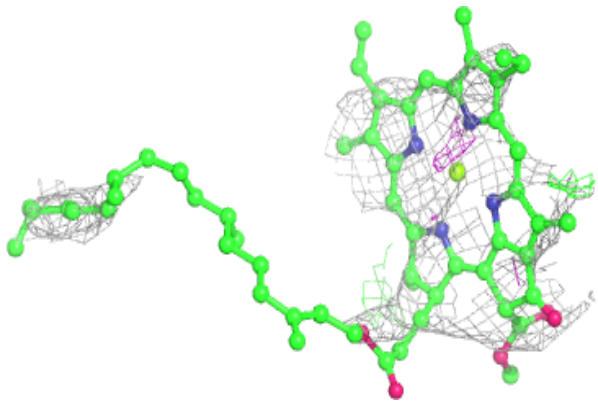
Electron density around CLA B 519:

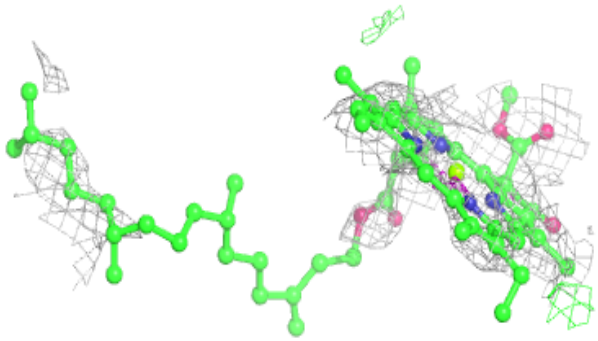
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

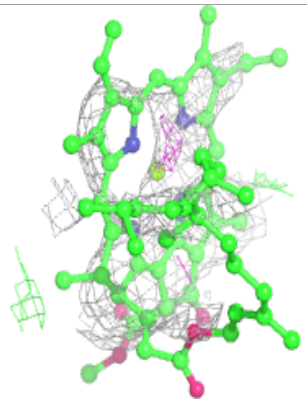


Electron density around CLA C 486:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

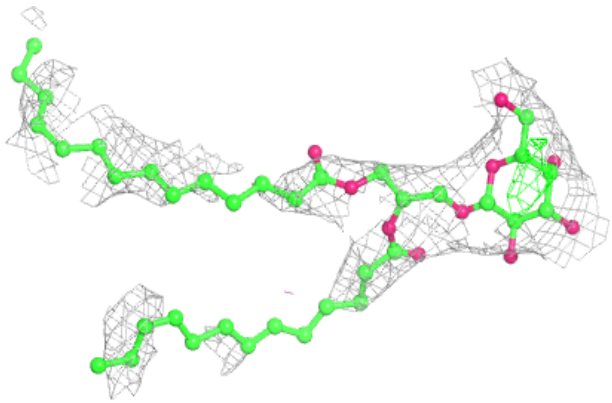


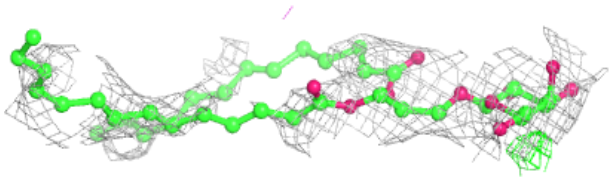


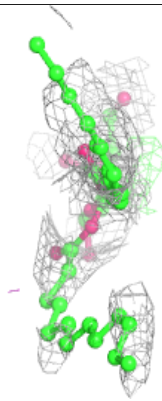


Electron density around LMG D 359:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

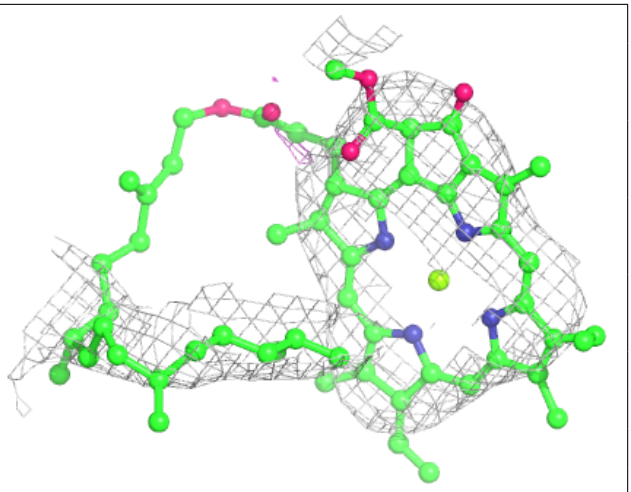


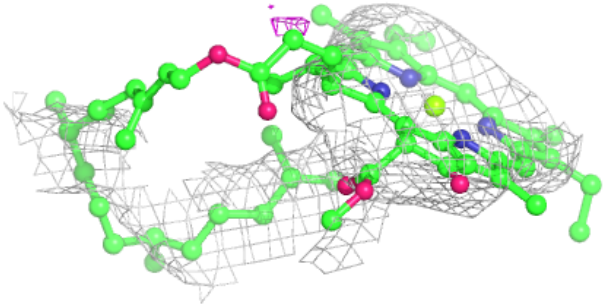


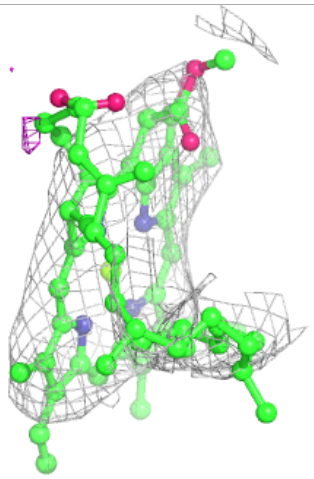


Electron density around CLA B 525:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

