Full wwPDB X-ray Structure Validation Report (i)

Mar 10, 2026 – 05:28 PM UTC

PDB ID	:	4V62 / pdb_00004v62
Title	:	Crystal Structure of cyanobacterial Photosystem II
Authors	:	Guskov, A.; Gabdulkhakov, A.; Kern, J.; Broser, M.; Zouni, A.; Saenger, W.
Deposited on	:	2008-01-17
Resolution	:	2.90 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:

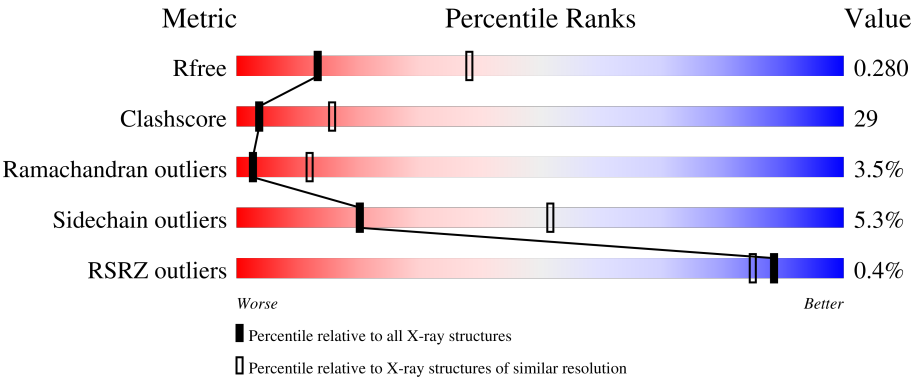
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 2.90 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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	AA	344	46% 46% 5% • •
1	BA	344	46% 45% 6% • •
2	AB	510	52% 37% 6% • •
2	BB	510	52% 37% 6% • •
3	AC	473	42% 46% 6% 5%

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Mol	Chain	Length	Quality of chain
3	BC	473	42% 46% 7% 5%
4	AD	352	51% 39% 7%
4	BD	352	49% 41% 7%
5	AE	84	29% 52% 14%
5	BE	84	27% 56% 13%
6	AF	45	29% 47% 22%
6	BF	45	29% 47% 22%
7	AH	66	38% 45% 14%
7	BH	66	38% 45% 15%
8	AI	38	32% 55% 5% 8%
8	BI	38	32% 58% 8%
9	AJ	40	32% 42% 10% 15%
9	BJ	40	32% 42% 10% 15%
10	AK	37	19% 68% 14%
10	BK	37	16% 73% 11%
11	AL	37	54% 35% 11%
11	BL	37	51% 41% 8%
12	AM	36	39% 53% 6%
12	BM	36	39% 53% 6%
13	AO	247	48% 45% 6%
13	BO	247	47% 45% 6%
14	AT	32	56% 41%
14	BT	32	56% 41%
15	AU	104	49% 37% 7% 7%
15	BU	104	51% 36% 6% 7%

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Mol	Chain	Length	Quality of chain
16	AV	137	58% 39%
16	BV	137	57% 39%
17	Ay	46	13% 35% 11% 39%
17	By	46	17% 28% 13% 39%
18	AX	50	38% 22% 10% 26%
18	BX	50	36% 24% 10% 26%
19	AY	28	75% 25%
19	BY	28	71% 29%
20	AZ	62	35% 48% 15%
20	BZ	62	35% 48% 15%

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
22	CLA	AA	402	X	-	-	-
22	CLA	AA	403	X	-	-	-
22	CLA	AA	404	X	-	-	-
22	CLA	AA	406	X	-	-	-
22	CLA	AB	601	X	-	-	-
22	CLA	AB	602	X	-	-	-
22	CLA	AB	603	X	-	-	-
22	CLA	AB	604	X	-	-	-
22	CLA	AB	605	X	-	-	-
22	CLA	AB	606	X	-	-	-
22	CLA	AB	607	X	-	-	-
22	CLA	AB	608	X	-	-	-
22	CLA	AB	609	X	-	-	-
22	CLA	AB	610	X	-	-	-
22	CLA	AB	611	X	-	-	-
22	CLA	AB	612	X	-	-	-
22	CLA	AB	613	X	-	-	-
22	CLA	AB	614	X	-	-	-
22	CLA	AB	615	X	-	-	-
22	CLA	AB	616	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	AC	501	X	-	-	-
22	CLA	AC	502	X	-	-	-
22	CLA	AC	503	X	-	-	-
22	CLA	AC	504	X	-	-	-
22	CLA	AC	505	X	-	-	-
22	CLA	AC	506	X	-	-	-
22	CLA	AC	507	X	-	-	-
22	CLA	AC	508	X	-	-	-
22	CLA	AC	509	X	-	-	-
22	CLA	AC	510	X	-	-	-
22	CLA	AC	511	X	-	-	-
22	CLA	AC	512	X	-	-	-
22	CLA	AC	513	X	-	-	-
22	CLA	AD	402	X	-	-	-
22	CLA	AD	404	X	-	-	-
22	CLA	BA	403	X	-	-	-
22	CLA	BA	404	X	-	-	-
22	CLA	BA	405	X	-	-	-
22	CLA	BA	407	X	-	-	-
22	CLA	BB	604	X	-	-	-
22	CLA	BB	605	X	-	-	-
22	CLA	BB	606	X	-	-	-
22	CLA	BB	607	X	-	-	-
22	CLA	BB	608	X	-	-	-
22	CLA	BB	609	X	-	-	-
22	CLA	BB	610	X	-	-	-
22	CLA	BB	611	X	-	-	-
22	CLA	BB	612	X	-	-	-
22	CLA	BB	613	X	-	-	-
22	CLA	BB	614	X	-	-	-
22	CLA	BB	615	X	-	-	-
22	CLA	BB	616	X	-	-	-
22	CLA	BB	617	X	-	-	-
22	CLA	BB	618	X	-	-	-
22	CLA	BB	619	X	-	-	-
22	CLA	BC	501	X	-	-	-
22	CLA	BC	502	X	-	-	-
22	CLA	BC	503	X	-	-	-
22	CLA	BC	504	X	-	-	-
22	CLA	BC	505	X	-	-	-
22	CLA	BC	506	X	-	-	-
22	CLA	BC	507	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	BC	508	X	-	-	-
22	CLA	BC	509	X	-	-	-
22	CLA	BC	510	X	-	-	-
22	CLA	BC	511	X	-	-	-
22	CLA	BC	512	X	-	-	-
22	CLA	BC	513	X	-	-	-
22	CLA	BD	402	X	-	-	-
22	CLA	BD	404	X	-	-	-
27	DGD	AA	410	X	-	-	-
27	DGD	AB	626	X	-	-	-
27	DGD	AC	516	X	-	-	-
27	DGD	AC	517	X	-	-	-
27	DGD	AC	518	X	-	-	-
27	DGD	AD	410	X	-	-	-
27	DGD	AH	102	X	-	-	-
27	DGD	BA	411	X	-	-	-
27	DGD	BB	602	X	-	-	-
27	DGD	BC	516	X	-	-	-
27	DGD	BC	517	X	-	-	-
27	DGD	BC	518	X	-	-	-
27	DGD	BD	410	X	-	-	-
27	DGD	BH	101	X	-	-	-
30	LMG	AA	413	X	-	-	-
30	LMG	AA	416	X	-	-	-
30	LMG	AB	621	X	-	-	-
30	LMG	AB	622	X	-	-	-
30	LMG	AB	623	X	-	-	-
30	LMG	AC	519	X	-	-	-
30	LMG	AC	520	X	-	-	-
30	LMG	AD	407	X	-	-	-
30	LMG	AD	408	X	-	-	-
30	LMG	AE	102	X	-	-	-
30	LMG	AI	101	X	-	-	-
30	LMG	AM	101	X	-	-	-
30	LMG	BA	414	X	-	-	-
30	LMG	BB	623	X	-	-	-
30	LMG	BB	624	X	-	-	-
30	LMG	BC	519	X	-	-	-
30	LMG	BC	520	X	-	-	-
30	LMG	BD	407	X	-	-	-
30	LMG	BD	408	X	-	-	-
30	LMG	BE	102	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	LMG	BI	101	X	-	-	-
30	LMG	BM	102	X	-	-	-

2 Entry composition (i)

There are 35 unique types of molecules in this entry. The entry contains 50234 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.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	490	Total	C	N	O	S	0	0	0
			3850	2528	641	668	13			
2	BB	490	Total	C	N	O	S	0	0	0
			3850	2528	641	668	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	447	Total	C	N	O	S	0	0	0
			3444	2256	576	599	13			
3	BC	447	Total	C	N	O	S	0	0	0
			3444	2256	576	599	13			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AC	2	LYS	-	SEE REMARK 999	UNP Q8DIF8
AC	3	THR	-	SEE REMARK 999	UNP Q8DIF8
AC	4	LEU	-	SEE REMARK 999	UNP Q8DIF8
AC	5	SER	-	SEE REMARK 999	UNP Q8DIF8
AC	6	SER	-	SEE REMARK 999	UNP Q8DIF8
AC	7	GLN	-	SEE REMARK 999	UNP Q8DIF8
AC	8	LYS	-	SEE REMARK 999	UNP Q8DIF8
AC	9	ARG	-	SEE REMARK 999	UNP Q8DIF8

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Chain	Residue	Modelled	Actual	Comment	Reference
AC	10	TYR	-	SEE REMARK 999	UNP Q8DIF8
AC	11	SER	-	SEE REMARK 999	UNP Q8DIF8
AC	12	PRO	-	SEE REMARK 999	UNP Q8DIF8
AC	13	VAL	-	SEE REMARK 999	UNP Q8DIF8
BC	2	LYS	-	SEE REMARK 999	UNP Q8DIF8
BC	3	THR	-	SEE REMARK 999	UNP Q8DIF8
BC	4	LEU	-	SEE REMARK 999	UNP Q8DIF8
BC	5	SER	-	SEE REMARK 999	UNP Q8DIF8
BC	6	SER	-	SEE REMARK 999	UNP Q8DIF8
BC	7	GLN	-	SEE REMARK 999	UNP Q8DIF8
BC	8	LYS	-	SEE REMARK 999	UNP Q8DIF8
BC	9	ARG	-	SEE REMARK 999	UNP Q8DIF8
BC	10	TYR	-	SEE REMARK 999	UNP Q8DIF8
BC	11	SER	-	SEE REMARK 999	UNP Q8DIF8
BC	12	PRO	-	SEE REMARK 999	UNP Q8DIF8
BC	13	VAL	-	SEE REMARK 999	UNP Q8DIF8

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	AE	82	Total	C	N	O	0	0	0
			666	434	108	124			
5	BE	82	Total	C	N	O	0	0	0
			666	434	108	124			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	35	Total	C	N	O	S	0	0	0
			282	192	46	43	1			
6	BF	35	Total	C	N	O	S	0	0	0
			282	192	46	43	1			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AT	32	Total	C	N	O	S	0	0	0
			275	192	40	41	2			
14	BT	32	Total	C	N	O	S	0	0	0
			275	192	40	41	2			

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

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

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

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

- Molecule 17 is a protein called Protein ycf12.

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

- Molecule 18 is a protein called Photosystem II PsbX protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AX	37	Total	C	N	O	0	0	0
			270	182	41	47			
18	BX	37	Total	C	N	O	0	0	0
			270	182	41	47			

- Molecule 19 is a protein called Photosystem II protein Y.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	AY	28	Total	C	N	O	0	0	0
			140	84	28	28			
19	BY	28	Total	C	N	O	0	0	0
			140	84	28	28			

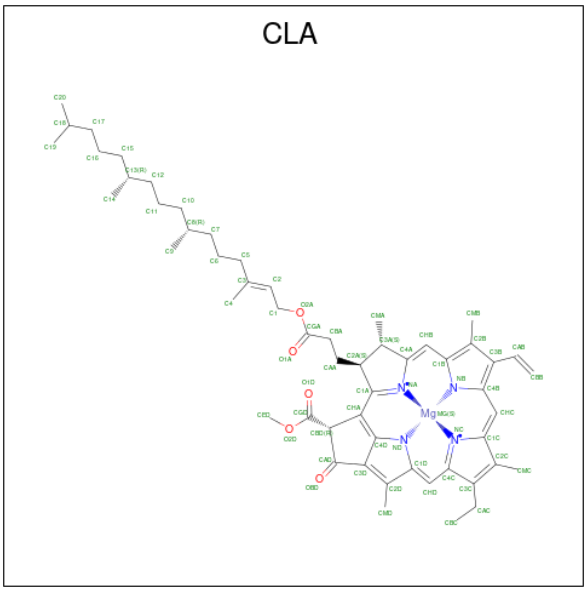
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AZ	62	Total	C	N	O	S	0	0	0
			479	328	72	77	2			
20	BZ	62	Total	C	N	O	S	0	0	0
			479	328	72	77	2			

- Molecule 21 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	AA	1	Total	Fe	0	0
			1	1		
21	BA	1	Total	Fe	0	0
			1	1		

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



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	AB	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	AB	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	AB	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	AB	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	AB	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	AB	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	AC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	AC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	AC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	AC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	AC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	AC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	AC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	AC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	AC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	AC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	AC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	AC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	AD	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	AD	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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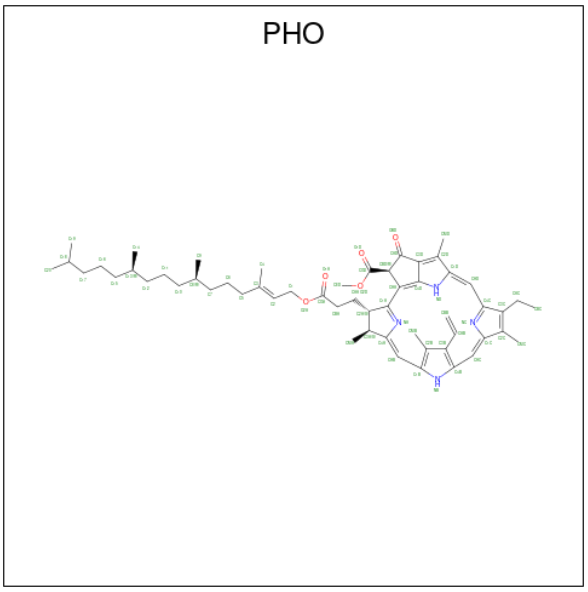
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	BA	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	BA	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	BA	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	BA	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	BB	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	BB	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	BB	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	BB	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	BB	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	BB	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	BB	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	BB	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	BB	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	BB	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	BB	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	BB	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	BB	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	BB	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	BB	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	BB	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	BC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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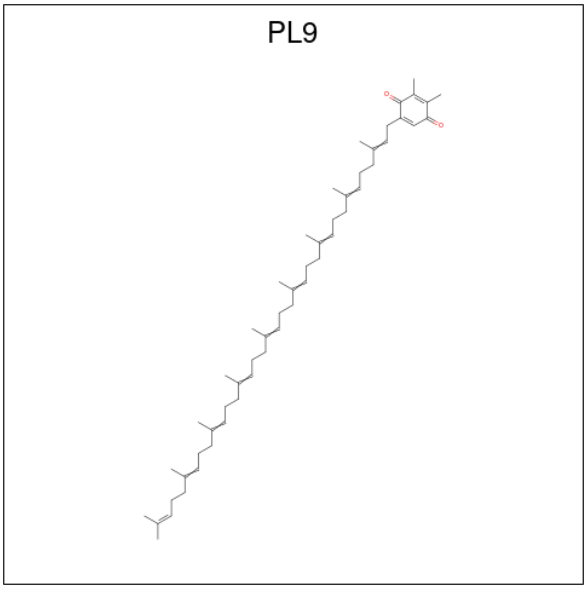
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	BC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	BC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	BC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	BC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	BC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	BC	1	Total	C	Mg	N	O	0	0
			65	55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

- Molecule 23 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



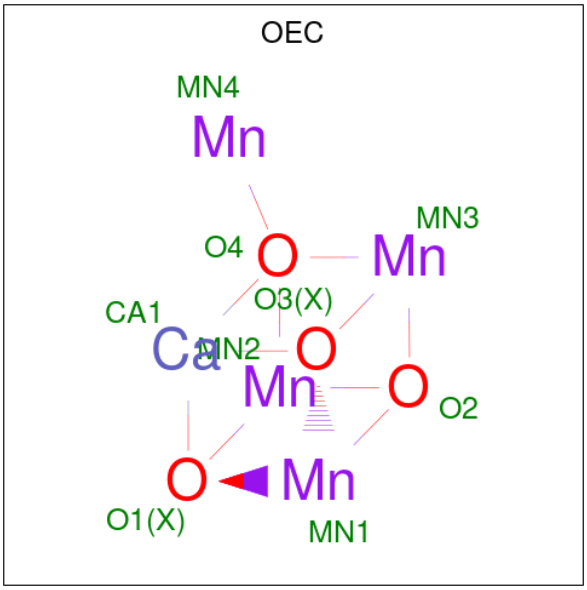
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
23	AA	1	Total	C	N	O	0	0
			64	55	4	5		
23	AD	1	Total	C	N	O	0	0
			64	55	4	5		
23	BA	1	Total	C	N	O	0	0
			64	55	4	5		
23	BD	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 24 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 (CCD ID: PL9) (formula: $C_{53}H_{80}O_2$).



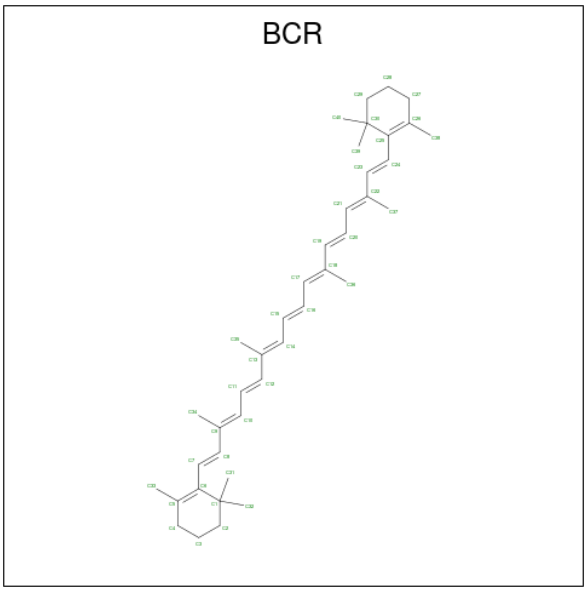
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	AA	1	Total C O 45 43 2	0	0
24	AD	1	Total C O 55 53 2	0	0
24	AJ	1	Total C O 35 33 2	0	0
24	BA	1	Total C O 45 43 2	0	0
24	BD	1	Total C O 55 53 2	0	0
24	BJ	1	Total C O 35 33 2	0	0

- Molecule 25 is OXYGEN EVOLVING SYSTEM (CCD ID: OEC) (formula: $CaMn_4O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	AA	1	Total Ca Mn 5 1 4	0	0
25	BA	1	Total Ca Mn 5 1 4	0	0

- Molecule 26 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



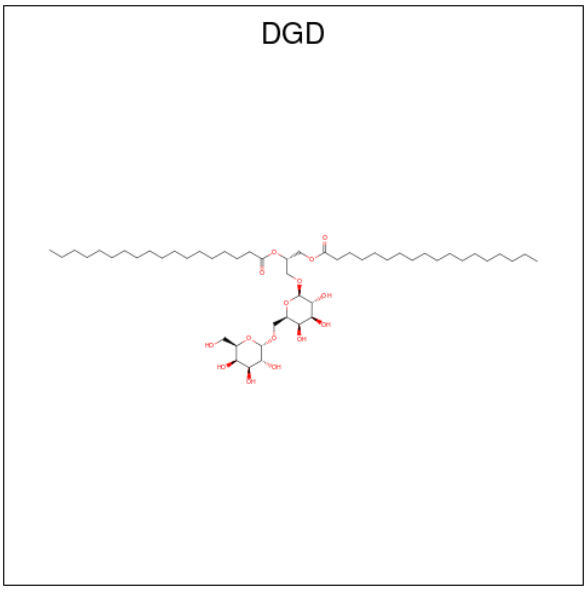
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	AA	1	Total C 40 40	0	0
26	AB	1	Total C 40 40	0	0
26	AB	1	Total C 40 40	0	0
26	AB	1	Total C 40 40	0	0
26	AB	1	Total C 40 40	0	0
26	AC	1	Total C 40 40	0	0
26	AC	1	Total C 40 40	0	0
26	AD	1	Total C 40 40	0	0
26	AH	1	Total C 40 40	0	0
26	AJ	1	Total C 40 40	0	0
26	AK	1	Total C 40 40	0	0
26	AT	1	Total C 40 40	0	0
26	AZ	1	Total C 40 40	0	0
26	BA	1	Total C 40 40	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	BB	1	Total C 40 40	0	0
26	BB	1	Total C 40 40	0	0
26	BB	1	Total C 40 40	0	0
26	BC	1	Total C 40 40	0	0
26	BC	1	Total C 40 40	0	0
26	BD	1	Total C 40 40	0	0
26	BJ	1	Total C 40 40	0	0
26	BK	1	Total C 40 40	0	0
26	BX	1	Total C 40 40	0	0
26	BZ	1	Total C 40 40	0	0

- Molecule 27 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



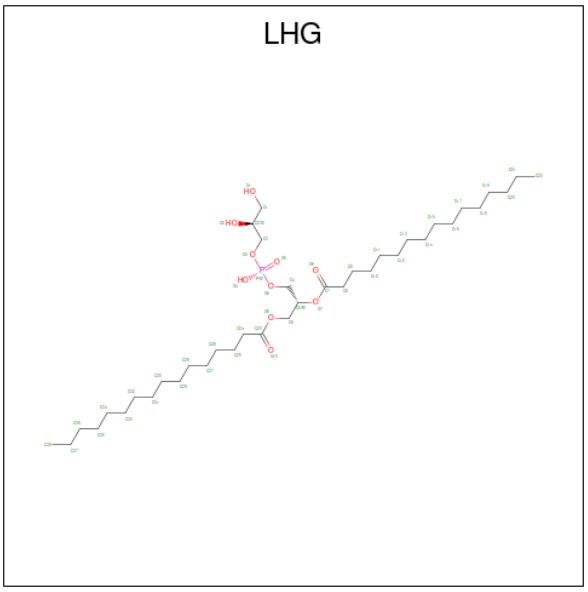
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	AA	1	Total C O 56 41 15	0	0

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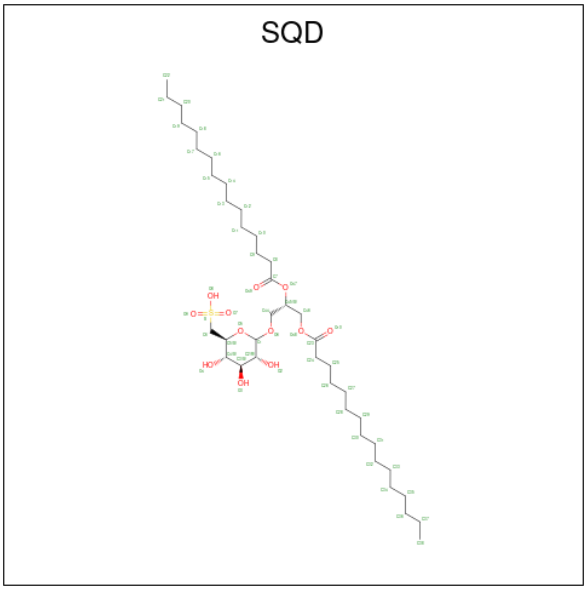
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	AB	1	Total C O 52 37 15	0	0
27	AC	1	Total C O 53 38 15	0	0
27	AC	1	Total C O 62 47 15	0	0
27	AC	1	Total C O 66 51 15	0	0
27	AD	1	Total C O 63 48 15	0	0
27	AH	1	Total C O 58 43 15	0	0
27	BA	1	Total C O 56 41 15	0	0
27	BB	1	Total C O 52 37 15	0	0
27	BC	1	Total C O 53 38 15	0	0
27	BC	1	Total C O 62 47 15	0	0
27	BC	1	Total C O 66 51 15	0	0
27	BD	1	Total C O 63 48 15	0	0
27	BH	1	Total C O 58 43 15	0	0

- Molecule 28 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



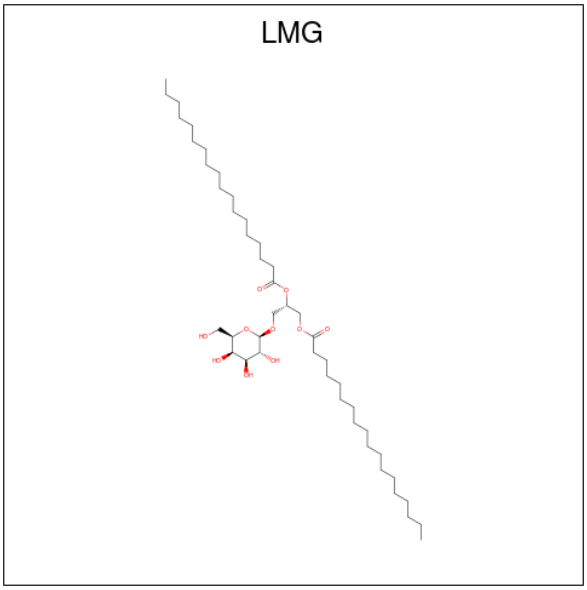
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	AA	1	Total	C	O	P	0	0
			39	28	10	1		
28	AC	1	Total	C	O	P	0	0
			37	26	10	1		
28	BA	1	Total	C	O	P	0	0
			39	28	10	1		
28	BC	1	Total	C	O	P	0	0
			37	26	10	1		

- Molecule 29 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	AA	1	Total	C	O	S	0	0
			51	38	12	1		
29	AA	1	Total	C	O	S	0	0
			54	41	12	1		
29	AD	1	Total	C	O	S	0	0
			43	30	12	1		
29	AF	1	Total	C	O	S	0	0
			45	32	12	1		
29	BA	1	Total	C	O	S	0	0
			54	41	12	1		
29	BA	1	Total	C	O	S	0	0
			51	38	12	1		
29	BB	1	Total	C	O	S	0	0
			47	34	12	1		
29	BD	1	Total	C	O	S	0	0
			43	30	12	1		
29	BF	1	Total	C	O	S	0	0
			45	32	12	1		
29	BL	1	Total	C	O	S	0	0
			47	34	12	1		

- Molecule 30 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	AA	1	Total	C	O	0	0
			51	41	10		

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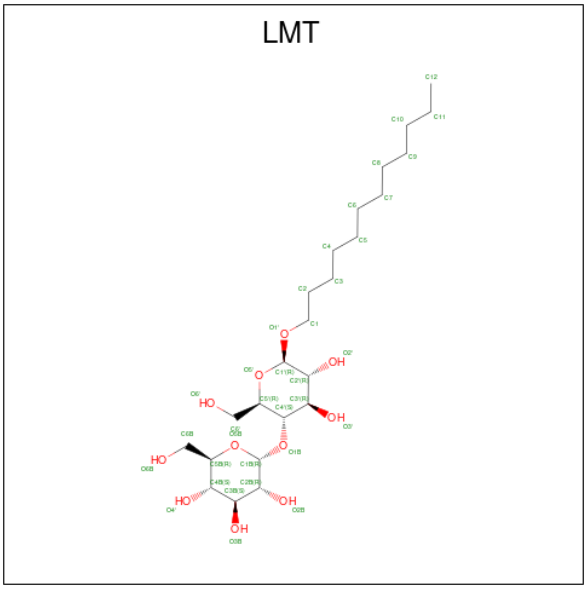
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	AA	1	Total C O 42 32 10	0	0
30	AB	1	Total C O 49 39 10	0	0
30	AB	1	Total C O 49 39 10	0	0
30	AB	1	Total C O 42 32 10	0	0
30	AC	1	Total C O 48 38 10	0	0
30	AC	1	Total C O 45 35 10	0	0
30	AD	1	Total C O 46 36 10	0	0
30	AD	1	Total C O 48 38 10	0	0
30	AE	1	Total C O 44 34 10	0	0
30	AI	1	Total C O 43 33 10	0	0
30	AM	1	Total C O 42 32 10	0	0
30	BA	1	Total C O 51 41 10	0	0
30	BB	1	Total C O 49 39 10	0	0
30	BB	1	Total C O 49 39 10	0	0
30	BC	1	Total C O 48 38 10	0	0
30	BC	1	Total C O 45 35 10	0	0
30	BD	1	Total C O 46 36 10	0	0
30	BD	1	Total C O 48 38 10	0	0
30	BE	1	Total C O 44 34 10	0	0
30	BI	1	Total C O 43 33 10	0	0
30	BM	1	Total C O 42 32 10	0	0

- Molecule 31 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	AA	1	Total Cl 1 1	0	0
31	BA	1	Total Cl 1 1	0	0

- Molecule 32 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



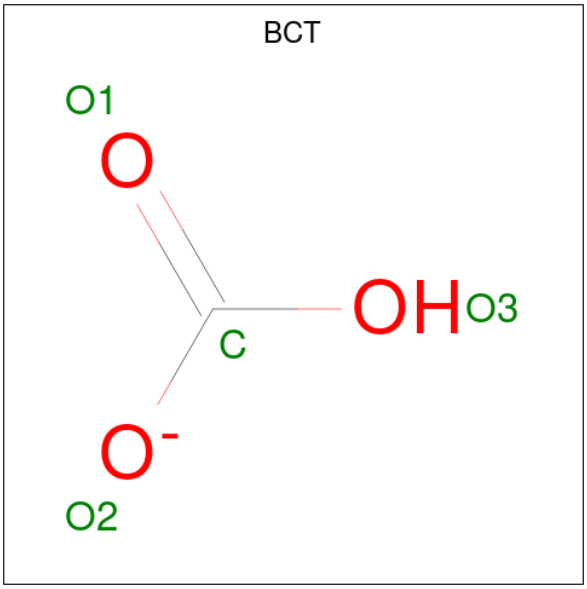
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	AB	1	Total C O 35 24 11	0	0
32	AB	1	Total C O 35 24 11	0	0
32	AB	1	Total C O 35 24 11	0	0
32	AD	1	Total C O 31 20 11	0	0
32	AI	1	Total C O 35 24 11	0	0
32	AM	1	Total C O 35 24 11	0	0
32	AT	1	Total C O 35 24 11	0	0
32	BB	1	Total C O 35 24 11	0	0
32	BB	1	Total C O 35 24 11	0	0

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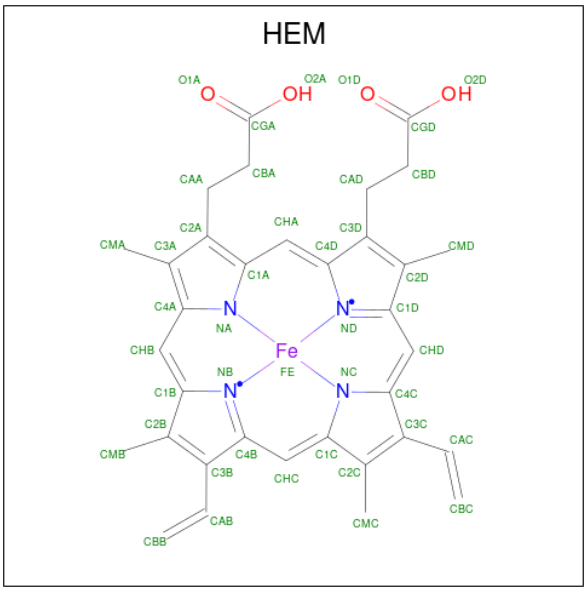
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	BB	1	Total C O 35 24 11	0	0
32	BD	1	Total C O 31 20 11	0	0
32	BI	1	Total C O 35 24 11	0	0
32	BM	1	Total C O 35 24 11	0	0
32	BT	1	Total C O 35 24 11	0	0

- Molecule 33 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	AD	1	Total C O 4 1 3	0	0
33	BD	1	Total C O 4 1 3	0	0

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
34	AE	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
34	AV	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
34	BE	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
34	BV	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 35 is CALCIUM ION (CCD ID: CA) (formula: Ca).

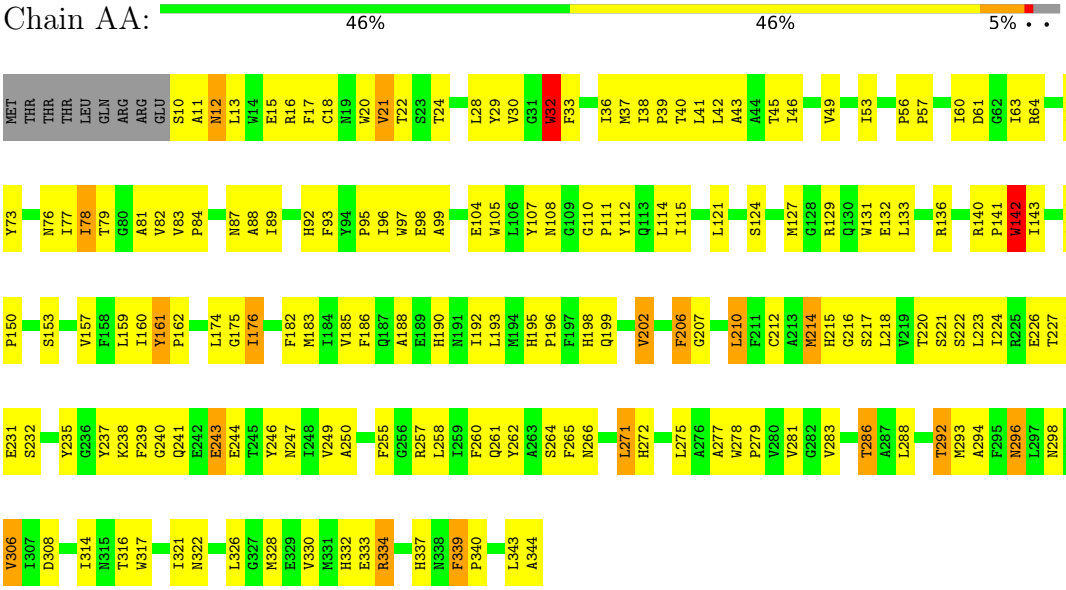
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	AK	1	Total	Ca	0	0
			1	1		
35	AO	1	Total	Ca	0	0
			1	1		
35	BK	1	Total	Ca	0	0
			1	1		
35	BO	1	Total	Ca	0	0
			1	1		

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.

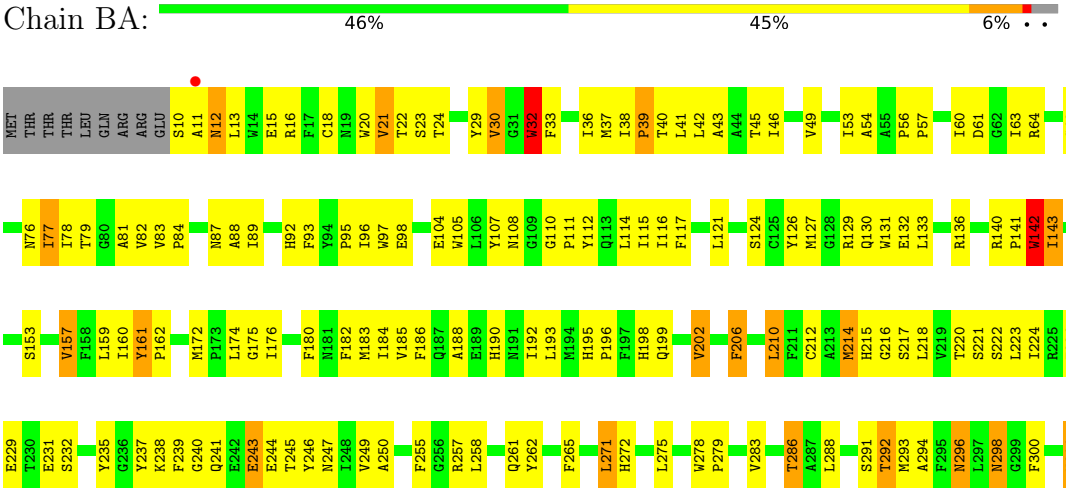
• Molecule 1: Photosystem Q(B) protein

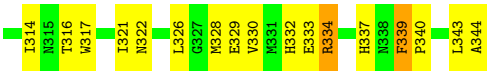
Chain AA:



• Molecule 1: Photosystem Q(B) protein

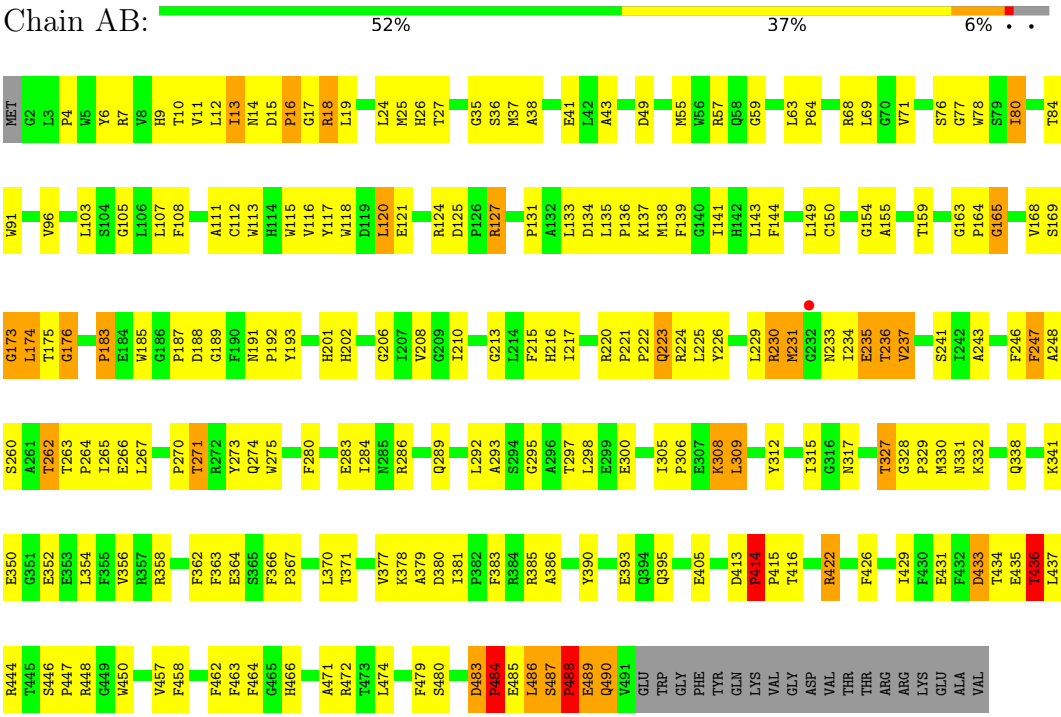
Chain BA:





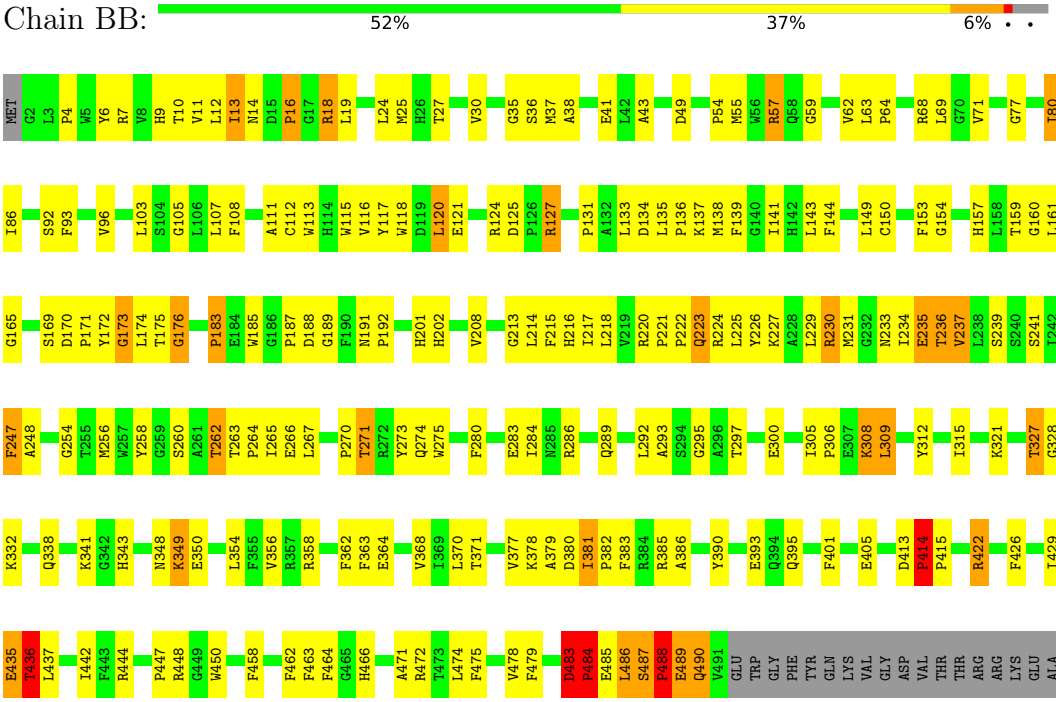
• Molecule 2: Photosystem II core light harvesting protein

Chain AB:



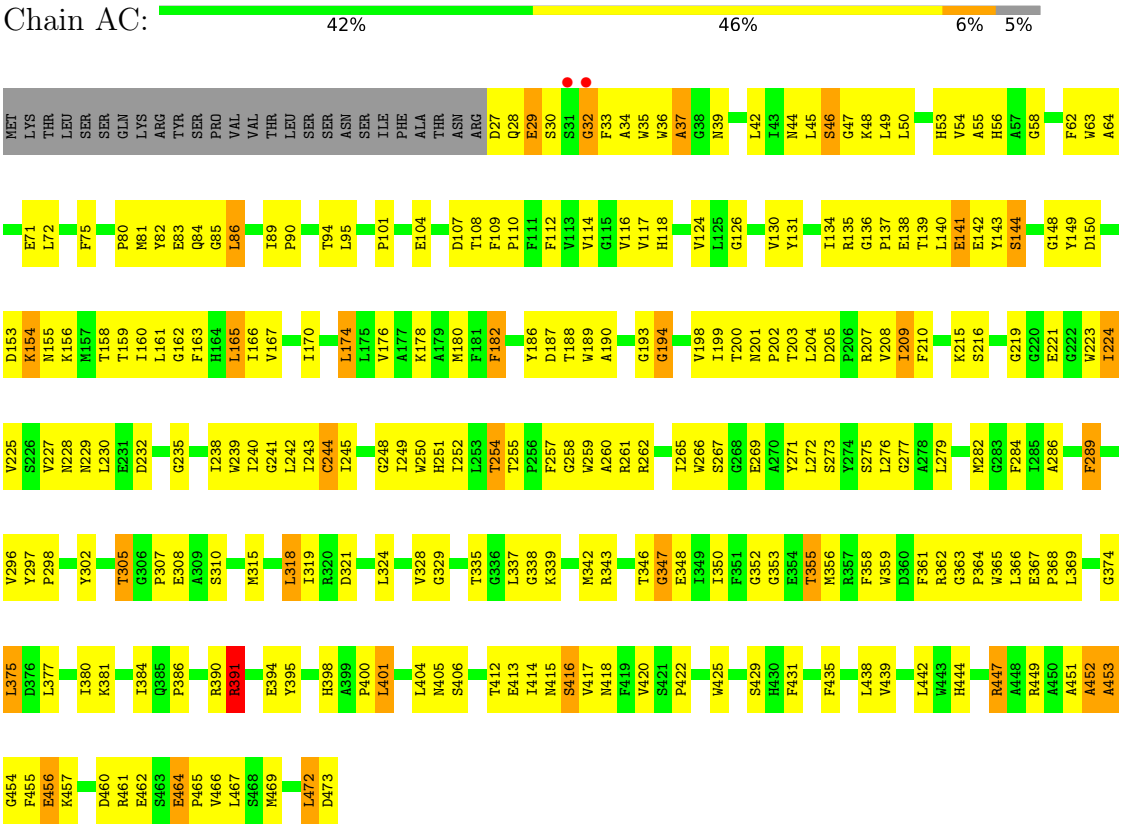
• Molecule 2: Photosystem II core light harvesting protein

Chain BB:



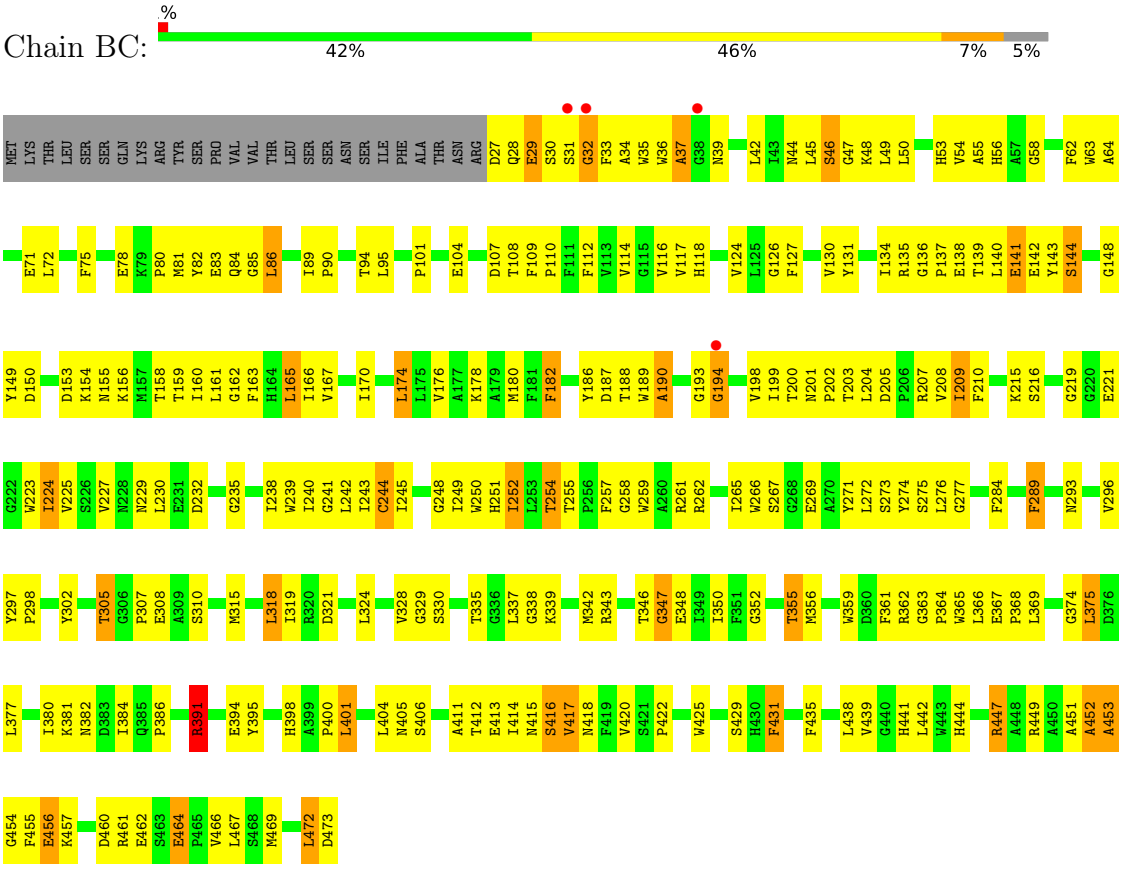
• Molecule 3: Photosystem II CP43 protein

Chain AC:



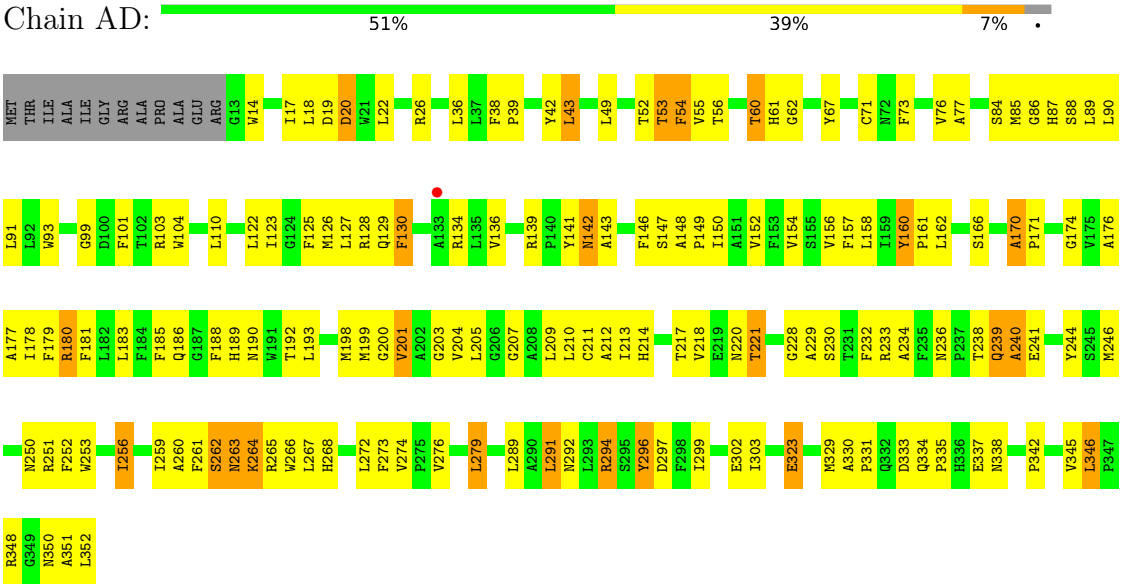
• Molecule 3: Photosystem II CP43 protein

Chain BC:



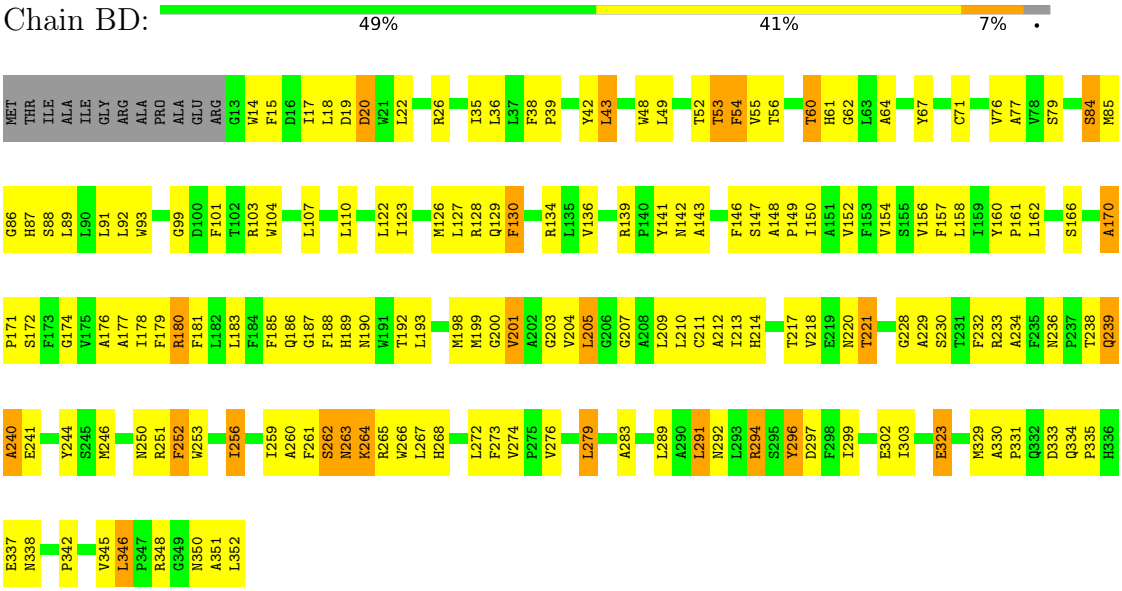
• Molecule 4: Photosystem II reaction center D2 protein

Chain AD:



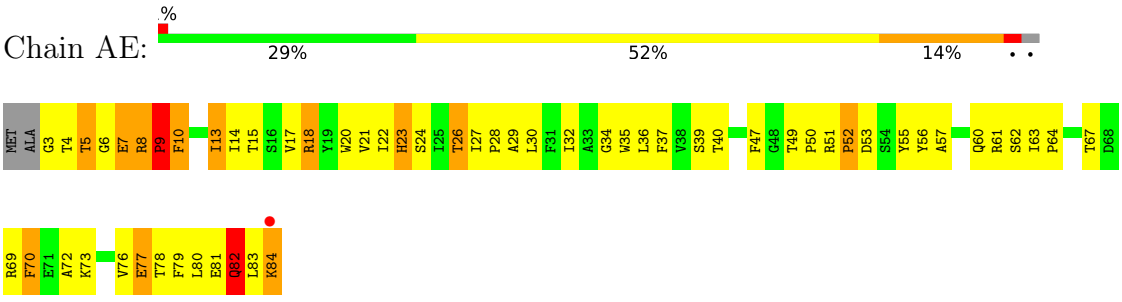
• Molecule 4: Photosystem II reaction center D2 protein

Chain BD:



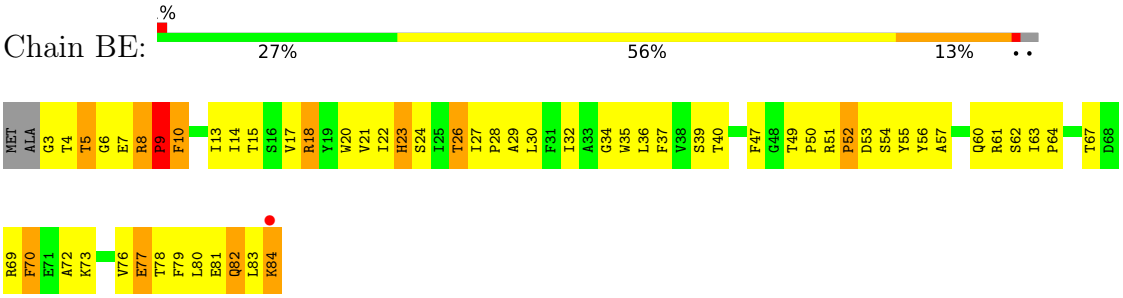
• Molecule 5: Cytochrome b559 subunit alpha

Chain AE:



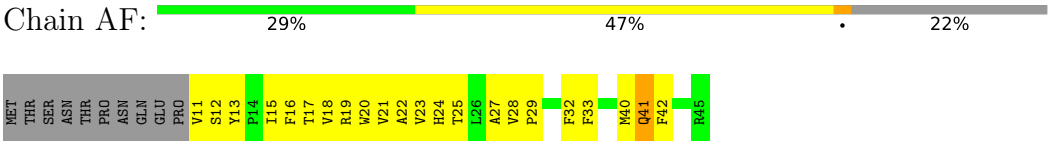
• Molecule 5: Cytochrome b559 subunit alpha

Chain BE:



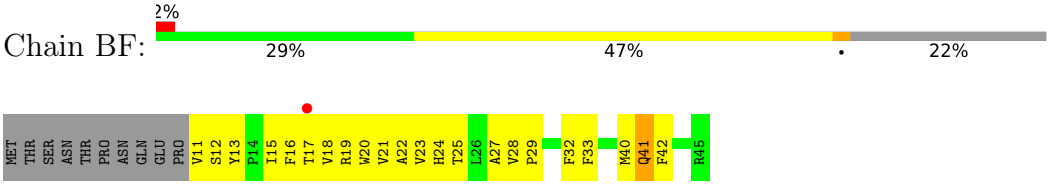
• Molecule 6: Cytochrome b559 subunit beta

Chain AF:



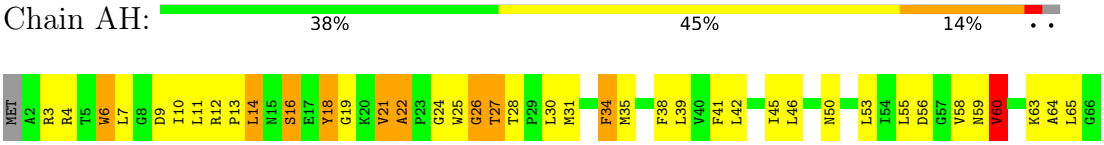
• Molecule 6: Cytochrome b559 subunit beta

Chain BF:



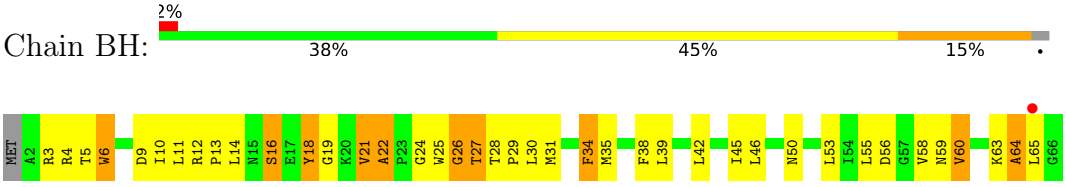
• Molecule 7: Photosystem II reaction center protein H

Chain AH:



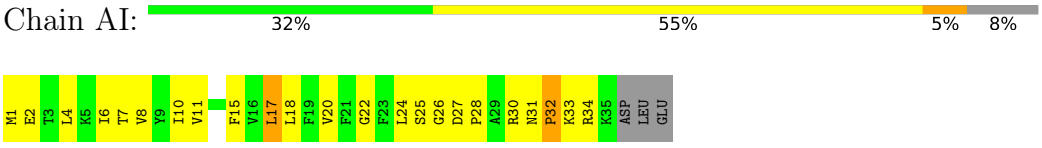
• Molecule 7: Photosystem II reaction center protein H

Chain BH:



• Molecule 8: Photosystem II reaction center protein I

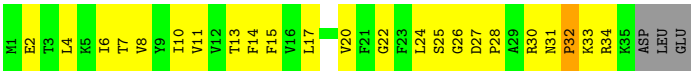
Chain AI:



• Molecule 8: Photosystem II reaction center protein I

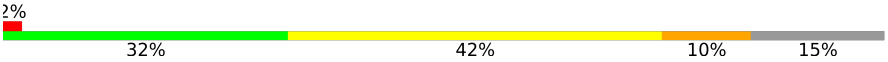
Chain BI:





• Molecule 9: Photosystem II reaction center protein J

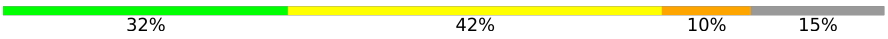
Chain AJ:

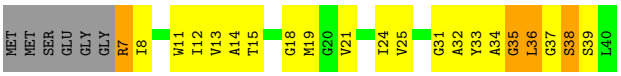




• Molecule 9: Photosystem II reaction center protein J

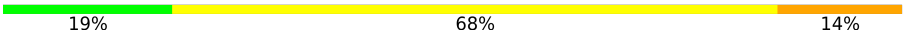
Chain BJ:





• Molecule 10: Photosystem II reaction center protein K

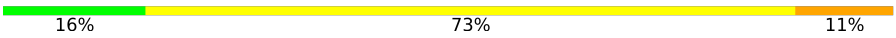
Chain AK:

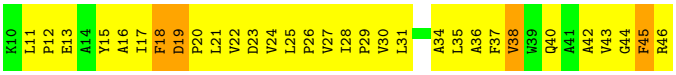




• Molecule 10: Photosystem II reaction center protein K

Chain BK:

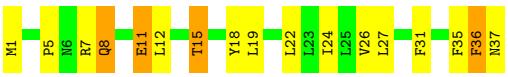




• Molecule 11: Photosystem II reaction center protein L

Chain AL:

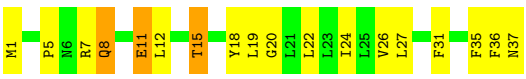




• Molecule 11: Photosystem II reaction center protein L

Chain BL:

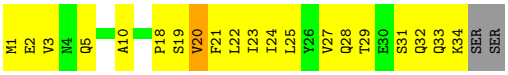




• Molecule 12: Photosystem II reaction center protein M

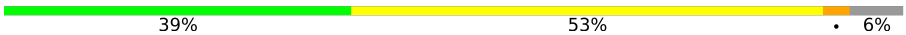
Chain AM:

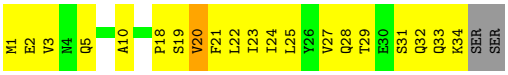




• Molecule 12: Photosystem II reaction center protein M

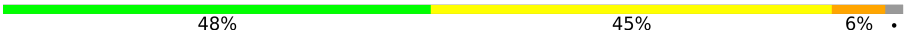
Chain BM:





• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain AO:

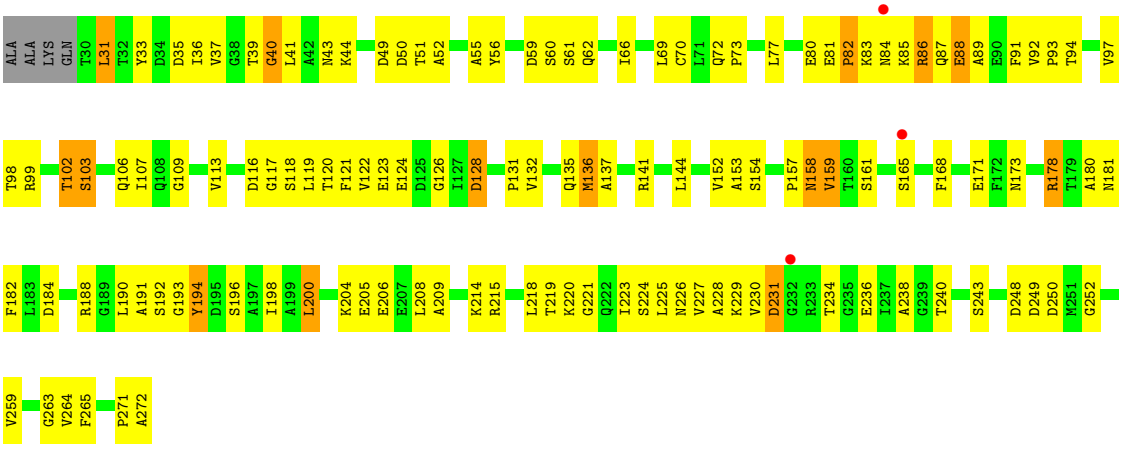




• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain BO:

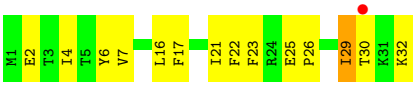




• Molecule 14: Photosystem II reaction center protein T

Chain AT:

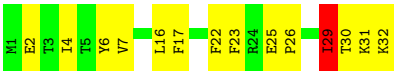




• Molecule 14: Photosystem II reaction center protein T

Chain BT:

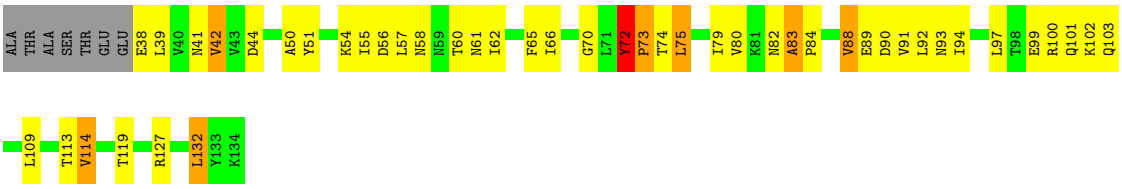




• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain AU:

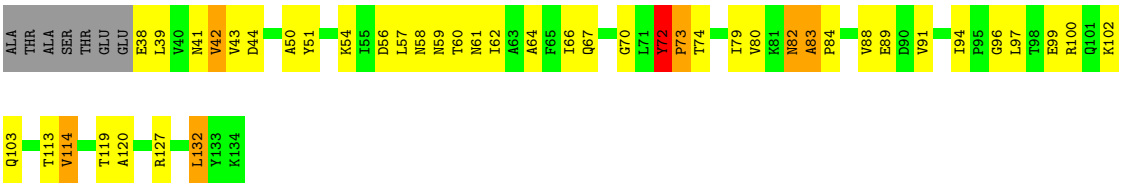




• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain BU:

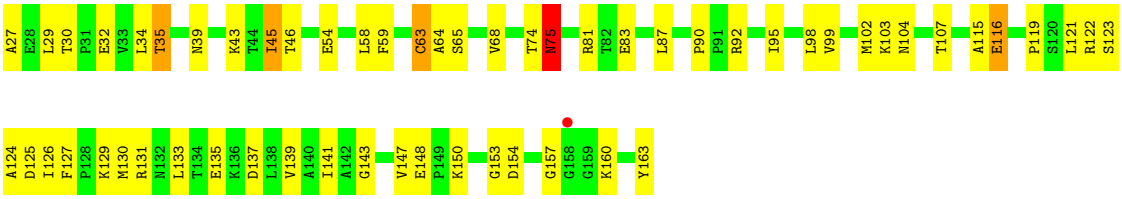




• Molecule 16: Cytochrome c-550

Chain AV:

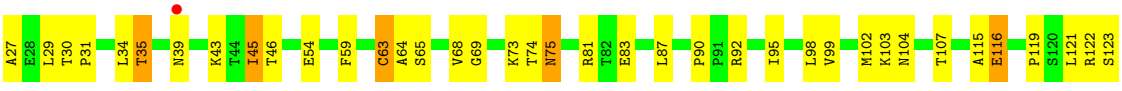


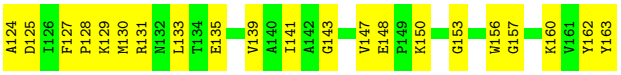


• Molecule 16: Cytochrome c-550

Chain BV:

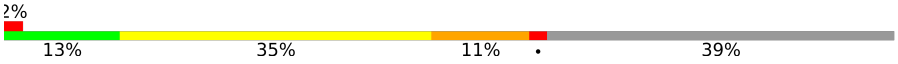


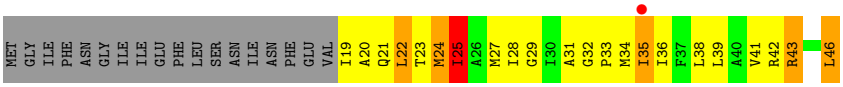




• Molecule 17: Protein ycf12

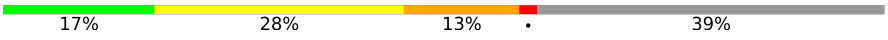
Chain Ay:





• Molecule 17: Protein ycf12

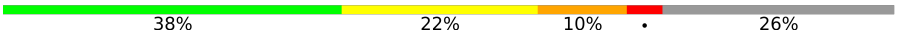
Chain By:

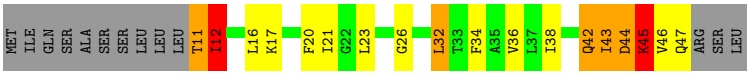




• Molecule 18: Photosystem II PsbX protein

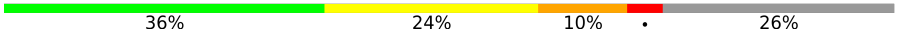
Chain AX:





• Molecule 18: Photosystem II PsbX protein

Chain BX:

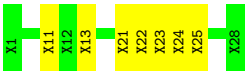




• Molecule 19: Photosystem II protein Y

Chain AY:

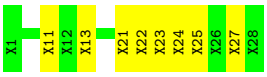




• Molecule 19: Photosystem II protein Y

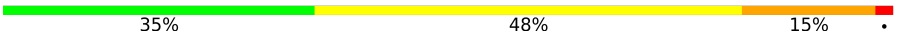
Chain BY:





• Molecule 20: Photosystem II reaction center protein Z

Chain AZ:





• Molecule 20: Photosystem II reaction center protein Z

Chain BZ:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	127.69Å 225.40Å 306.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.90 10.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.7 (10.00-2.90) 96.8 (10.00-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	1.81 (at 2.88Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.249 , 0.292 0.243 , 0.280	Depositor DCC
R_{free} test set	3869 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å^2)	78.2	Xtriage
Anisotropy	0.357	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 81.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	50234	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.57% 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: OEC, BCT, SQD, HEM, CL, LMG, CLA, LHG, LMT, FE2, CA, BCR, DGD, PL9, PHO

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	AA	0.55	0/2713	1.06	19/3700 (0.5%)
1	BA	0.53	0/2713	1.05	20/3700 (0.5%)
2	AB	0.55	0/3986	1.04	30/5433 (0.6%)
2	BB	0.54	0/3986	1.02	29/5433 (0.5%)
3	AC	0.50	0/3556	1.01	13/4842 (0.3%)
3	BC	0.47	0/3556	0.99	17/4842 (0.4%)
4	AD	0.58	0/2801	1.01	12/3818 (0.3%)
4	BD	0.52	0/2801	1.00	13/3818 (0.3%)
5	AE	0.52	0/685	1.20	11/933 (1.2%)
5	BE	0.49	0/685	1.18	9/933 (1.0%)
6	AF	0.53	0/291	0.85	0/397
6	BF	0.53	0/291	0.84	0/397
7	AH	0.50	0/520	1.01	3/709 (0.4%)
7	BH	0.49	0/520	0.99	3/709 (0.4%)
8	AI	0.54	0/293	1.08	2/395 (0.5%)
8	BI	0.53	0/293	1.05	2/395 (0.5%)
9	AJ	0.50	0/255	1.17	2/346 (0.6%)
9	BJ	0.53	0/255	1.12	2/346 (0.6%)
10	AK	0.52	0/303	0.96	1/416 (0.2%)
10	BK	0.51	0/303	0.93	1/416 (0.2%)
11	AL	0.52	0/311	1.02	1/422 (0.2%)
11	BL	0.52	0/311	1.00	0/422
12	AM	0.54	0/270	0.91	0/367
12	BM	0.56	0/270	0.88	0/367
13	AO	0.53	0/1876	1.03	11/2548 (0.4%)
13	BO	0.51	0/1876	1.02	12/2548 (0.5%)
14	AT	0.60	0/284	0.96	0/381
14	BT	0.59	0/284	1.00	1/381 (0.3%)
15	AU	0.55	0/785	1.11	6/1064 (0.6%)
15	BU	0.51	0/785	1.10	6/1064 (0.6%)
16	AV	0.50	0/1081	0.95	4/1468 (0.3%)
16	BV	0.46	0/1081	0.94	3/1468 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
17	Ay	0.66	0/202	1.23	1/272 (0.4%)
17	By	0.57	0/202	1.26	1/272 (0.4%)
18	AX	0.51	0/273	1.00	1/370 (0.3%)
18	BX	0.49	0/273	1.01	2/370 (0.5%)
20	AZ	0.48	0/490	1.12	4/669 (0.6%)
20	BZ	0.49	0/490	1.14	4/669 (0.6%)
All	All	0.52	0/41950	1.03	246/57100 (0.4%)

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	AA	0	1
1	BA	0	1
All	All	0	2

There are no bond length outliers.

All (246) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	AZ	34	ASP	N-CA-C	-9.30	101.71	113.43
20	BZ	34	ASP	N-CA-C	-9.13	101.92	113.43
17	Ay	22	LEU	N-CA-C	-9.06	101.48	112.54
17	By	22	LEU	N-CA-C	-8.92	101.66	112.54
3	AC	182	PHE	N-CA-C	8.81	123.86	113.20
13	AO	102	THR	N-CA-C	8.77	120.92	111.36
5	AE	57	ALA	N-CA-C	-8.70	99.31	110.53
15	AU	51	TYR	N-CA-C	-8.62	97.72	110.23
9	BJ	36	LEU	N-CA-C	-8.55	102.98	113.41
3	AC	439	VAL	N-CA-C	-8.45	102.62	110.82
3	BC	182	PHE	N-CA-C	8.42	123.38	113.20
5	BE	57	ALA	N-CA-C	-8.40	99.21	110.55
2	AB	483	ASP	CA-C-N	8.39	130.33	119.84
2	AB	483	ASP	C-N-CA	8.39	130.33	119.84
9	AJ	36	LEU	N-CA-C	-8.33	103.25	113.41
13	BO	102	THR	N-CA-C	8.27	120.37	111.36
3	BC	318	LEU	N-CA-C	-8.26	102.36	111.36
15	BU	51	TYR	N-CA-C	-8.25	98.27	110.23
2	BB	483	ASP	CA-C-N	8.17	130.05	119.84
2	BB	483	ASP	C-N-CA	8.17	130.05	119.84

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Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	BB	328	GLY	CA-C-N	8.17	128.05	120.21
2	BB	328	GLY	C-N-CA	8.17	128.05	120.21
15	AU	74	THR	N-CA-C	8.16	119.86	110.97
3	AC	318	LEU	N-CA-C	-8.07	102.56	111.36
3	BC	439	VAL	N-CA-C	-8.03	102.98	110.53
15	BU	74	THR	N-CA-C	7.98	119.67	110.97
13	BO	103	SER	N-CA-C	7.87	121.64	110.23
13	AO	103	SER	N-CA-C	7.85	121.61	110.23
5	BE	70	PHE	N-CA-C	7.74	119.35	111.07
18	BX	46	VAL	N-CA-C	7.68	120.50	109.51
8	AI	2	GLU	N-CA-C	-7.58	103.49	112.89
5	AE	24	SER	N-CA-C	-7.55	103.33	112.54
2	AB	328	GLY	CA-C-N	7.55	127.45	120.21
2	AB	328	GLY	C-N-CA	7.55	127.45	120.21
8	BI	2	GLU	N-CA-C	-7.53	103.55	112.89
18	AX	46	VAL	N-CA-C	7.51	120.25	109.51
5	AE	70	PHE	N-CA-C	7.42	119.01	111.07
2	AB	489	GLU	N-CA-C	7.40	126.56	110.80
2	AB	327	THR	N-CA-C	7.38	119.48	110.41
3	AC	347	GLY	N-CA-C	7.30	123.38	114.69
3	BC	347	GLY	N-CA-C	7.28	123.35	114.69
2	BB	489	GLU	N-CA-C	7.25	126.25	110.80
2	AB	488	PRO	N-CA-C	7.21	127.33	112.47
4	AD	54	PHE	N-CA-C	7.18	121.92	112.72
5	BE	24	SER	N-CA-C	-7.15	103.82	112.54
2	BB	236	THR	N-CA-C	-7.11	105.14	114.31
4	BD	54	PHE	N-CA-C	7.06	122.32	113.43
2	AB	236	THR	N-CA-C	-7.05	105.22	114.31
2	BB	488	PRO	N-CA-C	7.03	126.94	112.47
10	AK	38	VAL	N-CA-C	-7.00	103.69	110.42
2	BB	327	THR	N-CA-C	6.99	119.01	110.41
5	AE	6	GLY	N-CA-C	6.94	121.29	112.83
5	BE	6	GLY	N-CA-C	6.93	121.29	112.83
4	AD	296	TYR	N-CA-C	6.90	118.59	111.14
2	BB	363	PHE	N-CA-C	6.88	119.90	108.96
2	AB	363	PHE	N-CA-C	6.84	119.84	108.96
9	AJ	39	SER	N-CA-C	-6.83	104.06	114.16
3	AC	254	THR	N-CA-C	6.82	117.58	108.38
1	BA	339	PHE	CA-C-N	6.80	126.32	119.24
1	BA	339	PHE	C-N-CA	6.80	126.32	119.24
7	AH	64	ALA	N-CA-C	-6.78	105.44	113.38
4	AD	156	VAL	N-CA-C	6.77	117.39	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	AU	72	TYR	N-CA-C	6.71	124.63	109.81
2	BB	37	MET	N-CA-C	-6.65	104.11	111.82
4	BD	296	TYR	N-CA-C	6.64	118.31	111.14
5	AE	67	THR	N-CA-C	6.62	122.18	113.30
3	BC	254	THR	N-CA-C	6.62	117.32	108.38
13	AO	200	LEU	CA-C-N	6.62	128.11	119.84
13	AO	200	LEU	C-N-CA	6.62	128.11	119.84
20	AZ	37	LYS	N-CA-C	-6.59	104.97	112.87
2	BB	381	ILE	CA-C-N	6.58	126.56	119.78
2	BB	381	ILE	C-N-CA	6.58	126.56	119.78
20	BZ	37	LYS	N-CA-C	-6.58	104.98	112.87
1	AA	87	ASN	N-CA-C	-6.57	105.08	113.23
3	AC	37	ALA	N-CA-C	-6.57	103.36	112.30
15	AU	62	ILE	N-CA-C	6.56	118.10	110.62
13	BO	200	LEU	CA-C-N	6.54	128.01	119.84
13	BO	200	LEU	C-N-CA	6.54	128.01	119.84
15	BU	72	TYR	N-CA-C	6.53	124.24	109.81
15	BU	62	ILE	N-CA-C	6.52	118.06	110.62
5	BE	67	THR	N-CA-C	6.51	122.03	113.30
9	BJ	39	SER	N-CA-C	-6.43	104.64	114.16
16	AV	104	ASN	CA-C-N	6.43	126.19	119.76
16	AV	104	ASN	C-N-CA	6.43	126.19	119.76
3	BC	37	ALA	N-CA-C	-6.41	103.58	112.30
1	AA	36	ILE	N-CA-C	-6.36	106.34	111.81
2	AB	37	MET	N-CA-C	-6.34	104.47	111.82
10	BK	38	VAL	N-CA-C	-6.33	104.34	110.42
1	BA	142	TRP	N-CA-C	6.33	124.28	110.80
13	BO	196	SER	N-CA-C	6.31	116.39	108.45
4	AD	142	ASN	N-CA-C	-6.29	105.43	113.23
4	AD	272	LEU	N-CA-C	-6.29	103.73	111.40
7	BH	64	ALA	N-CA-C	-6.27	106.04	113.38
1	BA	32	TRP	N-CA-C	-6.25	104.00	111.69
16	BV	104	ASN	CA-C-N	6.25	126.01	119.76
16	BV	104	ASN	C-N-CA	6.25	126.01	119.76
2	AB	381	ILE	CA-C-N	6.21	126.17	119.78
2	AB	381	ILE	C-N-CA	6.21	126.17	119.78
2	AB	332	LYS	N-CA-C	-6.19	105.69	113.18
13	BO	249	ASP	N-CA-C	-6.17	105.39	113.17
1	AA	142	TRP	N-CA-C	6.15	123.91	110.80
13	AO	40	GLY	N-CA-C	-6.14	107.23	115.21
2	BB	484	PRO	N-CA-C	6.12	125.07	112.47
1	BA	87	ASN	N-CA-C	-6.02	105.77	113.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	AB	484	PRO	N-CA-C	6.00	124.83	112.47
13	AO	249	ASP	N-CA-C	-5.99	105.62	113.17
2	BB	332	LYS	N-CA-C	-5.99	105.93	113.18
4	AD	147	SER	N-CA-C	-5.99	104.83	111.36
4	BD	297	ASP	N-CA-C	5.92	118.41	109.41
13	AO	196	SER	N-CA-C	5.91	116.04	108.24
4	AD	273	PHE	N-CA-C	5.91	118.23	111.02
1	AA	32	TRP	N-CA-C	-5.90	104.43	111.69
4	BD	273	PHE	N-CA-C	5.89	118.21	111.02
1	BA	36	ILE	N-CA-C	-5.89	106.74	111.81
3	AC	32	GLY	N-CA-C	-5.88	99.24	113.18
4	BD	156	VAL	N-CA-C	5.86	117.39	111.00
3	BC	302	TYR	N-CA-C	-5.84	101.01	109.31
2	AB	174	LEU	N-CA-C	-5.80	108.01	114.62
2	AB	163	GLY	CA-C-N	5.80	127.09	119.84
2	AB	163	GLY	C-N-CA	5.80	127.09	119.84
4	BD	272	LEU	N-CA-C	-5.76	103.75	112.04
4	BD	294	ARG	N-CA-C	5.75	118.29	110.35
13	BO	181	ASN	N-CA-C	5.75	119.92	113.01
16	AV	75	ASN	CA-C-N	5.75	125.46	119.82
16	AV	75	ASN	C-N-CA	5.75	125.46	119.82
5	BE	8	ARG	CA-C-N	5.75	127.03	119.84
5	BE	8	ARG	C-N-CA	5.75	127.03	119.84
2	BB	77	GLY	N-CA-C	5.75	120.51	113.79
1	AA	78	ILE	N-CA-C	5.74	116.52	110.72
2	BB	163	GLY	CA-C-N	5.73	127.00	119.84
2	BB	163	GLY	C-N-CA	5.73	127.00	119.84
14	BT	29	ILE	N-CA-C	5.72	116.29	110.05
5	AE	8	ARG	CA-C-N	5.72	126.99	119.84
5	AE	8	ARG	C-N-CA	5.72	126.99	119.84
4	BD	181	PHE	N-CA-C	-5.69	105.16	111.36
13	AO	128	ASP	N-CA-C	5.64	119.25	112.93
1	BA	261	GLN	N-CA-C	5.64	122.81	110.80
3	AC	302	TYR	N-CA-C	-5.63	101.31	109.31
3	AC	224	ILE	CB-CA-C	-5.62	104.68	112.04
4	AD	297	ASP	N-CA-C	5.57	117.88	109.41
1	AA	261	GLN	N-CA-C	5.57	122.67	110.80
4	BD	147	SER	N-CA-C	-5.57	105.29	111.36
1	BA	56	PRO	CA-C-N	5.56	125.57	119.90
1	BA	56	PRO	C-N-CA	5.56	125.57	119.90
2	AB	49	ASP	CA-C-N	5.55	126.04	120.04
2	AB	49	ASP	C-N-CA	5.55	126.04	120.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	BA	195	HIS	CA-C-N	5.53	124.99	119.24
1	BA	195	HIS	C-N-CA	5.53	124.99	119.24
13	BO	128	ASP	N-CA-C	5.52	119.11	112.93
2	AB	80	ILE	N-CA-C	5.52	116.91	110.62
1	AA	339	PHE	CA-C-N	5.52	126.74	119.84
1	AA	339	PHE	C-N-CA	5.52	126.74	119.84
3	BC	224	ILE	CB-CA-C	-5.51	104.82	112.04
7	AH	34	PHE	N-CA-C	-5.51	105.27	111.28
2	BB	120	LEU	N-CA-C	-5.51	102.73	110.50
1	AA	146	ALA	N-CA-C	-5.50	105.37	111.36
4	AD	170	ALA	N-CA-C	-5.49	103.00	110.36
5	AE	23	HIS	N-CA-C	5.48	119.23	112.54
8	BI	17	LEU	N-CA-C	-5.48	104.95	111.03
5	AE	26	THR	N-CA-C	5.48	116.93	111.07
1	AA	88	ALA	N-CA-C	-5.47	105.47	111.82
1	BA	296	ASN	N-CA-C	5.47	119.24	112.24
7	BH	34	PHE	N-CA-C	-5.47	105.32	111.28
2	BB	57	ARG	N-CA-C	-5.46	106.79	113.50
4	BD	170	ALA	N-CA-C	-5.46	103.05	110.36
2	BB	487	SER	N-CA-C	5.45	121.86	109.81
1	BA	88	ALA	N-CA-C	-5.45	105.50	111.82
5	AE	13	ILE	N-CA-C	5.42	115.63	110.42
2	BB	49	ASP	CA-C-N	5.42	125.90	120.04
2	BB	49	ASP	C-N-CA	5.42	125.90	120.04
2	BB	321	LYS	N-CA-C	-5.42	102.02	110.42
4	AD	181	PHE	N-CA-C	-5.42	105.45	111.36
5	BE	23	HIS	N-CA-C	5.42	119.15	112.54
1	BA	83	VAL	CA-C-N	5.42	125.36	119.78
1	BA	83	VAL	C-N-CA	5.42	125.36	119.78
2	AB	487	SER	N-CA-C	5.41	121.77	109.81
3	BC	32	GLY	N-CA-C	-5.41	100.37	113.18
7	AH	22	ALA	N-CA-C	-5.40	102.30	110.39
3	BC	293	ASN	N-CA-C	5.39	118.05	110.23
3	AC	228	ASN	N-CA-C	5.38	119.62	112.30
2	AB	247	PHE	N-CA-C	-5.36	105.35	111.14
15	AU	70	GLY	N-CA-C	5.36	122.19	114.10
1	AA	83	VAL	CA-C-N	5.35	125.29	119.78
1	AA	83	VAL	C-N-CA	5.35	125.29	119.78
4	BD	299	ILE	N-CA-C	5.34	116.07	110.62
2	AB	19	LEU	N-CA-C	-5.32	105.15	111.69
2	AB	77	GLY	N-CA-C	5.31	120.01	113.79
13	AO	205	GLU	N-CA-C	5.31	120.03	113.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	BO	136	MET	N-CA-C	5.31	116.72	109.18
11	AL	36	PHE	N-CA-C	-5.30	106.32	112.89
8	AI	17	LEU	N-CA-C	-5.30	105.15	111.03
3	AC	464	GLU	CA-C-N	5.29	126.45	119.84
3	AC	464	GLU	C-N-CA	5.29	126.45	119.84
20	BZ	35	ARG	N-CA-C	-5.28	105.57	112.23
7	BH	22	ALA	N-CA-C	-5.28	102.47	110.39
3	BC	391	ARG	N-CA-C	-5.26	105.45	111.14
20	BZ	33	TRP	N-CA-C	-5.26	105.94	112.47
2	BB	237	VAL	N-CA-C	-5.26	104.48	111.05
1	BA	298	ASN	N-CA-C	5.24	117.99	109.86
1	BA	77	ILE	N-CA-C	5.24	115.86	110.36
15	BU	70	GLY	N-CA-C	5.22	121.98	114.10
13	BO	40	GLY	N-CA-C	-5.21	108.44	115.21
1	BA	33	PHE	N-CA-C	-5.21	105.78	111.82
20	AZ	35	ARG	N-CA-C	-5.20	105.67	112.23
3	BC	431	PHE	N-CA-C	-5.20	105.30	111.69
2	BB	80	ILE	N-CA-C	5.20	116.54	110.62
1	AA	56	PRO	CA-C-N	5.19	125.19	119.90
1	AA	56	PRO	C-N-CA	5.19	125.19	119.90
2	BB	247	PHE	N-CA-C	-5.19	105.54	111.14
3	AC	391	ARG	N-CA-C	-5.17	105.55	111.14
13	AO	181	ASN	N-CA-C	5.17	119.44	113.18
2	AB	237	VAL	N-CA-C	-5.17	104.59	111.05
2	AB	57	ARG	N-CA-C	-5.15	107.17	113.50
1	AA	33	PHE	N-CA-C	-5.14	105.85	111.82
4	BD	187	GLY	N-CA-C	5.14	118.86	112.64
1	BA	143	ILE	N-CA-C	-5.13	105.50	110.42
16	BV	73	LYS	N-CA-C	5.13	117.53	111.33
3	BC	464	GLU	CA-C-N	5.12	126.25	119.84
3	BC	464	GLU	C-N-CA	5.12	126.25	119.84
18	BX	30	LEU	N-CA-C	-5.12	105.70	111.28
13	BO	194	TYR	N-CA-C	5.12	117.72	110.50
13	AO	194	TYR	N-CA-C	5.12	117.72	110.50
15	AU	75	LEU	N-CA-C	5.11	116.66	111.14
2	AB	120	LEU	N-CA-C	-5.11	103.30	110.50
5	BE	26	THR	N-CA-C	5.10	116.53	111.07
13	BO	205	GLU	N-CA-C	5.10	119.77	113.50
2	AB	165	GLY	N-CA-C	-5.09	105.92	111.21
20	AZ	33	TRP	N-CA-C	-5.08	106.18	112.47
1	AA	266	ASN	N-CA-C	-5.07	107.03	114.39
1	BA	54	ALA	N-CA-C	5.07	121.22	113.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	195	HIS	CA-C-N	5.07	124.51	119.24
1	AA	195	HIS	C-N-CA	5.07	124.51	119.24
1	AA	296	ASN	N-CA-C	5.06	118.72	112.24
2	BB	19	LEU	N-CA-C	-5.06	105.46	111.69
2	AB	317	ASN	N-CA-C	-5.06	105.90	113.89
5	AE	7	GLU	N-CA-C	5.05	117.36	110.24
3	BC	252	ILE	N-CA-C	-5.04	105.58	110.42
15	BU	82	ASN	N-CA-C	5.04	117.68	110.68
2	BB	479	PHE	N-CA-C	-5.03	103.85	110.43
4	AD	294	ARG	N-CA-C	5.02	117.28	110.35
2	BB	382	PRO	N-CA-C	5.02	119.19	111.21
2	AB	155	ALA	N-CA-C	5.01	116.44	111.07
4	AD	299	ILE	N-CA-C	5.01	115.73	110.62
4	BD	64	ALA	N-CA-C	-5.01	101.80	109.76
3	BC	190	ALA	CA-C-N	5.00	124.44	119.24
3	BC	190	ALA	C-N-CA	5.00	124.44	119.24