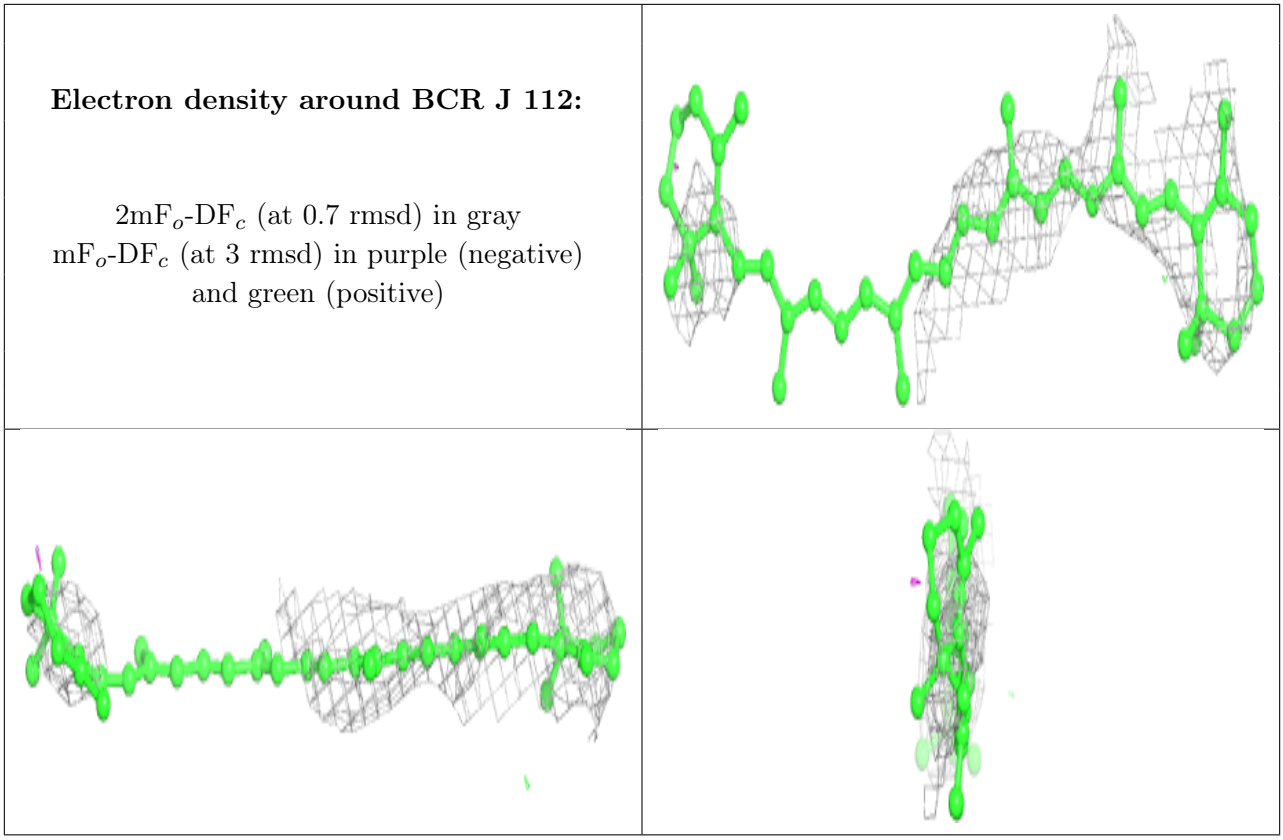






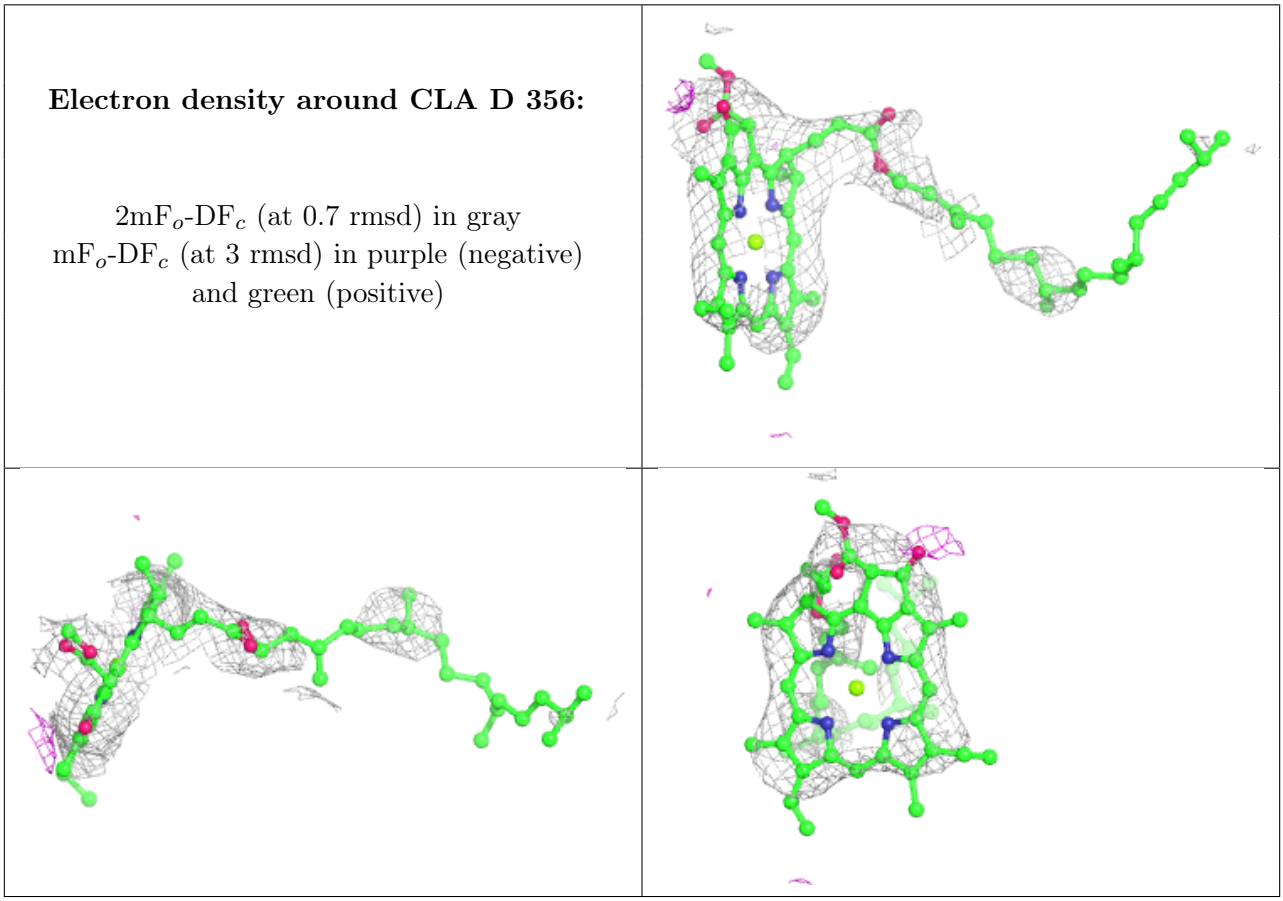
Electron density around BCR J 112:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



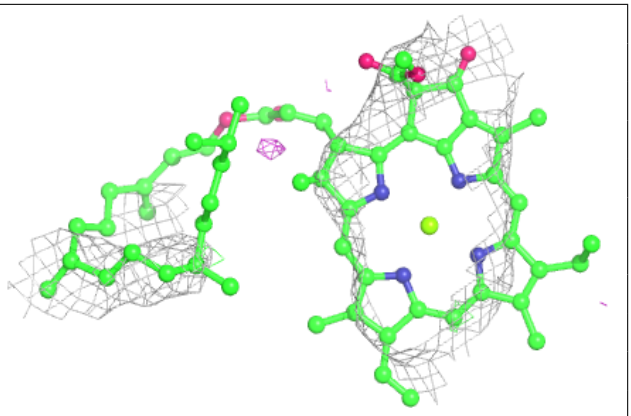
Electron density around CLA D 356:

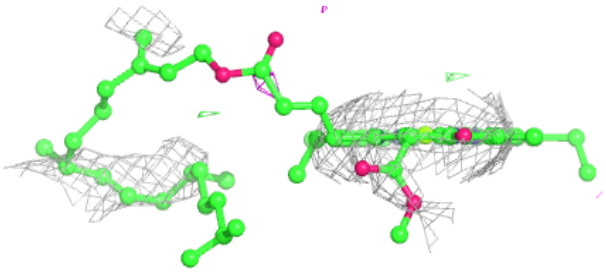
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

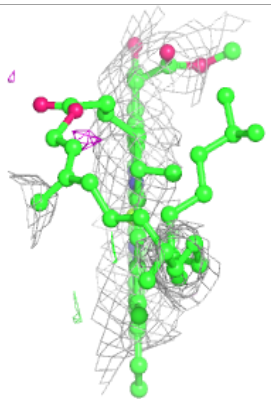


Electron density around CLA C 487:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

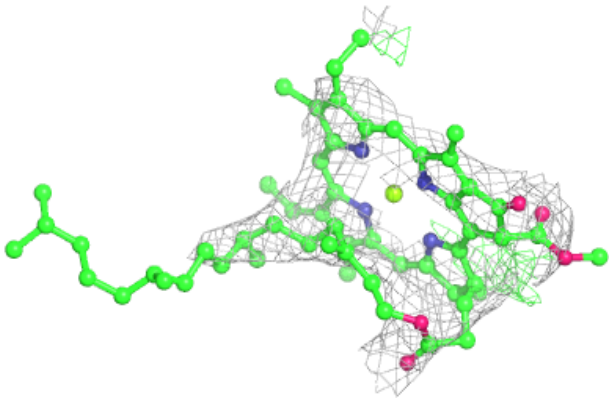


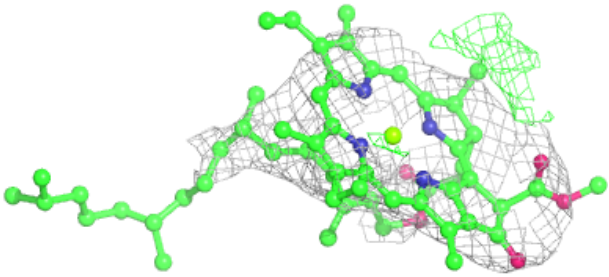


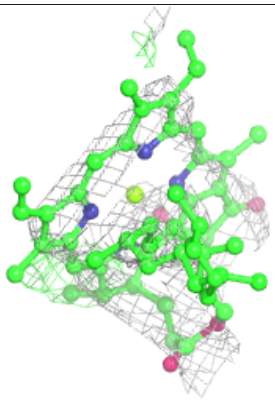


Electron density around CLA C 481:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