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	161	TYR	Sidechain
1	BA	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	AA	2628	0	2524	195	0
1	BA	2628	0	2524	192	0
2	AB	3850	0	3718	235	0
2	BB	3850	0	3718	238	0
3	AC	3444	0	3365	277	0
3	BC	3444	0	3365	277	0
4	AD	2706	0	2608	184	0
4	BD	2706	0	2608	192	0
5	AE	666	0	651	69	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	BE	666	0	651	74	0
6	AF	282	0	291	30	0
6	BF	282	0	291	31	0
7	AH	507	0	521	57	0
7	BH	507	0	521	55	0
8	AI	286	0	308	22	0
8	BI	286	0	308	21	0
9	AJ	249	0	262	30	0
9	BJ	249	0	262	28	0
10	AK	293	0	305	50	0
10	BK	293	0	305	52	0
11	AL	304	0	316	19	0
11	BL	304	0	316	21	0
12	AM	267	0	289	28	0
12	BM	267	0	289	27	0
13	AO	1845	0	1801	125	0
13	BO	1845	0	1801	127	0
14	AT	275	0	288	22	0
14	BT	275	0	288	21	0
15	AU	774	0	773	48	0
15	BU	774	0	773	48	0
16	AV	1060	0	1068	45	0
16	BV	1060	0	1068	45	0
17	Ay	201	0	226	36	0
17	By	201	0	226	36	0
18	AX	270	0	299	29	0
18	BX	270	0	299	27	0
19	AY	140	0	32	4	0
19	BY	140	0	32	6	0
20	AZ	479	0	516	60	0
20	BZ	479	0	516	61	0
21	AA	1	0	0	0	0
21	BA	1	0	0	0	0
22	AA	260	0	288	19	0
22	AB	1040	0	1152	71	0
22	AC	845	0	936	50	0
22	AD	130	0	144	10	0
22	BA	260	0	288	20	0
22	BB	1040	0	1152	76	0
22	BC	845	0	936	50	0
22	BD	130	0	144	11	0
23	AA	64	0	74	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	AD	64	0	74	3	0
23	BA	64	0	74	5	0
23	BD	64	0	74	6	0
24	AA	45	0	61	5	0
24	AD	55	0	80	9	0
24	AJ	35	0	45	0	0
24	BA	45	0	61	6	0
24	BD	55	0	80	8	0
24	BJ	35	0	45	0	0
25	AA	5	0	0	0	0
25	BA	5	0	0	0	0
26	AA	40	0	56	6	0
26	AB	160	0	224	9	0
26	AC	80	0	112	13	0
26	AD	40	0	56	3	0
26	AH	40	0	56	2	0
26	AJ	40	0	56	5	0
26	AK	40	0	56	13	0
26	AT	40	0	56	7	0
26	AZ	40	0	56	4	0
26	BA	40	0	56	3	0
26	BB	120	0	168	5	0
26	BC	80	0	112	16	0
26	BD	40	0	56	3	0
26	BJ	40	0	56	5	0
26	BK	40	0	56	13	0
26	BX	40	0	56	4	0
26	BZ	40	0	56	4	0
27	AA	56	0	70	0	0
27	AB	52	0	62	3	0
27	AC	181	0	245	19	0
27	AD	63	0	87	0	0
27	AH	58	0	74	1	0
27	BA	56	0	70	0	0
27	BB	52	0	62	3	0
27	BC	181	0	245	22	0
27	BD	63	0	87	0	0
27	BH	58	0	74	1	0
28	AA	39	0	51	3	0
28	AC	37	0	44	5	0
28	BA	39	0	51	4	0
28	BC	37	0	44	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	AA	105	0	145	10	0
29	AD	43	0	49	2	0
29	AF	45	0	53	2	0
29	BA	105	0	145	6	0
29	BB	47	0	60	2	0
29	BD	43	0	49	2	0
29	BF	45	0	53	1	0
29	BL	47	0	60	2	0
30	AA	93	0	126	5	0
30	AB	140	0	190	4	0
30	AC	93	0	126	6	0
30	AD	94	0	128	9	0
30	AE	44	0	58	4	0
30	AI	43	0	56	3	0
30	AM	42	0	54	4	0
30	BA	51	0	72	2	0
30	BB	98	0	136	2	0
30	BC	93	0	126	8	0
30	BD	94	0	128	10	0
30	BE	44	0	58	4	0
30	BI	43	0	56	3	0
30	BM	42	0	54	4	0
31	AA	1	0	0	0	0
31	BA	1	0	0	0	0
32	AB	105	0	138	7	0
32	AD	31	0	35	1	0
32	AI	35	0	46	4	0
32	AM	35	0	46	1	0
32	AT	35	0	46	3	0
32	BB	105	0	138	6	0
32	BD	31	0	35	0	0
32	BI	35	0	46	3	0
32	BM	35	0	46	1	0
32	BT	35	0	46	3	0
33	AD	4	0	0	1	0
33	BD	4	0	0	1	0
34	AE	43	0	30	5	0
34	AV	43	0	30	3	0
34	BE	43	0	30	6	0
34	BV	43	0	30	3	0
35	AK	1	0	0	0	0
35	AO	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	BK	1	0	0	0	0
35	BO	1	0	0	0	0
All	All	50234	0	51364	2938	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 29.

All (2938) 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)
16:AV:63:CYS:SG	34:AV:201:HEM:HAB	1.85	1.16
15:BU:83:ALA:HB1	15:BU:84:PRO:HD2	1.23	1.16
9:AJ:15:THR:HG21	10:AK:38:VAL:HG13	1.23	1.16
16:BV:63:CYS:SG	34:BV:201:HEM:HAB	1.85	1.15
9:BJ:15:THR:HG21	10:BK:38:VAL:HG13	1.24	1.13
2:BB:68:ARG:HH22	22:BB:607:CLA:HED1	1.13	1.11
15:AU:83:ALA:HB1	15:AU:84:PRO:HD2	1.22	1.09
2:AB:68:ARG:HH22	22:AB:604:CLA:HED1	1.12	1.07
1:AA:129:ARG:HH21	4:AD:256:ILE:HD12	1.19	1.06
2:BB:121:GLU:HG2	7:BH:4:ARG:HG2	1.36	1.05
2:AB:121:GLU:HG2	7:AH:4:ARG:HG2	1.36	1.04
1:BA:214:MET:HE2	1:BA:214:MET:HA	1.39	1.04
13:BO:178:ARG:HH11	13:BO:178:ARG:HG3	1.17	1.04
13:AO:178:ARG:HH11	13:AO:178:ARG:HG3	1.18	1.04
13:AO:82:PRO:HG3	13:AO:89:ALA:HB2	1.37	1.03
3:BC:254:THR:HG22	3:BC:255:THR:H	1.23	1.03
3:AC:254:THR:HG22	3:AC:255:THR:H	1.18	1.03
1:AA:214:MET:HE2	1:AA:214:MET:HA	1.39	1.01
1:BA:317:TRP:CZ3	4:BD:180:ARG:HD3	1.96	1.01
1:BA:129:ARG:HH21	4:BD:256:ILE:HD12	1.20	1.00
13:BO:82:PRO:HG3	13:BO:89:ALA:HB2	1.40	1.00
2:AB:149:LEU:HG	22:AB:603:CLA:HBC1	1.44	1.00
1:AA:317:TRP:CZ3	4:AD:180:ARG:HD3	1.95	0.99
17:Ay:35:ILE:HG22	20:AZ:21:ILE:HG23	1.43	0.99
17:By:35:ILE:HG22	20:BZ:21:ILE:HG23	1.44	0.97
12:AM:33:GLN:HB3	12:BM:33:GLN:HB3	1.43	0.97
4:AD:26:ARG:HD3	6:AF:18:VAL:HG11	1.47	0.97
13:AO:230:VAL:HG12	13:AO:231:ASP:H	1.30	0.97
2:BB:149:LEU:HG	22:BB:606:CLA:HBC1	1.45	0.96
13:BO:230:VAL:HG12	13:BO:231:ASP:H	1.32	0.94
13:AO:69:LEU:HB3	13:AO:107:ILE:HB	1.49	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:AU:83:ALA:HB1	15:AU:84:PRO:CD	1.98	0.93
14:AT:29:ILE:HD12	14:AT:29:ILE:H	1.33	0.92
4:BD:26:ARG:HD3	6:BF:18:VAL:HG11	1.48	0.92
2:BB:271:THR:HG22	2:BB:273:TYR:H	1.35	0.92
15:BU:83:ALA:HB1	15:BU:84:PRO:CD	2.00	0.91
13:BO:69:LEU:HB3	13:BO:107:ILE:HB	1.51	0.91
2:BB:414:PRO:HB2	2:BB:415:PRO:HD3	1.53	0.90
14:BT:29:ILE:H	14:BT:29:ILE:HD12	1.34	0.90
2:BB:68:ARG:NH2	22:BB:607:CLA:HED1	1.87	0.90
13:BO:178:ARG:HH11	13:BO:178:ARG:CG	1.84	0.90
3:BC:473:ASP:HB2	14:BT:26:PRO:HB3	1.54	0.90
3:AC:473:ASP:HB2	14:AT:26:PRO:HB3	1.53	0.89
1:AA:72:LEU:HD13	30:AA:416:LMG:H111	1.55	0.89
1:AA:317:TRP:HZ3	4:AD:180:ARG:HD3	1.37	0.89
22:AD:404:CLA:H42	18:AX:26:GLY:HA3	1.53	0.89
1:AA:214:MET:HE1	4:AD:142:ASN:ND2	1.88	0.88
13:BO:69:LEU:HD12	13:BO:70:CYS:H	1.37	0.88
3:AC:224:ILE:O	3:AC:227:VAL:HG23	1.73	0.88
1:BA:214:MET:HE1	4:BD:142:ASN:ND2	1.88	0.88
22:BD:404:CLA:H42	18:BX:26:GLY:HA3	1.56	0.88
2:AB:68:ARG:NH2	22:AB:604:CLA:HED1	1.88	0.88
13:AO:178:ARG:HH11	13:AO:178:ARG:CG	1.88	0.87
5:BE:18:ARG:HD2	5:BE:22:ILE:HD11	1.55	0.87
7:BH:12:ARG:O	7:BH:12:ARG:HD3	1.74	0.87
15:AU:72:TYR:HB3	15:AU:73:PRO:HD3	1.57	0.87
2:AB:414:PRO:HB2	2:AB:415:PRO:HD3	1.55	0.87
22:AB:608:CLA:HAB	4:AD:123:ILE:HG23	1.58	0.86
11:BL:5:PRO:HA	11:BL:7:ARG:HH22	1.38	0.86
2:AB:271:THR:HG22	2:AB:273:TYR:H	1.39	0.86
3:AC:305:THR:HG22	3:AC:308:GLU:H	1.40	0.86
4:AD:129:GLN:NE2	4:AD:143:ALA:HA	1.92	0.85
13:AO:69:LEU:HD12	13:AO:70:CYS:H	1.39	0.85
1:BA:317:TRP:HZ3	4:BD:180:ARG:HD3	1.36	0.85
3:AC:447:ARG:HG2	3:AC:447:ARG:HH11	1.40	0.85
18:AX:12:ILE:HG12	18:AX:16:LEU:HD12	1.56	0.85
3:BC:155:ASN:HD21	3:BC:255:THR:HB	1.39	0.85
3:BC:224:ILE:O	3:BC:227:VAL:HG23	1.76	0.85
7:AH:12:ARG:O	7:AH:12:ARG:HD3	1.76	0.84
34:BE:101:HEM:HBC2	6:BF:27:ALA:HB1	1.58	0.84
11:BL:8:GLN:N	11:BL:8:GLN:HE21	1.74	0.84
7:BH:31:MET:HE3	7:BH:35:MET:HE1	1.58	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:AE:101:HEM:HBC2	6:AF:27:ALA:HB1	1.59	0.84
5:AE:18:ARG:HD2	5:AE:22:ILE:HD11	1.60	0.84
11:AL:5:PRO:HA	11:AL:7:ARG:HH22	1.39	0.84
3:BC:447:ARG:HH11	3:BC:447:ARG:HG2	1.40	0.84
3:BC:39:ASN:HB2	22:BC:508:CLA:HBA1	1.57	0.84
3:BC:305:THR:HG23	3:BC:307:PRO:HD2	1.59	0.84
3:BC:449:ARG:HE	22:BC:505:CLA:HED1	1.42	0.84
3:AC:155:ASN:HD21	3:AC:255:THR:HB	1.40	0.84
3:AC:305:THR:HG23	3:AC:307:PRO:HD2	1.60	0.84
22:BB:611:CLA:HAB	4:BD:123:ILE:HG23	1.60	0.84
3:BC:305:THR:HG22	3:BC:308:GLU:H	1.40	0.84
15:BU:72:TYR:HB3	15:BU:73:PRO:HD3	1.59	0.83
4:BD:148:ALA:HB3	4:BD:149:PRO:HD3	1.60	0.83
20:BZ:36:SER:HA	20:BZ:39:LEU:HG	1.60	0.83
1:BA:192:ILE:HA	1:BA:293:MET:HE1	1.61	0.83
3:AC:39:ASN:HB2	22:AC:508:CLA:HBA1	1.58	0.83
11:AL:8:GLN:N	11:AL:8:GLN:HE21	1.75	0.83
3:AC:449:ARG:HE	22:AC:505:CLA:HED1	1.43	0.83
1:BA:190:HIS:HB3	1:BA:293:MET:HE2	1.61	0.83
22:BA:403:CLA:H152	23:BA:406:PHO:H51	1.60	0.83
3:BC:166:ILE:HG23	3:BC:245:ILE:HG23	1.60	0.83
2:BB:68:ARG:HH22	22:BB:607:CLA:CED	1.91	0.83
2:AB:68:ARG:HH22	22:AB:604:CLA:CED	1.92	0.83
2:BB:124:ARG:HE	2:BB:131:PRO:HD3	1.42	0.83
1:BA:41:LEU:HD13	23:BA:406:PHO:H2	1.61	0.82
18:BX:12:ILE:HG12	18:BX:16:LEU:HD12	1.61	0.82
2:AB:124:ARG:HE	2:AB:131:PRO:HD3	1.43	0.82
3:AC:166:ILE:HG23	3:AC:245:ILE:HG23	1.61	0.81
7:AH:31:MET:HE3	7:AH:35:MET:HE1	1.62	0.81
2:BB:489:GLU:HB2	5:BE:3:GLY:N	1.95	0.81
4:BD:129:GLN:NE2	4:BD:143:ALA:HA	1.97	0.80
3:BC:315:MET:HE1	3:BC:369:LEU:HD12	1.62	0.80
1:AA:192:ILE:HA	1:AA:293:MET:HE1	1.61	0.80
2:AB:489:GLU:HB2	5:AE:3:GLY:N	1.96	0.80
13:AO:83:LYS:HG2	13:AO:84:ASN:H	1.46	0.80
17:By:39:LEU:HB3	17:By:46:LEU:HD21	1.63	0.80
1:BA:214:MET:HE1	4:BD:142:ASN:HD21	1.47	0.80
22:AA:402:CLA:H152	23:AA:405:PHO:H51	1.63	0.80
26:AD:406:BCR:H403	9:AJ:25:VAL:HG21	1.64	0.80
20:AZ:36:SER:HA	20:AZ:39:LEU:HG	1.64	0.80
17:Ay:39:LEU:HB3	17:Ay:46:LEU:HD21	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:41:LEU:HD13	23:AA:405:PHO:H2	1.62	0.79
1:AA:214:MET:HE1	4:AD:142:ASN:HD21	1.46	0.79
3:AC:254:THR:HG22	3:AC:255:THR:N	1.96	0.79
2:AB:483:ASP:CG	2:AB:484:PRO:HD2	2.07	0.79
1:BA:258:LEU:HD12	4:BD:128:ARG:HD3	1.65	0.79
4:AD:148:ALA:HB3	4:AD:149:PRO:HD3	1.63	0.79
17:Ay:34:MET:HE1	17:Ay:38:LEU:HD21	1.65	0.79
13:AO:230:VAL:HG12	13:AO:231:ASP:N	1.98	0.79
13:BO:218:LEU:HD22	15:BU:119:THR:HG21	1.65	0.79
2:AB:348:ASN:HB3	2:AB:354:LEU:HD21	1.65	0.78
1:AA:12:ASN:HD22	1:AA:15:GLU:HB2	1.49	0.78
2:AB:24:LEU:HD21	22:AB:616:CLA:HAB	1.65	0.78
5:AE:84:LYS:HB2	5:AE:84:LYS:NZ	1.97	0.78
4:BD:60:THR:HG23	4:BD:61:HIS:CD2	2.18	0.78
2:AB:271:THR:HG22	2:AB:273:TYR:N	1.98	0.78
13:BO:31:LEU:HB2	13:BO:36:ILE:HD11	1.66	0.78
13:BO:83:LYS:HG2	13:BO:84:ASN:H	1.47	0.78
1:BA:12:ASN:HD22	1:BA:15:GLU:HB2	1.49	0.78
2:BB:271:THR:HG22	2:BB:273:TYR:N	1.98	0.78
2:BB:483:ASP:CG	2:BB:484:PRO:HD2	2.08	0.78
11:BL:5:PRO:HA	11:BL:7:ARG:NH2	1.99	0.78
13:BO:35:ASP:C	13:BO:36:ILE:HD12	2.09	0.78
24:BA:408:PL9:H33	4:BD:38:PHE:HD1	1.47	0.77
2:BB:124:ARG:HH11	2:BB:124:ARG:HG3	1.49	0.77
26:BD:406:BCR:H403	9:BJ:25:VAL:HG21	1.64	0.77
9:BJ:11:TRP:CH2	17:By:36:ILE:HD11	2.20	0.77
1:AA:190:HIS:HB3	1:AA:293:MET:HE2	1.64	0.77
24:AA:407:PL9:H33	4:AD:38:PHE:HD1	1.48	0.77
20:BZ:32:ASP:CG	20:BZ:33:TRP:H	1.92	0.77
3:AC:315:MET:HE1	3:AC:369:LEU:HD12	1.66	0.77
2:BB:24:LEU:HD21	22:BB:619:CLA:HAB	1.67	0.76
2:AB:329:PRO:HB3	22:AB:607:CLA:HED1	1.65	0.76
9:AJ:11:TRP:CH2	17:Ay:36:ILE:HD11	2.20	0.76
26:BC:514:BCR:H353	26:BK:102:BCR:H321	1.68	0.76
5:BE:84:LYS:HB2	5:BE:84:LYS:NZ	2.00	0.76
2:BB:188:ASP:HA	7:BH:58:VAL:HG23	1.68	0.76
2:BB:329:PRO:HB3	22:BB:610:CLA:HED1	1.67	0.76
7:AH:35:MET:HE2	26:AH:101:BCR:HC21	1.66	0.76
13:AO:31:LEU:HB2	13:AO:36:ILE:HD11	1.67	0.76
1:AA:258:LEU:HD12	4:AD:128:ARG:HD3	1.66	0.76
1:AA:57:PRO:HG3	1:AA:68:SER:HB3	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:BK:21:LEU:CD1	17:By:24:MET:HE2	2.15	0.76
20:AZ:32:ASP:CG	20:AZ:33:TRP:H	1.90	0.76
20:AZ:32:ASP:HB2	20:AZ:35:ARG:HG2	1.67	0.76
2:AB:134:ASP:OD2	2:AB:137:LYS:HE3	1.86	0.75
4:BD:244:TYR:OH	4:BD:264:LYS:HE3	1.86	0.75
3:AC:391:ARG:NH1	3:AC:391:ARG:HB2	2.02	0.75
7:AH:3:ARG:HH21	11:AL:1:MET:HE1	1.50	0.75
18:AX:12:ILE:HG23	18:AX:12:ILE:O	1.85	0.75
5:BE:18:ARG:HB3	5:BE:18:ARG:HH11	1.50	0.75
1:BA:57:PRO:HG3	1:BA:68:SER:HB3	1.68	0.75
2:BB:134:ASP:OD2	2:BB:137:LYS:HE3	1.87	0.75
4:BD:85:MET:HE1	5:BE:69:ARG:HA	1.69	0.75
3:BC:254:THR:HG22	3:BC:255:THR:N	2.00	0.75
20:AZ:49:ALA:O	20:AZ:53:VAL:HG23	1.86	0.75
13:AO:35:ASP:C	13:AO:36:ILE:HD12	2.12	0.74
1:BA:214:MET:HA	1:BA:214:MET:CE	2.17	0.74
11:AL:5:PRO:HA	11:AL:7:ARG:NH2	2.00	0.74
10:AK:21:LEU:HD13	17:Ay:24:MET:HE2	1.68	0.74
7:BH:3:ARG:HH21	11:BL:1:MET:HE1	1.51	0.74
3:AC:155:ASN:HA	3:AC:158:THR:HG22	1.69	0.74
3:AC:241:GLY:O	3:AC:245:ILE:HG13	1.88	0.74
13:BO:230:VAL:HG12	13:BO:231:ASP:N	2.02	0.74
2:AB:137:LYS:HD2	7:AH:14:LEU:O	1.87	0.74
4:AD:244:TYR:OH	4:AD:264:LYS:HE3	1.88	0.74
4:AD:148:ALA:HB2	4:AD:276:VAL:HG13	1.70	0.74
6:AF:17:THR:HG23	6:AF:20:TRP:H	1.53	0.74
5:BE:17:VAL:O	5:BE:21:VAL:HG23	1.87	0.74
5:AE:18:ARG:HB3	5:AE:18:ARG:HH11	1.52	0.73
13:BO:69:LEU:HD12	13:BO:70:CYS:N	2.03	0.73
17:By:34:MET:HE1	17:By:38:LEU:HD21	1.68	0.73
3:AC:240:ILE:O	3:AC:244:CYS:HB2	1.88	0.73
4:AD:60:THR:HG23	4:AD:61:HIS:CD2	2.23	0.73
26:AC:514:BCR:H353	26:AK:102:BCR:H321	1.69	0.73
10:BK:21:LEU:HD13	17:By:24:MET:HE2	1.71	0.73
13:AO:218:LEU:HD22	15:AU:119:THR:HG21	1.69	0.73
2:AB:483:ASP:CB	2:AB:484:PRO:HD2	2.17	0.73
2:BB:286:ARG:HH11	2:BB:286:ARG:HG2	1.54	0.73
3:BC:155:ASN:HA	3:BC:158:THR:HG22	1.70	0.73
3:BC:241:GLY:O	3:BC:245:ILE:HG13	1.87	0.73
5:AE:17:VAL:O	5:AE:21:VAL:HG23	1.88	0.73
12:AM:20:VAL:HG21	12:BM:20:VAL:HG21	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AO:92:VAL:CG1	13:AO:93:PRO:HD2	2.19	0.73
4:BD:88:SER:HB2	5:BE:69:ARG:NH2	2.02	0.73
10:AK:21:LEU:CD1	17:Ay:24:MET:HE2	2.17	0.73
18:AX:34:PHE:O	18:AX:38:ILE:HG12	1.88	0.73
7:BH:35:MET:HE2	26:BX:101:BCR:HC21	1.71	0.73
2:BB:348:ASN:HB3	2:BB:354:LEU:HD21	1.71	0.73
13:AO:206:GLU:H	13:AO:206:GLU:CD	1.97	0.73
2:BB:135:LEU:HA	2:BB:138:MET:HE3	1.70	0.73
22:BD:404:CLA:H43	18:BX:23:LEU:HA	1.71	0.73
1:AA:41:LEU:O	1:AA:45:THR:HG22	1.88	0.72
3:AC:254:THR:CG2	3:AC:255:THR:H	2.00	0.72
3:AC:305:THR:CG2	3:AC:308:GLU:H	2.02	0.72
16:BV:63:CYS:SG	34:BV:201:HEM:CAB	2.74	0.72
2:AB:135:LEU:HD23	2:AB:138:MET:HE3	1.71	0.72
20:BZ:32:ASP:HB2	20:BZ:35:ARG:HG2	1.71	0.72
3:AC:405:ASN:HD22	27:AC:518:DGD:HD5	1.54	0.72
3:AC:415:ASN:O	3:AC:416:SER:HB3	1.89	0.72
3:BC:240:ILE:O	3:BC:244:CYS:HB2	1.89	0.72
1:AA:129:ARG:NH2	4:AD:256:ILE:HD12	2.01	0.72
5:AE:81:GLU:C	5:AE:83:LEU:H	1.96	0.72
3:BC:391:ARG:NH1	3:BC:391:ARG:HB2	2.04	0.72
5:BE:81:GLU:C	5:BE:83:LEU:H	1.97	0.72
3:AC:361:PHE:HA	27:AC:516:DGD:HE61	1.72	0.72
1:BA:41:LEU:O	1:BA:45:THR:HG22	1.89	0.72
2:BB:483:ASP:CB	2:BB:484:PRO:HD2	2.19	0.72
3:BC:305:THR:CG2	3:BC:308:GLU:H	2.02	0.72
13:AO:69:LEU:HD12	13:AO:70:CYS:N	2.05	0.72
13:AO:86:ARG:NH1	13:AO:87:GLN:HA	2.05	0.72
13:BO:86:ARG:NH1	13:BO:87:GLN:HA	2.05	0.72
2:AB:27:THR:HG22	2:AB:107:LEU:HD13	1.72	0.71
3:AC:29:GLU:HB3	10:AK:46:ARG:NH1	2.04	0.71
3:AC:391:ARG:HB2	3:AC:391:ARG:HH11	1.55	0.71
2:AB:68:ARG:NH1	2:AB:262:THR:HG23	2.04	0.71
2:AB:188:ASP:HA	7:AH:58:VAL:HG23	1.72	0.71
5:AE:56:TYR:O	16:AV:27:ALA:HB2	1.90	0.71
12:AM:33:GLN:HB3	12:BM:33:GLN:CB	2.19	0.71
22:AD:404:CLA:H43	18:AX:23:LEU:HA	1.71	0.71
3:BC:405:ASN:HD22	27:BC:518:DGD:HD5	1.55	0.71
13:BO:206:GLU:CD	13:BO:206:GLU:H	1.97	0.71
1:AA:214:MET:HA	1:AA:214:MET:CE	2.17	0.71
13:BO:92:VAL:CG1	13:BO:93:PRO:HD2	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:124:ARG:HG3	2:AB:124:ARG:HH11	1.55	0.71
14:AT:29:ILE:H	14:AT:29:ILE:CD1	1.95	0.71
7:BH:3:ARG:NH2	11:BL:1:MET:HE1	2.05	0.71
1:BA:129:ARG:NH2	4:BD:256:ILE:HA	2.06	0.71
1:BA:193:LEU:HD11	22:BA:403:CLA:HMC2	1.73	0.71
2:BB:68:ARG:NH1	2:BB:262:THR:HG23	2.06	0.70
3:BC:29:GLU:HB3	10:BK:46:ARG:NH1	2.06	0.70
3:AC:277:GLY:C	22:AC:505:CLA:HBC2	2.15	0.70
2:BB:135:LEU:HD23	2:BB:138:MET:HE3	1.73	0.70
3:AC:348:GLU:OE2	13:AO:37:VAL:HA	1.91	0.70
5:AE:84:LYS:HB2	5:AE:84:LYS:HZ2	1.55	0.70
3:BC:277:GLY:C	22:BC:505:CLA:HBC2	2.16	0.70
4:BD:148:ALA:HB2	4:BD:276:VAL:HG13	1.71	0.70
3:AC:187:ASP:HB2	3:AC:230:LEU:HD12	1.73	0.70
7:AH:38:PHE:HB2	26:AH:101:BCR:H10C	1.74	0.70
15:AU:38:GLU:HG2	15:AU:39:LEU:N	2.05	0.70
13:BO:77:LEU:HD23	13:BO:93:PRO:HA	1.72	0.70
1:AA:129:ARG:NH2	4:AD:256:ILE:HA	2.06	0.70
7:AH:3:ARG:NH2	11:AL:1:MET:HE1	2.05	0.70
16:AV:63:CYS:SG	34:AV:201:HEM:CAB	2.74	0.70
1:BA:93:PHE:CD2	1:BA:95:PRO:HD3	2.26	0.70
2:BB:27:THR:HG22	2:BB:107:LEU:HD13	1.72	0.70
13:AO:77:LEU:HD23	13:AO:93:PRO:HA	1.74	0.70
3:BC:158:THR:O	3:BC:251:HIS:HB3	1.92	0.70
4:BD:39:PRO:O	4:BD:43:LEU:HD22	1.91	0.70
4:BD:192:THR:HG23	22:BD:402:CLA:HBC2	1.74	0.70
5:BE:26:THR:HB	34:BE:101:HEM:HBB2	1.74	0.70
13:AO:87:GLN:O	13:AO:88:GLU:HB3	1.91	0.70
4:AD:85:MET:HE1	5:AE:69:ARG:HA	1.74	0.70
16:AV:115:ALA:CB	16:AV:122:ARG:HD2	2.22	0.70
18:BX:12:ILE:HG23	18:BX:12:ILE:O	1.89	0.70
1:AA:93:PHE:CD2	1:AA:95:PRO:HD3	2.26	0.69
30:AB:623:LMG:H111	1:BA:72:LEU:HD13	1.74	0.69
2:BB:137:LYS:HD2	7:BH:14:LEU:O	1.92	0.69
4:AD:55:VAL:HG21	4:AD:110:LEU:HD12	1.74	0.69
1:BA:332:HIS:CD2	1:BA:333:GLU:HG3	2.27	0.69
3:BC:85:GLY:N	27:BC:517:DGD:HE4	2.06	0.69
6:BF:17:THR:HG23	6:BF:20:TRP:H	1.57	0.69
4:AD:122:LEU:HD11	23:AD:403:PHO:H92	1.74	0.69
4:AD:152:VAL:HG21	4:AD:279:LEU:HD12	1.72	0.69
13:AO:33:TYR:O	13:AO:37:VAL:HG23	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:BE:56:TYR:O	16:BV:27:ALA:HB2	1.92	0.69
7:BH:38:PHE:HB2	26:BX:101:BCR:H10C	1.73	0.69
3:AC:85:GLY:N	27:AC:517:DGD:HE4	2.07	0.69
3:AC:158:THR:O	3:AC:251:HIS:HB3	1.92	0.69
5:AE:26:THR:HB	34:AE:101:HEM:HBB2	1.74	0.69
5:AE:81:GLU:O	5:AE:83:LEU:N	2.24	0.69
4:BD:152:VAL:HG21	4:BD:279:LEU:HD12	1.74	0.69
16:BV:115:ALA:CB	16:BV:122:ARG:HD2	2.23	0.69
18:BX:34:PHE:O	18:BX:38:ILE:HG12	1.91	0.69
4:AD:39:PRO:O	4:AD:43:LEU:HD22	1.93	0.69
12:AM:33:GLN:CB	12:BM:33:GLN:HB3	2.19	0.69
3:BC:254:THR:CG2	3:BC:255:THR:H	2.04	0.69
3:BC:348:GLU:OE2	13:BO:37:VAL:HA	1.93	0.69
5:BE:84:LYS:HB2	5:BE:84:LYS:HZ2	1.58	0.69
4:AD:87:HIS:HD2	4:AD:162:LEU:HD23	1.58	0.69
4:AD:129:GLN:HE22	4:AD:143:ALA:HA	1.55	0.69
2:BB:264:PRO:HG2	2:BB:267:LEU:HD12	1.74	0.69
13:BO:33:TYR:O	13:BO:37:VAL:HG23	1.92	0.69
2:AB:135:LEU:HA	2:AB:138:MET:HE3	1.74	0.69
13:AO:86:ARG:HD2	13:AO:86:ARG:C	2.18	0.69
13:BO:178:ARG:CG	13:BO:178:ARG:NH1	2.53	0.68
15:BU:38:GLU:HG2	15:BU:39:LEU:N	2.08	0.68
15:BU:54:LYS:HB2	15:BU:113:THR:HG23	1.75	0.68
5:AE:15:THR:HG23	9:AJ:8:ILE:O	1.92	0.68
7:AH:6:TRP:CE2	7:AH:10:ILE:HD11	2.27	0.68
20:AZ:30:PRO:HG3	20:AZ:33:TRP:HZ3	1.58	0.68
1:BA:129:ARG:NH2	4:BD:256:ILE:HD12	2.02	0.68
1:AA:40:THR:HG21	1:AA:121:LEU:HD23	1.73	0.68
2:AB:4:PRO:HD2	2:AB:7:ARG:HD2	1.74	0.68
4:AD:192:THR:HG23	22:AD:402:CLA:HBC2	1.74	0.68
22:AC:511:CLA:H43	17:Ay:46:LEU:HD22	1.75	0.68
20:AZ:32:ASP:HB3	20:AZ:35:ARG:NH1	2.08	0.68
2:BB:284:ILE:HG12	2:BB:309:LEU:CD1	2.23	0.68
10:AK:19:ASP:N	10:AK:20:PRO:HD2	2.09	0.68
3:BC:166:ILE:O	3:BC:170:ILE:HG13	1.93	0.68
1:AA:238:LYS:HD2	14:AT:32:LYS:HB3	1.76	0.68
1:AA:332:HIS:CD2	1:AA:333:GLU:HG3	2.27	0.68
2:BB:135:LEU:HB2	2:BB:136:PRO:HD3	1.75	0.68
13:BO:86:ARG:C	13:BO:86:ARG:HD2	2.19	0.68
22:AA:404:CLA:HAB	22:AD:402:CLA:H72	1.76	0.68
20:AZ:28:ALA:O	20:AZ:30:PRO:HD3	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BB:4:PRO:HD2	2:BB:7:ARG:HD2	1.74	0.68
2:BB:315:ILE:HG22	2:BB:426:PHE:HB3	1.76	0.68
4:BD:122:LEU:HD11	23:BD:403:PHO:H92	1.76	0.68
12:BM:31:SER:HB3	30:BM:102:LMG:HC71	1.76	0.68
2:AB:284:ILE:HG12	2:AB:309:LEU:CD1	2.23	0.68
4:AD:279:LEU:HG	23:AD:403:PHO:HBC3	1.76	0.68
22:BA:405:CLA:HAB	22:BD:402:CLA:H72	1.76	0.68
2:BB:135:LEU:HD23	2:BB:138:MET:CE	2.24	0.68
3:BC:141:GLU:H	3:BC:141:GLU:CD	2.02	0.68
3:BC:305:THR:HG22	3:BC:308:GLU:CB	2.24	0.67
4:BD:250:ASN:HD22	4:BD:262:SER:HB3	1.58	0.67
4:AD:180:ARG:HH11	4:AD:180:ARG:CG	2.08	0.67
2:BB:331:ASN:HB3	2:BB:437:LEU:HD12	1.75	0.67
4:BD:180:ARG:CG	4:BD:180:ARG:HH11	2.07	0.67
20:BZ:33:TRP:O	20:BZ:37:LYS:HB2	1.93	0.67
1:AA:192:ILE:CA	1:AA:293:MET:HE1	2.23	0.67
2:AB:264:PRO:HG2	2:AB:267:LEU:HD12	1.75	0.67
2:AB:483:ASP:OD2	2:AB:484:PRO:HD2	1.94	0.67
3:AC:42:LEU:HD21	22:AC:511:CLA:H2A	1.74	0.67
20:AZ:33:TRP:CD1	20:AZ:33:TRP:O	2.48	0.67
3:BC:361:PHE:HA	27:BC:516:DGD:HE61	1.77	0.67
2:AB:135:LEU:HD23	2:AB:138:MET:CE	2.25	0.67
6:BF:11:VAL:HG12	6:BF:12:SER:N	2.09	0.67
7:BH:6:TRP:CE2	7:BH:10:ILE:HD11	2.29	0.67
10:BK:19:ASP:N	10:BK:20:PRO:HD2	2.10	0.67
2:AB:270:PRO:HG3	2:AB:312:TYR:HD2	1.59	0.67
24:BA:408:PL9:H33	4:BD:38:PHE:CD1	2.29	0.67
5:BE:27:ILE:HB	5:BE:28:PRO:HD3	1.77	0.67
3:AC:166:ILE:O	3:AC:170:ILE:HG13	1.94	0.67
3:AC:472:LEU:HD12	3:AC:473:ASP:H	1.59	0.67
3:BC:215:LYS:HB3	3:BC:223:TRP:HA	1.77	0.67
3:BC:391:ARG:HB2	3:BC:391:ARG:HH11	1.59	0.67
6:AF:11:VAL:HG12	6:AF:12:SER:H	1.59	0.67
12:AM:31:SER:HB3	30:AM:101:LMG:HC71	1.77	0.67
1:BA:192:ILE:CA	1:BA:293:MET:HE1	2.24	0.67
3:BC:75:PHE:HD1	3:BC:86:LEU:HD21	1.60	0.67
3:BC:415:ASN:O	3:BC:416:SER:HB3	1.94	0.67
2:AB:133:LEU:HB3	2:AB:138:MET:CE	2.24	0.67
2:AB:271:THR:CG2	2:AB:273:TYR:H	2.08	0.67
22:AB:602:CLA:H42	7:AH:45:ILE:HD11	1.76	0.67
3:AC:215:LYS:HB3	3:AC:223:TRP:HA	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:377:LEU:O	3:AC:381:LYS:HB2	1.95	0.67
1:BA:174:LEU:HD22	23:BA:406:PHO:H151	1.75	0.67
2:BB:356:VAL:HG22	2:BB:370:LEU:HD21	1.77	0.67
3:BC:155:ASN:HD21	3:BC:255:THR:CB	2.07	0.67
4:BD:186:GLN:HB2	22:BD:402:CLA:HBC1	1.77	0.67
5:AE:78:THR:O	5:AE:81:GLU:HB2	1.94	0.67
1:BA:32:TRP:HA	1:BA:32:TRP:CE3	2.30	0.67
1:AA:161:TYR:HB3	1:AA:162:PRO:HD3	1.77	0.66
3:AC:44:ASN:C	3:AC:45:LEU:HD12	2.20	0.66
3:AC:75:PHE:HD1	3:AC:86:LEU:HD21	1.59	0.66
4:AD:267:LEU:HD23	4:AD:267:LEU:C	2.20	0.66
2:BB:483:ASP:OD2	2:BB:484:PRO:HD2	1.95	0.66
3:BC:161:LEU:HG	3:BC:165:LEU:HD12	1.77	0.66
3:BC:377:LEU:O	3:BC:381:LYS:HB2	1.94	0.66
3:BC:449:ARG:HE	22:BC:505:CLA:CED	2.07	0.66
5:BE:81:GLU:O	5:BE:83:LEU:N	2.27	0.66
13:BO:92:VAL:HG12	13:BO:93:PRO:HD2	1.78	0.66
2:BB:284:ILE:HG23	2:BB:305:ILE:HD12	1.76	0.66
6:BF:11:VAL:HG12	6:BF:12:SER:H	1.59	0.66
3:AC:150:ASP:HB3	3:AC:153:ASP:HB2	1.77	0.66
22:AC:507:CLA:H112	26:AC:515:BCR:H362	1.78	0.66
12:AM:23:ILE:HD13	30:AM:101:LMG:H182	1.78	0.66
3:BC:42:LEU:HD21	22:BC:511:CLA:H2A	1.77	0.66
2:AB:141:ILE:CG2	22:AB:615:CLA:HBB1	2.26	0.66
22:AC:505:CLA:HBD	22:AC:505:CLA:HBA1	1.77	0.66
6:AF:11:VAL:HG12	6:AF:12:SER:N	2.09	0.66
15:AU:83:ALA:CB	15:AU:84:PRO:HD2	2.14	0.66
1:BA:238:LYS:HD2	14:BT:32:LYS:HB3	1.76	0.66
5:BE:15:THR:HG23	9:BJ:8:ILE:O	1.95	0.66
5:BE:18:ARG:O	5:BE:22:ILE:HG13	1.95	0.66
3:AC:305:THR:HG22	3:AC:308:GLU:CB	2.26	0.66
1:BA:40:THR:HG21	1:BA:121:LEU:HD23	1.77	0.66
3:BC:30:SER:HB2	10:BK:46:ARG:O	1.95	0.66
3:BC:114:VAL:HG22	30:BC:520:LMG:H152	1.77	0.66
11:BL:7:ARG:HD2	11:BL:7:ARG:O	1.96	0.66
1:BA:343:LEU:O	1:BA:344:ALA:HB2	1.96	0.66
3:BC:89:ILE:N	3:BC:90:PRO:HD2	2.11	0.66
22:BC:511:CLA:H43	17:By:46:LEU:HD22	1.76	0.66
20:BZ:30:PRO:HG3	20:BZ:33:TRP:HZ3	1.60	0.66
2:BB:133:LEU:HB3	2:BB:138:MET:CE	2.26	0.66
4:BD:279:LEU:HG	23:BD:403:PHO:HBC3	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:356:VAL:HG22	2:AB:370:LEU:CD2	2.26	0.66
1:BA:77:ILE:HD11	14:BT:6:TYR:HB3	1.78	0.66
13:BO:120:THR:HG22	13:BO:154:SER:OG	1.96	0.66
4:AD:209:LEU:HD23	4:AD:209:LEU:C	2.21	0.65
2:BB:490:GLN:OE1	2:BB:490:GLN:O	2.15	0.65
22:BC:505:CLA:HBA1	22:BC:505:CLA:HBD	1.78	0.65
1:AA:81:ALA:HB2	1:AA:175:GLY:HA3	1.78	0.65
24:AA:407:PL9:H33	4:AD:38:PHE:CD1	2.31	0.65
2:AB:224:ARG:HG2	7:AH:24:GLY:O	1.96	0.65
4:AD:250:ASN:HD22	4:AD:262:SER:HB3	1.62	0.65
20:AZ:33:TRP:O	20:AZ:37:LYS:HB2	1.95	0.65
2:BB:327:THR:HG22	22:BB:610:CLA:H12	1.78	0.65
4:BD:267:LEU:HD23	4:BD:267:LEU:C	2.21	0.65
5:BE:78:THR:O	5:BE:81:GLU:HB2	1.96	0.65
3:AC:89:ILE:N	3:AC:90:PRO:HD2	2.11	0.65
3:AC:161:LEU:HG	3:AC:165:LEU:HD12	1.78	0.65
1:AA:32:TRP:HA	1:AA:32:TRP:CE3	2.31	0.65
2:AB:331:ASN:HB3	2:AB:437:LEU:HD12	1.79	0.65
3:AC:55:ALA:HB1	26:AC:514:BCR:H373	1.78	0.65
13:AO:144:LEU:HD13	13:AO:259:VAL:HG11	1.78	0.65
2:BB:247:PHE:HE1	22:BB:605:CLA:H101	1.61	0.65
20:BZ:33:TRP:O	20:BZ:33:TRP:CD1	2.50	0.65
2:BB:86:ILE:HD12	2:BB:86:ILE:O	1.96	0.65
2:BB:270:PRO:HG3	2:BB:312:TYR:HD2	1.61	0.65
2:BB:386:ALA:HB3	15:BU:132:LEU:HD11	1.79	0.65
3:AC:30:SER:HB2	10:AK:46:ARG:O	1.95	0.65
3:AC:155:ASN:HD21	3:AC:255:THR:CB	2.07	0.65
13:AO:92:VAL:HG12	13:AO:93:PRO:HD2	1.78	0.65
2:BB:356:VAL:HG22	2:BB:370:LEU:CD2	2.27	0.65
4:BD:103:ARG:HG3	5:BE:73:LYS:HG3	1.78	0.65
7:BH:12:ARG:HD3	7:BH:12:ARG:C	2.22	0.65
9:BJ:11:TRP:CZ3	17:By:36:ILE:HD11	2.32	0.65
20:BZ:49:ALA:O	20:BZ:53:VAL:HG23	1.96	0.65
2:AB:222:PRO:HG3	7:AH:27:THR:H	1.61	0.65
9:AJ:14:ALA:CB	26:AK:102:BCR:H393	2.27	0.65
22:BC:507:CLA:H112	26:BC:515:BCR:H362	1.78	0.65
13:BO:87:GLN:O	13:BO:88:GLU:HB3	1.96	0.65
2:AB:271:THR:HB	2:AB:274:GLN:HG3	1.78	0.65
22:BC:512:CLA:H143	22:BC:513:CLA:H162	1.79	0.65
20:BZ:28:ALA:O	20:BZ:30:PRO:HD3	1.97	0.65
2:AB:248:ALA:HA	22:AB:603:CLA:H42	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:490:GLN:OE1	2:AB:490:GLN:O	2.15	0.65
11:AL:7:ARG:O	11:AL:7:ARG:HD2	1.97	0.65
13:AO:120:THR:HG22	13:AO:154:SER:OG	1.96	0.65
3:BC:187:ASP:HB2	3:BC:230:LEU:HD12	1.78	0.65
1:AA:193:LEU:HD11	22:AA:402:CLA:HMC2	1.79	0.64
1:AA:328:MET:HE1	4:AD:183:LEU:HD22	1.79	0.64
2:AB:247:PHE:HE1	22:AB:602:CLA:H101	1.62	0.64
2:AB:86:ILE:O	2:AB:86:ILE:HD12	1.97	0.64
3:AC:186:TYR:HE2	3:AC:188:THR:HG22	1.62	0.64
3:BC:55:ALA:HB1	26:BC:514:BCR:H373	1.77	0.64
22:BC:511:CLA:H151	20:BZ:20:VAL:HG13	1.78	0.64
27:BC:518:DGD:HD2	9:BJ:32:ALA:O	1.97	0.64
14:BT:29:ILE:HD12	14:BT:29:ILE:N	2.10	0.64
2:AB:139:PHE:CZ	2:AB:143:LEU:HD22	2.32	0.64
4:AD:88:SER:HB2	5:AE:69:ARG:NH2	2.11	0.64
2:BB:271:THR:CG2	2:BB:273:TYR:H	2.08	0.64
4:BD:87:HIS:HD2	4:BD:162:LEU:HD23	1.62	0.64
4:BD:209:LEU:C	4:BD:209:LEU:HD23	2.23	0.64
3:AC:449:ARG:HE	22:AC:505:CLA:CED	2.08	0.64
15:BU:94:ILE:O	15:BU:97:LEU:HG	1.98	0.64
3:BC:156:LYS:O	3:BC:160:ILE:HG13	1.97	0.64
3:BC:318:LEU:HD23	3:BC:318:LEU:C	2.23	0.64
3:BC:472:LEU:HD12	3:BC:473:ASP:H	1.62	0.64
2:AB:135:LEU:HB2	2:AB:136:PRO:HD3	1.79	0.64
2:AB:327:THR:HG22	22:AB:607:CLA:H12	1.78	0.64
2:BB:271:THR:HB	2:BB:274:GLN:HG3	1.80	0.64
1:AA:174:LEU:HD22	23:AA:405:PHO:H151	1.78	0.64
22:AC:511:CLA:H151	20:AZ:20:VAL:HG13	1.78	0.64
9:AJ:11:TRP:CZ3	17:Ay:36:ILE:HD11	2.32	0.64
4:BD:129:GLN:HE22	4:BD:143:ALA:HA	1.61	0.64
5:BE:26:THR:O	5:BE:29:ALA:HB3	1.97	0.64
15:BU:58:ASN:ND2	15:BU:114:VAL:HG13	2.13	0.64
22:BC:511:CLA:H171	20:BZ:20:VAL:HA	1.80	0.64
11:AL:7:ARG:C	11:AL:8:GLN:HE21	2.06	0.64
15:AU:66:ILE:O	15:AU:66:ILE:HG22	1.98	0.64
22:BC:505:CLA:CMD	22:BC:507:CLA:HAB	2.28	0.64
15:BU:66:ILE:O	15:BU:66:ILE:HG22	1.97	0.64
1:AA:57:PRO:HG3	1:AA:68:SER:CB	2.28	0.64
2:AB:286:ARG:HG2	2:AB:286:ARG:HH11	1.62	0.64
2:AB:379:ALA:HA	2:AB:390:TYR:HB3	1.80	0.64
13:AO:36:ILE:HG23	13:AO:41:LEU:HB3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AO:117:GLY:O	13:AO:159:VAL:HG12	1.98	0.64
2:AB:284:ILE:HG23	2:AB:305:ILE:HD12	1.80	0.63
16:AV:143:GLY:O	16:AV:147:VAL:HG23	1.97	0.63
2:BB:379:ALA:HA	2:BB:390:TYR:HB3	1.79	0.63
3:BC:204:LEU:HD21	3:BC:238:ILE:HG21	1.79	0.63
12:BM:23:ILE:HD13	30:BM:102:LMG:H182	1.79	0.63
3:AC:209:ILE:HG23	26:AC:515:BCR:H382	1.81	0.63
3:AC:310:SER:OG	3:AC:355:THR:HG23	1.98	0.63
13:BO:144:LEU:HD13	13:BO:259:VAL:HG11	1.80	0.63
2:AB:386:ALA:HB3	15:AU:132:LEU:HD11	1.80	0.63
2:BB:141:ILE:CG2	22:BB:618:CLA:HBB1	2.27	0.63
11:BL:7:ARG:C	11:BL:8:GLN:HE21	2.04	0.63
17:By:42:ARG:HH11	17:By:42:ARG:HG2	1.63	0.63
3:AC:318:LEU:HD23	3:AC:318:LEU:C	2.24	0.63
5:AE:36:LEU:O	5:AE:40:THR:HG23	1.98	0.63
2:BB:139:PHE:CZ	2:BB:143:LEU:HD22	2.32	0.63
2:AB:486:LEU:O	2:AB:486:LEU:HD13	1.98	0.63
22:AB:602:CLA:H61	7:AH:46:LEU:HD13	1.80	0.63
3:AC:141:GLU:CD	3:AC:141:GLU:H	2.05	0.63
4:AD:186:GLN:HB2	22:AD:402:CLA:HBC1	1.80	0.63
3:BC:150:ASP:HB3	3:BC:153:ASP:HB2	1.78	0.63
3:BC:223:TRP:CD2	3:BC:224:ILE:HG13	2.34	0.63
29:AA:412:SQD:H311	22:AC:508:CLA:H71	1.81	0.63
27:AC:518:DGD:HD2	9:AJ:32:ALA:O	1.99	0.63
9:BJ:14:ALA:CB	26:BK:102:BCR:H393	2.28	0.63
2:AB:297:THR:OG1	2:AB:300:GLU:HG3	1.98	0.63
3:AC:107:ASP:OD2	3:AC:110:PRO:HD3	1.99	0.63
22:AC:511:CLA:H171	20:AZ:20:VAL:HA	1.79	0.63
1:BA:81:ALA:HB2	1:BA:175:GLY:HA3	1.80	0.63
10:BK:18:PHE:HD2	10:BK:18:PHE:N	1.96	0.63
13:BO:36:ILE:HG23	13:BO:41:LEU:HB3	1.79	0.63
7:AH:12:ARG:HD3	7:AH:12:ARG:C	2.24	0.63
10:AK:18:PHE:N	10:AK:18:PHE:HD2	1.97	0.63
11:AL:1:MET:HA	11:AL:1:MET:HE2	1.79	0.63
17:Ay:41:VAL:C	17:Ay:43:ARG:H	2.06	0.63
4:BD:246:MET:HE3	4:BD:262:SER:HA	1.80	0.63
5:BE:36:LEU:O	5:BE:40:THR:HG23	1.99	0.63
5:BE:79:PHE:O	5:BE:84:LYS:HB3	1.99	0.63
13:AO:230:VAL:CG1	13:AO:231:ASP:H	2.10	0.62
5:AE:27:ILE:HB	5:AE:28:PRO:HD3	1.80	0.62
7:BH:19:GLY:O	7:BH:21:VAL:HG13	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:337:LEU:HD12	13:AO:131:PRO:HG3	1.81	0.62
5:AE:26:THR:O	5:AE:29:ALA:HB3	1.98	0.62
7:AH:19:GLY:O	7:AH:21:VAL:HG13	1.99	0.62
1:BA:57:PRO:HG3	1:BA:68:SER:CB	2.29	0.62