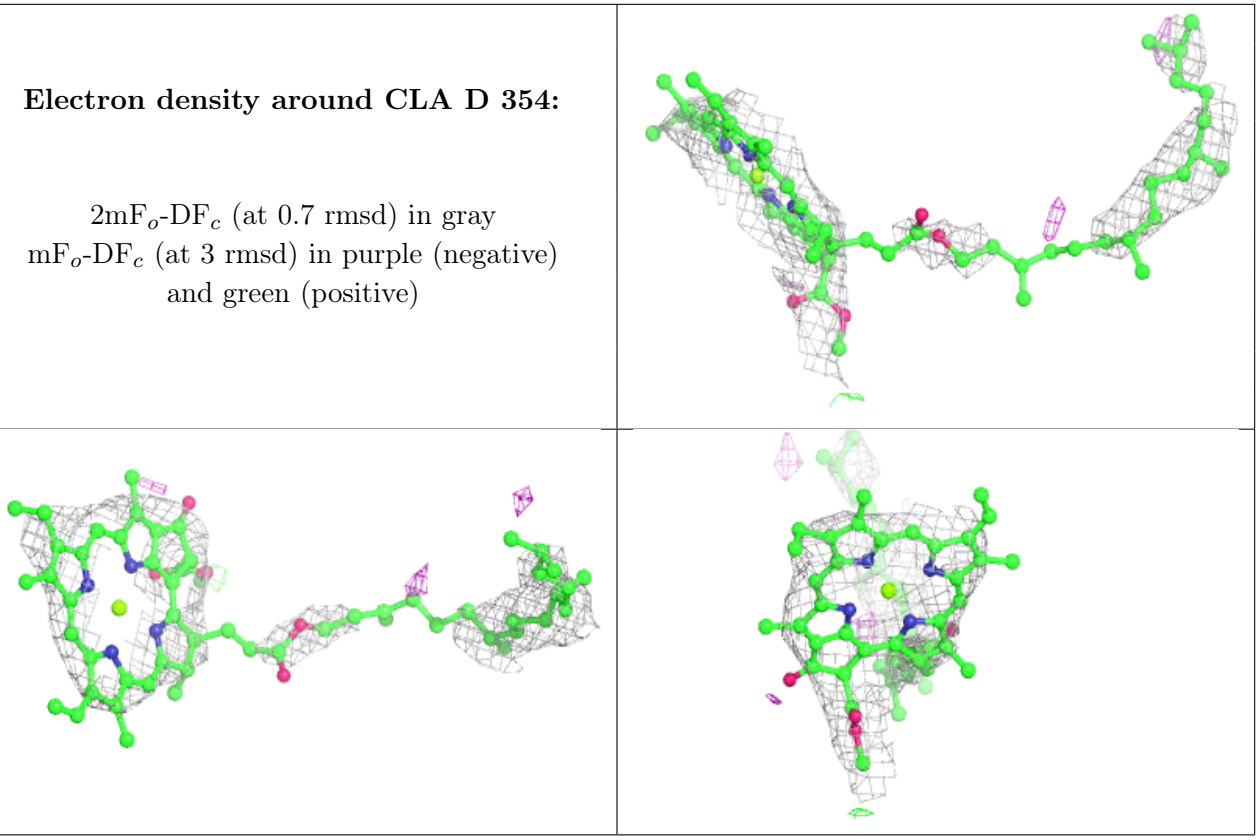






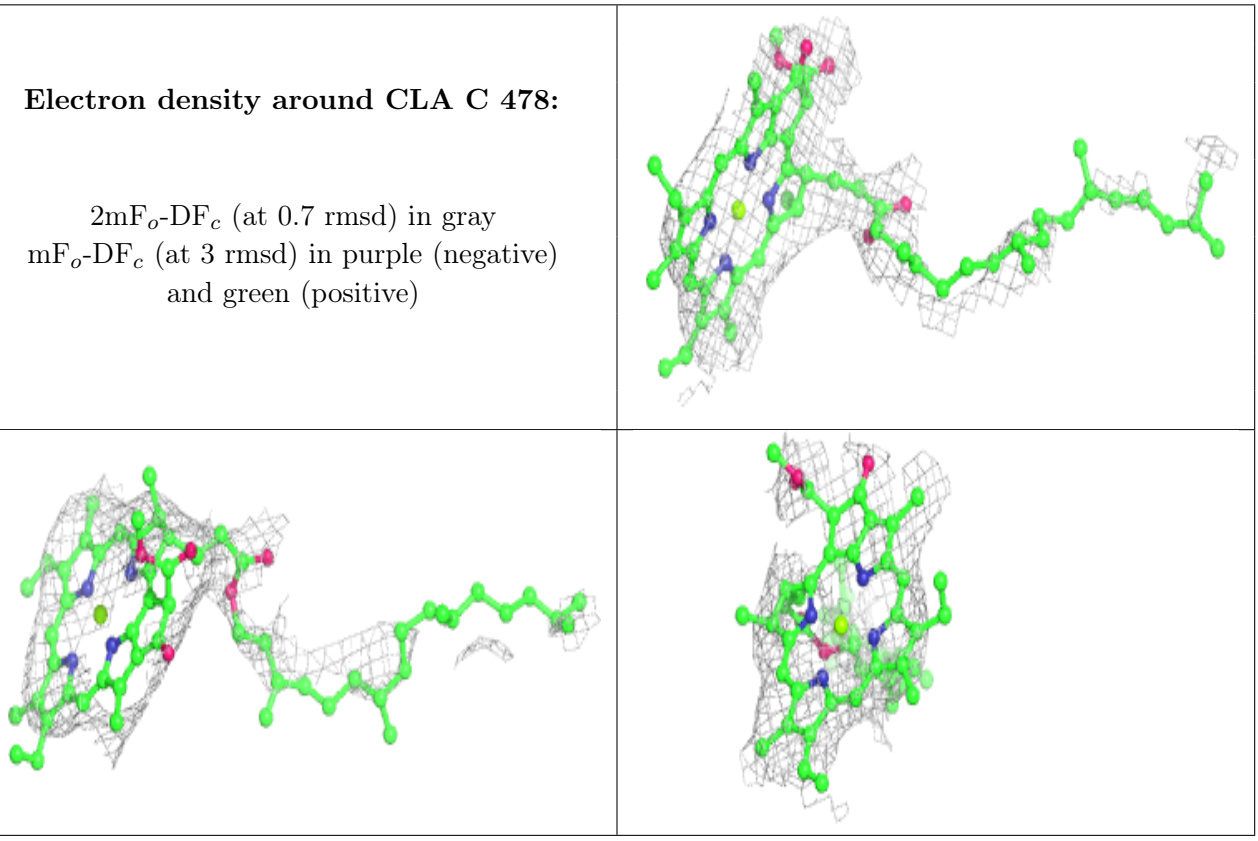
Electron density around CLA D 354:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



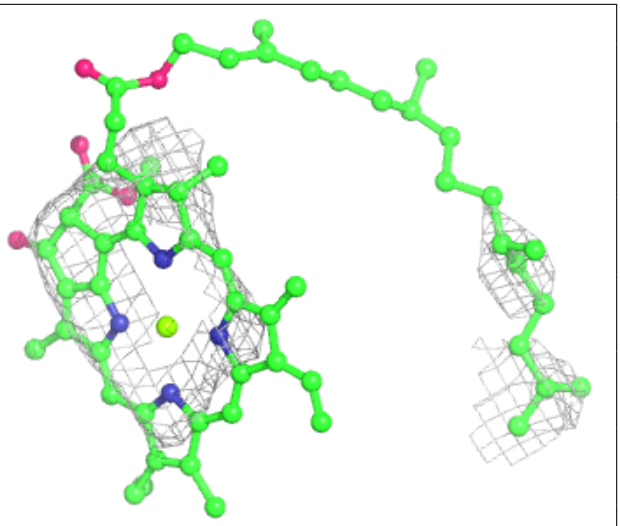
Electron density around CLA C 478:

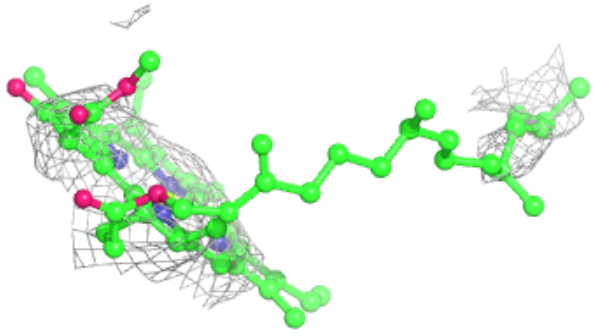
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

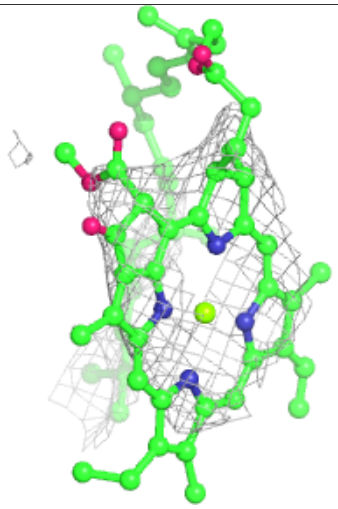


Electron density around CLA C 483:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

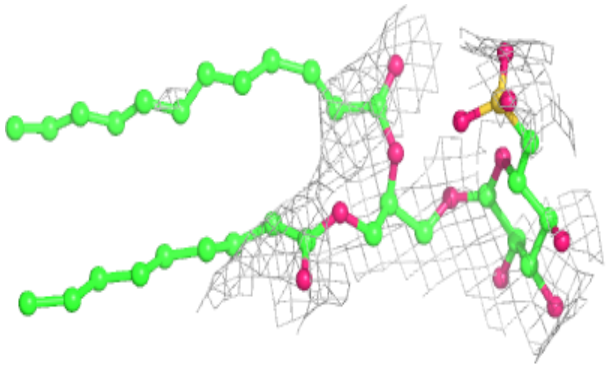


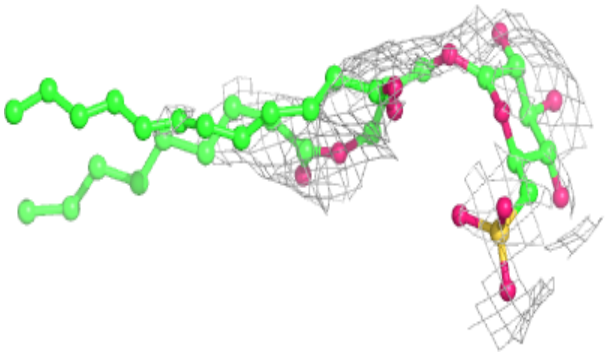


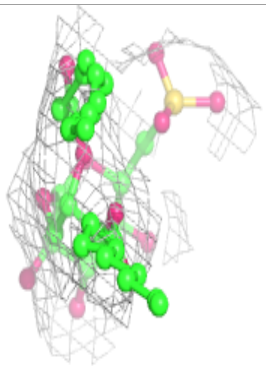


Electron density around SQD D 361:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

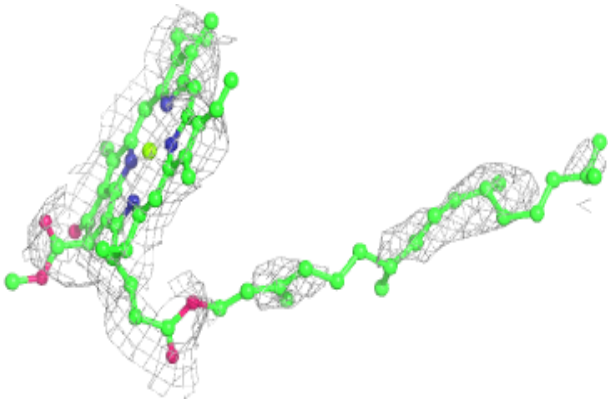


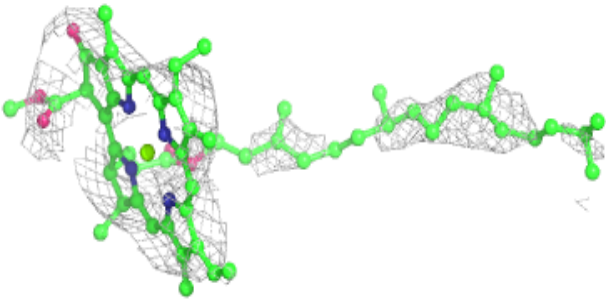


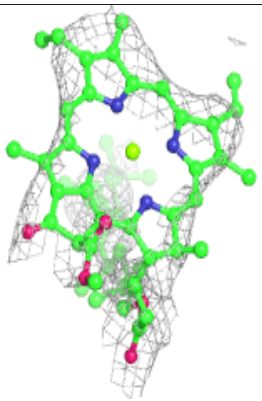


Electron density around CLA B 517:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

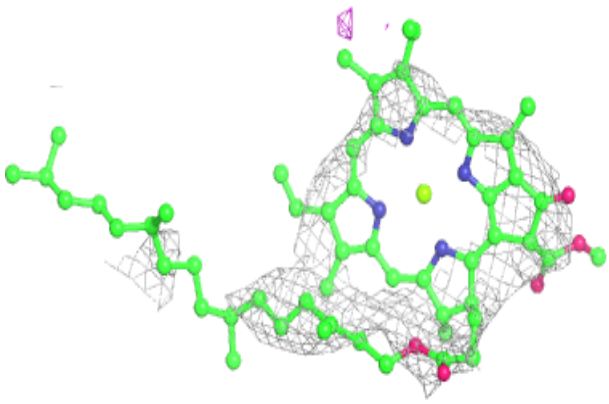


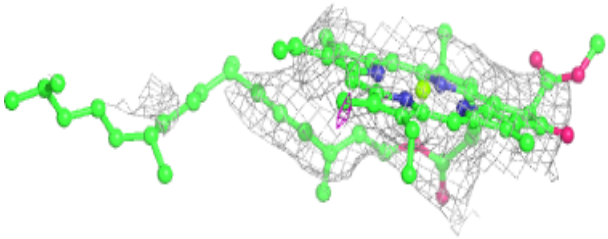


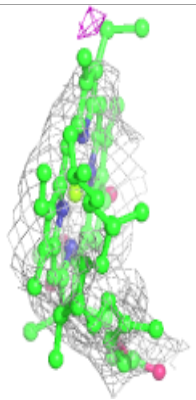


Electron density around CLA C 477:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