1:AA:29:TYR:CG	1:AA:133:LEU:HD13	2.34	0.62
10:AK:24:VAL:HG21	17:Ay:25:ILE:HG12	1.81	0.62
1:BA:89:ILE:HD11	1:BA:108:ASN:HB3	1.81	0.62
2:BB:124:ARG:NE	2:BB:131:PRO:HD3	2.14	0.62
20:BZ:32:ASP:HB3	20:BZ:35:ARG:NH1	2.13	0.62
26:BC:514:BCR:H312	20:BZ:9:LEU:HD11	1.80	0.62
26:BK:102:BCR:HC8	26:BK:102:BCR:H331	1.82	0.62
11:BL:1:MET:HE2	11:BL:1:MET:HA	1.81	0.62
3:AC:305:THR:HG22	3:AC:308:GLU:HB2	1.82	0.62
22:AC:505:CLA:CMD	22:AC:507:CLA:HAB	2.29	0.62
2:BB:224:ARG:HG2	7:BH:24:GLY:O	1.99	0.62
1:AA:142:TRP:HB2	4:AD:220:ASN:OD1	1.99	0.62
2:AB:356:VAL:HG22	2:AB:370:LEU:HD21	1.81	0.62
4:AD:160:TYR:HB3	4:AD:161:PRO:CD	2.30	0.62
14:AT:29:ILE:HD12	14:AT:29:ILE:N	2.10	0.62
3:BC:186:TYR:HE2	3:BC:188:THR:HG22	1.65	0.62
2:AB:124:ARG:NE	2:AB:131:PRO:HD3	2.13	0.62
30:AD:408:LMG:HC62	11:AL:15:THR:HG21	1.82	0.62
5:AE:64:PRO:HB3	5:AE:84:LYS:HE2	1.82	0.62
12:AM:28:GLN:HB3	12:BM:27:VAL:HG12	1.81	0.62
18:AX:11:THR:HG23	18:AX:12:ILE:HG22	1.81	0.62
1:BA:29:TYR:CG	1:BA:133:LEU:HD13	2.34	0.62
22:BB:605:CLA:H42	7:BH:45:ILE:HD11	1.82	0.62
3:BC:44:ASN:C	3:BC:45:LEU:HD12	2.25	0.62
3:BC:310:SER:OG	3:BC:355:THR:HG23	2.00	0.62
6:BF:28:VAL:HB	6:BF:29:PRO:HD3	1.81	0.62
2:BB:222:PRO:HG3	7:BH:27:THR:H	1.63	0.62
17:By:41:VAL:C	17:By:43:ARG:H	2.06	0.62
4:AD:26:ARG:CD	6:AF:18:VAL:HG11	2.27	0.62
26:AC:514:BCR:H312	20:AZ:9:LEU:HD11	1.80	0.61
7:AH:58:VAL:HG13	7:AH:58:VAL:O	2.00	0.61
15:AU:58:ASN:ND2	15:AU:114:VAL:HG13	2.15	0.61
15:AU:94:ILE:O	15:AU:97:LEU:HG	2.00	0.61
5:BE:64:PRO:HB3	5:BE:84:LYS:HE2	1.82	0.61
1:AA:18:CYS:O	1:AA:22:THR:HG22	2.00	0.61
1:AA:93:PHE:HZ	22:AA:406:CLA:HAA1	1.64	0.61
1:BA:93:PHE:HZ	22:BA:407:CLA:HAA1	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:328:MET:HE1	4:BD:183:LEU:HD22	1.82	0.61
10:BK:24:VAL:HG21	17:By:25:ILE:HG12	1.82	0.61
1:AA:228:THR:HG22	1:AA:229:GLU:H	1.65	0.61
5:AE:7:GLU:H	5:AE:7:GLU:CD	2.07	0.61
12:AM:27:VAL:HG12	12:BM:28:GLN:HB3	1.80	0.61
15:AU:54:LYS:HB2	15:AU:113:THR:HG23	1.82	0.61
1:BA:142:TRP:HB2	4:BD:220:ASN:OD1	2.01	0.61
3:BC:209:ILE:HG23	26:BC:515:BCR:H382	1.81	0.61
2:AB:192:PRO:HD2	7:AH:60:VAL:HG12	1.82	0.61
2:AB:371:THR:HG22	2:AB:377:VAL:HA	1.81	0.61
15:AU:89:GLU:H	15:AU:89:GLU:CD	2.09	0.61
1:BA:161:TYR:HB3	1:BA:162:PRO:HD3	1.82	0.61
1:BA:228:THR:HG22	1:BA:229:GLU:H	1.66	0.61
1:BA:257:ARG:HG3	1:BA:257:ARG:HH11	1.65	0.61
3:AC:44:ASN:O	3:AC:45:LEU:HD12	1.99	0.61
22:AC:512:CLA:H143	22:AC:513:CLA:H162	1.82	0.61
3:BC:107:ASP:OD2	3:BC:110:PRO:HD3	1.99	0.61
1:AA:89:ILE:HD11	1:AA:108:ASN:HB3	1.81	0.61
1:AA:343:LEU:O	1:AA:344:ALA:HB2	2.00	0.61
3:AC:248:GLY:O	3:AC:252:ILE:HG12	2.00	0.61
3:BC:83:GLU:CD	16:BV:129:LYS:HZ1	2.08	0.61
16:BV:143:GLY:O	16:BV:147:VAL:HG23	2.00	0.61
20:BZ:55:GLY:HA2	26:BZ:101:BCR:H312	1.83	0.61
1:AA:77:ILE:HD11	14:AT:6:TYR:HB3	1.82	0.61
2:BB:371:THR:HG22	2:BB:377:VAL:HA	1.82	0.61
2:BB:471:ALA:HB2	4:BD:130:PHE:CZ	2.36	0.61
3:BC:318:LEU:HG	3:BC:328:VAL:HG11	1.83	0.61
4:BD:55:VAL:HG21	4:BD:110:LEU:HD12	1.81	0.61
16:BV:81:ARG:CZ	16:BV:157:GLY:HA3	2.30	0.61
3:AC:180:MET:HE3	3:AC:202:PRO:HD3	1.82	0.61
4:AD:246:MET:HE3	4:AD:262:SER:HA	1.82	0.61
15:AU:97:LEU:O	15:AU:102:LYS:HE2	2.01	0.61
10:BK:17:ILE:N	10:BK:17:ILE:HD12	2.16	0.61
2:AB:264:PRO:CG	2:AB:267:LEU:HD12	2.31	0.61
3:AC:374:GLY:O	3:AC:375:LEU:C	2.44	0.61
4:AD:342:PRO:O	4:AD:345:VAL:HG12	2.01	0.61
6:AF:28:VAL:HB	6:AF:29:PRO:HD3	1.83	0.61
16:AV:90:PRO:O	16:AV:92:ARG:HD3	2.01	0.61
2:BB:172:TYR:O	2:BB:174:LEU:HG	2.00	0.61
3:BC:337:LEU:HD12	13:BO:131:PRO:HG3	1.83	0.61
17:By:19:ILE:HG23	17:By:20:ALA:H	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:BD:408:LMG:HC62	11:BL:15:THR:HG21	1.82	0.61
5:BE:18:ARG:HB3	5:BE:18:ARG:NH1	2.14	0.61
5:AE:18:ARG:O	5:AE:22:ILE:HG13	2.00	0.60
2:BB:486:LEU:O	2:BB:486:LEU:HD13	2.01	0.60
1:BA:202:VAL:HG11	22:BA:405:CLA:OBD	1.99	0.60
2:BB:68:ARG:HH11	2:BB:262:THR:HG23	1.67	0.60
3:BC:112:PHE:O	3:BC:116:VAL:HG13	2.01	0.60
3:BC:374:GLY:O	3:BC:375:LEU:C	2.44	0.60
10:BK:18:PHE:N	10:BK:18:PHE:CD2	2.68	0.60
1:AA:60:ILE:HD12	1:AA:84:PRO:HD2	1.83	0.60
4:AD:103:ARG:HG3	5:AE:73:LYS:HG3	1.83	0.60
10:AK:17:ILE:HD12	10:AK:17:ILE:N	2.17	0.60
13:AO:39:THR:OG1	13:AO:41:LEU:HB2	2.01	0.60
13:AO:234:THR:OG1	13:AO:236:GLU:HG2	2.00	0.60
29:BA:413:SQD:H311	22:BC:508:CLA:H71	1.83	0.60
18:BX:11:THR:HG23	18:BX:12:ILE:HG22	1.82	0.60
3:AC:143:TYR:O	3:AC:144:SER:HB2	2.00	0.60
3:AC:391:ARG:HD2	3:AC:395:TYR:CE2	2.36	0.60
3:AC:461:ARG:HG3	3:AC:461:ARG:HH11	1.65	0.60
4:BD:250:ASN:ND2	4:BD:262:SER:HB3	2.17	0.60
5:BE:4:THR:HG22	5:BE:5:THR:N	2.16	0.60
2:AB:471:ALA:HB2	4:AD:130:PHE:CZ	2.36	0.60
4:AD:199:MET:HB3	24:AD:405:PL9:H28	1.84	0.60
5:AE:23:HIS:HA	5:AE:26:THR:OG1	2.00	0.60
4:AD:49:LEU:O	4:AD:53:THR:HG23	2.01	0.60
26:AK:102:BCR:HC8	26:AK:102:BCR:H331	1.83	0.60
20:AZ:32:ASP:CB	20:AZ:35:ARG:HG2	2.30	0.60
1:BA:29:TYR:CD2	1:BA:133:LEU:HD13	2.37	0.60
2:BB:222:PRO:HG3	7:BH:26:GLY:HA3	1.83	0.60
3:BC:305:THR:HG22	3:BC:308:GLU:HB2	1.83	0.60
2:AB:213:GLY:O	2:AB:217:ILE:HG13	2.02	0.60
12:AM:20:VAL:HG22	12:BM:20:VAL:HG11	1.84	0.60
3:BC:143:TYR:O	3:BC:144:SER:HB2	2.01	0.60
2:AB:41:GLU:OE1	2:AB:63:LEU:HB2	2.02	0.60
2:AB:315:ILE:HG22	2:AB:426:PHE:HB3	1.82	0.60
3:AC:186:TYR:CE2	3:AC:188:THR:HG22	2.37	0.60
3:AC:318:LEU:HG	3:AC:328:VAL:HG11	1.82	0.60
13:AO:31:LEU:HD12	13:AO:31:LEU:N	2.17	0.60
1:BA:306:VAL:HG13	1:BA:314:ILE:O	2.01	0.60
20:AZ:33:TRP:O	20:AZ:33:TRP:HD1	1.84	0.60
22:BB:609:CLA:HMD3	32:BB:625:LMT:H1'	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BD:239:GLN:O	4:BD:240:ALA:HB3	2.02	0.60
13:BO:39:THR:OG1	13:BO:41:LEU:HB2	2.02	0.60
13:BO:117:GLY:O	13:BO:159:VAL:HG12	2.01	0.60
1:AA:153:SER:CB	22:AA:402:CLA:H11	2.32	0.60
1:AA:202:VAL:HG11	22:AA:404:CLA:OBD	2.02	0.60
3:AC:114:VAL:HG22	30:AC:520:LMG:H152	1.83	0.60
4:AD:56:THR:HG21	5:AE:50:PRO:HD3	1.84	0.60
5:AE:4:THR:HG22	5:AE:5:THR:N	2.17	0.60
16:BV:90:PRO:O	16:BV:92:ARG:HD3	2.02	0.60
1:AA:306:VAL:HG13	1:AA:314:ILE:O	2.01	0.59
3:AC:223:TRP:CD2	3:AC:224:ILE:HG13	2.37	0.59
2:BB:213:GLY:O	2:BB:217:ILE:HG13	2.02	0.59
5:AE:79:PHE:O	5:AE:84:LYS:HB3	2.01	0.59
12:AM:20:VAL:HG11	12:BM:20:VAL:HG22	1.83	0.59
17:Ay:19:ILE:HG23	17:Ay:20:ALA:H	1.68	0.59
22:AB:606:CLA:HMD3	32:AB:624:LMT:H1'	1.84	0.59
5:AE:18:ARG:HB3	5:AE:18:ARG:NH1	2.17	0.59
15:BU:97:LEU:O	15:BU:102:LYS:HE2	2.02	0.59
17:Ay:42:ARG:HG2	17:Ay:42:ARG:HH11	1.66	0.59
3:BC:155:ASN:O	3:BC:158:THR:HG22	2.03	0.59
3:BC:461:ARG:HH11	3:BC:461:ARG:HG3	1.68	0.59
5:BE:26:THR:HB	34:BE:101:HEM:CBB	2.32	0.59
17:By:39:LEU:CB	17:By:46:LEU:HD21	2.32	0.59
10:AK:18:PHE:N	10:AK:18:PHE:CD2	2.69	0.59
10:AK:21:LEU:HD11	26:AK:102:BCR:HC32	1.84	0.59
10:AK:40:GLN:HA	10:AK:43:VAL:HG12	1.83	0.59
26:AT:102:BCR:H393	22:BB:610:CLA:HAC2	1.83	0.59
1:BA:13:LEU:H	1:BA:13:LEU:HD12	1.68	0.59
4:BD:87:HIS:CD2	4:BD:162:LEU:HD23	2.38	0.59
15:BU:113:THR:O	15:BU:114:VAL:HG23	2.02	0.59
1:AA:257:ARG:HH11	1:AA:257:ARG:HG3	1.66	0.59
2:AB:222:PRO:HG3	7:AH:26:GLY:HA3	1.83	0.59
1:BA:153:SER:CB	22:BA:403:CLA:H11	2.33	0.59
16:BV:125:ASP:HA	16:BV:131:ARG:HH21	1.68	0.59
1:BA:272:HIS:CD2	4:BD:218:VAL:HG21	2.38	0.59
5:BE:76:VAL:O	5:BE:80:LEU:HD22	2.03	0.59
2:AB:68:ARG:HH11	2:AB:262:THR:HG23	1.68	0.59
3:AC:124:VAL:HB	26:AZ:101:BCR:H362	1.84	0.59
3:BC:343:ARG:NH1	3:BC:347:GLY:O	2.35	0.59
13:AO:86:ARG:C	13:AO:86:ARG:HH11	2.11	0.59
15:AU:113:THR:O	15:AU:114:VAL:HG23	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BB:605:CLA:H61	7:BH:46:LEU:HD13	1.84	0.59
15:BU:83:ALA:CB	15:BU:84:PRO:CD	2.78	0.59
5:AE:26:THR:HB	34:AE:101:HEM:CBB	2.33	0.59
5:AE:76:VAL:O	5:AE:80:LEU:HD22	2.03	0.59
2:BB:264:PRO:CG	2:BB:267:LEU:HD12	2.32	0.59
3:BC:124:VAL:HB	26:BZ:101:BCR:H362	1.84	0.59
4:BD:274:VAL:HA	24:BD:405:PL9:H253	1.85	0.59
13:BO:123:GLU:HG2	13:BO:124:GLU:N	2.17	0.59
20:BZ:32:ASP:CB	20:BZ:35:ARG:HG2	2.32	0.59
2:AB:133:LEU:HB3	2:AB:138:MET:HE2	1.85	0.58
4:AD:55:VAL:HG21	4:AD:110:LEU:CD1	2.33	0.58
2:BB:192:PRO:HD2	7:BH:60:VAL:HG12	1.85	0.58
4:BD:18:LEU:HD22	18:BX:38:ILE:CD1	2.32	0.58
17:By:19:ILE:HG23	17:By:20:ALA:N	2.18	0.58
17:By:33:PRO:O	17:By:36:ILE:HG13	2.02	0.58
20:BZ:33:TRP:O	20:BZ:33:TRP:HD1	1.86	0.58
20:BZ:36:SER:OG	20:BZ:39:LEU:HD12	2.03	0.58
3:BC:248:GLY:O	3:BC:252:ILE:HG12	2.02	0.58
1:AA:13:LEU:H	1:AA:13:LEU:HD12	1.69	0.58
3:AC:204:LEU:HD21	3:AC:238:ILE:HG21	1.84	0.58
3:AC:305:THR:HG23	3:AC:307:PRO:CD	2.32	0.58
13:AO:123:GLU:HG2	13:AO:124:GLU:N	2.18	0.58
22:BB:611:CLA:HMD1	22:BB:613:CLA:HAB	1.84	0.58
10:BK:40:GLN:HA	10:BK:43:VAL:HG12	1.85	0.58
2:AB:55:MET:HE2	2:AB:80:ILE:HD12	1.85	0.58
3:AC:112:PHE:O	3:AC:116:VAL:HG13	2.03	0.58
16:BV:135:GLU:O	16:BV:139:VAL:HG23	2.03	0.58
2:AB:188:ASP:OD1	7:AH:58:VAL:HA	2.03	0.58
22:AB:607:CLA:HAC2	26:AB:618:BCR:H393	1.84	0.58
6:AF:19:ARG:O	6:AF:23:VAL:HG23	2.03	0.58
15:AU:38:GLU:HG2	15:AU:39:LEU:H	1.68	0.58
20:AZ:32:ASP:CG	20:AZ:33:TRP:N	2.60	0.58
1:BA:82:VAL:HB	1:BA:174:LEU:HB2	1.85	0.58
1:BA:143:ILE:HD11	4:BD:217:THR:HA	1.86	0.58
1:BA:249:VAL:HG11	2:BB:486:LEU:HD23	1.86	0.58
2:BB:112:CYS:HB3	26:BB:622:BCR:H393	1.85	0.58
32:BB:626:LMT:H102	7:BH:35:MET:SD	2.43	0.58
3:BC:165:LEU:HD21	22:BC:506:CLA:HHC	1.85	0.58
4:BD:342:PRO:O	4:BD:345:VAL:HG12	2.04	0.58
10:BK:18:PHE:CE1	20:BZ:9:LEU:HG	2.39	0.58
3:AC:156:LYS:O	3:AC:160:ILE:HG13	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:369:LEU:HD21	3:AC:384:ILE:HD13	1.85	0.58
3:AC:380:ILE:HA	3:AC:384:ILE:HD11	1.85	0.58
1:BA:49:VAL:O	1:BA:53:ILE:HG13	2.04	0.58
4:BD:18:LEU:O	4:BD:22:LEU:HG	2.02	0.58
7:BH:58:VAL:HG13	7:BH:58:VAL:O	2.02	0.58
4:BD:160:TYR:HB3	4:BD:161:PRO:CD	2.33	0.58
2:AB:329:PRO:HD3	22:AB:607:CLA:HED2	1.86	0.58
3:AC:131:TYR:HE1	3:AC:135:ARG:HD2	1.68	0.58
4:AD:18:LEU:HD22	18:AX:38:ILE:CD1	2.34	0.58
4:AD:239:GLN:O	4:AD:240:ALA:HB3	2.03	0.58
1:BA:60:ILE:HD12	1:BA:84:PRO:HD2	1.86	0.58
2:BB:188:ASP:OD1	7:BH:58:VAL:HA	2.04	0.58
22:BC:505:CLA:H92	22:BC:505:CLA:HAB	1.85	0.58
4:AD:87:HIS:CD2	4:AD:162:LEU:HD23	2.37	0.58
16:AV:74:THR:O	16:AV:75:ASN:HB2	2.04	0.58
20:AZ:16:SER:O	20:AZ:20:VAL:HG23	2.04	0.58
3:BC:44:ASN:O	3:BC:45:LEU:HD12	2.04	0.58
15:BU:57:LEU:HD22	15:BU:79:ILE:HG21	1.86	0.58
1:AA:238:LYS:O	1:AA:241:GLN:HG3	2.03	0.57
2:AB:6:TYR:HA	22:AB:611:CLA:H11	1.85	0.57
3:AC:42:LEU:HD13	22:AC:511:CLA:HMA2	1.86	0.57
3:AC:447:ARG:HG2	3:AC:447:ARG:NH1	2.16	0.57
17:Ay:39:LEU:CB	17:Ay:46:LEU:HD21	2.32	0.57
2:BB:103:LEU:HD21	22:BB:608:CLA:HMC3	1.86	0.57
10:BK:31:LEU:O	10:BK:34:ALA:HB3	2.04	0.57
20:BZ:5:PHE:HA	20:BZ:57:LEU:CD2	2.34	0.57
2:AB:149:LEU:HG	22:AB:603:CLA:CBC	2.29	0.57
2:AB:172:TYR:O	2:AB:174:LEU:HG	2.02	0.57
4:AD:188:PHE:HE2	4:AD:329:MET:CE	2.17	0.57
16:AV:81:ARG:CZ	16:AV:157:GLY:HA3	2.34	0.57
5:BE:7:GLU:CD	5:BE:7:GLU:H	2.12	0.57
13:BO:180:ALA:HB1	13:BO:191:ALA:HB2	1.86	0.57
4:AD:36:LEU:O	4:AD:39:PRO:HD2	2.05	0.57
11:AL:11:GLU:HG2	11:AL:12:LEU:N	2.19	0.57
20:AZ:14:ILE:O	20:AZ:18:VAL:HG23	2.04	0.57
1:BA:140:ARG:HH22	28:BA:412:LHG:P	2.27	0.57
15:BU:89:GLU:CD	15:BU:89:GLU:H	2.11	0.57
3:AC:130:VAL:O	3:AC:134:ILE:HG12	2.04	0.57
10:AK:17:ILE:HD12	10:AK:17:ILE:H	1.69	0.57
18:AX:45:LYS:HD3	18:AX:45:LYS:N	2.20	0.57
6:BF:19:ARG:O	6:BF:23:VAL:HG23	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:BZ:16:SER:O	20:BZ:20:VAL:HG23	2.04	0.57
1:AA:38:ILE:O	1:AA:42:LEU:HG	2.05	0.57
2:AB:25:MET:HE3	26:AB:617:BCR:H23C	1.87	0.57
3:AC:83:GLU:CD	16:AV:129:LYS:HZ1	2.13	0.57
4:AD:18:LEU:O	4:AD:22:LEU:HG	2.05	0.57
4:AD:252:PHE:O	4:AD:256:ILE:HG22	2.05	0.57
10:AK:31:LEU:O	10:AK:34:ALA:HB3	2.04	0.57
13:AO:80:GLU:O	13:AO:89:ALA:HB1	2.05	0.57
15:AU:57:LEU:HD22	15:AU:79:ILE:HG21	1.87	0.57
4:BD:36:LEU:O	4:BD:39:PRO:HD2	2.05	0.57
4:BD:188:PHE:HE2	4:BD:329:MET:CE	2.17	0.57
13:BO:118:SER:HB3	13:BO:157:PRO:HA	1.87	0.57
1:AA:11:ALA:O	1:AA:12:ASN:CB	2.53	0.57
3:AC:37:ALA:HA	22:AC:508:CLA:O1A	2.04	0.57
22:AC:505:CLA:H92	22:AC:505:CLA:HAB	1.87	0.57
20:AZ:30:PRO:C	20:AZ:32:ASP:H	2.12	0.57
3:BC:180:MET:HE3	3:BC:202:PRO:HD3	1.86	0.57
4:BD:346:LEU:O	4:BD:348:ARG:HG3	2.05	0.57
10:AK:26:PRO:O	10:AK:29:PRO:HD2	2.05	0.57
12:AM:29:THR:O	12:AM:32:GLN:HG3	2.05	0.57
2:BB:248:ALA:HA	22:BB:606:CLA:H42	1.86	0.57
2:AB:174:LEU:HD23	2:AB:308:LYS:HG2	1.87	0.57
10:AK:18:PHE:CE1	20:AZ:9:LEU:HG	2.40	0.57
3:BC:130:VAL:O	3:BC:134:ILE:HG12	2.04	0.57
10:BK:26:PRO:O	10:BK:29:PRO:HD2	2.04	0.57
20:BZ:36:SER:HA	20:BZ:39:LEU:CG	2.31	0.57
2:AB:256:MET:HA	2:AB:263:THR:HG21	1.87	0.57
3:AC:343:ARG:NH1	3:AC:347:GLY:O	2.38	0.57
3:BC:37:ALA:HA	22:BC:508:CLA:O1A	2.05	0.57
4:BD:18:LEU:HD22	18:BX:38:ILE:HD13	1.85	0.57
4:BD:56:THR:HG21	5:BE:50:PRO:HD3	1.86	0.57
17:Ay:19:ILE:HG23	17:Ay:20:ALA:N	2.19	0.57
2:BB:41:GLU:OE1	2:BB:63:LEU:HB2	2.04	0.57
18:BX:45:LYS:HD3	18:BX:45:LYS:N	2.19	0.57
2:AB:10:THR:C	2:AB:12:LEU:H	2.12	0.56
2:AB:191:ASN:ND2	7:AH:60:VAL:HA	2.20	0.56
3:AC:165:LEU:HD21	22:AC:506:CLA:HHC	1.85	0.56
4:AD:266:TRP:CD1	30:AD:408:LMG:HC3	2.40	0.56
24:AD:405:PL9:H13	30:AD:408:LMG:H132	1.87	0.56
17:Ay:33:PRO:O	17:Ay:36:ILE:HG13	2.05	0.56
3:BC:186:TYR:CE2	3:BC:188:THR:HG22	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BC:391:ARG:HD2	3:BC:395:TYR:CE2	2.40	0.56
4:BD:157:PHE:CE1	4:BD:171:PRO:HG2	2.40	0.56
4:BD:199:MET:HB3	24:BD:405:PL9:H28	1.86	0.56
13:BO:31:LEU:HD12	13:BO:31:LEU:N	2.19	0.56
13:BO:230:VAL:CG1	13:BO:231:ASP:H	2.12	0.56
15:BU:100:ARG:HH11	15:BU:103:GLN:HG2	1.70	0.56
1:AA:249:VAL:HG11	2:AB:486:LEU:HD23	1.87	0.56
1:AA:272:HIS:CD2	4:AD:218:VAL:HG21	2.40	0.56
2:AB:230:ARG:O	2:AB:233:ASN:HB3	2.05	0.56
2:BB:10:THR:C	2:BB:12:LEU:H	2.11	0.56
2:BB:414:PRO:HB2	2:BB:415:PRO:CD	2.33	0.56
3:BC:305:THR:HG22	3:BC:308:GLU:N	2.16	0.56
6:BF:21:VAL:O	6:BF:25:THR:HG23	2.06	0.56
20:BZ:29:SER:HB2	20:BZ:31:GLN:HG3	1.88	0.56
3:AC:193:GLY:O	3:AC:194:GLY:C	2.49	0.56
16:AV:87:LEU:N	16:AV:87:LEU:HD12	2.20	0.56
2:BB:286:ARG:HG2	2:BB:286:ARG:NH1	2.17	0.56
2:BB:297:THR:OG1	2:BB:300:GLU:HG3	2.04	0.56
3:BC:42:LEU:HD13	22:BC:511:CLA:HMA2	1.86	0.56
22:BC:501:CLA:HMB3	26:BC:515:BCR:H403	1.88	0.56
5:BE:23:HIS:HA	5:BE:26:THR:OG1	2.05	0.56
20:BZ:26:ALA:CB	20:BZ:40:ILE:HD11	2.36	0.56
1:AA:265:PHE:CD1	1:AA:271:LEU:HA	2.41	0.56
30:AA:416:LMG:H112	2:BB:43:ALA:HA	1.87	0.56
4:AD:274:VAL:HA	24:AD:405:PL9:H253	1.86	0.56
20:AZ:55:GLY:HA2	26:AZ:101:BCR:H312	1.87	0.56
2:BB:133:LEU:HB3	2:BB:138:MET:HE2	1.87	0.56
3:BC:305:THR:HG23	3:BC:307:PRO:CD	2.32	0.56
9:BJ:14:ALA:HB3	26:BK:102:BCR:H393	1.88	0.56
10:BK:21:LEU:HD11	26:BK:102:BCR:HC32	1.87	0.56
13:BO:80:GLU:O	13:BO:89:ALA:HB1	2.05	0.56
26:AA:409:BCR:H321	29:AA:415:SQD:H321	1.87	0.56
20:AZ:32:ASP:C	20:AZ:34:ASP:N	2.60	0.56
1:BA:18:CYS:O	1:BA:22:THR:HG22	2.05	0.56
12:BM:29:THR:O	12:BM:32:GLN:HG3	2.06	0.56
13:BO:154:SER:O	13:BO:168:PHE:HA	2.05	0.56
20:BZ:23:VAL:O	20:BZ:26:ALA:HB3	2.06	0.56
1:AA:244:GLU:HG3	1:AA:246:TYR:H	1.70	0.56
2:AB:293:ALA:C	2:AB:295:GLY:H	2.14	0.56
4:AD:152:VAL:HG21	4:AD:279:LEU:CD1	2.35	0.56
7:AH:58:VAL:O	7:AH:58:VAL:CG1	2.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:20:TRP:O	1:BA:21:VAL:C	2.49	0.56
30:BD:408:LMG:H111	11:BL:19:LEU:HD21	1.87	0.56
10:BK:24:VAL:O	10:BK:27:VAL:HG12	2.06	0.56
13:BO:178:ARG:HG3	13:BO:178:ARG:NH1	2.00	0.56
16:BV:59:PHE:HA	16:BV:63:CYS:SG	2.46	0.56
20:BZ:30:PRO:C	20:BZ:32:ASP:H	2.12	0.56
1:AA:140:ARG:HH22	28:AA:411:LHG:P	2.28	0.56
3:AC:149:TYR:HA	3:AC:156:LYS:HD3	1.88	0.56
3:BC:239:TRP:CE3	3:BC:243:ILE:HD11	2.40	0.56
4:BD:26:ARG:CD	6:BF:18:VAL:HG11	2.29	0.56
13:BO:141:ARG:HG2	13:BO:141:ARG:HH11	1.71	0.56
17:By:39:LEU:CD2	20:BZ:25:VAL:HG12	2.35	0.56
1:AA:84:PRO:HA	1:AA:112:TYR:CG	2.40	0.56
1:AA:240:GLY:HA3	14:AT:29:ILE:HG22	1.88	0.56
2:AB:191:ASN:HD21	7:AH:60:VAL:HA	1.70	0.56
3:AC:250:TRP:CD1	3:AC:250:TRP:C	2.84	0.56
4:AD:199:MET:HG2	24:AD:405:PL9:H322	1.86	0.56
1:BA:265:PHE:CD1	1:BA:271:LEU:HA	2.41	0.56
2:BB:434:THR:HG23	13:BO:204:LYS:HE3	1.86	0.56
3:BC:429:SER:HB3	27:BC:517:DGD:HA81	1.88	0.56
20:BZ:32:ASP:C	20:BZ:34:ASP:N	2.60	0.56
2:AB:12:LEU:HD22	2:AB:18:ARG:HB2	1.87	0.56
2:AB:112:CYS:HB3	26:AB:620:BCR:H393	1.88	0.56
2:AB:191:ASN:HB2	7:AH:58:VAL:CG2	2.36	0.56
22:AB:608:CLA:HMD1	22:AB:610:CLA:HAB	1.86	0.56
13:AO:31:LEU:HD12	13:AO:31:LEU:H	1.71	0.56
18:AX:12:ILE:HG12	18:AX:16:LEU:CD1	2.31	0.56
20:AZ:29:SER:HB2	20:AZ:31:GLN:HG3	1.88	0.56
1:BA:11:ALA:O	1:BA:12:ASN:CB	2.53	0.56
2:BB:170:ASP:HB2	2:BB:171:PRO:CD	2.36	0.56
2:BB:191:ASN:HB2	7:BH:58:VAL:CG2	2.36	0.56
22:BB:611:CLA:H42	4:BD:127:LEU:HD11	1.86	0.56
13:BO:59:ASP:C	13:BO:61:SER:H	2.13	0.56
1:AA:104:GLU:OE2	13:AO:99:ARG:HD3	2.06	0.56
9:AJ:14:ALA:HB1	26:AK:102:BCR:H393	1.88	0.56
16:AV:125:ASP:HA	16:AV:131:ARG:HH21	1.70	0.56
17:Ay:39:LEU:CD2	20:AZ:25:VAL:HG12	2.36	0.56
29:BA:413:SQD:H223	27:BC:518:DGD:HAE1	1.88	0.56
2:BB:25:MET:HE3	26:BB:620:BCR:H23C	1.88	0.56
10:BK:17:ILE:HD12	10:BK:17:ILE:H	1.71	0.56
3:AC:199:ILE:N	3:AC:199:ILE:HD12	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:AZ:23:VAL:O	20:AZ:26:ALA:HB3	2.07	0.55
3:BC:223:TRP:CG	3:BC:224:ILE:H	2.24	0.55
4:BD:60:THR:HG23	4:BD:61:HIS:HD2	1.70	0.55
16:BV:29:LEU:HD11	16:BV:34:LEU:HD21	1.87	0.55
2:AB:43:ALA:HA	30:AB:623:LMG:H112	1.87	0.55
4:AD:250:ASN:ND2	4:AD:262:SER:HB3	2.21	0.55
4:AD:267:LEU:HD23	4:AD:267:LEU:O	2.06	0.55
8:AI:11:VAL:O	8:AI:15:PHE:HD2	1.89	0.55
14:AT:7:VAL:HG12	32:AT:101:LMT:H122	1.89	0.55
20:AZ:26:ALA:CB	20:AZ:40:ILE:HD11	2.36	0.55
24:BD:405:PL9:H13	30:BD:408:LMG:H132	1.87	0.55
13:BO:83:LYS:HG2	13:BO:84:ASN:N	2.20	0.55
20:BZ:5:PHE:HA	20:BZ:57:LEU:HD21	1.88	0.55
3:AC:305:THR:HG22	3:AC:308:GLU:N	2.16	0.55
13:AO:83:LYS:HE2	2:BB:338:GLN:HA	1.87	0.55
1:BA:104:GLU:OE2	13:BO:99:ARG:HD3	2.06	0.55
4:BD:221:THR:HG23	4:BD:244:TYR:HB2	1.87	0.55
4:BD:267:LEU:HD23	4:BD:267:LEU:O	2.07	0.55
15:BU:38:GLU:HG2	15:BU:39:LEU:H	1.71	0.55
2:BB:55:MET:HE2	2:BB:80:ILE:HD12	1.89	0.55
4:BD:53:THR:HG22	4:BD:67:TYR:CD2	2.41	0.55
6:BF:16:PHE:CD2	29:BF:101:SQD:H262	2.41	0.55
13:BO:86:ARG:HH11	13:BO:87:GLN:HA	1.71	0.55
2:AB:170:ASP:HB2	2:AB:171:PRO:CD	2.36	0.55
3:AC:350:ILE:HG21	3:AC:359:TRP:HB2	1.88	0.55
3:BC:193:GLY:O	3:BC:194:GLY:C	2.48	0.55
3:BC:350:ILE:HG21	3:BC:359:TRP:HB2	1.89	0.55
4:BD:49:LEU:O	4:BD:53:THR:HG23	2.06	0.55
1:AA:29:TYR:CD2	1:AA:133:LEU:HD13	2.41	0.55
4:AD:157:PHE:CE1	4:AD:171:PRO:HG2	2.41	0.55
30:AD:407:LMG:O3	9:AJ:37:GLY:HA3	2.07	0.55
13:AO:66:ILE:HD12	13:AO:121:PHE:CD1	2.42	0.55
18:AX:16:LEU:C	18:AX:16:LEU:HD13	2.31	0.55
1:BA:131:TRP:CE3	1:BA:132:GLU:N	2.74	0.55
1:BA:140:ARG:NH2	1:BA:142:TRP:HZ3	2.05	0.55
1:BA:238:LYS:O	1:BA:241:GLN:HG3	2.07	0.55
1:BA:244:GLU:HG3	1:BA:246:TYR:H	1.71	0.55
2:BB:6:TYR:HA	22:BB:614:CLA:H11	1.88	0.55
3:BC:107:ASP:OD2	3:BC:109:PHE:HB3	2.06	0.55
3:BC:346:THR:O	13:BO:40:GLY:HA2	2.07	0.55
1:AA:37:MET:HG2	1:AA:41:LEU:HD12	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:AB:608:CLA:H42	4:AD:127:LEU:HD11	1.88	0.55
3:AC:95:LEU:HD13	22:AC:502:CLA:H143	1.89	0.55
5:AE:55:TYR:O	5:AE:84:LYS:HE3	2.07	0.55
2:BB:174:LEU:HD23	2:BB:308:LYS:HG2	1.87	0.55
2:BB:183:PRO:HB2	2:BB:185:TRP:CH2	2.41	0.55
18:BX:12:ILE:CG1	18:BX:16:LEU:HD12	2.36	0.55
1:AA:131:TRP:CE3	1:AA:132:GLU:N	2.75	0.55
3:AC:45:LEU:HD23	3:AC:48:LYS:HD2	1.89	0.55
1:BA:64:ARG:NH1	13:BO:98:THR:HG21	2.22	0.55
1:BA:183:MET:HE1	22:BA:404:CLA:HMD2	1.89	0.55
4:BD:77:ALA:HB2	4:BD:174:GLY:HA3	1.88	0.55
13:BO:66:ILE:HD12	13:BO:121:PHE:CD1	2.41	0.55
20:BZ:21:ILE:O	20:BZ:25:VAL:HG22	2.07	0.55
2:AB:25:MET:HE1	2:AB:108:PHE:CE1	2.42	0.55
2:AB:133:LEU:HB3	2:AB:138:MET:HE1	1.88	0.55
4:AD:189:HIS:HA	4:AD:294:ARG:HD2	1.88	0.55
20:AZ:36:SER:HA	20:AZ:39:LEU:CG	2.35	0.55
4:BD:53:THR:HG22	4:BD:67:TYR:CE2	2.42	0.55
1:AA:20:TRP:O	1:AA:21:VAL:C	2.50	0.55
3:AC:107:ASP:OD2	3:AC:109:PHE:HB3	2.06	0.55
4:AD:180:ARG:CG	4:AD:180:ARG:NH1	2.70	0.55
13:AO:59:ASP:C	13:AO:61:SER:H	2.14	0.55
16:AV:59:PHE:HA	16:AV:63:CYS:SG	2.47	0.55
18:AX:32:LEU:N	18:AX:32:LEU:HD23	2.22	0.55
3:BC:239:TRP:HE3	3:BC:243:ILE:HD11	1.71	0.55
4:BD:88:SER:HB2	5:BE:69:ARG:CZ	2.36	0.55
4:BD:152:VAL:HG21	4:BD:279:LEU:CD1	2.36	0.55
1:AA:217:SER:HA	1:AA:220:THR:HG22	1.88	0.54
9:AJ:14:ALA:HB3	26:AK:102:BCR:H393	1.89	0.54
1:BA:38:ILE:O	1:BA:42:LEU:HG	2.06	0.54
1:BA:243:GLU:H	1:BA:243:GLU:CD	2.12	0.54
3:BC:425:TRP:CE2	22:BC:504:CLA:HBA1	2.42	0.54
1:AA:235:TYR:C	1:AA:237:TYR:H	2.16	0.54
13:AO:180:ALA:HB1	13:AO:191:ALA:HB2	1.89	0.54
2:BB:154:GLY:O	2:BB:159:THR:HG23	2.07	0.54
2:BB:246:PHE:CD1	2:BB:246:PHE:C	2.85	0.54
3:BC:250:TRP:CD1	3:BC:250:TRP:C	2.85	0.54
4:BD:85:MET:CE	5:BE:69:ARG:HA	2.35	0.54
4:BD:199:MET:HG2	24:BD:405:PL9:H322	1.89	0.54
4:BD:334:GLN:N	4:BD:335:PRO:HD3	2.22	0.54
16:BV:35:THR:HG23	16:BV:46:THR:OG1	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:221:SER:HB3	4:AD:141:TYR:HB2	1.89	0.54
3:AC:29:GLU:HB3	10:AK:46:ARG:HH11	1.70	0.54
5:AE:8:ARG:NE	5:AE:13:ILE:HG12	2.22	0.54
3:BC:95:LEU:HD13	22:BC:502:CLA:H143	1.88	0.54
3:BC:473:ASP:HB2	14:BT:26:PRO:CB	2.33	0.54
4:BD:76:VAL:O	4:BD:77:ALA:HB2	2.07	0.54
4:BD:180:ARG:HG3	4:BD:180:ARG:NH1	2.22	0.54
11:BL:11:GLU:HG2	11:BL:12:LEU:N	2.22	0.54
1:AA:64:ARG:NH1	13:AO:98:THR:HG21	2.22	0.54
3:AC:155:ASN:O	3:AC:158:THR:HG22	2.07	0.54
4:AD:86:GLY:O	4:AD:166:SER:HB2	2.08	0.54
15:AU:72:TYR:O	15:AU:73:PRO:C	2.48	0.54
15:AU:100:ARG:O	15:AU:103:GLN:HB3	2.07	0.54
20:AZ:21:ILE:O	20:AZ:25:VAL:HG22	2.07	0.54
20:AZ:35:ARG:O	20:AZ:38:GLN:HB3	2.07	0.54
22:BA:404:CLA:HED1	24:BD:405:PL9:H372	1.89	0.54
2:BB:224:ARG:NE	7:BH:25:TRP:NE1	2.55	0.54
2:BB:293:ALA:C	2:BB:295:GLY:H	2.15	0.54
15:BU:66:ILE:O	15:BU:66:ILE:CG2	2.56	0.54
2:AB:235:GLU:HG2	2:AB:235:GLU:O	2.08	0.54
3:AC:239:TRP:CE3	3:AC:243:ILE:HD11	2.42	0.54
3:AC:425:TRP:CE2	22:AC:504:CLA:HBA1	2.42	0.54
4:AD:18:LEU:HD22	18:AX:38:ILE:HD13	1.89	0.54
13:AO:141:ARG:HG2	13:AO:141:ARG:HH11	1.71	0.54
13:AO:227:VAL:HG12	13:AO:228:ALA:N	2.22	0.54
3:BC:135:ARG:HB2	20:BZ:27:TYR:HB3	1.90	0.54
3:BC:149:TYR:HA	3:BC:156:LYS:HD3	1.89	0.54
3:BC:158:THR:HG21	3:BC:254:THR:O	2.08	0.54
3:BC:369:LEU:HD21	3:BC:384:ILE:HD13	1.89	0.54
2:AB:150:CYS:HA	22:AB:603:CLA:HBC2	1.89	0.54
3:AC:135:ARG:HB2	20:AZ:27:TYR:HB3	1.89	0.54
3:AC:178:LYS:HA	3:AC:182:PHE:HB2	1.90	0.54
2:BB:12:LEU:HD22	2:BB:18:ARG:HB2	1.89	0.54
14:BT:25:GLU:O	14:BT:26:PRO:C	2.50	0.54
20:BZ:29:SER:C	20:BZ:31:GLN:H	2.16	0.54
20:BZ:32:ASP:CG	20:BZ:33:TRP:N	2.62	0.54
1:AA:76:ASN:OD1	1:AA:79:THR:HG23	2.07	0.54
1:AA:82:VAL:HB	1:AA:174:LEU:HB2	1.88	0.54
2:AB:487:SER:N	2:AB:488:PRO:HD2	2.23	0.54
15:AU:58:ASN:OD1	15:AU:84:PRO:HA	2.07	0.54
1:BA:217:SER:HA	1:BA:220:THR:HG22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:BO:271:PRO:HG2	13:BO:272:ALA:H	1.73	0.54
3:AC:155:ASN:HA	3:AC:158:THR:CG2	2.38	0.54
13:AO:154:SER:O	13:AO:168:PHE:HA	2.07	0.54
2:BB:487:SER:N	2:BB:488:PRO:HD2	2.22	0.54
27:BB:602:DGD:HD3	32:BB:603:LMT:H32	1.89	0.54
3:BC:453:ALA:O	8:BI:34:ARG:HB2	2.07	0.54
5:BE:55:TYR:O	5:BE:84:LYS:HE3	2.07	0.54
15:BU:100:ARG:O	15:BU:103:GLN:HB3	2.08	0.54
7:AH:12:ARG:N	7:AH:13:PRO:HD2	2.23	0.54
16:AV:35:THR:HG23	16:AV:46:THR:OG1	2.08	0.54
1:BA:190:HIS:CB	1:BA:293:MET:HE2	2.37	0.54
2:BB:133:LEU:HB3	2:BB:138:MET:HE1	1.88	0.54
2:BB:191:ASN:HD21	7:BH:60:VAL:HA	1.72	0.54
2:BB:230:ARG:O	2:BB:233:ASN:HB3	2.08	0.54
4:BD:239:GLN:O	4:BD:240:ALA:CB	2.56	0.54
5:BE:8:ARG:NE	5:BE:13:ILE:HG12	2.23	0.54
9:BJ:15:THR:O	9:BJ:19:MET:HG3	2.08	0.54
30:AD:408:LMG:H111	11:AL:19:LEU:HD21	1.88	0.54
13:AO:190:LEU:HB2	13:AO:214:LYS:HB2	1.90	0.54
3:BC:45:LEU:HD23	3:BC:48:LYS:HD2	1.90	0.54
3:BC:276:LEU:HD11	3:BC:444:HIS:HD2	1.73	0.54
1:AA:81:ALA:CB	1:AA:175:GLY:HA3	2.37	0.53
3:AC:30:SER:OG	4:AD:233:ARG:NH2	2.40	0.53
3:AC:276:LEU:HD11	3:AC:444:HIS:HD2	1.73	0.53
16:AV:116:GLU:O	16:AV:116:GLU:HG3	2.08	0.53
20:AZ:36:SER:OG	20:AZ:39:LEU:HD12	2.07	0.53
1:BA:114:LEU:HD23	1:BA:114:LEU:C	2.33	0.53
2:BB:191:ASN:ND2	7:BH:60:VAL:HA	2.23	0.53
3:BC:36:TRP:O	22:BC:508:CLA:H11	2.08	0.53
3:BC:118:HIS:CE1	30:BC:520:LMG:H192	2.42	0.53
3:BC:135:ARG:HE	20:BZ:33:TRP:HE1	1.56	0.53
3:BC:380:ILE:HA	3:BC:384:ILE:HD11	1.88	0.53
4:BD:238:THR:O	4:BD:239:GLN:O	2.26	0.53
10:BK:37:PHE:HB3	26:BK:102:BCR:C40	2.39	0.53
20:BZ:14:ILE:O	20:BZ:18:VAL:HG23	2.08	0.53
3:AC:453:ALA:O	8:AI:34:ARG:HB2	2.08	0.53
12:AM:25:LEU:O	12:AM:28:GLN:HG3	2.08	0.53
13:AO:92:VAL:HG13	13:AO:93:PRO:HD2	1.90	0.53
1:BA:240:GLY:HA3	14:BT:29:ILE:HG22	1.90	0.53
2:BB:329:PRO:HD3	22:BB:610:CLA:HED2	1.91	0.53
3:BC:447:ARG:HG2	3:BC:447:ARG:NH1	2.16	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BD:266:TRP:CD1	30:BD:408:LMG:HC3	2.42	0.53
6:BF:18:VAL:HG13	6:BF:19:ARG:N	2.23	0.53
7:BH:12:ARG:N	7:BH:13:PRO:HD2	2.23	0.53