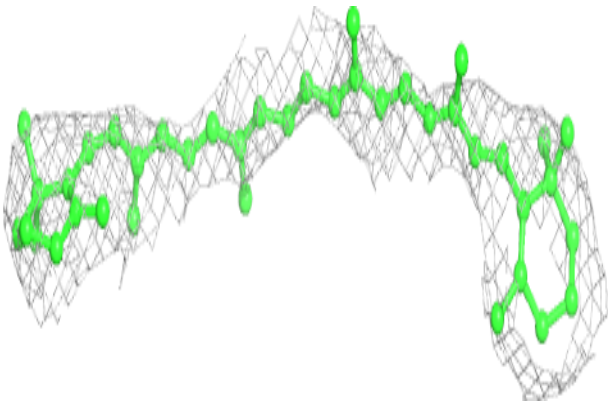


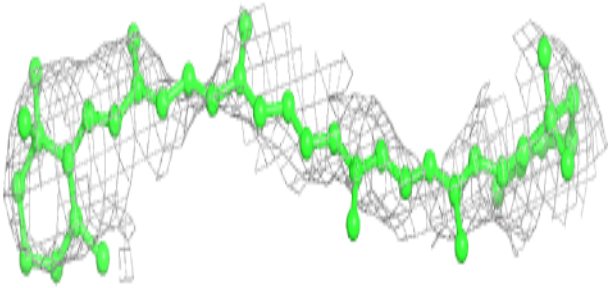


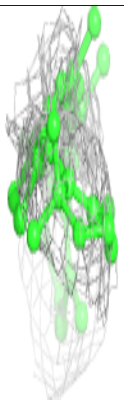


Electron density around BCR D 358:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

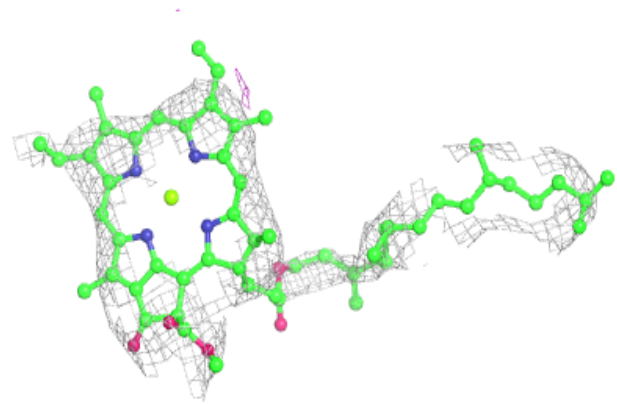


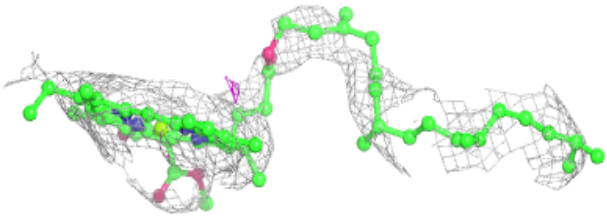


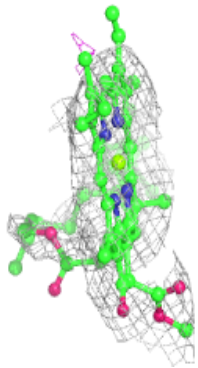


Electron density around CLA A 364:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

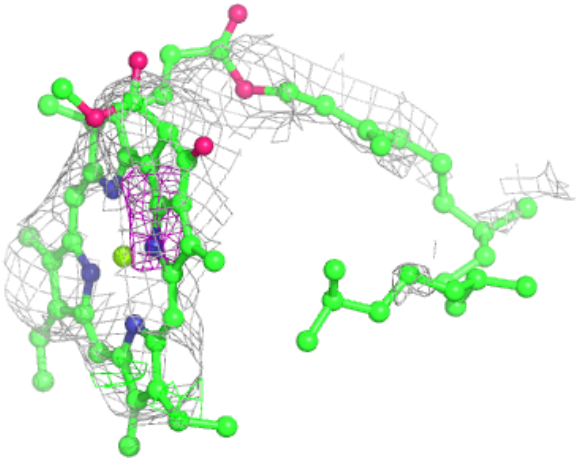


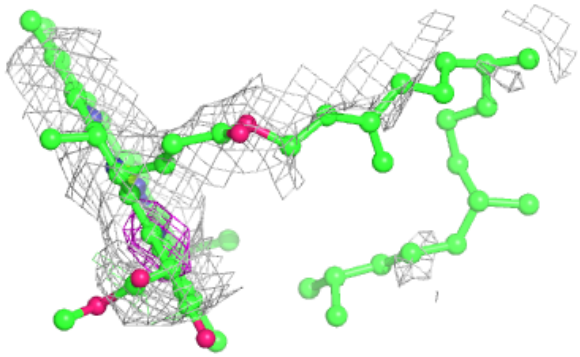


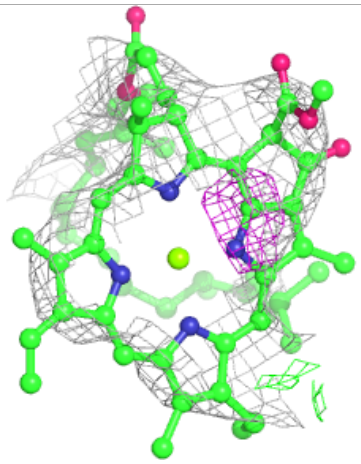


Electron density around CLA C 479:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

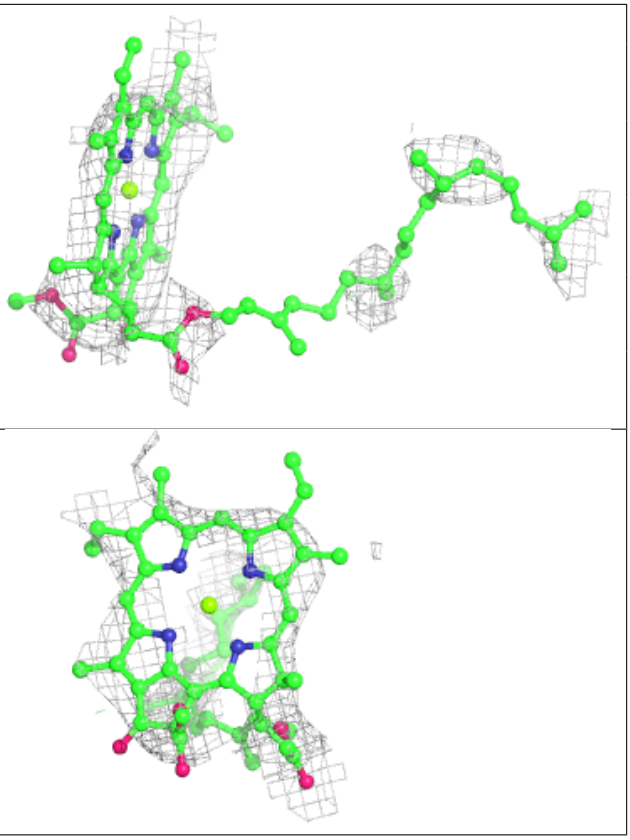


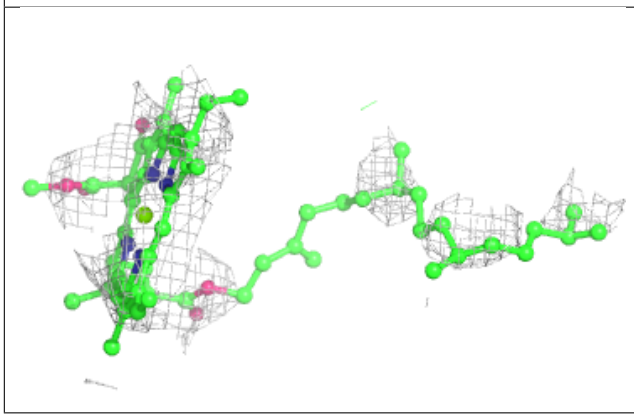




Electron density around CLA C 484:

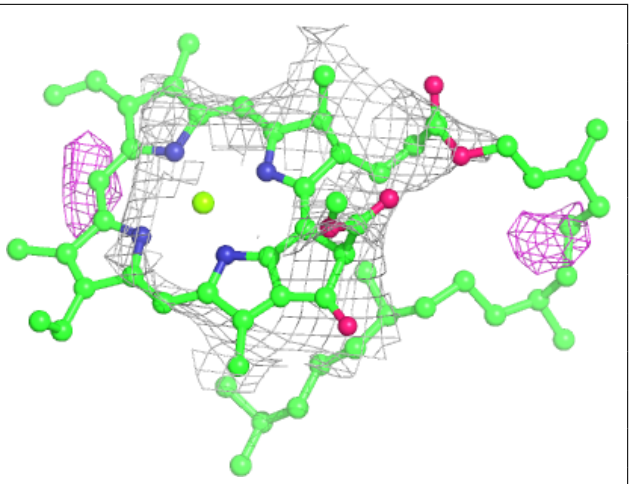
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

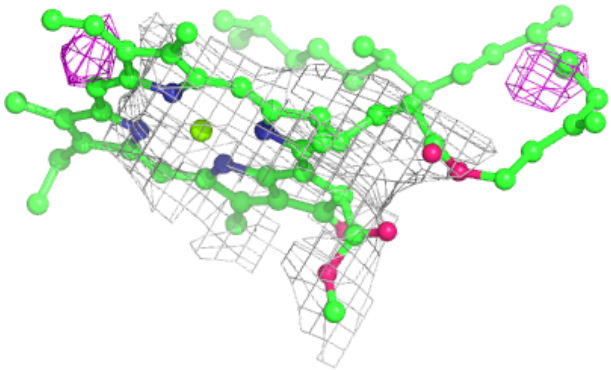


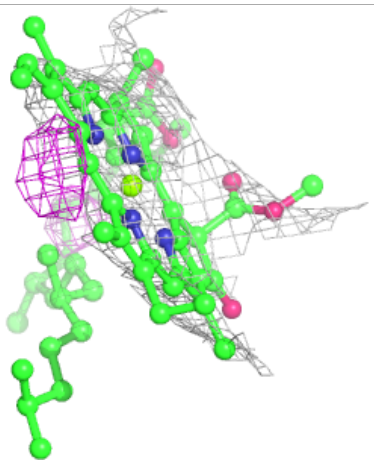


Electron density around CLA C 485:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

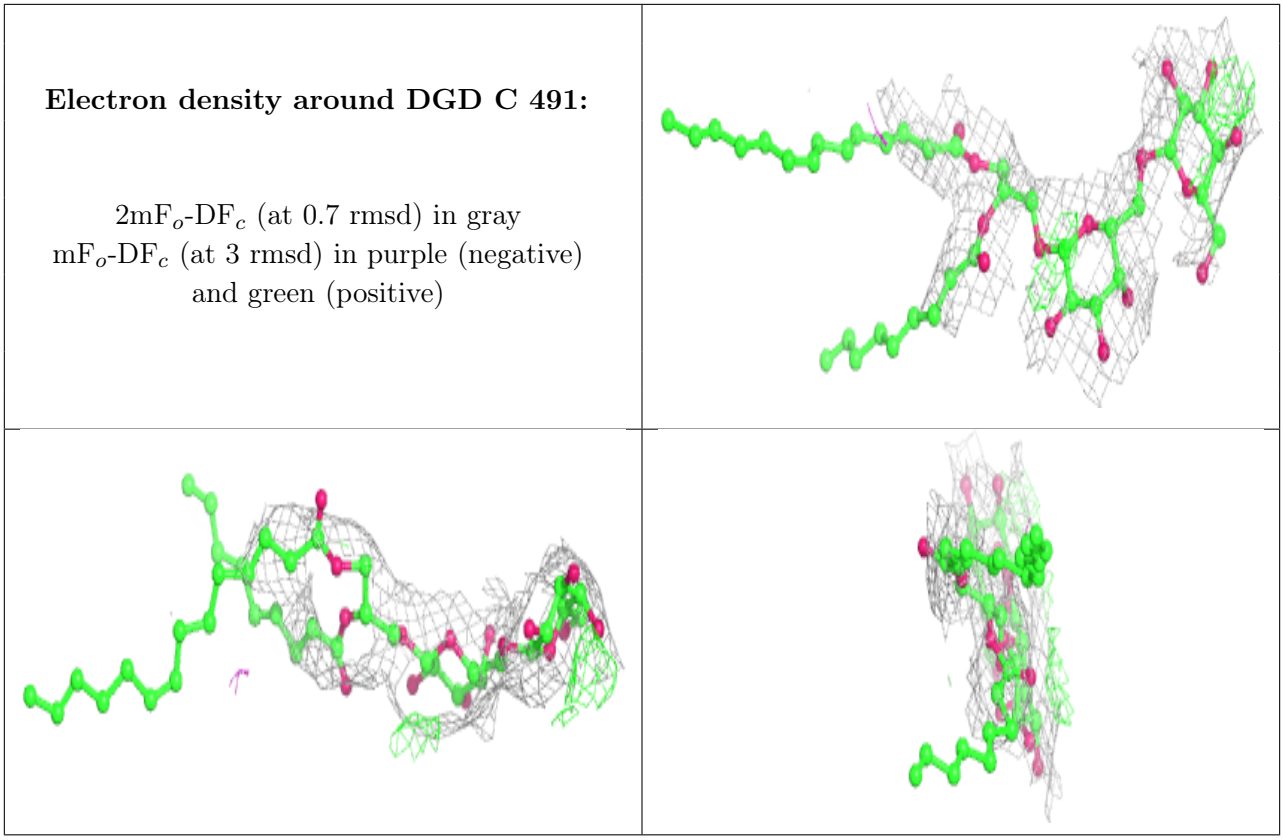






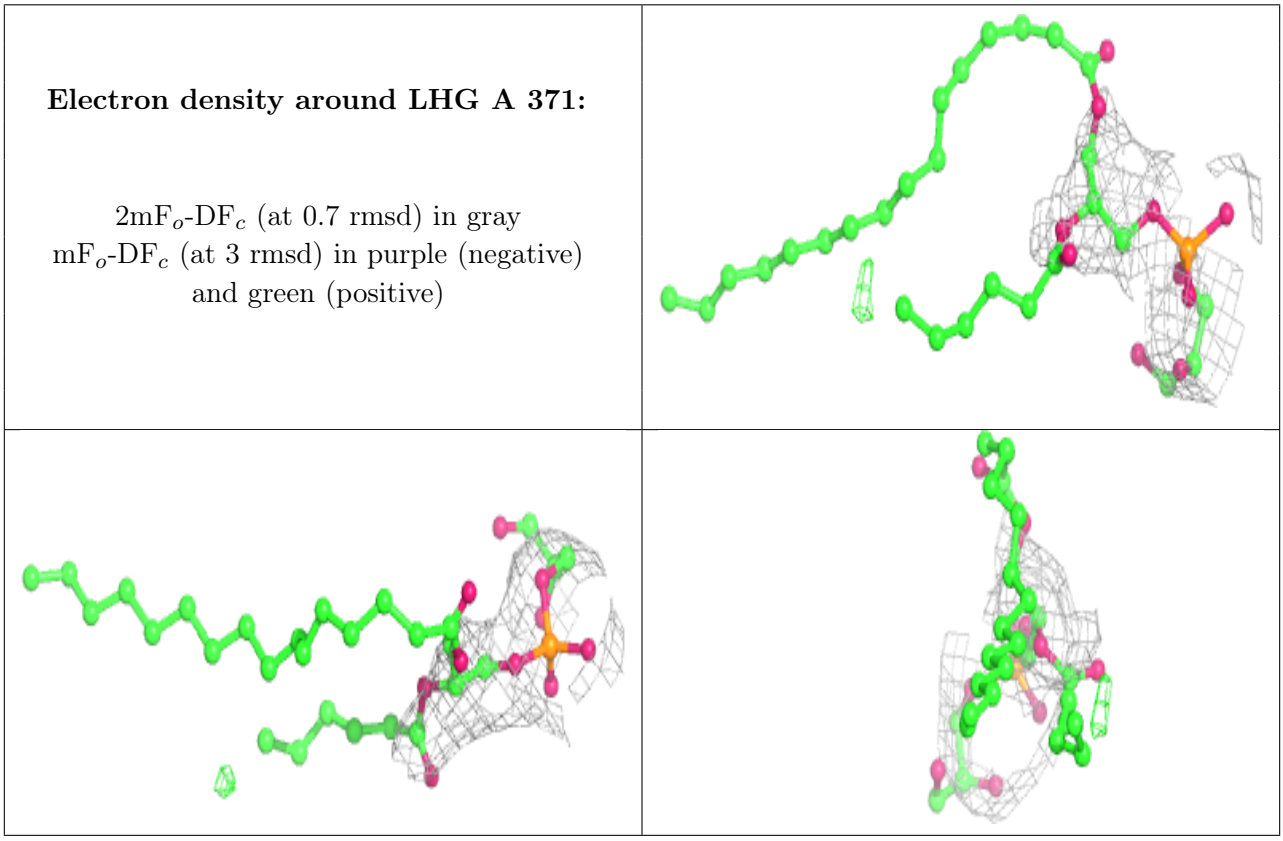
Electron density around DGD C 491:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



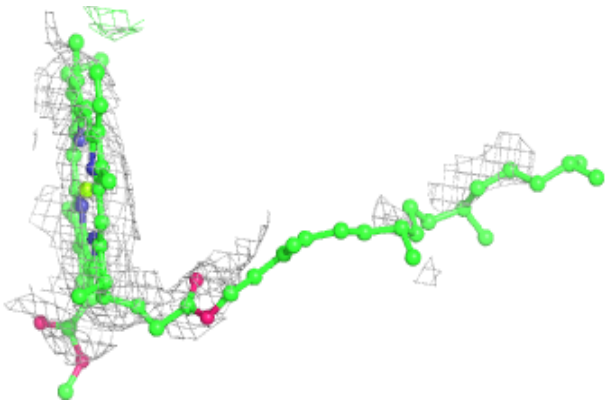
Electron density around LHG A 371:

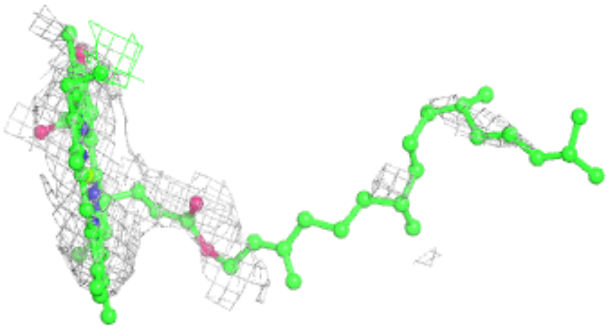
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

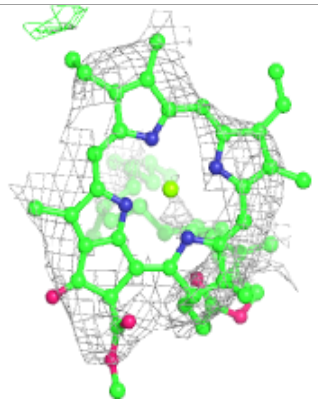


Electron density around CLA B 516:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

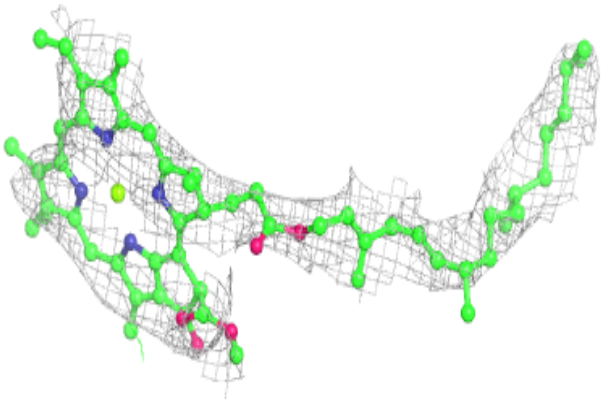


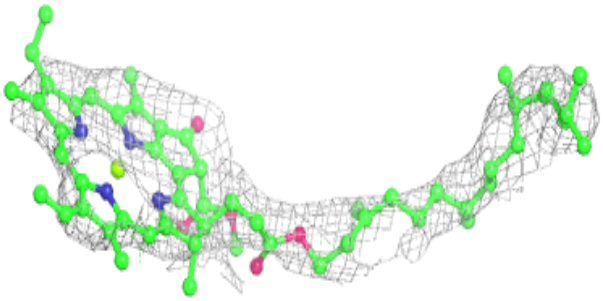


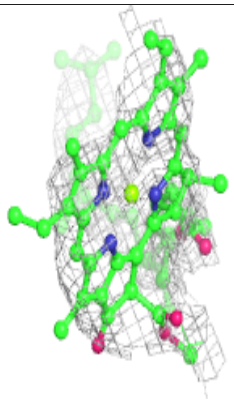


Electron density around CLA A 362:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