8:BI:11:VAL:O	8:BI:15:PHE:HD2	1.91	0.53
10:BK:43:VAL:O	10:BK:43:VAL:HG13	2.08	0.53
3:AC:223:TRP:CG	3:AC:224:ILE:H	2.25	0.53
4:AD:279:LEU:HD11	22:AD:402:CLA:O1A	2.09	0.53
22:BB:610:CLA:H42	30:BB:624:LMG:H131	1.90	0.53
4:BD:189:HIS:HA	4:BD:294:ARG:HD2	1.90	0.53
7:BH:58:VAL:O	7:BH:58:VAL:CG1	2.56	0.53
2:AB:434:THR:HG23	13:AO:204:LYS:HE3	1.91	0.53
3:AC:118:HIS:CE1	30:AC:520:LMG:H192	2.43	0.53
13:AO:83:LYS:HG2	13:AO:84:ASN:N	2.19	0.53
2:BB:341:LYS:HD2	2:BB:429:ILE:HG22	1.90	0.53
3:BC:30:SER:OG	4:BD:233:ARG:NH2	2.41	0.53
3:BC:137:PRO:HB2	3:BC:139:THR:O	2.09	0.53
3:BC:418:ASN:HD21	27:BC:517:DGD:HD4	1.74	0.53
13:BO:178:ARG:HD2	13:BO:182:PHE:CD1	2.43	0.53
15:BU:58:ASN:OD1	15:BU:84:PRO:HA	2.07	0.53
16:BV:87:LEU:HD12	16:BV:87:LEU:N	2.22	0.53
18:BX:16:LEU:HD13	18:BX:16:LEU:C	2.33	0.53
20:BZ:3:ILE:O	20:BZ:7:LEU:HG	2.08	0.53
3:AC:36:TRP:O	22:AC:508:CLA:H11	2.08	0.53
3:AC:473:ASP:HB2	14:AT:26:PRO:CB	2.33	0.53
4:AD:180:ARG:NH1	4:AD:180:ARG:HG3	2.23	0.53
4:AD:239:GLN:O	4:AD:240:ALA:CB	2.55	0.53
1:BA:283:VAL:O	1:BA:286:THR:HG22	2.08	0.53
3:BC:178:LYS:HA	3:BC:182:PHE:HB2	1.89	0.53
1:AA:143:ILE:HD11	4:AD:217:THR:HA	1.89	0.53
3:AC:174:LEU:HG	22:AC:512:CLA:H92	1.90	0.53
1:BA:322:ASN:OD1	3:BC:412:THR:HA	2.08	0.53
3:BC:131:TYR:HE1	3:BC:135:ARG:HD2	1.74	0.53
5:BE:28:PRO:O	5:BE:32:ILE:HG13	2.08	0.53
13:BO:227:VAL:HG12	13:BO:228:ALA:N	2.23	0.53
14:BT:29:ILE:H	14:BT:29:ILE:CD1	1.98	0.53
27:AC:517:DGD:HB62	26:AJ:102:BCR:H352	1.91	0.53
13:AO:178:ARG:CG	13:AO:178:ARG:NH1	2.55	0.53
1:BA:76:ASN:OD1	1:BA:79:THR:HG23	2.08	0.53
1:BA:107:TYR:CD1	13:BO:141:ARG:NH1	2.77	0.53
3:BC:117:VAL:HG12	30:BC:520:LMG:H191	1.91	0.53
3:BC:337:LEU:CD1	13:BO:131:PRO:HG3	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:BO:31:LEU:HB2	13:BO:36:ILE:CD1	2.37	0.53
13:BO:86:ARG:C	13:BO:86:ARG:HH11	2.16	0.53
17:By:21:GLN:HA	17:By:23:THR:HG22	1.91	0.53
4:AD:330:ALA:HB3	4:AD:331:PRO:HD3	1.91	0.53
4:AD:337:GLU:O	4:AD:338:ASN:C	2.51	0.53
15:AU:66:ILE:O	15:AU:66:ILE:CG2	2.56	0.53
2:BB:235:GLU:O	2:BB:235:GLU:HG2	2.09	0.53
3:BC:33:PHE:CE1	4:BD:229:ALA:CB	2.92	0.53
3:BC:342:MET:HE3	3:BC:352:GLY:HA2	1.91	0.53
9:BJ:14:ALA:HB1	26:BK:102:BCR:H393	1.91	0.53
27:AB:626:DGD:HD3	32:AB:627:LMT:H32	1.90	0.53
3:AC:259:TRP:CD1	3:AC:259:TRP:H	2.26	0.53
22:AC:501:CLA:HMB3	26:AC:515:BCR:H403	1.90	0.53
4:AD:238:THR:O	4:AD:239:GLN:O	2.27	0.53
9:AJ:15:THR:O	9:AJ:19:MET:HG3	2.08	0.53
10:AK:37:PHE:HB3	26:AK:102:BCR:C40	2.39	0.53
3:BC:117:VAL:CG1	30:BC:520:LMG:H191	2.39	0.53
4:BD:161:PRO:HG3	4:BD:170:ALA:HB2	1.91	0.53
20:BZ:35:ARG:O	20:BZ:38:GLN:HB3	2.09	0.53
26:AA:409:BCR:H312	8:AI:15:PHE:CE1	2.44	0.53
2:AB:172:TYR:O	2:AB:173:GLY:C	2.52	0.53
22:AB:608:CLA:H12	4:AD:127:LEU:HD21	1.91	0.53
6:AF:21:VAL:O	6:AF:25:THR:HG23	2.09	0.53
2:BB:120:LEU:HD13	22:BB:619:CLA:CMD	2.40	0.53
13:BO:92:VAL:HG13	13:BO:93:PRO:HD2	1.92	0.53
1:AA:114:LEU:C	1:AA:114:LEU:HD23	2.34	0.52
2:AB:341:LYS:HD2	2:AB:429:ILE:HG22	1.90	0.52
3:AC:391:ARG:HH11	3:AC:391:ARG:CB	2.19	0.52
7:AH:55:LEU:O	7:AH:58:VAL:HG12	2.09	0.52
13:AO:225:LEU:C	13:AO:226:ASN:HD22	2.17	0.52
15:AU:100:ARG:HH11	15:AU:103:GLN:HG2	1.73	0.52
1:BA:43:ALA:HB1	26:BA:410:BCR:H362	1.91	0.52
1:BA:300:PHE:CZ	3:BC:404:LEU:HD23	2.45	0.52
3:BC:71:GLU:OE1	3:BC:89:ILE:HG13	2.08	0.52
3:BC:167:VAL:HG12	22:BC:512:CLA:H2	1.89	0.52
4:BD:55:VAL:HG21	4:BD:110:LEU:CD1	2.39	0.52
18:BX:12:ILE:HG12	18:BX:16:LEU:CD1	2.35	0.52
1:AA:49:VAL:O	1:AA:53:ILE:HG13	2.10	0.52
1:AA:196:PRO:HA	1:AA:199:GLN:OE1	2.09	0.52
3:AC:80:PRO:HB2	3:AC:83:GLU:HG3	1.90	0.52
3:AC:466:VAL:HG13	4:AD:251:ARG:HD2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AD:71:CYS:HB2	4:AD:76:VAL:HG12	1.91	0.52
4:AD:221:THR:HG23	4:AD:244:TYR:HB2	1.91	0.52
4:AD:334:GLN:N	4:AD:335:PRO:HD3	2.24	0.52
1:BA:232:SER:HB3	1:BA:235:TYR:CD1	2.44	0.52
13:BO:234:THR:OG1	13:BO:236:GLU:HG2	2.09	0.52
15:BU:72:TYR:CB	15:BU:73:PRO:HD3	2.34	0.52
1:AA:22:THR:HG21	8:AI:30:ARG:HD3	1.90	0.52
1:AA:215:HIS:O	1:AA:216:GLY:C	2.53	0.52
3:AC:33:PHE:CE1	4:AD:229:ALA:CB	2.92	0.52
4:AD:161:PRO:HG3	4:AD:170:ALA:HB2	1.91	0.52
6:AF:18:VAL:HG13	6:AF:19:ARG:N	2.25	0.52
15:AU:66:ILE:HG13	15:AU:72:TYR:CD1	2.44	0.52
16:BV:74:THR:O	16:BV:75:ASN:HB2	2.09	0.52
1:AA:326:LEU:HD21	3:AC:412:THR:HB	1.91	0.52
3:AC:216:SER:HB3	3:AC:221:GLU:HB2	1.90	0.52
3:AC:429:SER:HB3	27:AC:517:DGD:HA81	1.91	0.52
3:AC:452:ALA:O	3:AC:454:GLY:N	2.42	0.52
13:AO:141:ARG:HG2	13:AO:141:ARG:NH1	2.24	0.52
16:AV:135:GLU:O	16:AV:139:VAL:HG23	2.08	0.52
17:Ay:21:GLN:HA	17:Ay:23:THR:HG22	1.90	0.52
3:BC:269:GLU:OE1	22:BC:508:CLA:HED1	2.08	0.52
30:BD:407:LMG:O3	9:BJ:37:GLY:HA3	2.09	0.52
14:BT:7:VAL:HG12	32:BT:101:LMT:H122	1.91	0.52
15:BU:83:ALA:CB	15:BU:84:PRO:HD2	2.15	0.52
2:AB:246:PHE:C	2:AB:246:PHE:CD1	2.88	0.52
3:AC:163:PHE:CD1	22:AC:512:CLA:HAB	2.45	0.52
26:AT:102:BCR:C40	2:BB:36:SER:HB2	2.40	0.52
20:AZ:32:ASP:C	20:AZ:34:ASP:H	2.17	0.52
1:BA:81:ALA:CB	1:BA:175:GLY:HA3	2.39	0.52
2:BB:220:ARG:HB3	2:BB:221:PRO:HD2	1.92	0.52
3:BC:116:VAL:HG21	26:BZ:101:BCR:H323	1.91	0.52
4:BD:87:HIS:CD2	4:BD:162:LEU:HA	2.45	0.52
9:BJ:18:GLY:HA3	26:BK:102:BCR:H371	1.92	0.52
30:AD:408:LMG:H392	26:AT:102:BCR:HC32	1.92	0.52
10:AK:24:VAL:O	10:AK:27:VAL:HG12	2.10	0.52
22:BC:504:CLA:H202	27:BC:518:DGD:HAF2	1.92	0.52
27:BC:517:DGD:HB62	26:BJ:102:BCR:H352	1.91	0.52
1:AA:232:SER:HB3	1:AA:235:TYR:CD1	2.45	0.52
3:AC:269:GLU:OE1	3:AC:447:ARG:HG2	2.10	0.52
3:AC:337:LEU:CD1	13:AO:131:PRO:HG3	2.39	0.52
5:AE:9:PRO:O	5:AE:10:PHE:C	2.53	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AO:178:ARG:HD2	13:AO:182:PHE:CD1	2.45	0.52
13:AO:223:ILE:HG13	13:AO:243:SER:HB3	1.92	0.52
17:Ay:36:ILE:C	17:Ay:36:ILE:HD12	2.35	0.52
1:BA:317:TRP:CD1	4:BD:177:ALA:HB2	2.44	0.52
3:BC:29:GLU:HB3	10:BK:46:ARG:HH11	1.74	0.52
3:BC:466:VAL:HG13	4:BD:251:ARG:HD2	1.92	0.52
20:BZ:31:GLN:O	20:BZ:32:ASP:HB3	2.10	0.52
1:AA:78:ILE:O	1:AA:176:ILE:HB	2.10	0.52
22:AB:604:CLA:H101	22:AB:615:CLA:H42	1.91	0.52
4:AD:88:SER:HB2	5:AE:69:ARG:CZ	2.40	0.52
10:AK:43:VAL:HG13	10:AK:43:VAL:O	2.09	0.52
16:AV:147:VAL:O	16:AV:150:LYS:HB2	2.10	0.52
3:BC:155:ASN:CA	3:BC:158:THR:HG22	2.39	0.52
3:BC:163:PHE:CD1	22:BC:512:CLA:HAB	2.44	0.52
1:AA:10:SER:C	1:AA:12:ASN:H	2.16	0.52
1:AA:232:SER:HB3	1:AA:235:TYR:HD1	1.75	0.52
1:AA:322:ASN:OD1	3:AC:412:THR:HA	2.09	0.52
3:AC:47:GLY:O	3:AC:50:LEU:HB3	2.10	0.52
3:AC:415:ASN:O	3:AC:416:SER:CB	2.57	0.52
17:Ay:20:ALA:C	17:Ay:22:LEU:H	2.15	0.52
3:BC:47:GLY:O	3:BC:50:LEU:HB3	2.10	0.52
3:BC:135:ARG:HE	20:BZ:33:TRP:NE1	2.07	0.52
3:BC:199:ILE:HD12	3:BC:199:ILE:N	2.25	0.52
7:BH:25:TRP:O	7:BH:26:GLY:C	2.53	0.52
12:BM:25:LEU:O	12:BM:28:GLN:HG3	2.10	0.52
1:AA:188:ALA:HB2	1:AA:328:MET:HB2	1.92	0.52
2:AB:224:ARG:NE	7:AH:25:TRP:NE1	2.58	0.52
4:AD:77:ALA:HB2	4:AD:174:GLY:HA3	1.91	0.52
4:AD:266:TRP:HD1	30:AD:408:LMG:HC3	1.74	0.52
18:AX:17:LYS:O	18:AX:21:ILE:HG13	2.10	0.52
20:AZ:17:PHE:CE2	20:AZ:21:ILE:HD11	2.45	0.52
2:BB:25:MET:HE1	2:BB:108:PHE:CE1	2.44	0.52
3:BC:296:VAL:HG23	3:BC:297:TYR:CD2	2.45	0.52
13:BO:31:LEU:HD12	13:BO:31:LEU:H	1.75	0.52
20:BZ:17:PHE:CE2	20:BZ:21:ILE:HD11	2.45	0.52
1:AA:183:MET:HE1	22:AA:403:CLA:HMD2	1.91	0.51
1:AA:227:THR:HA	1:AA:231:GLU:OE2	2.10	0.51
1:AA:279:PRO:CG	4:AD:212:ALA:HB2	2.40	0.51
22:AB:603:CLA:H193	7:AH:42:LEU:HD12	1.92	0.51
1:BA:22:THR:HG21	8:BI:30:ARG:HD3	1.91	0.51
22:BB:607:CLA:H101	22:BB:618:CLA:H42	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BB:611:CLA:H12	4:BD:127:LEU:HD21	1.92	0.51
4:BD:252:PHE:O	4:BD:256:ILE:HG22	2.10	0.51
4:BD:350:ASN:O	4:BD:352:LEU:N	2.42	0.51
13:BO:141:ARG:HG2	13:BO:141:ARG:NH1	2.24	0.51
15:BU:72:TYR:O	15:BU:73:PRO:C	2.51	0.51
1:AA:43:ALA:HB1	26:AA:409:BCR:H362	1.92	0.51
3:AC:418:ASN:HD21	27:AC:517:DGD:HD4	1.74	0.51
28:AC:521:LHG:H162	26:AJ:102:BCR:H313	1.91	0.51
13:AO:178:ARG:HG3	13:AO:178:ARG:NH1	2.01	0.51
20:AZ:3:ILE:O	20:AZ:7:LEU:HG	2.09	0.51
3:BC:116:VAL:CG2	26:BZ:101:BCR:H323	2.41	0.51
4:BD:136:VAL:O	4:BD:136:VAL:HG12	2.10	0.51
20:BZ:32:ASP:C	20:BZ:34:ASP:H	2.17	0.51
1:AA:228:THR:HG22	1:AA:229:GLU:N	2.25	0.51
3:AC:239:TRP:HE3	3:AC:243:ILE:HD11	1.74	0.51
4:AD:85:MET:CE	5:AE:69:ARG:HA	2.41	0.51
1:BA:190:HIS:O	1:BA:298:ASN:HB3	2.11	0.51
2:BB:9:HIS:HB2	22:BB:614:CLA:HBA1	1.91	0.51
3:BC:391:ARG:HH11	3:BC:391:ARG:CB	2.22	0.51
10:BK:35:LEU:HA	10:BK:38:VAL:HG23	1.92	0.51
17:By:20:ALA:C	17:By:22:LEU:H	2.18	0.51
1:AA:140:ARG:NH2	1:AA:142:TRP:HZ3	2.07	0.51
1:AA:334:ARG:NH1	13:AO:184:ASP:C	2.69	0.51
4:AD:87:HIS:CD2	4:AD:162:LEU:HA	2.45	0.51
4:AD:221:THR:HG23	4:AD:221:THR:O	2.10	0.51
13:AO:271:PRO:HG2	13:AO:272:ALA:H	1.76	0.51
20:AZ:31:GLN:O	20:AZ:32:ASP:HB3	2.10	0.51
20:AZ:32:ASP:OD1	20:AZ:36:SER:HB2	2.11	0.51
10:BK:20:PRO:O	10:BK:23:ASP:HB2	2.10	0.51
13:BO:225:LEU:C	13:BO:226:ASN:HD22	2.18	0.51
20:BZ:5:PHE:CE1	20:BZ:54:VAL:HG13	2.46	0.51
2:AB:229:LEU:O	2:AB:231:MET:N	2.43	0.51
4:AD:136:VAL:HG12	4:AD:136:VAL:O	2.10	0.51
5:AE:36:LEU:HA	5:AE:39:SER:OG	2.11	0.51
20:AZ:29:SER:C	20:AZ:31:GLN:H	2.17	0.51
26:BA:410:BCR:H312	8:BI:15:PHE:CE1	2.45	0.51
2:BB:434:THR:CG2	13:BO:204:LYS:HE3	2.40	0.51
2:AB:12:LEU:CD2	2:AB:18:ARG:HB2	2.40	0.51
2:AB:125:ASP:OD2	2:AB:127:ARG:HB3	2.11	0.51
3:AC:62:PHE:HE2	10:AK:29:PRO:HD3	1.76	0.51
2:BB:150:CYS:HA	22:BB:606:CLA:HBC2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BB:613:CLA:H12	22:BB:613:CLA:H112	1.92	0.51
16:BV:95:ILE:O	16:BV:99:VAL:HG23	2.09	0.51
1:AA:214:MET:O	1:AA:215:HIS:C	2.54	0.51
2:AB:27:THR:HG22	2:AB:107:LEU:CD1	2.40	0.51
2:AB:36:SER:HB2	26:AB:618:BCR:C40	2.40	0.51
3:AC:117:VAL:HG12	30:AC:520:LMG:H191	1.92	0.51
1:BA:196:PRO:HA	1:BA:199:GLN:OE1	2.10	0.51
2:BB:55:MET:CE	2:BB:80:ILE:HD12	2.41	0.51
3:BC:72:LEU:HD11	3:BC:108:THR:HB	1.93	0.51
7:BH:55:LEU:HB2	7:BH:58:VAL:HG12	1.93	0.51
13:BO:223:ILE:HG12	13:BO:224:SER:N	2.25	0.51
1:AA:92:HIS:CD2	3:AC:219:GLY:HA3	2.46	0.51
22:AB:610:CLA:H12	22:AB:610:CLA:H112	1.93	0.51
3:AC:452:ALA:C	3:AC:454:GLY:N	2.68	0.51
4:AD:86:GLY:HA2	4:AD:166:SER:HB3	1.93	0.51
7:AH:25:TRP:O	7:AH:26:GLY:C	2.53	0.51
7:AH:55:LEU:HB2	7:AH:58:VAL:HG12	1.92	0.51
13:AO:240:THR:HA	13:AO:264:VAL:HA	1.91	0.51
3:BC:62:PHE:HE2	10:BK:29:PRO:HD3	1.75	0.51
26:BC:514:BCR:H391	10:BK:36:ALA:HB2	1.93	0.51
20:BZ:32:ASP:OD1	20:BZ:36:SER:HB2	2.11	0.51
32:AB:625:LMT:H102	7:AH:35:MET:SD	2.51	0.51
3:AC:135:ARG:HE	20:AZ:33:TRP:NE1	2.09	0.51
6:AF:16:PHE:CD2	29:AF:101:SQD:H262	2.46	0.51
13:AO:118:SER:HB3	13:AO:157:PRO:HA	1.93	0.51
18:AX:12:ILE:CG1	18:AX:16:LEU:HD12	2.33	0.51
1:BA:306:VAL:HG11	1:BA:316:THR:HG23	1.92	0.51
3:BC:155:ASN:HA	3:BC:158:THR:CG2	2.38	0.51
3:BC:460:ASP:O	3:BC:461:ARG:C	2.54	0.51
4:BD:86:GLY:O	4:BD:166:SER:HB2	2.11	0.51
4:BD:221:THR:HG23	4:BD:221:THR:O	2.10	0.51
1:AA:29:TYR:OH	1:AA:132:GLU:OE2	2.25	0.51
4:AD:53:THR:HG22	4:AD:67:TYR:CD2	2.46	0.51
2:BB:256:MET:HA	2:BB:263:THR:HG21	1.93	0.51
3:BC:269:GLU:OE1	3:BC:447:ARG:HG2	2.11	0.51
17:By:21:GLN:HG2	17:By:21:GLN:O	2.10	0.51
2:AB:183:PRO:HB2	2:AB:185:TRP:CH2	2.46	0.50
3:AC:116:VAL:HG21	26:AZ:101:BCR:H323	1.92	0.50
8:AI:27:ASP:N	8:AI:28:PRO:CD	2.74	0.50
15:AU:83:ALA:CB	15:AU:84:PRO:CD	2.77	0.50
1:BA:10:SER:C	1:BA:12:ASN:H	2.19	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:BA:408:PL9:H301	4:BD:42:TYR:HA	1.94	0.50
3:BC:80:PRO:HB2	3:BC:83:GLU:HG3	1.91	0.50
3:BC:135:ARG:HB2	20:BZ:27:TYR:CG	2.46	0.50
3:BC:447:ARG:HH11	3:BC:447:ARG:CG	2.14	0.50
1:AA:149:ALA:HB3	1:AA:150:PRO:CD	2.41	0.50
3:AC:116:VAL:CG2	26:AZ:101:BCR:H323	2.41	0.50
3:AC:158:THR:HG21	3:AC:254:THR:O	2.10	0.50
4:AD:346:LEU:O	4:AD:348:ARG:HG3	2.10	0.50
10:AK:17:ILE:H	10:AK:17:ILE:CD1	2.24	0.50
20:AZ:5:PHE:HA	20:AZ:57:LEU:CD2	2.40	0.50
29:BA:413:SQD:H5	4:BD:232:PHE:HB3	1.93	0.50
2:BB:63:LEU:N	2:BB:64:PRO:HD2	2.27	0.50
3:BC:259:TRP:CD1	3:BC:259:TRP:H	2.27	0.50
22:BC:504:CLA:HED1	30:BC:519:LMG:O3	2.11	0.50
13:BO:190:LEU:HB2	13:BO:214:LYS:HB2	1.93	0.50
16:BV:147:VAL:O	16:BV:150:LYS:HB2	2.11	0.50
1:AA:283:VAL:O	1:AA:286:THR:HG22	2.11	0.50
3:AC:167:VAL:HG12	22:AC:512:CLA:H2	1.94	0.50
4:AD:76:VAL:O	4:AD:77:ALA:HB2	2.10	0.50
10:AK:25:LEU:HB2	10:AK:26:PRO:HD3	1.93	0.50
13:AO:86:ARG:HH11	13:AO:87:GLN:HA	1.75	0.50
13:AO:223:ILE:HG12	13:AO:224:SER:N	2.27	0.50
18:AX:12:ILE:O	18:AX:12:ILE:CG2	2.58	0.50
1:BA:232:SER:HB3	1:BA:235:TYR:HD1	1.75	0.50
2:BB:149:LEU:HG	22:BB:606:CLA:CBC	2.30	0.50
4:BD:62:GLY:HA3	5:BE:63:ILE:HD13	1.94	0.50
8:BI:27:ASP:N	8:BI:28:PRO:CD	2.74	0.50
3:AC:159:THR:HG23	3:AC:252:ILE:HD13	1.93	0.50
22:AC:504:CLA:H202	27:AC:518:DGD:HAF2	1.94	0.50
4:AD:53:THR:HG22	4:AD:67:TYR:CE2	2.47	0.50
5:BE:8:ARG:HB2	6:BF:13:TYR:HB3	1.92	0.50
18:BX:17:LYS:O	18:BX:21:ILE:HG13	2.11	0.50
29:AA:412:SQD:H223	27:AC:518:DGD:HAE1	1.92	0.50
2:AB:134:ASP:OD2	2:AB:137:LYS:HB2	2.11	0.50
22:AB:605:CLA:HBB1	22:AB:606:CLA:H51	1.92	0.50
22:AB:607:CLA:H42	30:AB:622:LMG:H131	1.92	0.50
3:AC:81:MET:CE	3:AC:89:ILE:HG22	2.42	0.50
3:AC:418:ASN:HB2	27:AC:518:DGD:HE2	1.92	0.50
5:AE:34:GLY:HA2	6:AF:32:PHE:CE1	2.46	0.50
17:Ay:39:LEU:HD21	20:AZ:25:VAL:HA	1.93	0.50
20:AZ:5:PHE:CE1	20:AZ:54:VAL:HG13	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:AZ:12:LEU:HB2	20:AZ:50:LEU:HD22	1.93	0.50
1:BA:334:ARG:NH1	13:BO:184:ASP:C	2.69	0.50
3:BC:413:GLU:HG3	3:BC:414:ILE:N	2.27	0.50
4:BD:134:ARG:HA	4:BD:134:ARG:HE	1.76	0.50
13:BO:223:ILE:HG13	13:BO:243:SER:HB3	1.93	0.50
18:BX:32:LEU:HD23	18:BX:32:LEU:N	2.26	0.50
1:AA:63:ILE:HB	3:AC:335:THR:HG21	1.92	0.50
22:AA:403:CLA:HED2	4:AD:198:MET:SD	2.51	0.50
2:AB:9:HIS:HB2	22:AB:611:CLA:HBA1	1.93	0.50
22:AB:612:CLA:H171	22:AB:613:CLA:HBB2	1.94	0.50
30:AI:101:LMG:H181	32:AI:102:LMT:H42	1.94	0.50
20:AZ:47:TRP:O	20:AZ:50:LEU:HB2	2.11	0.50
28:BA:412:LHG:HC12	22:BC:508:CLA:O1D	2.12	0.50
2:BB:12:LEU:CD2	2:BB:18:ARG:HB2	2.41	0.50
2:BB:471:ALA:HB2	4:BD:130:PHE:HZ	1.76	0.50
22:BB:611:CLA:H151	22:BB:612:CLA:H203	1.93	0.50
3:BC:154:LYS:HE2	3:BC:261:ARG:HD2	1.93	0.50
34:BE:101:HEM:HBC2	6:BF:27:ALA:CB	2.37	0.50
14:BT:22:PHE:C	14:BT:23:PHE:HD2	2.20	0.50
18:BX:43:ILE:O	18:BX:43:ILE:HG22	2.11	0.50
1:AA:10:SER:C	1:AA:12:ASN:N	2.69	0.50
29:AA:415:SQD:H2	22:BB:619:CLA:H43	1.94	0.50
2:AB:55:MET:CE	2:AB:80:ILE:HD12	2.42	0.50
2:AB:229:LEU:O	2:AB:230:ARG:C	2.54	0.50
3:AC:89:ILE:N	3:AC:90:PRO:CD	2.75	0.50
3:AC:117:VAL:CG1	30:AC:520:LMG:H191	2.41	0.50
3:AC:266:TRP:HB3	3:AC:271:TYR:OH	2.11	0.50
13:AO:59:ASP:HB3	13:AO:62:GLN:HB3	1.93	0.50
1:BA:235:TYR:C	1:BA:237:TYR:H	2.20	0.50
2:BB:124:ARG:HG3	2:BB:124:ARG:NH1	2.22	0.50
2:BB:172:TYR:O	2:BB:173:GLY:C	2.52	0.50
4:BD:217:THR:O	4:BD:221:THR:HB	2.11	0.50
2:AB:286:ARG:HG2	2:AB:286:ARG:NH1	2.26	0.50
22:AB:616:CLA:H43	29:BA:401:SQD:H2	1.94	0.50
16:AV:95:ILE:O	16:AV:99:VAL:HG23	2.12	0.50
1:BA:159:LEU:C	1:BA:162:PRO:HD2	2.37	0.50
3:BC:275:SER:HB3	22:BC:509:CLA:HED3	1.94	0.50
27:BC:517:DGD:HBV1	28:BC:521:LHG:H151	1.93	0.50
1:AA:192:ILE:CB	1:AA:293:MET:HE1	2.42	0.50
2:AB:141:ILE:HG23	22:AB:615:CLA:HBB1	1.92	0.50
32:AB:627:LMT:H11	30:BI:101:LMG:HC2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:265:ILE:HG12	22:AC:505:CLA:HED1	1.94	0.50
3:AC:269:GLU:OE1	22:AC:508:CLA:HED1	2.12	0.50
4:AD:19:ASP:O	4:AD:20:ASP:C	2.55	0.50
4:AD:54:PHE:HB3	5:AE:47:PHE:CD2	2.46	0.50
30:AI:101:LMG:HC2	32:BB:603:LMT:H11	1.93	0.50
1:BA:221:SER:HB3	4:BD:141:TYR:HB2	1.94	0.50
2:BB:96:VAL:HG22	22:BB:609:CLA:HBA1	1.94	0.50
2:BB:187:PRO:HB3	22:BB:604:CLA:HMB1	1.94	0.50
16:BV:45:ILE:HG12	16:BV:46:THR:N	2.26	0.50
1:AA:96:ILE:HG12	1:AA:105:TRP:CE2	2.47	0.49
1:AA:107:TYR:CD1	13:AO:141:ARG:NH1	2.80	0.49
2:AB:349:LYS:HG3	2:AB:350:GLU:OE1	2.12	0.49
6:AF:11:VAL:CG1	6:AF:12:SER:H	2.25	0.49
1:BA:96:ILE:HG12	1:BA:105:TRP:CE2	2.47	0.49
1:BA:206:PHE:CE2	22:BD:402:CLA:HBA1	2.47	0.49
1:BA:330:VAL:HG12	4:BD:348:ARG:HA	1.93	0.49
2:BB:86:ILE:HD12	2:BB:86:ILE:C	2.37	0.49
5:BE:8:ARG:HB2	6:BF:13:TYR:CB	2.42	0.49
14:BT:22:PHE:C	14:BT:23:PHE:CD2	2.89	0.49
2:AB:471:ALA:HB2	4:AD:130:PHE:HZ	1.78	0.49
3:AC:72:LEU:HD11	3:AC:108:THR:HB	1.93	0.49
3:AC:137:PRO:HB2	3:AC:139:THR:O	2.12	0.49
3:AC:315:MET:O	3:AC:319:ILE:HG13	2.12	0.49
3:AC:391:ARG:HD2	3:AC:395:TYR:CZ	2.47	0.49
4:AD:36:LEU:C	4:AD:39:PRO:HD2	2.37	0.49
4:AD:350:ASN:O	4:AD:352:LEU:N	2.42	0.49
9:AJ:18:GLY:HA3	26:AK:102:BCR:H371	1.93	0.49
13:AO:31:LEU:HB2	13:AO:36:ILE:CD1	2.38	0.49
17:Ay:24:MET:O	17:Ay:25:ILE:C	2.55	0.49
18:AX:42:GLN:O	18:AX:43:ILE:HG13	2.12	0.49
1:BA:84:PRO:HA	1:BA:112:TYR:CG	2.47	0.49
3:BC:418:ASN:HB2	27:BC:518:DGD:HE2	1.93	0.49
3:BC:452:ALA:O	3:BC:454:GLY:N	2.44	0.49
4:BD:180:ARG:CG	4:BD:180:ARG:NH1	2.69	0.49
4:BD:337:GLU:O	4:BD:338:ASN:C	2.55	0.49
18:BX:32:LEU:O	18:BX:36:VAL:HG23	2.11	0.49
1:AA:224:ILE:O	1:AA:226:GLU:OE2	2.30	0.49
2:AB:220:ARG:HB3	2:AB:221:PRO:HD2	1.93	0.49
3:AC:135:ARG:HE	20:AZ:33:TRP:HE1	1.59	0.49
3:AC:275:SER:HB3	22:AC:509:CLA:HED3	1.94	0.49
3:AC:473:ASP:CB	14:AT:26:PRO:HB3	2.36	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:AV:29:LEU:HD11	16:AV:34:LEU:HD21	1.92	0.49
2:BB:10:THR:C	2:BB:12:LEU:N	2.70	0.49
22:BC:504:CLA:H151	27:BC:517:DGD:HBW1	1.93	0.49
4:BD:54:PHE:HB3	5:BE:47:PHE:CD2	2.47	0.49
2:AB:462:PHE:HA	22:AB:611:CLA:HMC2	1.94	0.49
4:AD:210:LEU:HA	4:AD:213:ILE:HG22	1.95	0.49
6:AF:23:VAL:O	6:AF:27:ALA:CB	2.60	0.49
11:AL:12:LEU:HD22	12:AM:25:LEU:HD12	1.93	0.49
32:BB:626:LMT:H3'	29:BD:409:SQD:H62	1.95	0.49
3:BC:116:VAL:HG23	3:BC:117:VAL:N	2.28	0.49
4:BD:176:ALA:HA	4:BD:179:PHE:CD2	2.47	0.49
4:BD:279:LEU:HD11	22:BD:402:CLA:O1A	2.13	0.49
5:BE:9:PRO:O	5:BE:10:PHE:C	2.55	0.49
5:BE:34:GLY:HA2	6:BF:32:PHE:CE1	2.48	0.49
10:BK:25:LEU:HB2	10:BK:26:PRO:HD3	1.94	0.49
2:AB:173:GLY:HA3	2:AB:265:ILE:HD11	1.93	0.49
22:AB:608:CLA:H151	22:AB:609:CLA:H203	1.93	0.49
3:AC:109:PHE:HB3	3:AC:110:PRO:HD3	1.94	0.49
26:AC:514:BCR:H391	10:AK:36:ALA:HB2	1.95	0.49
16:AV:63:CYS:O	16:AV:64:ALA:C	2.55	0.49
1:BA:24:THR:OG1	3:BC:469:MET:HE2	2.13	0.49
2:BB:24:LEU:HB3	2:BB:111:ALA:HB2	1.94	0.49
3:BC:174:LEU:HG	22:BC:512:CLA:H92	1.93	0.49
26:BC:514:BCR:HC22	10:BK:18:PHE:HD1	1.77	0.49
5:BE:4:THR:CG2	5:BE:5:THR:N	2.76	0.49
5:BE:81:GLU:C	5:BE:83:LEU:N	2.65	0.49
17:By:36:ILE:C	17:By:36:ILE:HD12	2.37	0.49
22:AB:608:CLA:H51	22:AB:609:CLA:H101	1.94	0.49
3:AC:413:GLU:HG3	3:AC:414:ILE:N	2.28	0.49
3:AC:452:ALA:O	3:AC:453:ALA:C	2.56	0.49
13:AO:43:ASN:OD1	13:AO:103:SER:HB2	2.12	0.49
18:AX:43:ILE:O	18:AX:43:ILE:HG22	2.12	0.49
1:BA:124:SER:O	1:BA:127:MET:HB3	2.12	0.49
2:BB:134:ASP:OD2	2:BB:137:LYS:HB2	2.12	0.49
22:BC:501:CLA:HMB2	22:BC:501:CLA:H51	1.93	0.49
4:BD:266:TRP:HD1	30:BD:408:LMG:HC3	1.76	0.49
9:BJ:34:ALA:O	9:BJ:35:GLY:O	2.31	0.49
13:BO:43:ASN:OD1	13:BO:103:SER:HB2	2.11	0.49
1:AA:243:GLU:CD	1:AA:243:GLU:H	2.16	0.49
24:AA:407:PL9:H301	4:AD:42:TYR:HA	1.94	0.49
2:AB:137:LYS:O	2:AB:141:ILE:HG13	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:56:HIS:C	3:AC:58:GLY:N	2.68	0.49
3:AC:126:GLY:O	3:AC:130:VAL:HG23	2.12	0.49
3:AC:154:LYS:HE2	3:AC:261:ARG:HD2	1.94	0.49
3:AC:405:ASN:HD22	27:AC:518:DGD:C5D	2.25	0.49
22:AD:404:CLA:C4	18:AX:26:GLY:HA3	2.34	0.49
1:BA:32:TRP:HA	1:BA:32:TRP:HE3	1.75	0.49
2:BB:435:GLU:O	2:BB:436:THR:C	2.56	0.49
3:BC:56:HIS:C	3:BC:58:GLY:N	2.70	0.49
3:BC:90:PRO:O	3:BC:94:THR:HG23	2.12	0.49
3:BC:473:ASP:CB	14:BT:26:PRO:HB3	2.37	0.49
29:BL:101:SQD:H45	14:BT:23:PHE:CD1	2.47	0.49
20:BZ:36:SER:C	20:BZ:38:GLN:N	2.70	0.49
1:AA:190:HIS:O	1:AA:298:ASN:HB3	2.13	0.49
1:AA:300:PHE:CZ	3:AC:404:LEU:HD23	2.48	0.49
3:AC:135:ARG:HB2	20:AZ:27:TYR:CG	2.48	0.49
3:AC:155:ASN:CA	3:AC:158:THR:HG22	2.39	0.49
3:AC:346:THR:O	13:AO:40:GLY:HA2	2.13	0.49
4:AD:323:GLU:HG2	13:AO:194:TYR:OH	2.12	0.49
13:AO:126:GLY:O	13:AO:128:ASP:N	2.45	0.49
15:AU:72:TYR:CB	15:AU:73:PRO:HD3	2.34	0.49
4:BD:87:HIS:ND1	27:BH:101:DGD:HD2	2.27	0.49
5:BE:9:PRO:HB3	30:BE:102:LMG:HC4	1.95	0.49
17:By:39:LEU:HD21	20:BZ:25:VAL:HA	1.93	0.49
3:AC:363:GLY:O	3:AC:364:PRO:C	2.56	0.49
3:AC:447:ARG:NH1	3:AC:447:ARG:CG	2.74	0.49
5:AE:9:PRO:HB3	30:AE:102:LMG:HC4	1.95	0.49
8:AI:6:ILE:O	8:AI:10:ILE:HG12	2.13	0.49
16:AV:45:ILE:HG12	16:AV:46:THR:N	2.28	0.49
17:Ay:21:GLN:O	17:Ay:21:GLN:HG2	2.13	0.49
1:BA:215:HIS:O	1:BA:216:GLY:C	2.56	0.49
22:BB:608:CLA:HBB1	22:BB:609:CLA:H51	1.95	0.49
1:AA:13:LEU:HD12	1:AA:13:LEU:N	2.28	0.49
1:AA:28:LEU:HD12	29:AA:415:SQD:H111	1.94	0.49
22:AA:403:CLA:HED1	24:AD:405:PL9:H372	1.95	0.49
2:AB:69:LEU:HD21	22:AB:603:CLA:HED3	1.95	0.49
2:AB:270:PRO:HG3	2:AB:312:TYR:CD2	2.43	0.49
2:AB:435:GLU:O	2:AB:436:THR:C	2.56	0.49
3:AC:90:PRO:O	3:AC:94:THR:HG23	2.12	0.49
3:AC:347:GLY:HA3	13:AO:43:ASN:HB2	1.95	0.49
3:AC:405:ASN:HB2	27:AC:518:DGD:HG31	1.95	0.49
9:AJ:11:TRP:CG	10:AK:42:ALA:HA	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:AK:15:TYR:HE2	20:AZ:62:VAL:HG21	1.78	0.49
3:BC:94:THR:HG22	3:BC:298:PRO:HD2	1.95	0.49
4:BD:67:TYR:CE1	4:BD:76:VAL:HG11	2.47	0.49
4:BD:86:GLY:HA2	4:BD:166:SER:HB3	1.94	0.49
5:BE:22:ILE:O	5:BE:26:THR:HG23	2.13	0.49
10:BK:18:PHE:O	10:BK:22:VAL:HG23	2.13	0.49
13:BO:86:ARG:C	13:BO:86:ARG:CD	2.84	0.49
13:BO:92:VAL:HG12	13:BO:93:PRO:CD	2.43	0.49
2:AB:69:LEU:HD12	22:AB:605:CLA:HBA1	1.95	0.48
7:AH:30:LEU:HD11	7:AH:34:PHE:HE1	1.78	0.48
13:AO:94:THR:HB	13:AO:135:GLN:O	2.12	0.48
1:BA:228:THR:HG22	1:BA:229:GLU:N	2.27	0.48
1:BA:278:TRP:HB3	1:BA:279:PRO:CD	2.42	0.48
1:BA:283:VAL:HG21	23:BA:406:PHO:HBC3	1.95	0.48
2:BB:35:GLY:O	2:BB:38:ALA:HB3	2.12	0.48
2:BB:413:ASP:O	2:BB:414:PRO:C	2.55	0.48
3:BC:35:TRP:CG	3:BC:36:TRP:N	2.81	0.48
3:BC:135:ARG:NE	20:BZ:33:TRP:HE1	2.11	0.48
3:BC:452:ALA:C	3:BC:454:GLY:N	2.68	0.48
4:BD:71:CYS:HB2	4:BD:76:VAL:HG12	1.95	0.48
7:BH:39:LEU:C	7:BH:39:LEU:HD23	2.38	0.48
22:AA:402:CLA:H202	22:AA:403:CLA:H93	1.96	0.48
2:AB:35:GLY:O	2:AB:38:ALA:HB3	2.13	0.48
26:AB:617:BCR:HC31	12:AM:10:ALA:HB2	1.94	0.48
32:AB:625:LMT:H3'	29:AD:409:SQD:H62	1.95	0.48
3:AC:208:VAL:O	3:AC:209:ILE:C	2.56	0.48
13:AO:159:VAL:HG13	13:AO:159:VAL:O	2.12	0.48
20:AZ:5:PHE:HA	20:AZ:57:LEU:HD21	1.95	0.48
1:BA:13:LEU:HD12	1:BA:13:LEU:N	2.27	0.48
1:BA:37:MET:HG2	1:BA:41:LEU:HD12	1.94	0.48
2:BB:125:ASP:OD2	2:BB:127:ARG:HB3	2.13	0.48
3:BC:89:ILE:N	3:BC:90:PRO:CD	2.74	0.48
3:BC:159:THR:HG23	3:BC:252:ILE:HD13	1.94	0.48
3:BC:258:GLY:C	3:BC:262:ARG:NH1	2.71	0.48
3:BC:342:MET:HE1	3:BC:356:MET:HE2	1.95	0.48
22:BC:503:CLA:H172	22:BC:510:CLA:HBB2	1.94	0.48
4:BD:49:LEU:HD13	26:BD:406:BCR:C15	2.43	0.48
10:BK:44:GLY:O	10:BK:45:PHE:C	2.56	0.48
13:BO:240:THR:HA	13:BO:264:VAL:HA	1.95	0.48
2:AB:175:THR:O	2:AB:176:GLY:O	2.31	0.48
2:AB:414:PRO:HB2	2:AB:415:PRO:CD	2.35	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:62:PHE:CE2	10:AK:29:PRO:HD3	2.48	0.48
4:AD:134:ARG:HA	4:AD:134:ARG:HE	1.78	0.48
4:AD:201:VAL:O	4:AD:205:LEU:HB2	2.13	0.48
5:AE:28:PRO:O	5:AE:32:ILE:HG13	2.13	0.48
1:BA:45:THR:HG23	1:BA:46:ILE:N	2.28	0.48
1:BA:214:MET:O	1:BA:215:HIS:C	2.54	0.48
1:BA:326:LEU:HD21	3:BC:412:THR:HB	1.94	0.48
3:BC:33:PHE:CD1	4:BD:229:ALA:HB3	2.48	0.48
3:BC:258:GLY:CA	3:BC:262:ARG:HH12	2.26	0.48
3:BC:425:TRP:CZ2	22:BC:504:CLA:HBA1	2.48	0.48
7:BH:30:LEU:HD11	7:BH:34:PHE:HE1	1.78	0.48
9:BJ:11:TRP:CG	10:BK:42:ALA:HA	2.48	0.48
13:BO:59:ASP:HB3	13:BO:62:GLN:HB3	1.95	0.48
13:BO:73:PRO:HG2	13:BO:102:THR:HB	1.95	0.48
1:AA:221:SER:HB2	4:AD:139:ARG:O	2.13	0.48
2:AB:154:GLY:O	2:AB:159:THR:HG23	2.13	0.48
2:AB:256:MET:O	2:AB:448:ARG:NH1	2.42	0.48
3:AC:413:GLU:HG3	3:AC:414:ILE:H	1.79	0.48
3:AC:425:TRP:CZ2	22:AC:504:CLA:HBA1	2.48	0.48
22:AC:501:CLA:HMB2	22:AC:501:CLA:H51	1.95	0.48
22:AC:504:CLA:H151	27:AC:517:DGD:HBW1	1.95	0.48
4:AD:193:LEU:HG	4:AD:193:LEU:O	2.14	0.48
5:AE:14:ILE:CG2	9:AJ:13:VAL:HG11	2.44	0.48
9:AJ:34:ALA:O	9:AJ:35:GLY:O	2.31	0.48
10:AK:17:ILE:C	10:AK:18:PHE:HD2	2.21	0.48
13:AO:77:LEU:HB3	13:AO:91:PHE:HB3	1.96	0.48
13:AO:226:ASN:HD22	13:AO:226:ASN:N	2.11	0.48
26:AA:409:BCR:H312	8:AI:15:PHE:HE1	1.79	0.48
3:AC:71:GLU:OE1	3:AC:89:ILE:HG13	2.13	0.48
22:AC:504:CLA:HED1	30:AC:519:LMG:O3	2.13	0.48
4:AD:62:GLY:HA3	5:AE:63:ILE:HD13	1.96	0.48
16:AV:64:ALA:O	16:AV:65:SER:C	2.56	0.48
34:AV:201:HEM:HHA	34:AV:201:HEM:HAD2	1.61	0.48
1:BA:72:LEU:HD21	32:BT:101:LMT:H31	1.96	0.48
2:BB:141:ILE:HG23	22:BB:618:CLA:HBB1	1.94	0.48
2:BB:262:THR:HG22	2:BB:263:THR:HG23	1.96	0.48
10:BK:17:ILE:H	10:BK:17:ILE:CD1	2.26	0.48
20:BZ:35:ARG:HG3	20:BZ:36:SER:N	2.28	0.48
2:AB:187:PRO:HB3	22:AB:601:CLA:HMB1	1.95	0.48
10:AK:20:PRO:O	10:AK:23:ASP:HB2	2.13	0.48
13:AO:86:ARG:NH1	13:AO:86:ARG:O	2.37	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:63:ILE:HB	3:BC:335:THR:HG21	1.94	0.48
1:BA:214:MET:HE3	23:BD:403:PHO:HMD2	1.96	0.48