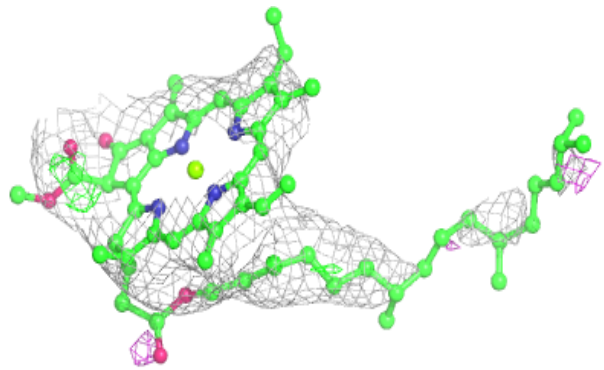


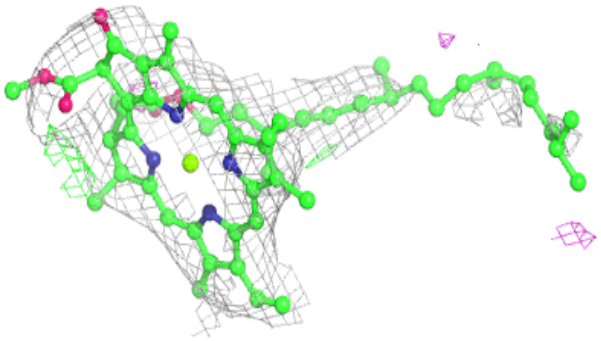


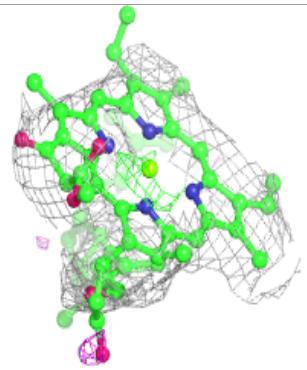


Electron density around CLA B 518:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

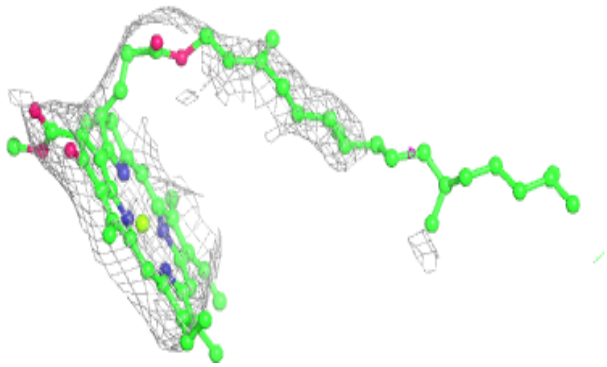


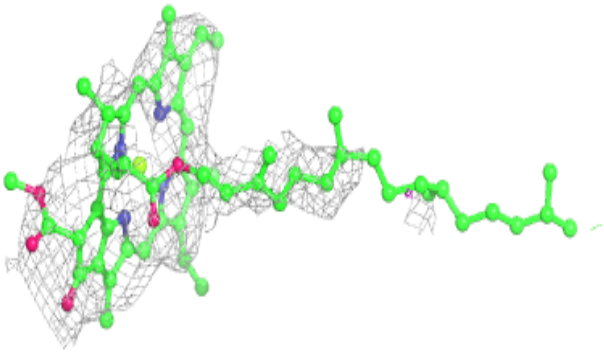


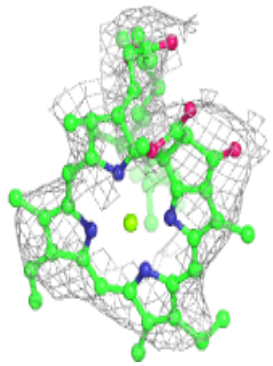


Electron density around CLA C 480:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

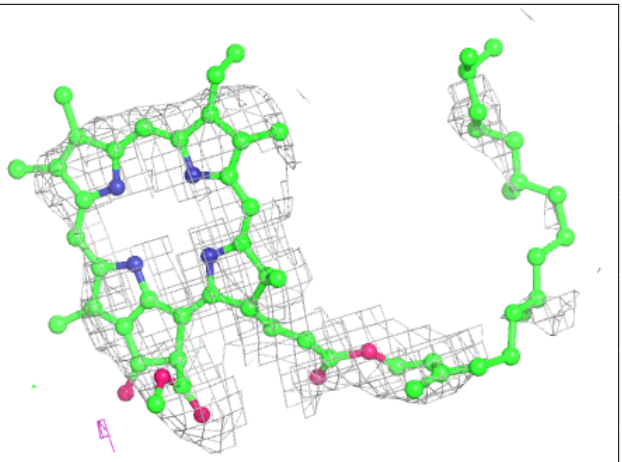


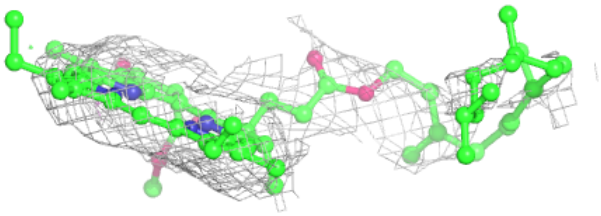


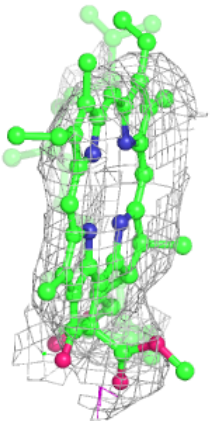


Electron density around PHO A 365:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

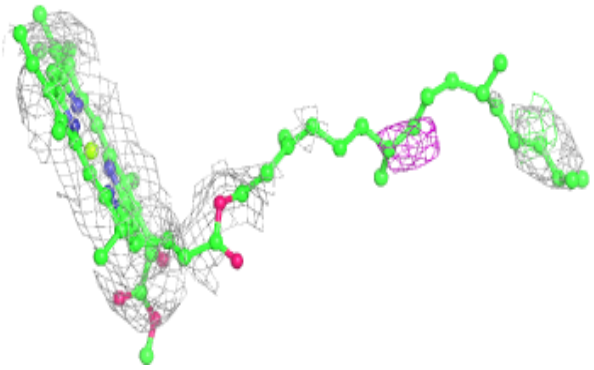


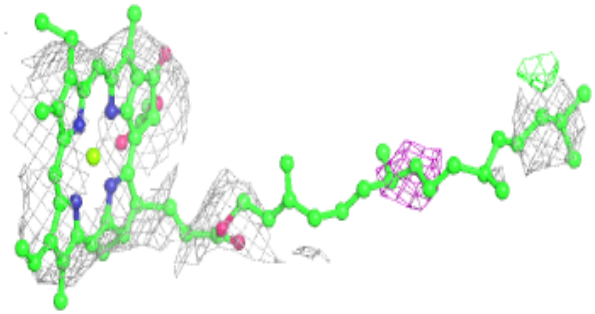


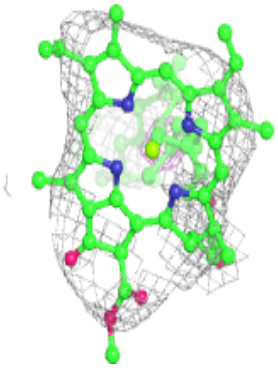


Electron density around CLA B 514:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

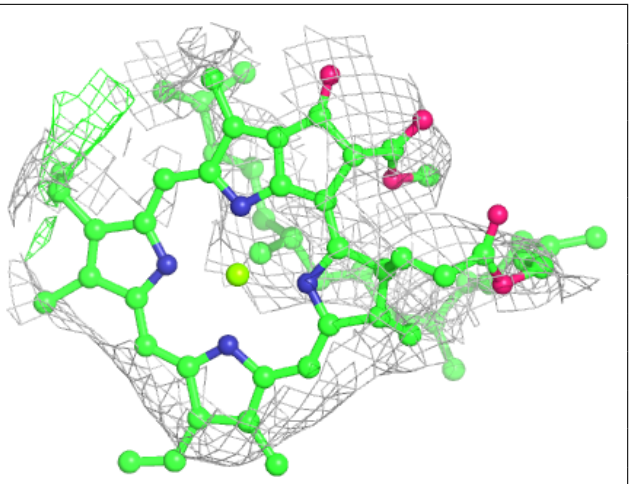


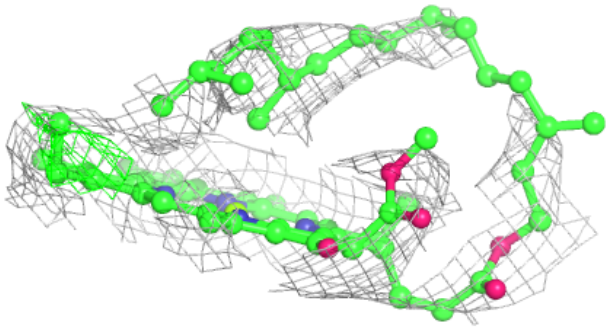


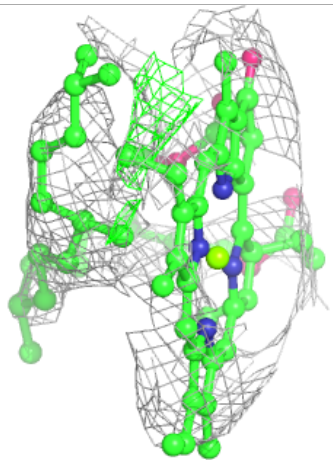


Electron density around CLA K 483:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

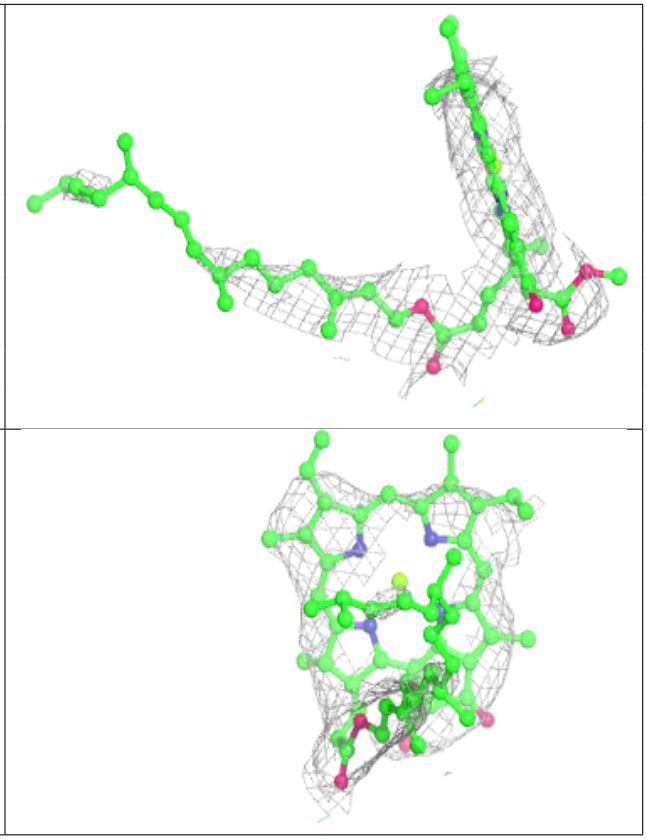






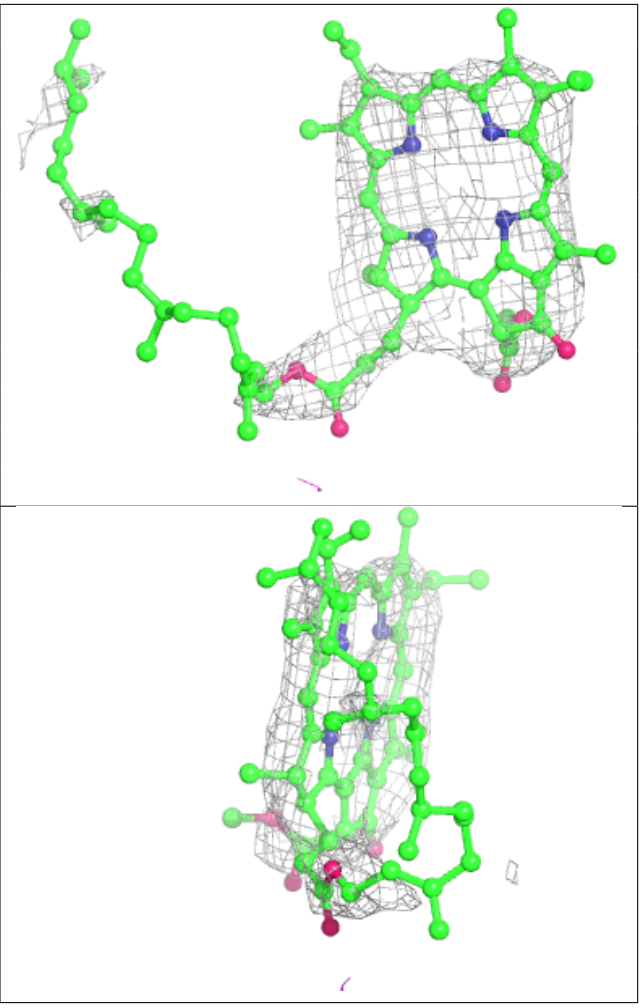
Electron density around CLA B 515:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



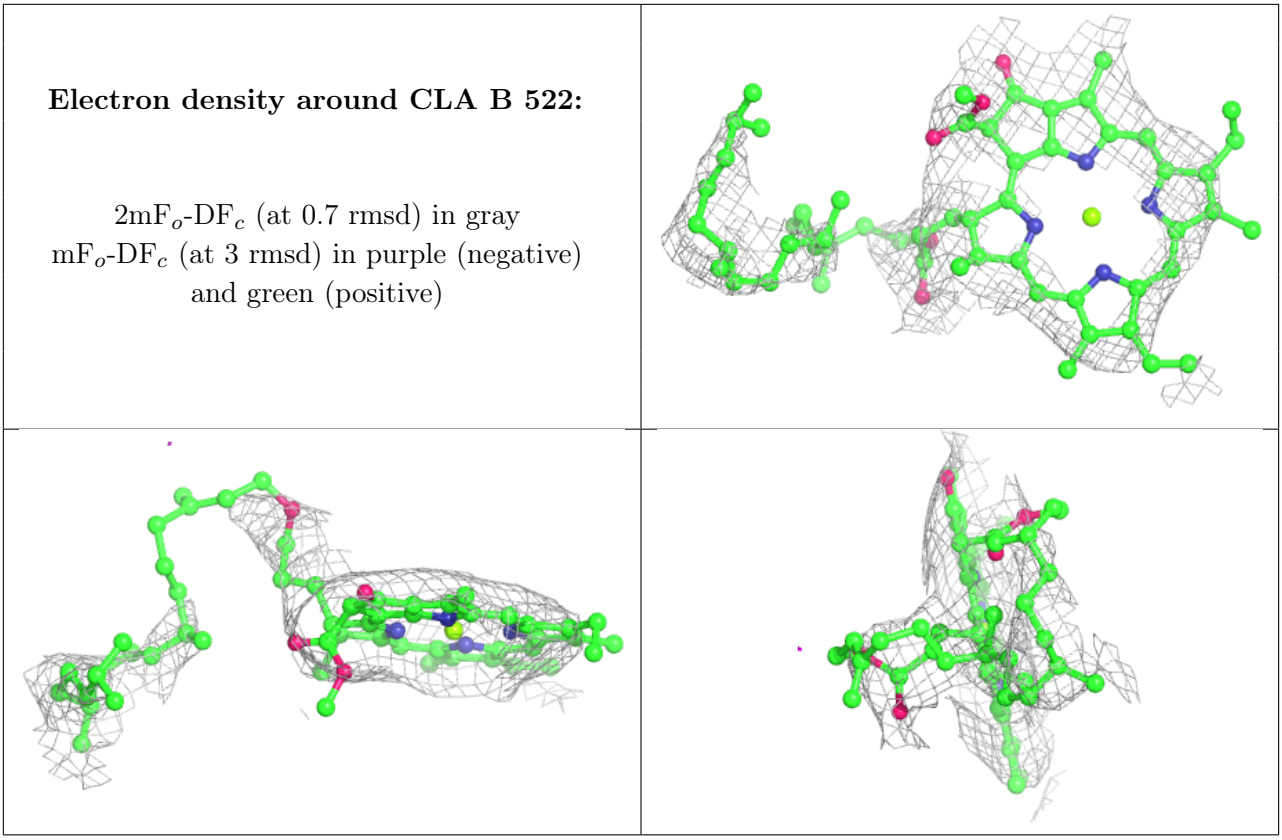
Electron density around PHO D 355:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



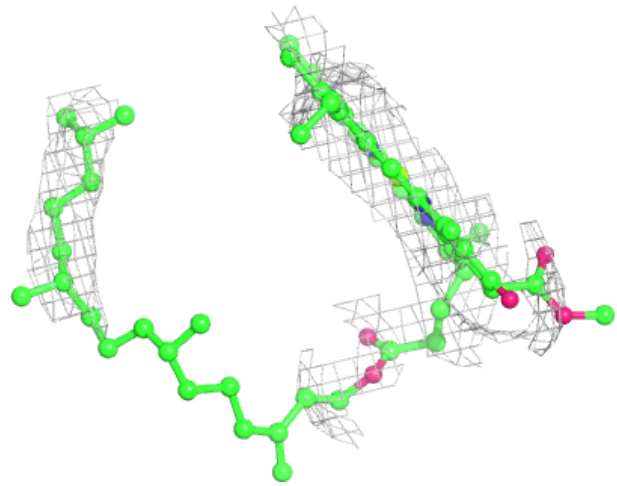
Electron density around CLA B 522:

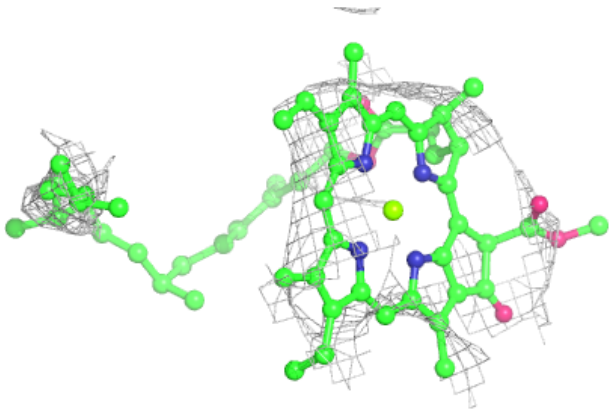
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

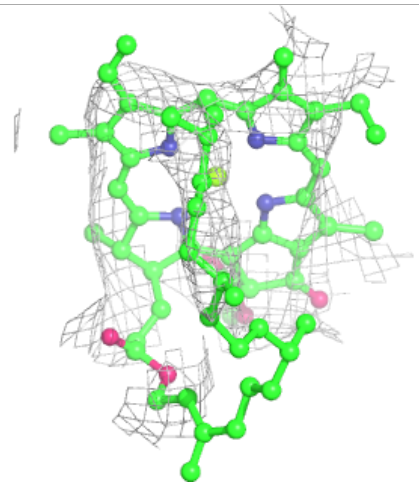


Electron density around CLA B 521:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

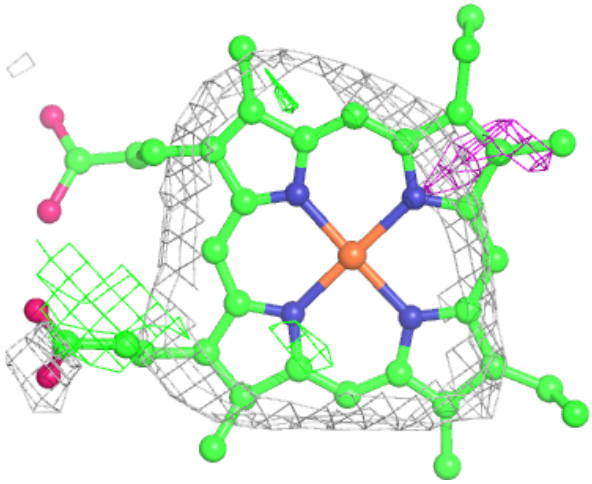


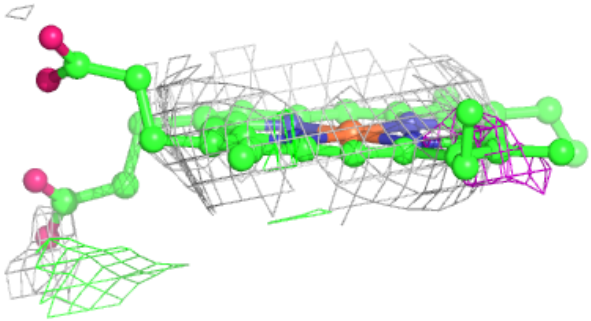


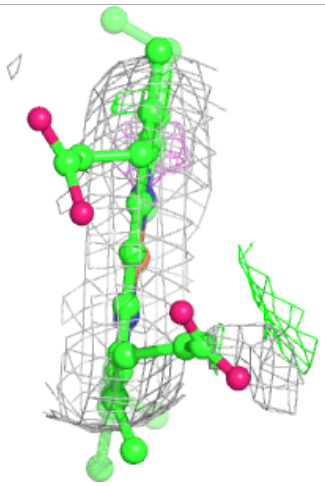


Electron density around HEM F 85:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