2:BB:222:PRO:O	2:BB:223:GLN:C	2.56	0.48
22:BB:606:CLA:H193	7:BH:42:LEU:HD12	1.95	0.48
3:BC:216:SER:HB3	3:BC:221:GLU:HB2	1.95	0.48
7:BH:55:LEU:O	7:BH:58:VAL:HG12	2.12	0.48
13:BO:159:VAL:HG13	13:BO:159:VAL:O	2.13	0.48
16:BV:148:GLU:OE1	16:BV:148:GLU:HA	2.13	0.48
20:BZ:47:TRP:O	20:BZ:50:LEU:HB2	2.13	0.48
2:AB:86:ILE:HD12	2:AB:86:ILE:C	2.38	0.48
2:AB:224:ARG:HG3	7:AH:25:TRP:CD1	2.48	0.48
3:AC:315:MET:CE	3:AC:366:LEU:HD13	2.44	0.48
3:AC:367:GLU:HB2	3:AC:368:PRO:HD3	1.95	0.48
17:Ay:41:VAL:C	17:Ay:43:ARG:N	2.71	0.48
1:BA:258:LEU:HD12	4:BD:128:ARG:CD	2.42	0.48
1:BA:343:LEU:O	1:BA:344:ALA:CB	2.60	0.48
28:BC:521:LHG:H271	28:BC:521:LHG:H101	1.95	0.48
10:BK:46:ARG:NH1	10:BK:46:ARG:HB2	2.28	0.48
15:BU:72:TYR:HB3	15:BU:73:PRO:CD	2.37	0.48
3:AC:48:LYS:HD2	3:AC:138:GLU:HG3	1.94	0.48
3:AC:296:VAL:HG23	3:AC:297:TYR:CD2	2.49	0.48
5:AE:77:GLU:HA	5:AE:80:LEU:HD23	1.95	0.48
13:AO:194:TYR:CE1	13:AO:198:ILE:HD13	2.49	0.48
14:AT:25:GLU:O	14:AT:26:PRO:C	2.54	0.48
2:BB:137:LYS:O	2:BB:141:ILE:HG13	2.14	0.48
3:BC:452:ALA:O	3:BC:453:ALA:C	2.57	0.48
5:BE:10:PHE:HB2	30:BE:102:LMG:O2	2.14	0.48
6:BF:23:VAL:O	6:BF:27:ALA:CB	2.61	0.48
13:BO:173:ASN:ND2	13:BO:220:LYS:HD3	2.29	0.48
15:BU:66:ILE:HG13	15:BU:72:TYR:CD1	2.49	0.48
1:AA:13:LEU:H	1:AA:13:LEU:CD1	2.27	0.48
1:AA:159:LEU:C	1:AA:162:PRO:HD2	2.38	0.48
2:AB:120:LEU:HD13	22:AB:616:CLA:CMD	2.44	0.48
2:AB:434:THR:CG2	13:AO:204:LYS:HE3	2.44	0.48
22:AC:503:CLA:H172	22:AC:510:CLA:HBB2	1.95	0.48
11:AL:24:ILE:N	11:AL:24:ILE:HD12	2.29	0.48
2:BB:229:LEU:O	2:BB:230:ARG:C	2.56	0.48
3:BC:126:GLY:O	3:BC:130:VAL:HG23	2.13	0.48
3:BC:308:GLU:HB2	3:BC:361:PHE:CE1	2.49	0.48
11:BL:22:LEU:O	11:BL:26:VAL:HG13	2.14	0.48
13:BO:36:ILE:HD12	13:BO:36:ILE:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:111:PRO:O	1:AA:115:ILE:HG13	2.14	0.48
2:AB:329:PRO:CB	22:AB:607:CLA:HED1	2.39	0.48
3:AC:460:ASP:O	3:AC:461:ARG:C	2.55	0.48
4:AD:87:HIS:ND1	27:AH:102:DGD:HD2	2.29	0.48
4:AD:126:MET:CE	4:AD:150:ILE:HG13	2.43	0.48
4:AD:261:PHE:HB2	24:AD:405:PL9:H521	1.96	0.48
20:AZ:30:PRO:C	20:AZ:32:ASP:N	2.72	0.48
3:BC:81:MET:CE	3:BC:89:ILE:HG22	2.44	0.48
3:BC:265:ILE:HG12	22:BC:505:CLA:HED1	1.95	0.48
4:BD:210:LEU:HA	4:BD:213:ILE:HG22	1.96	0.48
5:BE:15:THR:O	9:BJ:8:ILE:HD12	2.14	0.48
10:BK:15:TYR:HE2	20:BZ:62:VAL:HG21	1.77	0.48
10:BK:37:PHE:HB3	26:BK:102:BCR:H402	1.95	0.48
29:BL:101:SQD:H45	14:BT:23:PHE:HD1	1.79	0.48
3:AC:116:VAL:HG23	3:AC:117:VAL:N	2.28	0.47
7:AH:39:LEU:HD23	7:AH:39:LEU:C	2.39	0.47
13:AO:184:ASP:OD2	13:AO:188:ARG:HB2	2.14	0.47
1:BA:13:LEU:H	1:BA:13:LEU:CD1	2.26	0.47
1:BA:279:PRO:CG	4:BD:212:ALA:HB2	2.44	0.47
2:BB:348:ASN:O	2:BB:349:LYS:C	2.56	0.47
2:BB:462:PHE:HA	22:BB:614:CLA:HMC2	1.96	0.47
3:BC:266:TRP:HB3	3:BC:271:TYR:OH	2.14	0.47
4:BD:126:MET:CE	4:BD:150:ILE:HG13	2.44	0.47
4:BD:261:PHE:O	4:BD:262:SER:HB3	2.14	0.47
30:BD:408:LMG:O10	11:BL:18:TYR:HB3	2.13	0.47
7:BH:63:LYS:C	7:BH:65:LEU:N	2.71	0.47
13:BO:157:PRO:O	13:BO:158:ASN:O	2.32	0.47
16:BV:81:ARG:HH11	16:BV:81:ARG:HG2	1.78	0.47
20:BZ:12:LEU:HB2	20:BZ:50:LEU:HD22	1.96	0.47
5:AE:8:ARG:HB2	6:AF:13:TYR:HB3	1.95	0.47
10:AK:44:GLY:O	10:AK:45:PHE:C	2.57	0.47
13:AO:36:ILE:HD12	13:AO:36:ILE:N	2.29	0.47
18:AX:32:LEU:O	18:AX:36:VAL:HG23	2.13	0.47
1:BA:188:ALA:HB2	1:BA:328:MET:HB2	1.94	0.47
2:BB:27:THR:HG22	2:BB:107:LEU:CD1	2.40	0.47
2:BB:224:ARG:HG3	7:BH:25:TRP:CD1	2.48	0.47
2:BB:349:LYS:HG3	2:BB:350:GLU:OE1	2.14	0.47
5:BE:51:ARG:O	5:BE:53:ASP:N	2.47	0.47
7:BH:31:MET:HE3	7:BH:35:MET:CE	2.37	0.47
8:BI:6:ILE:O	8:BI:10:ILE:HG12	2.14	0.47
10:BK:17:ILE:C	10:BK:18:PHE:HD2	2.20	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AE:22:ILE:O	5:AE:26:THR:HG23	2.14	0.47
1:BA:78:ILE:O	1:BA:176:ILE:HB	2.13	0.47
3:BC:391:ARG:HD2	3:BC:395:TYR:CZ	2.49	0.47
4:BD:36:LEU:C	4:BD:39:PRO:HD2	2.37	0.47
1:AA:136:ARG:NH2	8:AI:27:ASP:OD1	2.47	0.47
28:AA:411:LHG:HC12	22:AC:508:CLA:O1D	2.13	0.47
2:AB:235:GLU:OE1	2:AB:472:ARG:NH1	2.47	0.47
2:AB:265:ILE:HG13	2:AB:266:GLU:N	2.30	0.47
3:AC:33:PHE:CD1	4:AD:229:ALA:HB3	2.49	0.47
19:AY:11:UNK:C	19:AY:13:UNK:N	2.75	0.47
2:BB:124:ARG:HD3	2:BB:131:PRO:N	2.30	0.47
2:BB:256:MET:O	2:BB:448:ARG:NH1	2.45	0.47
3:BC:347:GLY:HA3	13:BO:43:ASN:HB2	1.95	0.47
4:BD:93:TRP:HA	4:BD:99:GLY:H	1.80	0.47
19:BY:11:UNK:C	19:BY:13:UNK:N	2.76	0.47
1:AA:12:ASN:O	1:AA:16:ARG:HG3	2.15	0.47
1:AA:124:SER:O	1:AA:127:MET:HB3	2.15	0.47
1:AA:255:PHE:HD2	1:AA:264:SER:HG	1.60	0.47
2:AB:10:THR:C	2:AB:12:LEU:N	2.71	0.47
2:AB:24:LEU:HB3	2:AB:111:ALA:HB2	1.96	0.47
2:AB:124:ARG:HG3	2:AB:124:ARG:NH1	2.26	0.47
14:AT:23:PHE:CD1	29:BB:601:SQD:H45	2.49	0.47
20:AZ:5:PHE:HE1	20:AZ:54:VAL:HG13	1.80	0.47
3:BC:55:ALA:HB1	26:BC:514:BCR:C37	2.44	0.47
3:BC:367:GLU:HB2	3:BC:368:PRO:HD3	1.97	0.47
3:BC:413:GLU:HG3	3:BC:414:ILE:H	1.80	0.47
2:AB:141:ILE:HG21	22:AB:615:CLA:HBB1	1.97	0.47
3:AC:135:ARG:NE	20:AZ:33:TRP:HE1	2.12	0.47
6:AF:23:VAL:O	6:AF:27:ALA:HB2	2.14	0.47
2:BB:234:ILE:C	2:BB:236:THR:H	2.23	0.47
2:BB:235:GLU:OE1	2:BB:472:ARG:NH1	2.48	0.47
3:BC:62:PHE:CE2	10:BK:29:PRO:HD3	2.49	0.47
28:BC:521:LHG:H162	26:BJ:102:BCR:H313	1.95	0.47
4:BD:263:ASN:O	4:BD:266:TRP:N	2.47	0.47
7:BH:11:LEU:C	7:BH:13:PRO:HD2	2.40	0.47
8:BI:30:ARG:O	8:BI:31:ASN:HB3	2.13	0.47
15:BU:100:ARG:NH1	15:BU:103:GLN:HG2	2.29	0.47
1:AA:206:PHE:CE2	22:AD:402:CLA:HBA1	2.50	0.47
2:AB:7:ARG:NH2	30:AB:621:LMG:O3	2.46	0.47
2:AB:124:ARG:HD3	2:AB:131:PRO:N	2.30	0.47
2:AB:234:ILE:C	2:AB:236:THR:H	2.23	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:458:PHE:HB3	22:AB:604:CLA:HBC2	1.97	0.47
3:AC:94:THR:HG22	3:AC:298:PRO:HD2	1.96	0.47
3:AC:250:TRP:HE1	22:AC:506:CLA:HED1	1.80	0.47
5:AE:35:TRP:CD1	5:AE:35:TRP:C	2.93	0.47
6:AF:41:GLN:OE1	9:AJ:31:GLY:HA3	2.15	0.47
15:AU:56:ASP:HB3	15:AU:60:THR:H	1.80	0.47
16:AV:148:GLU:OE1	16:AV:148:GLU:HA	2.15	0.47
1:BA:296:ASN:HB2	3:BC:400:PRO:O	2.14	0.47
2:BB:69:LEU:HD12	22:BB:608:CLA:HBA1	1.97	0.47
2:BB:175:THR:O	2:BB:176:GLY:O	2.33	0.47
2:BB:341:LYS:HA	2:BB:405:GLU:HB2	1.97	0.47
22:BB:615:CLA:H171	22:BB:616:CLA:HBB2	1.96	0.47
3:BC:205:ASP:OD1	3:BC:207:ARG:HB3	2.15	0.47
3:BC:365:TRP:CB	3:BC:391:ARG:HG2	2.44	0.47
4:BD:185:PHE:CE2	4:BD:289:LEU:HD12	2.49	0.47
5:BE:7:GLU:HB3	6:BF:19:ARG:CZ	2.45	0.47
7:BH:18:TYR:CG	7:BH:19:GLY:N	2.83	0.47
9:BJ:36:LEU:C	9:BJ:38:SER:H	2.22	0.47
10:BK:18:PHE:O	10:BK:19:ASP:C	2.57	0.47
13:BO:194:TYR:CE1	13:BO:198:ILE:HD13	2.50	0.47
16:BV:63:CYS:O	16:BV:64:ALA:C	2.56	0.47
17:By:24:MET:O	17:By:25:ILE:C	2.58	0.47
29:AA:412:SQD:H5	4:AD:232:PHE:HB3	1.96	0.47
2:AB:215:PHE:C	2:AB:215:PHE:CD2	2.93	0.47
4:AD:49:LEU:HD13	26:AD:406:BCR:C15	2.45	0.47
5:AE:4:THR:CG2	5:AE:5:THR:N	2.77	0.47
1:BA:107:TYR:HD1	13:BO:141:ARG:NH1	2.13	0.47
2:BB:173:GLY:HA3	2:BB:265:ILE:HD11	1.95	0.47
22:BB:611:CLA:CMD	22:BB:613:CLA:HAB	2.44	0.47
3:BC:109:PHE:HB3	3:BC:110:PRO:HD3	1.96	0.47
5:BE:14:ILE:CG2	9:BJ:13:VAL:HG11	2.45	0.47
13:BO:135:GLN:HG2	13:BO:141:ARG:HG3	1.96	0.47
16:BV:39:ASN:HD21	16:BV:43:LYS:HB3	1.79	0.47
16:BV:130:MET:SD	16:BV:133:LEU:HD12	2.54	0.47
20:BZ:30:PRO:C	20:BZ:32:ASP:N	2.72	0.47
1:AA:190:HIS:CB	1:AA:293:MET:HE2	2.38	0.47
2:AB:413:ASP:O	2:AB:414:PRO:C	2.57	0.47
22:AB:607:CLA:H193	11:AL:27:LEU:HD11	1.95	0.47
3:AC:27:ASP:OD1	3:AC:28:GLN:HG2	2.14	0.47
3:AC:33:PHE:HE1	4:AD:229:ALA:CB	2.27	0.47
3:AC:229:ASN:ND2	3:AC:232:ASP:OD1	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:365:TRP:CB	3:AC:391:ARG:HG2	2.45	0.47
4:AD:176:ALA:HA	4:AD:179:PHE:CD2	2.49	0.47
5:AE:15:THR:O	9:AJ:8:ILE:HD12	2.15	0.47
14:AT:4:ILE:HD13	26:AT:102:BCR:C38	2.44	0.47
14:AT:22:PHE:C	14:AT:23:PHE:CD2	2.93	0.47
16:AV:98:LEU:O	16:AV:102:MET:HG3	2.15	0.47
2:BB:150:CYS:HB2	22:BB:606:CLA:CMC	2.45	0.47
3:BC:34:ALA:HB2	4:BD:230:SER:CB	2.44	0.47
4:BD:303:ILE:CD1	12:BM:2:GLU:HG2	2.45	0.47
30:BI:101:LMG:H181	32:BI:102:LMT:H42	1.97	0.47
1:AA:306:VAL:HG11	1:AA:316:THR:HG23	1.96	0.47
3:AC:193:GLY:O	3:AC:194:GLY:O	2.33	0.47
4:AD:93:TRP:HA	4:AD:99:GLY:H	1.80	0.47
4:AD:122:LEU:HB3	4:AD:150:ILE:CD1	2.45	0.47
4:AD:261:PHE:O	4:AD:262:SER:HB3	2.14	0.47
4:AD:274:VAL:HG13	24:AD:405:PL9:H211	1.97	0.47
8:AI:30:ARG:O	8:AI:31:ASN:HB3	2.14	0.47
1:BA:11:ALA:HB1	1:BA:15:GLU:OE1	2.15	0.47
1:BA:12:ASN:O	1:BA:16:ARG:HG3	2.14	0.47
1:BA:258:LEU:O	4:BD:128:ARG:NH1	2.48	0.47
1:BA:317:TRP:O	1:BA:321:ILE:HG13	2.15	0.47
2:BB:463:PHE:C	2:BB:463:PHE:CD2	2.92	0.47
3:BC:405:ASN:HB2	27:BC:518:DGD:HG31	1.97	0.47
4:BD:89:LEU:HG	7:BH:50:ASN:OD1	2.15	0.47
8:BI:27:ASP:O	8:BI:28:PRO:C	2.56	0.47
17:By:42:ARG:HG2	17:By:42:ARG:NH1	2.27	0.47
1:AA:32:TRP:HA	1:AA:32:TRP:HE3	1.76	0.46
3:AC:53:HIS:HB3	22:AC:512:CLA:OBD	2.15	0.46
4:AD:14:TRP:CE3	18:AX:38:ILE:HD12	2.50	0.46
5:AE:8:ARG:HB2	6:AF:13:TYR:CB	2.45	0.46
13:AO:92:VAL:HG12	13:AO:93:PRO:CD	2.43	0.46
16:AV:102:MET:HE1	16:AV:141:ILE:CD1	2.45	0.46
2:BB:458:PHE:HB3	22:BB:607:CLA:HBC2	1.97	0.46
30:BE:102:LMG:O9	30:BE:102:LMG:HC71	2.15	0.46
13:BO:77:LEU:HB3	13:BO:91:PHE:HB3	1.97	0.46
16:BV:102:MET:HE1	16:BV:141:ILE:CD1	2.44	0.46
1:AA:96:ILE:C	1:AA:98:GLU:H	2.23	0.46
2:AB:348:ASN:O	2:AB:349:LYS:C	2.57	0.46
3:AC:258:GLY:CA	3:AC:262:ARG:HH12	2.28	0.46
7:AH:63:LYS:C	7:AH:65:LEU:N	2.70	0.46
13:AO:135:GLN:HG2	13:AO:141:ARG:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:40:THR:HG23	22:BA:407:CLA:HBB1	1.96	0.46
1:BA:60:ILE:HG23	1:BA:61:ASP:N	2.30	0.46
6:BF:11:VAL:CG1	6:BF:12:SER:N	2.77	0.46
1:AA:278:TRP:HB3	1:AA:279:PRO:CD	2.46	0.46
2:AB:216:HIS:HE1	22:AB:609:CLA:C1A	2.29	0.46
22:AB:606:CLA:H72	26:AB:620:BCR:H311	1.97	0.46
3:AC:328:VAL:HG23	3:AC:329:GLY:N	2.31	0.46
4:AD:60:THR:HG23	4:AD:61:HIS:HD2	1.75	0.46
13:AO:83:LYS:CG	13:AO:84:ASN:H	2.23	0.46
16:AV:68:VAL:HG13	16:AV:68:VAL:O	2.15	0.46
18:AX:12:ILE:C	18:AX:12:ILE:HD13	2.40	0.46
1:BA:92:HIS:CD2	3:BC:219:GLY:HA3	2.49	0.46
22:BB:611:CLA:H51	22:BB:612:CLA:H101	1.97	0.46
26:BB:620:BCR:HC31	12:BM:10:ALA:HB2	1.97	0.46
3:BC:258:GLY:HA3	3:BC:262:ARG:HH12	1.80	0.46
4:BD:122:LEU:HB3	4:BD:150:ILE:CD1	2.46	0.46
13:BO:72:GLN:O	13:BO:263:GLY:HA3	2.14	0.46
16:BV:98:LEU:O	16:BV:102:MET:HG3	2.16	0.46
2:AB:474:LEU:O	4:AD:134:ARG:NH1	2.48	0.46
27:AC:517:DGD:HBV1	28:AC:521:LHG:H151	1.98	0.46
4:AD:146:PHE:O	4:AD:150:ILE:HG12	2.14	0.46
2:BB:201:HIS:HD2	2:BB:202:HIS:ND1	2.13	0.46
2:BB:225:LEU:O	2:BB:226:TYR:C	2.59	0.46
2:BB:422:ARG:HG2	2:BB:422:ARG:HH11	1.80	0.46
27:BB:602:DGD:HD5	27:BB:602:DGD:HE1	1.66	0.46
4:BD:14:TRP:CE3	18:BX:38:ILE:HD12	2.51	0.46
13:BO:94:THR:HB	13:BO:135:GLN:O	2.14	0.46
17:By:24:MET:O	17:By:28:ILE:HG23	2.15	0.46
20:BZ:22:GLY:O	20:BZ:23:VAL:C	2.58	0.46
1:AA:239:PHE:O	14:AT:29:ILE:HA	2.14	0.46
1:AA:283:VAL:HG21	23:AA:405:PHO:HBC3	1.97	0.46
2:AB:341:LYS:HA	2:AB:405:GLU:HB2	1.98	0.46
3:AC:45:LEU:O	3:AC:46:SER:C	2.58	0.46
10:AK:35:LEU:HA	10:AK:38:VAL:HG23	1.96	0.46
12:AM:24:ILE:HG12	12:BM:24:ILE:HG12	1.98	0.46
1:BA:149:ALA:HB3	1:BA:150:PRO:CD	2.45	0.46
22:BA:403:CLA:H202	22:BA:404:CLA:H93	1.98	0.46
2:BB:265:ILE:HG13	2:BB:266:GLU:N	2.30	0.46
22:BD:404:CLA:C4	18:BX:26:GLY:HA3	2.36	0.46
5:BE:78:THR:HA	5:BE:81:GLU:HG2	1.98	0.46
13:BO:113:VAL:HA	13:BO:119:LEU:HD23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:BO:120:THR:HA	13:BO:153:ALA:O	2.15	0.46
13:BO:226:ASN:HD22	13:BO:226:ASN:N	2.13	0.46
3:AC:189:TRP:O	3:AC:190:ALA:C	2.59	0.46
9:AJ:36:LEU:C	9:AJ:38:SER:H	2.23	0.46
13:AO:113:VAL:HA	13:AO:119:LEU:HD23	1.97	0.46
1:BA:216:GLY:O	1:BA:220:THR:HG22	2.16	0.46
3:BC:33:PHE:HE1	4:BD:229:ALA:CB	2.28	0.46
3:BC:315:MET:O	3:BC:319:ILE:HG13	2.16	0.46
5:BE:64:PRO:HD3	5:BE:84:LYS:HE2	1.97	0.46
15:BU:56:ASP:HB3	15:BU:60:THR:H	1.80	0.46
1:AA:183:MET:HA	22:AA:402:CLA:HMD2	1.97	0.46
1:AA:216:GLY:O	1:AA:220:THR:HG22	2.16	0.46
2:AB:10:THR:O	2:AB:13:ILE:HG13	2.16	0.46
3:AC:34:ALA:HB2	4:AD:230:SER:CB	2.46	0.46
3:AC:258:GLY:HA3	3:AC:262:ARG:HH12	1.81	0.46
5:AE:17:VAL:HG22	9:AJ:8:ILE:HD11	1.97	0.46
10:AK:11:LEU:O	10:AK:12:PRO:C	2.59	0.46
16:AV:83:GLU:H	16:AV:83:GLU:CD	2.23	0.46
20:AZ:35:ARG:HG3	20:AZ:36:SER:N	2.30	0.46
1:BA:96:ILE:C	1:BA:98:GLU:H	2.24	0.46
2:BB:7:ARG:NH2	30:BB:623:LMG:O3	2.49	0.46
3:BC:223:TRP:CE3	3:BC:224:ILE:HG13	2.51	0.46
3:BC:362:ARG:O	27:BC:516:DGD:O4E	2.33	0.46
4:BD:26:ARG:HD3	6:BF:18:VAL:CG1	2.34	0.46
7:BH:16:SER:C	7:BH:18:TYR:H	2.23	0.46
18:BX:12:ILE:C	18:BX:12:ILE:HD13	2.40	0.46
2:AB:59:GLY:HA3	22:AB:607:CLA:HED1	1.98	0.46
2:AB:96:VAL:HG22	22:AB:606:CLA:HBA1	1.97	0.46
3:AC:342:MET:HE1	3:AC:356:MET:HE2	1.98	0.46
4:AD:217:THR:O	4:AD:221:THR:HB	2.15	0.46
8:AI:24:LEU:O	8:AI:26:GLY:N	2.41	0.46
12:AM:18:PRO:O	12:AM:21:PHE:HB3	2.16	0.46
20:AZ:23:VAL:HB	20:AZ:24:PRO:HD3	1.97	0.46
20:AZ:36:SER:C	20:AZ:38:GLN:H	2.24	0.46
1:BA:10:SER:C	1:BA:12:ASN:N	2.71	0.46
1:BA:192:ILE:CB	1:BA:293:MET:HE1	2.44	0.46
3:BC:318:LEU:HD23	3:BC:318:LEU:O	2.16	0.46
3:BC:328:VAL:HG23	3:BC:329:GLY:N	2.30	0.46
3:BC:405:ASN:HD22	27:BC:518:DGD:C5D	2.25	0.46
1:AA:24:THR:OG1	3:AC:469:MET:HE2	2.15	0.46
1:AA:40:THR:HG23	22:AA:406:CLA:HBB1	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:330:VAL:HG11	4:AD:348:ARG:HG2	1.98	0.46
2:AB:63:LEU:N	2:AB:64:PRO:HD2	2.30	0.46
2:AB:208:VAL:HG21	22:AB:602:CLA:HMC3	1.98	0.46
2:AB:463:PHE:C	2:AB:463:PHE:CD2	2.94	0.46
3:AC:342:MET:HE3	3:AC:352:GLY:HA2	1.98	0.46
22:AC:509:CLA:HBD	22:AC:509:CLA:H121	1.97	0.46
10:AK:37:PHE:HB3	26:AK:102:BCR:H402	1.97	0.46
14:AT:22:PHE:C	14:AT:23:PHE:HD2	2.24	0.46
16:AV:54:GLU:OE1	16:AV:54:GLU:HA	2.16	0.46
1:BA:221:SER:HB2	4:BD:139:ARG:O	2.15	0.46
2:BB:12:LEU:O	2:BB:14:ASN:N	2.49	0.46
2:BB:141:ILE:O	2:BB:144:PHE:HB3	2.16	0.46
3:BC:101:PRO:O	3:BC:104:GLU:HB2	2.16	0.46
3:BC:142:GLU:C	3:BC:144:SER:H	2.22	0.46
3:BC:202:PRO:HB2	3:BC:235:GLY:HA2	1.97	0.46
4:BD:19:ASP:O	4:BD:20:ASP:C	2.57	0.46
16:BV:54:GLU:OE1	16:BV:54:GLU:HA	2.15	0.46
17:By:32:GLY:N	17:By:33:PRO:HD2	2.30	0.46
2:AB:71:VAL:HG21	2:AB:96:VAL:HG21	1.98	0.46
2:AB:329:PRO:HD3	22:AB:607:CLA:CED	2.46	0.46
2:AB:444:ARG:HH11	2:AB:444:ARG:HG3	1.81	0.46
14:AT:23:PHE:HD1	29:BB:601:SQD:H45	1.81	0.46
22:BB:609:CLA:H3A	22:BB:609:CLA:HBA2	1.55	0.46
3:BC:315:MET:CE	3:BC:366:LEU:HD13	2.46	0.46
4:BD:128:ARG:O	4:BD:129:GLN:C	2.59	0.46
4:BD:154:VAL:O	4:BD:158:LEU:HB2	2.16	0.46
15:BU:72:TYR:CB	15:BU:73:PRO:CD	2.94	0.46
1:AA:262:TYR:O	30:AE:102:LMG:H112	2.16	0.45
22:AB:608:CLA:H92	29:AD:409:SQD:H172	1.97	0.45
3:AC:258:GLY:C	3:AC:262:ARG:NH1	2.74	0.45
4:AD:128:ARG:O	4:AD:129:GLN:C	2.59	0.45
7:AH:31:MET:HE3	7:AH:35:MET:CE	2.40	0.45
13:AO:86:ARG:HD2	13:AO:87:GLN:N	2.31	0.45
13:AO:116:ASP:OD2	13:AO:116:ASP:C	2.58	0.45
20:AZ:36:SER:C	20:AZ:38:GLN:N	2.69	0.45
1:BA:42:LEU:HD23	29:BA:401:SQD:H192	1.98	0.45
3:BC:82:TYR:HA	3:BC:422:PRO:HG2	1.98	0.45
3:BC:163:PHE:CD1	3:BC:252:ILE:HD11	2.51	0.45
3:BC:235:GLY:O	3:BC:238:ILE:HB	2.15	0.45
3:BC:435:PHE:O	3:BC:438:LEU:N	2.47	0.45
4:BD:274:VAL:HG13	24:BD:405:PL9:H211	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BH:21:VAL:HG23	7:BH:22:ALA:O	2.15	0.45
8:BI:24:LEU:O	8:BI:26:GLY:N	2.41	0.45
18:BX:44:ASP:O	18:BX:45:LYS:HB3	2.16	0.45
2:AB:450:TRP:NE1	22:AB:607:CLA:HBA1	2.32	0.45
22:AB:608:CLA:CMD	22:AB:610:CLA:HAB	2.46	0.45
7:AH:21:VAL:HG23	7:AH:22:ALA:O	2.16	0.45
17:Ay:42:ARG:HG2	17:Ay:42:ARG:NH1	2.30	0.45
2:BB:215:PHE:C	2:BB:215:PHE:CD2	2.95	0.45
2:BB:444:ARG:HH11	2:BB:444:ARG:HG3	1.82	0.45
2:BB:484:PRO:O	2:BB:485:GLU:HG2	2.16	0.45
22:BB:609:CLA:H72	26:BB:622:BCR:H311	1.98	0.45
3:BC:455:PHE:C	3:BC:457:LYS:H	2.24	0.45
22:BC:509:CLA:HBD	22:BC:509:CLA:H121	1.97	0.45
4:BD:221:THR:CG2	4:BD:244:TYR:HB2	2.45	0.45
2:AB:447:PRO:O	2:AB:448:ARG:C	2.59	0.45
3:AC:49:LEU:O	3:AC:53:HIS:ND1	2.43	0.45
3:AC:142:GLU:C	3:AC:144:SER:H	2.24	0.45
3:AC:210:PHE:HZ	3:AC:243:ILE:HD11	1.81	0.45
11:AL:31:PHE:HB3	11:AL:35:PHE:CE1	2.51	0.45
15:AU:99:GLU:HA	15:AU:102:LYS:HE3	1.99	0.45
22:BA:403:CLA:HBB1	22:BD:402:CLA:NC	2.32	0.45
2:BB:289:GLN:OE1	2:BB:292:LEU:HD12	2.17	0.45
34:BE:101:HEM:CBC	6:BF:27:ALA:HB1	2.39	0.45
13:BO:56:TYR:O	13:BO:161:SER:HA	2.17	0.45
13:BO:116:ASP:OD1	13:BO:157:PRO:HB3	2.16	0.45
1:AA:45:THR:HG23	1:AA:46:ILE:N	2.31	0.45
1:AA:258:LEU:HD12	4:AD:128:ARG:CD	2.42	0.45
2:AB:241:SER:HB3	22:AB:612:CLA:HED3	1.97	0.45
30:AD:408:LMG:O10	11:AL:18:TYR:HB3	2.16	0.45
26:AJ:102:BCR:H361	26:AJ:102:BCR:H20C	1.83	0.45
12:AM:3:VAL:HG11	14:AT:2:GLU:HG2	1.99	0.45
1:BA:10:SER:OG	1:BA:13:LEU:HD12	2.16	0.45
26:BA:410:BCR:H312	8:BI:15:PHE:HE1	1.82	0.45
2:BB:187:PRO:C	2:BB:189:GLY:H	2.24	0.45
2:BB:270:PRO:HG3	2:BB:312:TYR:CD2	2.45	0.45
3:BC:53:HIS:HB3	22:BC:512:CLA:OBD	2.16	0.45
3:BC:406:SER:HA	3:BC:420:VAL:CG2	2.46	0.45
5:BE:77:GLU:HA	5:BE:80:LEU:HD23	1.97	0.45
1:AA:129:ARG:C	1:AA:131:TRP:H	2.23	0.45
1:AA:317:TRP:CD1	4:AD:177:ALA:HB2	2.52	0.45
1:AA:330:VAL:HG12	4:AD:348:ARG:HA	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:318:LEU:HD23	3:AC:318:LEU:O	2.16	0.45
4:AD:185:PHE:CE2	4:AD:289:LEU:HD12	2.52	0.45
4:AD:213:ILE:HG23	4:AD:214:HIS:N	2.30	0.45
5:AE:7:GLU:HB3	6:AF:19:ARG:CZ	2.47	0.45
5:AE:10:PHE:HB2	30:AE:102:LMG:O2	2.16	0.45
13:AO:144:LEU:CD1	13:AO:259:VAL:HG11	2.45	0.45
15:AU:100:ARG:NH1	15:AU:103:GLN:HG2	2.31	0.45
2:BB:141:ILE:HG21	22:BB:618:CLA:HBB1	1.97	0.45
2:BB:208:VAL:HG21	22:BB:605:CLA:HMC3	1.99	0.45
4:BD:302:GLU:OE1	4:BD:302:GLU:HA	2.17	0.45
4:BD:303:ILE:HD13	12:BM:2:GLU:HG2	1.99	0.45
5:BE:61:ARG:HH22	16:BV:153:GLY:HA3	1.82	0.45
10:BK:21:LEU:HD11	26:BK:102:BCR:C3	2.46	0.45
11:BL:31:PHE:HB3	11:BL:35:PHE:CE1	2.51	0.45
13:BO:70:CYS:O	13:BO:265:PHE:HB2	2.15	0.45
13:BO:184:ASP:OD2	13:BO:188:ARG:HB2	2.16	0.45
16:BV:116:GLU:O	16:BV:116:GLU:HG3	2.16	0.45
1:AA:11:ALA:HB1	1:AA:15:GLU:OE1	2.17	0.45
1:AA:202:VAL:O	1:AA:206:PHE:HB2	2.17	0.45
1:AA:212:CYS:HB2	4:AD:211:CYS:HB2	1.99	0.45
3:AC:284:PHE:HB3	27:AC:516:DGD:HA51	1.99	0.45
3:AC:308:GLU:HB2	3:AC:361:PHE:CE1	2.51	0.45
7:AH:63:LYS:C	7:AH:65:LEU:H	2.24	0.45
13:AO:56:TYR:O	13:AO:161:SER:HA	2.17	0.45
13:AO:132:VAL:O	13:AO:144:LEU:HD23	2.17	0.45
15:AU:80:VAL:HG22	15:AU:127:ARG:NH2	2.31	0.45
1:BA:227:THR:HA	1:BA:231:GLU:OE2	2.17	0.45
2:BB:59:GLY:HA3	22:BB:610:CLA:HED1	1.98	0.45
11:BL:24:ILE:HD12	11:BL:24:ILE:N	2.31	0.45
13:BO:120:THR:HG22	13:BO:154:SER:CB	2.47	0.45
13:BO:126:GLY:O	13:BO:128:ASP:N	2.50	0.45
15:BU:58:ASN:HD22	15:BU:114:VAL:HG13	1.82	0.45
17:By:41:VAL:C	17:By:43:ARG:N	2.72	0.45
1:AA:258:LEU:O	4:AD:128:ARG:NH1	2.49	0.45
1:AA:317:TRP:HZ3	4:AD:180:ARG:CD	2.19	0.45
2:AB:306:PRO:HG2	2:AB:309:LEU:HB2	1.98	0.45
7:AH:9:ASP:O	7:AH:12:ARG:HB3	2.17	0.45
7:AH:11:LEU:C	7:AH:13:PRO:HD2	2.42	0.45
10:AK:18:PHE:O	10:AK:22:VAL:HG23	2.16	0.45
1:BA:182:PHE:O	1:BA:186:PHE:HB2	2.17	0.45
30:BA:414:LMG:H421	22:BB:614:CLA:H142	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BB:216:HIS:HE1	22:BB:612:CLA:C1A	2.30	0.45
2:BB:229:LEU:O	2:BB:231:MET:N	2.50	0.45
2:BB:284:ILE:HG23	2:BB:305:ILE:CD1	2.44	0.45
2:BB:474:LEU:O	4:BD:134:ARG:NH1	2.49	0.45
3:BC:176:VAL:HG11	3:BC:238:ILE:HG12	1.99	0.45
3:BC:457:LYS:HE3	4:BD:228:GLY:O	2.17	0.45
4:BD:238:THR:O	4:BD:239:GLN:C	2.59	0.45
5:BE:17:VAL:HG22	9:BJ:8:ILE:HD11	1.98	0.45
5:BE:72:ALA:O	5:BE:76:VAL:HG23	2.16	0.45
8:BI:7:THR:O	8:BI:8:VAL:C	2.59	0.45
1:AA:72:LEU:HD21	32:AT:101:LMT:H31	1.99	0.45
3:AC:176:VAL:HG11	3:AC:238:ILE:HG12	1.99	0.45
3:AC:451:ALA:HA	3:AC:456:GLU:CD	2.41	0.45
4:AD:67:TYR:CE1	4:AD:76:VAL:HG11	2.51	0.45
4:AD:90:LEU:HD23	4:AD:90:LEU:HA	1.79	0.45
12:AM:28:GLN:CB	12:BM:27:VAL:HG12	2.47	0.45
17:Ay:32:GLY:N	17:Ay:33:PRO:HD2	2.32	0.45
22:BA:404:CLA:HED2	4:BD:198:MET:SD	2.57	0.45
2:BB:306:PRO:HG2	2:BB:309:LEU:HB2	1.99	0.45
2:BB:380:ASP:C	2:BB:380:ASP:OD1	2.59	0.45
2:BB:385:ARG:O	2:BB:386:ALA:C	2.60	0.45
3:BC:49:LEU:O	3:BC:53:HIS:ND1	2.43	0.45
3:BC:143:TYR:O	3:BC:144:SER:CB	2.65	0.45
3:BC:193:GLY:O	3:BC:194:GLY:O	2.34	0.45
3:BC:208:VAL:O	3:BC:209:ILE:C	2.60	0.45
6:BF:23:VAL:O	6:BF:27:ALA:HB2	2.17	0.45
7:BH:63:LYS:C	7:BH:65:LEU:H	2.23	0.45
13:BO:184:ASP:C	13:BO:184:ASP:OD1	2.59	0.45
20:BZ:5:PHE:HE1	20:BZ:54:VAL:HG13	1.80	0.45
20:BZ:36:SER:HA	20:BZ:39:LEU:CD1	2.46	0.45
2:AB:474:LEU:HD11	22:AB:608:CLA:HAA1	1.98	0.45
22:AB:607:CLA:HBA2	22:AB:607:CLA:H3A	1.68	0.45
3:AC:245:ILE:O	3:AC:249:ILE:HG12	2.16	0.45
3:AC:457:LYS:HE3	4:AD:228:GLY:O	2.17	0.45
4:AD:303:ILE:HD13	12:AM:2:GLU:HG2	1.97	0.45
5:AE:51:ARG:O	5:AE:53:ASP:N	2.49	0.45
15:AU:72:TYR:HB3	15:AU:73:PRO:CD	2.34	0.45
15:AU:80:VAL:HG22	15:AU:127:ARG:HH21	1.82	0.45
1:BA:183:MET:HA	22:BA:403:CLA:HMD2	1.98	0.45
1:BA:222:SER:O	1:BA:246:TYR:HB2	2.16	0.45
1:BA:292:THR:C	1:BA:294:ALA:H	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BB:10:THR:O	2:BB:13:ILE:HG13	2.17	0.45
3:BC:284:PHE:HB3	27:BC:516:DGD:HA51	1.99	0.45
30:BC:519:LMG:H172	10:BK:27:VAL:HG11	1.99	0.45
4:BD:146:PHE:O	4:BD:150:ILE:HG12	2.17	0.45
4:BD:239:GLN:HB3	4:BD:240:ALA:H	1.34	0.45
7:BH:63:LYS:O	7:BH:64:ALA:HB3	2.17	0.45
13:BO:248:ASP:CG	13:BO:250:ASP:H	2.24	0.45
2:AB:141:ILE:O	2:AB:144:PHE:HB3	2.17	0.45
2:AB:169:SER:O	7:AH:65:LEU:HG	2.16	0.45
2:AB:225:LEU:O	2:AB:226:TYR:C	2.60	0.45
3:AC:225:VAL:HG13	3:AC:289:PHE:HA	1.99	0.45
3:AC:435:PHE:O	3:AC:438:LEU:N	2.49	0.45
4:AD:199:MET:O	4:AD:200:GLY:C	2.59	0.45
13:AO:120:THR:HG22	13:AO:154:SER:CB	2.47	0.45
16:AV:119:PRO:HG3	16:AV:127:PHE:CD1	2.52	0.45
2:BB:187:PRO:HB3	22:BB:604:CLA:CMB	2.47	0.45
2:BB:237:VAL:HG22	22:BB:613:CLA:HBC2	2.00	0.45
2:BB:329:PRO:HD3	22:BB:610:CLA:CED	2.46	0.45
22:BB:611:CLA:HMA1	4:BD:130:PHE:CE1	2.51	0.45
3:BC:27:ASP:OD1	3:BC:28:GLN:HG2	2.17	0.45
4:BD:253:TRP:HB2	4:BD:260:ALA:HB2	1.99	0.45
5:BE:63:ILE:HG23	5:BE:64:PRO:HD2	1.99	0.45
5:BE:69:ARG:HG3	5:BE:70:PHE:N	2.32	0.45
12:BM:33:GLN:HG2	12:BM:34:LYS:N	2.30	0.45
13:BO:81:GLU:C	13:BO:83:LYS:H	2.25	0.45
1:AA:183:MET:HG2	22:AA:403:CLA:HBC1	1.98	0.44
3:AC:35:TRP:CG	3:AC:36:TRP:N	2.84	0.44
3:AC:110:PRO:O	3:AC:114:VAL:HG23	2.17	0.44
5:AE:64:PRO:HD3	5:AE:84:LYS:HE2	1.98	0.44
10:AK:23:ASP:CB	17:Ay:21:GLN:HE21	2.30	0.44
1:BA:129:ARG:C	1:BA:131:TRP:H	2.25	0.44
1:BA:238:LYS:HD3	1:BA:238:LYS:HA	1.86	0.44
1:BA:262:TYR:O	30:BE:102:LMG:H112	2.17	0.44
27:BB:602:DGD:HA21	32:BB:603:LMT:H121	1.98	0.44
3:BC:425:TRP:HE1	27:BC:517:DGD:HE62	1.82	0.44
26:BJ:102:BCR:H20C	26:BJ:102:BCR:H361	1.81	0.44
15:BU:82:ASN:ND2	15:BU:94:ILE:HG23	2.32	0.44
15:BU:89:GLU:C	15:BU:91:VAL:N	2.75	0.44
16:BV:64:ALA:O	16:BV:65:SER:C	2.60	0.44
2:AB:191:ASN:HB2	7:AH:58:VAL:HG22	1.98	0.44
22:AC:505:CLA:H42	26:AC:515:BCR:H342	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AE:63:ILE:HG23	5:AE:64:PRO:HD2	1.99	0.44
8:AI:4:LEU:O	8:AI:8:VAL:HG23	2.17	0.44
13:AO:173:ASN:ND2	13:AO:220:LYS:HD3	2.32	0.44
16:AV:39:ASN:HD21	16:AV:43:LYS:HB3	1.82	0.44
1:BA:210:LEU:HG	23:BD:403:PHO:NC	2.33	0.44
2:BB:191:ASN:HB2	7:BH:58:VAL:HG22	1.98	0.44
3:BC:84:GLN:C	3:BC:86:LEU:HD13	2.43	0.44
3:BC:155:ASN:C	3:BC:158:THR:HG22	2.42	0.44
4:BD:201:VAL:O	4:BD:205:LEU:HB2	2.17	0.44
5:BE:51:ARG:O	5:BE:54:SER:N	2.50	0.44
6:BF:11:VAL:CG1	6:BF:12:SER:H	2.25	0.44
13:BO:109:GLY:HA3	13:BO:122:VAL:O	2.16	0.44
1:AA:12:ASN:O	1:AA:13:LEU:C	2.60	0.44
1:AA:214:MET:HE3	23:AD:403:PHO:HMD2	1.99	0.44
22:AA:402:CLA:HBB1	22:AD:402:CLA:NC	2.32	0.44
2:AB:222:PRO:O	2:AB:223:GLN:C	2.59	0.44
2:AB:283:GLU:HA	2:AB:283:GLU:OE1	2.17	0.44
3:AC:170:ILE:HD13	22:AC:513:CLA:H201	1.98	0.44
3:AC:276:LEU:CD1	3:AC:444:HIS:HD2	2.30	0.44
3:AC:425:TRP:HE1	27:AC:517:DGD:HE62	1.81	0.44
30:AC:519:LMG:H172	10:AK:27:VAL:HG11	1.99	0.44
10:AK:18:PHE:O	10:AK:19:ASP:C	2.60	0.44
13:AO:72:GLN:O	13:AO:263:GLY:HA3	2.17	0.44
13:AO:218:LEU:HD22	15:AU:119:THR:CG2	2.45	0.44
18:AX:16:LEU:HD11	18:AX:20:PHE:CE2	2.53	0.44
18:AX:44:ASP:O	18:AX:45:LYS:HB3	2.17	0.44
2:BB:450:TRP:NE1	22:BB:610:CLA:HBA1	2.33	0.44
22:BB:617:CLA:H51	26:BB:620:BCR:H372	2.00	0.44
3:BC:50:LEU:O	3:BC:54:VAL:HG23	2.18	0.44
3:BC:210:PHE:HZ	3:BC:243:ILE:HD11	1.82	0.44
26:BC:514:BCR:H11C	26:BK:102:BCR:H322	1.99	0.44
13:BO:132:VAL:O	13:BO:144:LEU:HD23	2.17	0.44
13:BO:171:GLU:HA	13:BO:221:GLY:O	2.17	0.44
2:AB:15:ASP:O	2:AB:17:GLY:N	2.50	0.44
2:AB:187:PRO:HB3	22:AB:601:CLA:CMB	2.47	0.44
22:AB:614:CLA:H51	26:AB:617:BCR:H372	1.99	0.44
3:AC:33:PHE:CE1	4:AD:229:ALA:HB3	2.53	0.44
1:BA:185:VAL:O	1:BA:186:PHE:C	2.59	0.44
1:BA:224:ILE:O	1:BA:226:GLU:OE2	2.36	0.44
22:BC:508:CLA:H172	27:BC:517:DGD:HBW2	2.00	0.44
4:BD:176:ALA:C	4:BD:178:ILE:H	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BD:330:ALA:HB3	4:BD:331:PRO:HD3	1.99	0.44
7:BH:53:LEU:HD21	7:BH:55:LEU:HD21	1.99	0.44
10:BK:43:VAL:O	10:BK:46:ARG:HG3	2.18	0.44
14:BT:16:LEU:O	14:BT:17:PHE:C	2.60	0.44
20:BZ:24:PRO:C	20:BZ:26:ALA:N	2.75	0.44