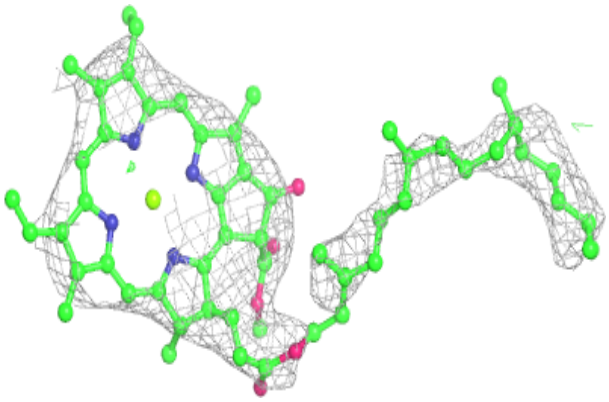


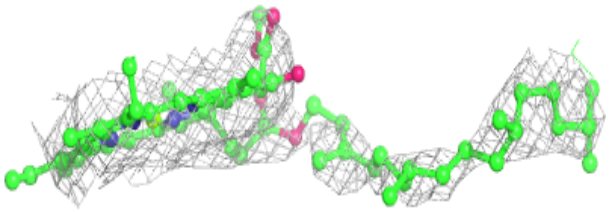


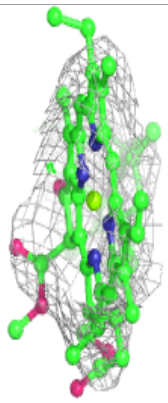


Electron density around CLA B 512:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

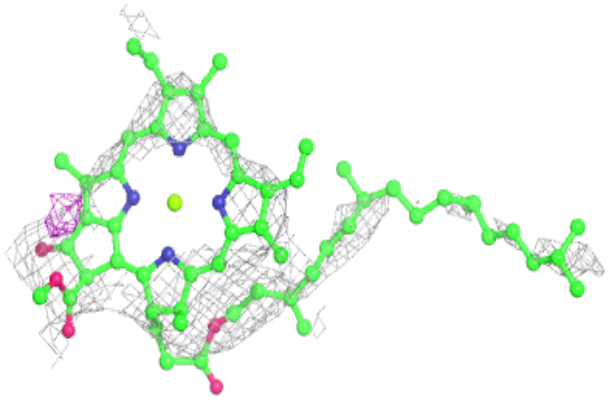


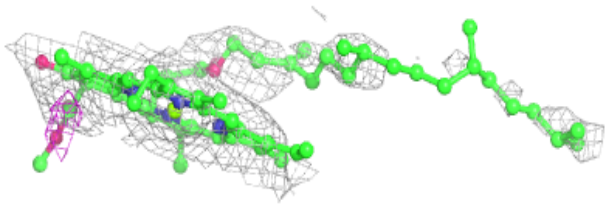


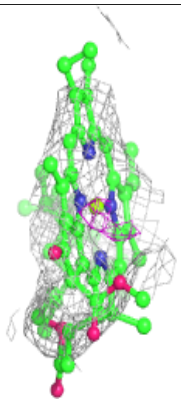


Electron density around CLA B 513:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

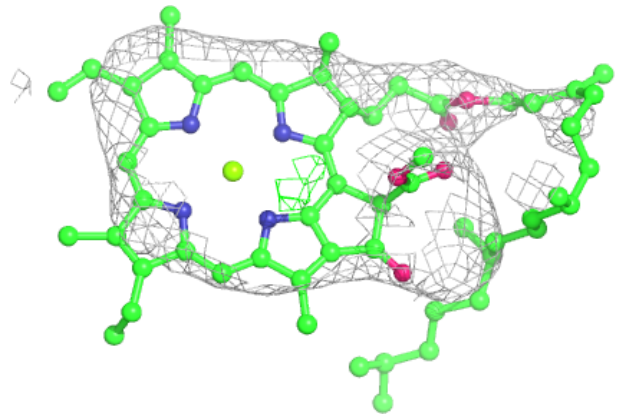


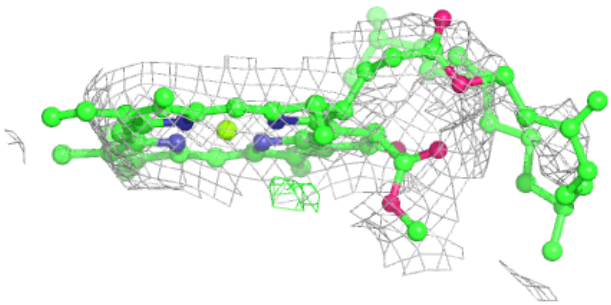


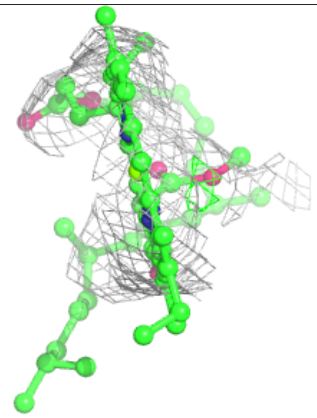


Electron density around CLA B 520:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

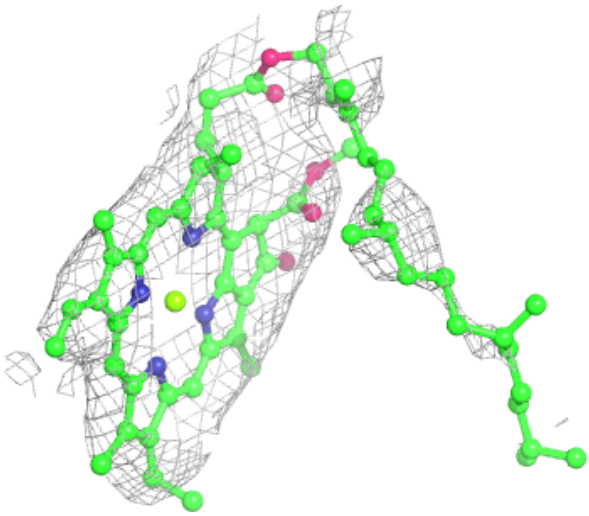


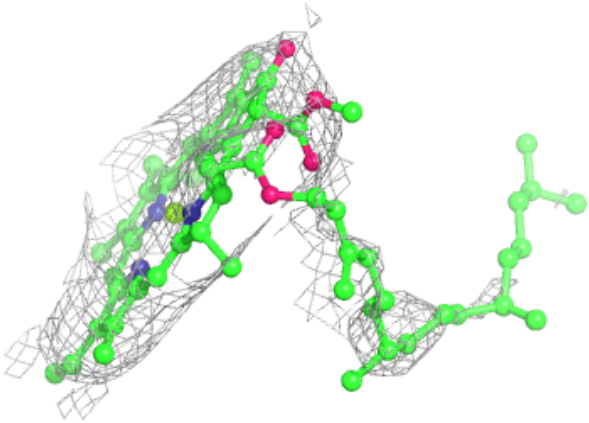


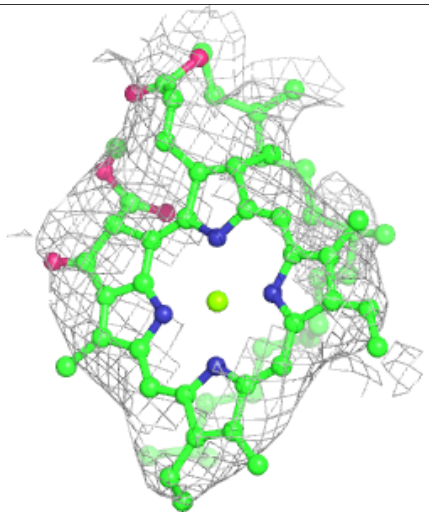


Electron density around CLA B 523:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

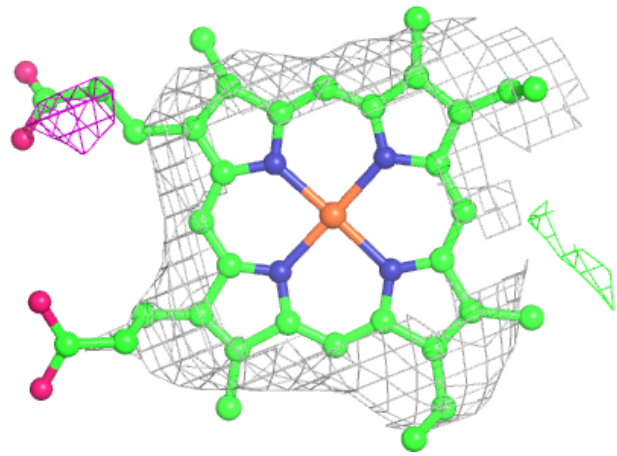


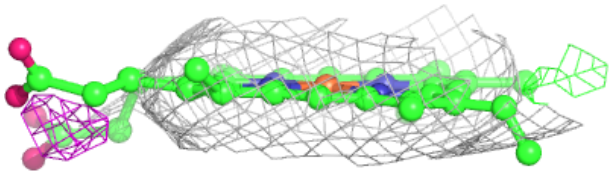


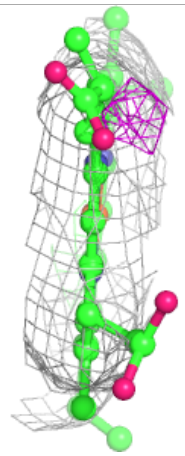


Electron density around HEM V 164:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.