20:BZ:36:SER:C	20:BZ:38:GLN:H	2.25	0.44
1:AA:99:ALA:O	8:AI:1:MET:HE3	2.17	0.44
1:AA:296:ASN:HB2	3:AC:400:PRO:O	2.17	0.44
2:AB:71:VAL:HG21	2:AB:96:VAL:CG2	2.47	0.44
3:AC:235:GLY:O	3:AC:238:ILE:HB	2.18	0.44
3:AC:449:ARG:NE	22:AC:505:CLA:HED1	2.22	0.44
7:AH:28:THR:O	7:AH:31:MET:HB3	2.18	0.44
8:AI:11:VAL:HG22	32:AI:102:LMT:H82	2.00	0.44
11:AL:36:PHE:O	11:AL:37:ASN:C	2.61	0.44
13:AO:116:ASP:OD1	13:AO:157:PRO:HB3	2.18	0.44
1:BA:39:PRO:HB2	22:BA:407:CLA:CBB	2.48	0.44
3:BC:363:GLY:O	3:BC:367:GLU:HG2	2.17	0.44
4:BD:333:ASP:C	4:BD:335:PRO:HD3	2.42	0.44
12:BM:33:GLN:CG	12:BM:34:LYS:N	2.81	0.44
1:AA:110:GLY:O	1:AA:111:PRO:C	2.60	0.44
2:AB:18:ARG:HD2	2:AB:115:TRP:CE3	2.52	0.44
2:AB:271:THR:CG2	2:AB:273:TYR:HB2	2.48	0.44
3:AC:163:PHE:CD1	3:AC:252:ILE:HD11	2.52	0.44
28:AC:521:LHG:H101	28:AC:521:LHG:H271	2.00	0.44
4:AD:126:MET:HE3	4:AD:150:ILE:HG13	1.99	0.44
4:AD:209:LEU:O	4:AD:213:ILE:HG22	2.18	0.44
6:AF:16:PHE:O	29:AF:101:SQD:H461	2.18	0.44
26:AJ:102:BCR:H24C	26:AJ:102:BCR:H371	1.79	0.44
13:AO:230:VAL:CG1	13:AO:231:ASP:N	2.70	0.44
16:AV:59:PHE:CD1	16:AV:63:CYS:SG	3.08	0.44
1:BA:21:VAL:HG11	1:BA:32:TRP:CE3	2.53	0.44
1:BA:77:ILE:HG12	14:BT:6:TYR:CD1	2.53	0.44
2:BB:329:PRO:CB	22:BB:610:CLA:HED1	2.43	0.44
22:BB:610:CLA:H193	11:BL:27:LEU:HD11	1.99	0.44
3:BC:225:VAL:HG13	3:BC:289:PHE:HA	1.99	0.44
4:BD:180:ARG:HH11	4:BD:180:ARG:HG3	1.78	0.44
4:BD:253:TRP:HA	4:BD:256:ILE:HG23	1.99	0.44
13:BO:69:LEU:HB3	13:BO:107:ILE:CB	2.36	0.44
13:BO:178:ARG:HD2	13:BO:182:PHE:CG	2.53	0.44
1:AA:107:TYR:HD1	13:AO:141:ARG:NH1	2.16	0.44
1:AA:129:ARG:C	1:AA:131:TRP:N	2.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:15:ASP:O	2:AB:16:PRO:C	2.61	0.44
2:AB:27:THR:CG2	2:AB:107:LEU:HD13	2.45	0.44
3:AC:55:ALA:HB1	26:AC:514:BCR:C37	2.46	0.44
3:AC:338:GLY:O	3:AC:339:LYS:C	2.60	0.44
1:BA:153:SER:HB2	22:BA:403:CLA:H43	2.00	0.44
1:BA:244:GLU:CD	1:BA:245:THR:H	2.26	0.44
2:BB:7:ARG:HG2	22:BB:614:CLA:CED	2.48	0.44
3:BC:45:LEU:O	3:BC:46:SER:C	2.60	0.44
4:BD:101:PHE:O	4:BD:104:TRP:HB3	2.17	0.44
5:BE:20:TRP:HD1	9:BJ:8:ILE:HD13	1.83	0.44
13:BO:86:ARG:HD2	13:BO:87:GLN:N	2.32	0.44
13:BO:86:ARG:O	13:BO:86:ARG:HG3	2.16	0.44
1:AA:42:LEU:HA	1:AA:45:THR:HG22	2.00	0.44
2:AB:185:TRP:CE3	22:AB:601:CLA:H61	2.53	0.44
2:AB:206:GLY:O	2:AB:210:ILE:HG13	2.18	0.44
2:AB:263:THR:HB	2:AB:448:ARG:HH12	1.82	0.44
2:AB:422:ARG:HG2	2:AB:422:ARG:HH11	1.81	0.44
3:AC:50:LEU:O	3:AC:54:VAL:HG23	2.17	0.44
3:AC:143:TYR:O	3:AC:144:SER:CB	2.64	0.44
26:AC:514:BCR:H11C	26:AK:102:BCR:H322	2.00	0.44
7:AH:16:SER:C	7:AH:18:TYR:H	2.25	0.44
3:BC:245:ILE:O	3:BC:249:ILE:HG12	2.18	0.44
5:BE:34:GLY:O	5:BE:37:PHE:HB3	2.17	0.44
5:BE:35:TRP:C	5:BE:35:TRP:CD1	2.95	0.44
1:AA:64:ARG:O	13:AO:178:ARG:NH2	2.51	0.44
1:AA:220:THR:O	1:AA:223:LEU:HG	2.18	0.44
1:AA:247:ASN:HB3	1:AA:250:ALA:HB3	2.00	0.44
2:AB:298:LEU:HD12	2:AB:298:LEU:HA	1.75	0.44
2:AB:380:ASP:C	2:AB:380:ASP:OD1	2.60	0.44
3:AC:82:TYR:HA	3:AC:422:PRO:HG2	2.00	0.44
3:AC:269:GLU:O	3:AC:272:LEU:HB3	2.18	0.44
4:AD:253:TRP:HB2	4:AD:260:ALA:HB2	2.00	0.44
16:AV:81:ARG:HG2	16:AV:81:ARG:HH11	1.83	0.44
1:BA:12:ASN:O	1:BA:15:GLU:HB3	2.18	0.44
2:BB:59:GLY:HA3	22:BB:610:CLA:CED	2.48	0.44
2:BB:137:LYS:NZ	7:BH:14:LEU:O	2.51	0.44
3:BC:140:LEU:HB2	3:BC:148:GLY:HA2	2.00	0.44
3:BC:229:ASN:ND2	3:BC:232:ASP:OD1	2.43	0.44
4:BD:213:ILE:HG23	4:BD:214:HIS:N	2.32	0.44
30:BI:101:LMG:H132	32:BI:102:LMT:O2'	2.18	0.44
1:AA:182:PHE:O	1:AA:186:PHE:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:238:LYS:HA	1:AA:238:LYS:HD3	1.86	0.43
2:AB:118:TRP:CH2	11:AL:5:PRO:HD2	2.53	0.43
3:AC:148:GLY:O	3:AC:156:LYS:NZ	2.51	0.43
3:AC:472:LEU:HD12	3:AC:473:ASP:N	2.28	0.43
34:AE:101:HEM:HBC2	6:AF:27:ALA:CB	2.39	0.43
13:AO:59:ASP:C	13:AO:61:SER:N	2.76	0.43
20:AZ:5:PHE:CG	20:AZ:61:VAL:HG21	2.53	0.43
1:BA:183:MET:HG2	22:BA:404:CLA:HBC1	1.99	0.43
2:BB:383:PHE:O	13:BO:192:SER:HA	2.18	0.43
22:BB:611:CLA:H92	29:BD:409:SQD:H172	2.00	0.43
4:BD:176:ALA:C	4:BD:178:ILE:N	2.76	0.43
5:BE:36:LEU:HA	5:BE:39:SER:OG	2.18	0.43
8:BI:6:ILE:CD1	32:BI:102:LMT:H5'	2.48	0.43
15:BU:73:PRO:HG2	16:BV:107:THR:HB	2.00	0.43
20:BZ:5:PHE:CD2	20:BZ:61:VAL:HG21	2.53	0.43
1:AA:217:SER:O	1:AA:220:THR:HG22	2.18	0.43
2:AB:442:ILE:HD11	13:AO:200:LEU:HD23	2.00	0.43
2:AB:484:PRO:O	2:AB:485:GLU:HG2	2.18	0.43
3:AC:386:PRO:HB3	16:AV:116:GLU:HG2	2.00	0.43
26:AC:514:BCR:HC22	10:AK:18:PHE:HD1	1.83	0.43
4:AD:190:ASN:HB2	4:AD:296:TYR:CD1	2.52	0.43
4:AD:303:ILE:CD1	12:AM:2:GLU:HG2	2.48	0.43
4:AD:329:MET:O	4:AD:330:ALA:C	2.61	0.43
4:AD:333:ASP:C	4:AD:335:PRO:HD3	2.43	0.43
7:AH:18:TYR:CG	7:AH:19:GLY:N	2.85	0.43
17:Ay:42:ARG:O	17:Ay:43:ARG:C	2.61	0.43
18:AX:32:LEU:HD23	18:AX:32:LEU:H	1.83	0.43
2:BB:120:LEU:HD13	22:BB:619:CLA:HMD1	1.99	0.43
2:BB:243:ALA:HB2	2:BB:466:HIS:CE1	2.53	0.43
2:BB:343:HIS:O	2:BB:401:PHE:HA	2.18	0.43
3:BC:163:PHE:CG	22:BC:512:CLA:HAB	2.52	0.43
3:BC:365:TRP:HB3	3:BC:391:ARG:HG2	1.99	0.43
12:BM:3:VAL:HG11	14:BT:2:GLU:HG2	2.00	0.43
12:BM:18:PRO:O	12:BM:21:PHE:HB3	2.18	0.43
15:BU:64:ALA:O	15:BU:67:GLN:HG2	2.18	0.43
15:BU:89:GLU:CD	15:BU:89:GLU:N	2.76	0.43
15:BU:99:GLU:HA	15:BU:102:LYS:HE3	1.99	0.43
1:AA:333:GLU:HB2	1:AA:337:HIS:HE1	1.83	0.43
2:AB:164:PRO:HG2	2:AB:165:GLY:H	1.82	0.43
2:AB:187:PRO:C	2:AB:189:GLY:H	2.26	0.43
2:AB:229:LEU:HD11	22:AB:609:CLA:O1A	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:260:SER:C	2:AB:262:THR:N	2.76	0.43
26:AB:618:BCR:C38	14:BT:4:ILE:HD13	2.48	0.43
3:AC:362:ARG:H	27:AC:516:DGD:HE4	1.83	0.43
3:AC:455:PHE:C	3:AC:457:LYS:H	2.26	0.43
4:AD:152:VAL:HG12	22:AD:402:CLA:H43	2.00	0.43
4:AD:238:THR:O	4:AD:239:GLN:C	2.60	0.43
5:AE:72:ALA:O	5:AE:76:VAL:HG23	2.18	0.43
10:AK:17:ILE:O	10:AK:17:ILE:HG22	2.17	0.43
12:AM:33:GLN:HG2	12:AM:34:LYS:N	2.33	0.43
15:AU:54:LYS:HD2	15:AU:113:THR:CG2	2.49	0.43
2:BB:113:TRP:CE2	2:BB:117:TYR:CD2	3.06	0.43
2:BB:170:ASP:HB2	2:BB:171:PRO:HD2	2.01	0.43
2:BB:474:LEU:HD11	22:BB:611:CLA:HAA1	1.99	0.43
3:BC:456:GLU:OE1	3:BC:456:GLU:N	2.52	0.43
26:BD:406:BCR:H363	6:BF:33:PHE:HB3	2.01	0.43
7:BH:9:ASP:O	7:BH:12:ARG:HB3	2.18	0.43
10:BK:16:ALA:O	10:BK:19:ASP:HB2	2.18	0.43
13:BO:86:ARG:NH1	13:BO:86:ARG:O	2.44	0.43
13:BO:135:GLN:HE21	13:BO:135:GLN:HB3	1.57	0.43
16:BV:83:GLU:CD	16:BV:83:GLU:H	2.25	0.43
17:By:42:ARG:O	17:By:43:ARG:C	2.60	0.43
1:AA:60:ILE:HG23	1:AA:61:ASP:N	2.32	0.43
2:AB:348:ASN:OD1	2:AB:352:GLU:HB2	2.18	0.43
22:AB:602:CLA:H122	22:AB:602:CLA:H162	1.79	0.43
3:AC:318:LEU:HG	3:AC:328:VAL:CG1	2.48	0.43
4:AD:161:PRO:HB3	4:AD:170:ALA:HB2	2.01	0.43
5:AE:69:ARG:HG3	5:AE:70:PHE:N	2.34	0.43
8:AI:6:ILE:CD1	32:AI:102:LMT:H5'	2.48	0.43
15:AU:73:PRO:HG2	16:AV:107:THR:HB	2.01	0.43
15:AU:89:GLU:CD	15:AU:89:GLU:N	2.73	0.43
1:BA:212:CYS:HB2	4:BD:211:CYS:HB2	2.01	0.43
1:BA:329:GLU:O	1:BA:332:HIS:ND1	2.48	0.43
2:BB:368:VAL:HG21	2:BB:381:ILE:HD12	2.01	0.43
2:BB:447:PRO:O	2:BB:448:ARG:C	2.60	0.43
5:BE:49:THR:HA	5:BE:50:PRO:HD3	1.84	0.43
6:BF:41:GLN:OE1	9:BJ:31:GLY:HA3	2.18	0.43
20:BZ:23:VAL:HB	20:BZ:24:PRO:HD3	2.00	0.43
1:AA:39:PRO:HB2	22:AA:406:CLA:CBB	2.48	0.43
30:AA:413:LMG:H421	22:AB:611:CLA:H142	2.00	0.43
2:AB:284:ILE:HG23	2:AB:305:ILE:CD1	2.48	0.43
2:AB:366:PHE:CD1	2:AB:367:PRO:HD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:AB:607:CLA:CAC	26:AB:618:BCR:H393	2.49	0.43
3:AC:223:TRP:CE3	3:AC:224:ILE:HG13	2.53	0.43
4:AD:154:VAL:O	4:AD:158:LEU:HB2	2.18	0.43
5:AE:20:TRP:HD1	9:AJ:8:ILE:HD13	1.82	0.43
10:AK:28:ILE:O	10:AK:29:PRO:C	2.61	0.43
10:AK:46:ARG:NH1	10:AK:46:ARG:HB2	2.34	0.43
14:AT:4:ILE:HD13	26:AT:102:BCR:H381	2.00	0.43
2:BB:433:ASP:OD1	2:BB:433:ASP:C	2.61	0.43
3:BC:453:ALA:HA	8:BI:34:ARG:O	2.18	0.43
13:BO:208:LEU:O	13:BO:209:ALA:C	2.61	0.43
18:BX:42:GLN:O	18:BX:43:ILE:HG13	2.18	0.43
1:AA:198:HIS:O	1:AA:202:VAL:HG12	2.18	0.43
2:AB:191:ASN:ND2	7:AH:59:ASN:C	2.76	0.43
3:AC:160:ILE:HA	3:AC:163:PHE:CD2	2.53	0.43
3:AC:353:GLY:C	3:AC:355:THR:N	2.77	0.43
8:AI:17:LEU:O	8:AI:18:LEU:C	2.61	0.43
20:AZ:24:PRO:C	20:AZ:26:ALA:N	2.76	0.43
20:AZ:36:SER:HA	20:AZ:39:LEU:CD1	2.48	0.43
3:BC:203:THR:O	3:BC:235:GLY:HA3	2.19	0.43
10:BK:17:ILE:N	10:BK:17:ILE:CD1	2.80	0.43
13:BO:225:LEU:N	13:BO:225:LEU:HD12	2.34	0.43
17:By:36:ILE:O	17:By:39:LEU:HB2	2.18	0.43
19:BY:23:UNK:O	19:BY:24:UNK:C	2.67	0.43
1:AA:153:SER:HB2	22:AA:402:CLA:H43	2.00	0.43
3:AC:162:GLY:O	3:AC:166:ILE:HG13	2.18	0.43
3:AC:163:PHE:CG	22:AC:512:CLA:HAB	2.54	0.43
4:AD:101:PHE:O	4:AD:104:TRP:HB3	2.18	0.43
4:AD:253:TRP:HA	4:AD:256:ILE:HG23	2.01	0.43
4:AD:263:ASN:O	4:AD:265:ARG:N	2.52	0.43
26:AD:406:BCR:H363	6:AF:33:PHE:HB3	2.00	0.43
5:AE:20:TRP:CD1	9:AJ:8:ILE:HD13	2.53	0.43
13:AO:171:GLU:HA	13:AO:221:GLY:O	2.19	0.43
20:AZ:22:GLY:O	20:AZ:23:VAL:C	2.61	0.43
1:BA:220:THR:O	1:BA:223:LEU:HG	2.19	0.43
1:BA:330:VAL:HG11	4:BD:348:ARG:HG2	1.99	0.43
2:BB:69:LEU:HD21	22:BB:606:CLA:HED3	2.00	0.43
2:BB:472:ARG:HG2	2:BB:472:ARG:HH11	1.84	0.43
3:BC:110:PRO:O	3:BC:114:VAL:HG23	2.19	0.43
6:BF:40:MET:C	6:BF:42:PHE:H	2.26	0.43
7:BH:55:LEU:O	7:BH:56:ASP:C	2.59	0.43
10:BK:23:ASP:CB	17:By:21:GLN:HE21	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:BT:29:ILE:O	14:BT:31:LYS:N	2.52	0.43
16:BV:81:ARG:HG2	16:BV:81:ARG:NH1	2.34	0.43
18:BX:44:ASP:C	18:BX:45:LYS:CD	2.91	0.43
20:BZ:17:PHE:HE2	20:BZ:21:ILE:HD11	1.83	0.43
2:AB:349:LYS:HG2	2:AB:395:GLN:O	2.19	0.43
3:AC:259:TRP:C	3:AC:261:ARG:N	2.74	0.43
6:AF:24:HIS:HA	6:AF:27:ALA:HB3	2.00	0.43
10:AK:20:PRO:O	17:Ay:21:GLN:HG3	2.18	0.43
12:AM:31:SER:HA	30:AM:101:LMG:HC3	2.01	0.43
13:AO:81:GLU:C	13:AO:83:LYS:H	2.26	0.43
14:AT:21:ILE:HD12	26:AT:102:BCR:H332	2.01	0.43
17:Ay:20:ALA:HA	17:Ay:22:LEU:HD12	2.01	0.43
1:BA:239:PHE:O	14:BT:29:ILE:HA	2.19	0.43
28:BA:412:LHG:HC92	29:BA:413:SQD:O10	2.19	0.43
28:BA:412:LHG:HC81	3:BC:36:TRP:CZ3	2.54	0.43
2:BB:260:SER:C	2:BB:262:THR:N	2.76	0.43
2:BB:354:LEU:HD12	2:BB:378:LYS:HB2	2.01	0.43
22:BB:605:CLA:H122	22:BB:605:CLA:H162	1.80	0.43
3:BC:28:GLN:HB2	22:BC:511:CLA:HED3	2.01	0.43
22:BC:505:CLA:H42	26:BC:515:BCR:H342	2.01	0.43
4:BD:323:GLU:HG2	13:BO:194:TYR:OH	2.19	0.43
15:BU:54:LYS:HD2	15:BU:113:THR:CG2	2.48	0.43
16:BV:119:PRO:HG3	16:BV:127:PHE:CD1	2.53	0.43
1:AA:185:VAL:O	1:AA:186:PHE:C	2.61	0.43
3:AC:259:TRP:O	3:AC:260:ALA:C	2.62	0.43
3:AC:464:GLU:O	3:AC:467:LEU:HB2	2.19	0.43
4:AD:203:GLY:O	4:AD:207:GLY:N	2.52	0.43
10:AK:43:VAL:O	10:AK:46:ARG:HG3	2.19	0.43
13:AO:70:CYS:O	13:AO:265:PHE:HB2	2.18	0.43
13:AO:86:ARG:O	13:AO:86:ARG:HG3	2.18	0.43
13:AO:168:PHE:O	13:AO:224:SER:HA	2.19	0.43
15:AU:89:GLU:C	15:AU:91:VAL:N	2.76	0.43
1:BA:111:PRO:O	1:BA:115:ILE:HG13	2.19	0.43
1:BA:131:TRP:CE3	1:BA:132:GLU:CA	3.02	0.43
1:BA:198:HIS:O	1:BA:202:VAL:HG12	2.19	0.43
1:BA:288:LEU:O	1:BA:292:THR:HB	2.18	0.43
5:BE:20:TRP:CD1	9:BJ:8:ILE:HD13	2.54	0.43
26:BJ:102:BCR:H24C	26:BJ:102:BCR:H371	1.78	0.43
13:BO:59:ASP:C	13:BO:61:SER:N	2.74	0.43
13:BO:168:PHE:O	13:BO:224:SER:HA	2.19	0.43
1:AA:222:SER:O	1:AA:246:TYR:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:289:GLN:OE1	2:AB:292:LEU:HD12	2.19	0.43
3:AC:242:LEU:O	3:AC:243:ILE:C	2.61	0.43
3:AC:394:GLU:OE2	3:AC:398:HIS:CD2	2.71	0.43
4:AD:180:ARG:HH11	4:AD:180:ARG:HG3	1.79	0.43
7:AH:55:LEU:O	7:AH:56:ASP:C	2.62	0.43
13:AO:225:LEU:HD12	13:AO:225:LEU:N	2.33	0.43
13:AO:227:VAL:CG1	13:AO:228:ALA:N	2.82	0.43
18:AX:44:ASP:C	18:AX:45:LYS:CD	2.92	0.43
2:BB:92:SER:O	2:BB:93:PHE:C	2.62	0.43
2:BB:164:PRO:HG2	2:BB:165:GLY:H	1.83	0.43
2:BB:280:PHE:O	2:BB:284:ILE:HG13	2.19	0.43
2:BB:289:GLN:OE1	2:BB:289:GLN:HA	2.19	0.43
3:BC:165:LEU:HG	22:BC:507:CLA:HED1	2.00	0.43
3:BC:386:PRO:HB3	16:BV:116:GLU:HG2	2.00	0.43
3:BC:415:ASN:O	3:BC:416:SER:CB	2.64	0.43
4:BD:126:MET:HE3	4:BD:150:ILE:HG13	2.01	0.43
4:BD:189:HIS:O	4:BD:190:ASN:C	2.61	0.43
4:BD:204:VAL:HG22	4:BD:279:LEU:HD21	2.01	0.43
19:BY:23:UNK:O	19:BY:25:UNK:N	2.52	0.43
2:AB:222:PRO:CG	7:AH:27:THR:H	2.28	0.42
2:AB:243:ALA:HB2	2:AB:466:HIS:CE1	2.54	0.42
2:AB:275:TRP:CH2	2:AB:358:ARG:HD3	2.54	0.42
2:AB:385:ARG:O	2:AB:386:ALA:C	2.60	0.42
3:AC:28:GLN:HB2	22:AC:511:CLA:HED3	2.00	0.42
4:AD:217:THR:HG21	24:AD:405:PL9:C1	2.49	0.42
7:AH:41:PHE:O	7:AH:45:ILE:HG23	2.18	0.42
10:AK:21:LEU:HD11	26:AK:102:BCR:C3	2.47	0.42
12:AM:19:SER:O	12:AM:23:ILE:HG13	2.18	0.42
15:AU:82:ASN:ND2	15:AU:94:ILE:HG23	2.34	0.42
2:BB:247:PHE:CE1	22:BB:605:CLA:H101	2.48	0.42
2:BB:464:PHE:HD2	22:BB:614:CLA:HAC2	1.84	0.42
22:BB:615:CLA:H162	22:BB:615:CLA:H122	1.84	0.42
3:BC:273:SER:OG	3:BC:274:TYR:N	2.52	0.42
4:BD:193:LEU:O	4:BD:193:LEU:HG	2.19	0.42
4:BD:291:LEU:O	4:BD:292:ASN:HB2	2.19	0.42
10:BK:28:ILE:O	10:BK:29:PRO:C	2.60	0.42
10:BK:46:ARG:HH11	10:BK:46:ARG:CB	2.32	0.42
15:BU:59:ASN:O	15:BU:60:THR:C	2.62	0.42
15:BU:96:GLY:O	15:BU:97:LEU:C	2.62	0.42
16:BV:68:VAL:O	16:BV:68:VAL:HG13	2.19	0.42
17:By:46:LEU:N	17:By:46:LEU:HD23	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:73:TYR:CE2	30:AA:416:LMG:HC61	2.53	0.42
1:AA:215:HIS:CD2	4:AD:268:HIS:HD2	2.37	0.42
1:AA:255:PHE:CE2	24:AA:407:PL9:H111	2.54	0.42
2:AB:464:PHE:HD2	22:AB:611:CLA:HAC2	1.84	0.42
3:AC:48:LYS:CD	3:AC:138:GLU:HG3	2.49	0.42
3:AC:155:ASN:C	3:AC:158:THR:HG22	2.45	0.42
22:AC:508:CLA:H172	27:AC:517:DGD:HBW2	2.01	0.42
4:AD:291:LEU:O	4:AD:292:ASN:HB2	2.18	0.42
9:AJ:15:THR:HG23	26:AK:102:BCR:H392	2.01	0.42
12:AM:5:GLN:NE2	32:AM:102:LMT:O2B	2.52	0.42
12:AM:33:GLN:CG	12:AM:34:LYS:N	2.82	0.42
13:AO:109:GLY:HA3	13:AO:122:VAL:O	2.18	0.42
1:BA:317:TRP:HZ3	4:BD:180:ARG:CD	2.20	0.42
2:BB:71:VAL:HG21	2:BB:96:VAL:HG21	2.01	0.42
3:BC:127:PHE:HE1	20:BZ:23:VAL:HG21	1.84	0.42
3:BC:259:TRP:C	3:BC:261:ARG:N	2.76	0.42
6:BF:24:HIS:HA	6:BF:27:ALA:HB3	2.02	0.42
32:BT:101:LMT:H3'	32:BT:101:LMT:H1B	1.63	0.42
15:BU:80:VAL:HG22	15:BU:127:ARG:NH2	2.34	0.42
18:BX:45:LYS:N	18:BX:45:LYS:CD	2.82	0.42
19:BY:21:UNK:O	19:BY:22:UNK:C	2.66	0.42
1:AA:42:LEU:HA	1:AA:45:THR:CG2	2.49	0.42
1:AA:92:HIS:HD2	3:AC:219:GLY:HA3	1.84	0.42
1:AA:160:ILE:HD12	3:AC:431:PHE:CE1	2.54	0.42
2:AB:471:ALA:HB2	4:AD:130:PHE:CE2	2.53	0.42
3:AC:406:SER:HA	3:AC:420:VAL:CG2	2.49	0.42
3:AC:456:GLU:N	3:AC:456:GLU:OE1	2.53	0.42
4:AD:52:THR:HG22	4:AD:67:TYR:CE2	2.54	0.42
4:AD:56:THR:HB	5:AE:49:THR:HG23	2.01	0.42
5:AE:60:GLN:HG2	5:AE:62:SER:H	1.84	0.42
6:AF:40:MET:C	6:AF:42:PHE:H	2.28	0.42
9:AJ:12:ILE:O	9:AJ:16:VAL:HG23	2.19	0.42
13:AO:248:ASP:CG	13:AO:250:ASP:H	2.27	0.42
2:BB:225:LEU:C	2:BB:227:LYS:N	2.77	0.42
2:BB:393:GLU:HG2	15:BU:44:ASP:O	2.19	0.42
3:BC:170:ILE:HD13	22:BC:513:CLA:H201	2.00	0.42
3:BC:451:ALA:HA	3:BC:456:GLU:CD	2.44	0.42
4:BD:294:ARG:H	4:BD:294:ARG:HG2	1.65	0.42
30:BD:408:LMG:HC2	30:BD:408:LMG:HC71	1.82	0.42
26:BJ:102:BCR:H15C	26:BJ:102:BCR:H351	1.91	0.42
10:BK:46:ARG:NH1	10:BK:46:ARG:CB	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:BL:12:LEU:HD22	12:BM:25:LEU:HD12	1.99	0.42
13:BO:144:LEU:CD1	13:BO:259:VAL:HG11	2.48	0.42
13:BO:218:LEU:HD22	15:BU:119:THR:CG2	2.40	0.42
15:BU:50:ALA:HB1	15:BU:113:THR:HG21	2.01	0.42
20:BZ:5:PHE:CG	20:BZ:61:VAL:HG21	2.54	0.42
2:AB:327:THR:O	2:AB:444:ARG:NE	2.46	0.42
27:AB:626:DGD:HA21	32:AB:627:LMT:H121	2.01	0.42
3:AC:174:LEU:HD12	22:AC:512:CLA:H71	2.01	0.42
3:AC:205:ASP:OD1	3:AC:207:ARG:HB3	2.19	0.42
4:AD:160:TYR:CB	4:AD:161:PRO:CD	2.96	0.42
4:AD:221:THR:CG2	4:AD:244:TYR:HB2	2.48	0.42
5:AE:34:GLY:O	5:AE:37:PHE:HB3	2.19	0.42
7:AH:55:LEU:HB2	7:AH:58:VAL:CG1	2.49	0.42
13:AO:69:LEU:HB3	13:AO:107:ILE:CB	2.35	0.42
15:AU:72:TYR:CG	15:AU:73:PRO:N	2.87	0.42
18:AX:44:ASP:C	18:AX:45:LYS:HD3	2.45	0.42
3:BC:33:PHE:CE1	4:BD:229:ALA:HB3	2.54	0.42
22:BC:505:CLA:HMD2	22:BC:507:CLA:HAB	2.01	0.42
4:BD:52:THR:HG22	4:BD:67:TYR:CE2	2.54	0.42
4:BD:84:SER:HB2	4:BD:85:MET:HE2	2.02	0.42
9:BJ:15:THR:HG23	26:BK:102:BCR:H392	2.01	0.42
10:BK:28:ILE:O	10:BK:31:LEU:HB2	2.20	0.42
11:BL:36:PHE:O	11:BL:37:ASN:C	2.62	0.42
17:By:31:ALA:O	17:By:35:ILE:HG23	2.19	0.42
1:AA:77:ILE:HG12	14:AT:6:TYR:CD1	2.54	0.42
1:AA:207:GLY:O	1:AA:210:LEU:HB3	2.19	0.42
1:AA:210:LEU:C	1:AA:210:LEU:CD2	2.92	0.42
1:AA:228:THR:HB	1:AA:231:GLU:HB3	2.01	0.42
26:AA:409:BCR:H342	29:AA:415:SQD:H342	2.02	0.42
3:AC:63:TRP:O	3:AC:64:ALA:C	2.62	0.42
4:AD:89:LEU:HG	7:AH:50:ASN:OD1	2.20	0.42
8:AI:20:VAL:C	8:AI:22:GLY:H	2.26	0.42
10:AK:19:ASP:N	10:AK:20:PRO:CD	2.80	0.42
20:AZ:5:PHE:CD2	20:AZ:61:VAL:HG21	2.54	0.42
1:BA:42:LEU:HA	1:BA:45:THR:CG2	2.50	0.42
1:BA:136:ARG:NH2	8:BI:27:ASP:OD1	2.49	0.42
1:BA:217:SER:O	1:BA:220:THR:HG22	2.18	0.42
2:BB:169:SER:O	7:BH:65:LEU:HG	2.20	0.42
3:BC:321:ASP:HA	3:BC:324:LEU:HD23	2.01	0.42
4:BD:35:ILE:O	4:BD:39:PRO:HG2	2.20	0.42
4:BD:161:PRO:HB3	4:BD:170:ALA:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:BO:59:ASP:O	13:BO:61:SER:N	2.53	0.42
16:BV:121:LEU:C	16:BV:123:SER:H	2.27	0.42
2:AB:354:LEU:HD12	2:AB:378:LYS:HB2	2.02	0.42
2:AB:433:ASP:OD1	2:AB:433:ASP:C	2.61	0.42
2:AB:457:VAL:O	2:AB:458:PHE:C	2.62	0.42
2:AB:472:ARG:HG2	2:AB:472:ARG:HH11	1.84	0.42
3:AC:276:LEU:HD21	22:AC:508:CLA:HBB1	2.01	0.42
3:AC:315:MET:HE1	3:AC:369:LEU:CD1	2.45	0.42
4:AD:263:ASN:O	4:AD:266:TRP:N	2.50	0.42
5:AE:15:THR:CG2	9:AJ:7:ARG:HG3	2.49	0.42
34:AE:101:HEM:HHA	34:AE:101:HEM:HAD2	1.57	0.42
8:AI:20:VAL:C	8:AI:22:GLY:N	2.77	0.42
9:AJ:7:ARG:HA	9:AJ:7:ARG:HE	1.83	0.42
16:AV:103:LYS:O	16:AV:122:ARG:HG2	2.19	0.42
1:BA:255:PHE:CE2	24:BA:408:PL9:H111	2.55	0.42
22:BB:612:CLA:NB	26:BX:101:BCR:H312	2.35	0.42
3:BC:35:TRP:CD2	3:BC:36:TRP:N	2.88	0.42
3:BC:189:TRP:O	3:BC:190:ALA:C	2.61	0.42
7:BH:28:THR:N	7:BH:29:PRO:HD2	2.35	0.42
13:BO:192:SER:OG	13:BO:193:GLY:N	2.53	0.42
16:BV:124:ALA:HB1	16:BV:131:ARG:CG	2.50	0.42
1:AA:22:THR:HG21	8:AI:30:ARG:CD	2.50	0.42
1:AA:73:TYR:CD2	30:AA:416:LMG:HC3	2.55	0.42
2:AB:59:GLY:HA3	22:AB:607:CLA:CED	2.50	0.42
22:AB:612:CLA:H162	22:AB:612:CLA:H122	1.84	0.42
3:AC:279:LEU:HD23	3:AC:282:MET:HE3	2.01	0.42
3:AC:321:ASP:HA	3:AC:324:LEU:HD23	2.01	0.42
3:AC:390:ARG:CZ	16:AV:126:ILE:HD13	2.50	0.42
4:AD:125:PHE:O	4:AD:128:ARG:HB3	2.19	0.42
4:AD:176:ALA:C	4:AD:178:ILE:H	2.26	0.42
4:AD:204:VAL:HG22	4:AD:279:LEU:HD21	2.01	0.42
5:AE:61:ARG:HH22	16:AV:153:GLY:HA3	1.85	0.42
6:AF:16:PHE:CD1	6:AF:16:PHE:N	2.88	0.42
10:AK:16:ALA:O	10:AK:19:ASP:HB2	2.20	0.42
12:AM:1:MET:HG2	12:AM:2:GLU:H	1.84	0.42
15:AU:91:VAL:HG13	15:AU:92:LEU:N	2.33	0.42
2:BB:9:HIS:HB2	22:BB:614:CLA:CBA	2.49	0.42
2:BB:71:VAL:HG21	2:BB:96:VAL:CG2	2.50	0.42
3:BC:48:LYS:HD2	3:BC:138:GLU:HG3	1.99	0.42
4:BD:77:ALA:CB	4:BD:174:GLY:HA3	2.50	0.42
5:BE:18:ARG:CD	5:BE:22:ILE:HD11	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:BK:11:LEU:O	10:BK:12:PRO:C	2.60	0.42
13:BO:215:ARG:NH1	13:BO:252:GLY:O	2.53	0.42
16:BV:59:PHE:CD1	16:BV:63:CYS:SG	3.08	0.42
34:BV:201:HEM:HHA	34:BV:201:HEM:HAD2	1.61	0.42
18:BX:16:LEU:HD11	18:BX:20:PHE:CE2	2.55	0.42
28:AA:411:LHG:HC92	29:AA:412:SQD:O10	2.20	0.42
2:AB:201:HIS:HD2	2:AB:202:HIS:ND1	2.16	0.42
3:AC:84:GLN:C	3:AC:86:LEU:HD13	2.44	0.42
4:AD:17:ILE:HG21	18:AX:42:GLN:HG3	2.02	0.42
5:AE:30:LEU:HD11	6:AF:28:VAL:HG13	2.02	0.42
6:AF:22:ALA:O	6:AF:23:VAL:C	2.62	0.42
6:AF:25:THR:O	6:AF:29:PRO:HG2	2.19	0.42
15:AU:41:ASN:O	15:AU:42:VAL:C	2.62	0.42
17:Ay:31:ALA:O	17:Ay:35:ILE:HG23	2.19	0.42
1:BA:42:LEU:HA	1:BA:45:THR:HG22	2.01	0.42
2:BB:263:THR:HB	2:BB:448:ARG:HH12	1.84	0.42
2:BB:442:ILE:HD11	13:BO:200:LEU:HD23	2.01	0.42
3:BC:429:SER:HA	27:BC:517:DGD:HAT1	2.02	0.42
26:BC:514:BCR:H341	26:BK:102:BCR:H322	2.00	0.42
26:BC:515:BCR:C33	8:BI:20:VAL:HG13	2.50	0.42
4:BD:17:ILE:HG21	18:BX:42:GLN:HG3	2.01	0.42
4:BD:92:LEU:HA	4:BD:104:TRP:CD1	2.55	0.42
34:BE:101:HEM:HHA	34:BE:101:HEM:HAD2	1.57	0.42
6:BF:22:ALA:O	6:BF:23:VAL:C	2.62	0.42
12:BM:31:SER:HA	30:BM:102:LMG:HC3	2.01	0.42
1:AA:127:MET:HE3	3:AC:442:LEU:HD11	2.01	0.42
1:AA:279:PRO:HG2	4:AD:212:ALA:HB2	2.00	0.42
2:AB:18:ARG:HD3	2:AB:118:TRP:HB3	2.01	0.42
2:AB:377:VAL:HG11	4:AD:342:PRO:HG2	2.01	0.42
2:AB:413:ASP:O	2:AB:413:ASP:CG	2.63	0.42
3:AC:140:LEU:HB2	3:AC:148:GLY:HA2	2.02	0.42
6:AF:15:ILE:HG22	6:AF:16:PHE:N	2.34	0.42
13:AO:59:ASP:O	13:AO:61:SER:N	2.53	0.42
16:AV:119:PRO:HA	16:AV:127:PHE:CD2	2.55	0.42
16:AV:130:MET:SD	16:AV:133:LEU:HD12	2.60	0.42
20:AZ:17:PHE:HE2	20:AZ:21:ILE:HD11	1.83	0.42
1:BA:306:VAL:CG1	1:BA:316:THR:HG23	2.49	0.42
2:BB:260:SER:C	2:BB:262:THR:H	2.28	0.42
2:BB:275:TRP:CH2	2:BB:358:ARG:HD3	2.55	0.42
2:BB:283:GLU:OE1	2:BB:283:GLU:HA	2.19	0.42
3:BC:249:ILE:O	3:BC:252:ILE:HB	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BC:276:LEU:CD1	3:BC:444:HIS:HD2	2.33	0.42
4:BD:203:GLY:O	4:BD:207:GLY:N	2.51	0.42
8:BI:20:VAL:C	8:BI:22:GLY:N	2.78	0.42
9:BJ:7:ARG:HA	9:BJ:7:ARG:HE	1.85	0.42
13:BO:80:GLU:O	13:BO:89:ALA:CB	2.66	0.42
13:BO:227:VAL:CG1	13:BO:228:ALA:N	2.83	0.42
1:AA:12:ASN:O	1:AA:15:GLU:HB3	2.20	0.42
2:AB:237:VAL:HG22	22:AB:610:CLA:HBC2	2.01	0.42
2:AB:330:MET:SD	2:AB:446:SER:HB3	2.59	0.42
2:AB:338:GLN:HB2	2:AB:431:GLU:O	2.20	0.42
2:AB:364:GLU:HG3	4:AD:296:TYR:CE2	2.55	0.42
27:AB:626:DGD:HE1	27:AB:626:DGD:HD5	1.66	0.42
30:AE:102:LMG:O9	30:AE:102:LMG:HC71	2.19	0.42
7:AH:13:PRO:HG2	7:AH:14:LEU:H	1.85	0.42
30:AI:101:LMG:H132	32:AI:102:LMT:O2'	2.20	0.42
9:AJ:11:TRP:CE2	9:AJ:12:ILE:HG12	2.55	0.42
16:AV:121:LEU:C	16:AV:123:SER:H	2.28	0.42
1:BA:160:ILE:HD12	3:BC:431:PHE:CE1	2.55	0.42
1:BA:180:PHE:O	1:BA:184:ILE:HG13	2.20	0.42
1:BA:215:HIS:HA	24:BA:408:PL9:O1	2.20	0.42
1:BA:339:PHE:HB3	1:BA:340:PRO:HD2	2.02	0.42
2:BB:16:PRO:HG3	2:BB:133:LEU:HD11	2.01	0.42
2:BB:135:LEU:HD23	2:BB:138:MET:HE1	2.00	0.42
2:BB:241:SER:HB3	22:BB:615:CLA:HED3	2.01	0.42
3:BC:335:THR:HA	13:BO:178:ARG:CD	2.50	0.42
5:BE:60:GLN:HG2	5:BE:62:SER:H	1.84	0.42
6:BF:18:VAL:CG1	6:BF:19:ARG:N	2.82	0.42
8:BI:20:VAL:C	8:BI:22:GLY:H	2.27	0.42
2:AB:150:CYS:HB2	22:AB:603:CLA:CMC	2.49	0.41
2:AB:175:THR:O	2:AB:176:GLY:C	2.63	0.41
22:AB:615:CLA:H162	7:AH:7:LEU:HD21	2.02	0.41
13:AO:92:VAL:HG11	2:BB:84:THR:HG21	2.03	0.41
15:AU:50:ALA:HB1	15:AU:113:THR:HG21	2.01	0.41
1:BA:64:ARG:O	13:BO:178:ARG:NH2	2.53	0.41
1:BA:339:PHE:HB3	1:BA:340:PRO:CD	2.50	0.41
2:BB:127:ARG:HD2	2:BB:127:ARG:C	2.44	0.41
2:BB:153:PHE:O	2:BB:157:HIS:HB3	2.20	0.41
2:BB:349:LYS:HG2	2:BB:395:GLN:O	2.19	0.41
3:BC:269:GLU:O	3:BC:272:LEU:HB3	2.20	0.41
3:BC:363:GLY:O	3:BC:364:PRO:C	2.62	0.41
22:BC:513:CLA:H3A	22:BC:513:CLA:HBA2	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BD:190:ASN:HB2	4:BD:296:TYR:CD1	2.55	0.41
5:BE:15:THR:O	9:BJ:8:ILE:CD1	2.68	0.41
6:BF:15:ILE:HG22	6:BF:16:PHE:N	2.34	0.41
9:BJ:11:TRP:CE2	9:BJ:12:ILE:HG12	2.55	0.41
30:BM:102:LMG:HC2	30:BM:102:LMG:HC72	1.96	0.41
18:BX:42:GLN:HE21	18:BX:42:GLN:HB2	1.63	0.41
1:AA:296:ASN:HB3	3:AC:401:LEU:HA	2.01	0.41
2:AB:76:SER:HG	2:AB:78:TRP:CD1	2.38	0.41
2:AB:260:SER:C	2:AB:262:THR:H	2.28	0.41
13:AO:88:GLU:C	13:AO:88:GLU:CD	2.89	0.41
13:AO:157:PRO:O	13:AO:158:ASN:O	2.38	0.41
17:Ay:36:ILE:O	17:Ay:39:LEU:HB2	2.20	0.41
1:BA:333:GLU:HB2	1:BA:337:HIS:HE1	1.85	0.41
2:BB:18:ARG:HD2	2:BB:115:TRP:CE3	2.55	0.41
2:BB:124:ARG:NH1	2:BB:124:ARG:CG	2.82	0.41
22:BC:502:CLA:HBD	22:BC:503:CLA:H43	2.02	0.41
4:BD:185:PHE:HE2	4:BD:289:LEU:HD12	1.85	0.41
4:BD:261:PHE:HB2	24:BD:405:PL9:H521	2.02	0.41
4:BD:267:LEU:C	4:BD:267:LEU:CD2	2.91	0.41
7:BH:55:LEU:HB2	7:BH:58:VAL:CG1	2.50	0.41
16:BV:69:GLY:O	16:BV:156:TRP:O	2.38	0.41
16:BV:160:LYS:HA	16:BV:163:TYR:CD2	2.56	0.41
17:By:22:LEU:HA	17:By:25:ILE:CD1	2.50	0.41
1:AA:21:VAL:HG11	1:AA:32:TRP:CE3	2.55	0.41
2:AB:12:LEU:O	2:AB:14:ASN:N	2.53	0.41
3:AC:188:THR:CG2	3:AC:298:PRO:HB3	2.51	0.41
30:AD:407:LMG:O4	9:AJ:31:GLY:O	2.39	0.41
15:AU:75:LEU:O	15:AU:79:ILE:HG13	2.21	0.41
1:BA:157:VAL:HG13	1:BA:172:MET:HB3	2.01	0.41
2:BB:7:ARG:HG2	22:BB:614:CLA:HED1	2.01	0.41
2:BB:239:SER:O	2:BB:466:HIS:ND1	2.49	0.41
4:BD:192:THR:CG2	22:BD:402:CLA:HBC2	2.48	0.41
10:BK:43:VAL:CG2	10:BK:46:ARG:HE	2.33	0.41
13:BO:36:ILE:O	13:BO:37:VAL:C	2.62	0.41
13:BO:55:ALA:HA	13:BO:230:VAL:HG11	2.03	0.41
16:BV:103:LYS:O	16:BV:122:ARG:HG2	2.20	0.41
1:AA:317:TRP:O	1:AA:321:ILE:HG13	2.20	0.41
1:AA:343:LEU:O	1:AA:344:ALA:CB	2.66	0.41
26:AA:409:BCR:H342	29:AA:415:SQD:H311	2.02	0.41
2:AB:16:PRO:HB3	2:AB:133:LEU:HD21	2.02	0.41
2:AB:413:ASP:OD1	2:AB:416:THR:HB	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:448:ARG:HH11	2:AB:448:ARG:HG3	1.84	0.41
3:AC:199:ILE:N	3:AC:199:ILE:CD1	2.83	0.41
3:AC:365:TRP:HB3	3:AC:391:ARG:HG2	2.02	0.41
8:AI:27:ASP:O	8:AI:28:PRO:C	2.59	0.41
13:AO:36:ILE:O	13:AO:37:VAL:C	2.64	0.41
13:AO:80:GLU:O	13:AO:89:ALA:CB	2.66	0.41
13:AO:147:THR:OG1	13:AO:148:VAL:N	2.54	0.41
13:AO:184:ASP:C	13:AO:184:ASP:OD1	2.63	0.41
32:AT:101:LMT:H1B	32:AT:101:LMT:H3'	1.64	0.41
19:AY:21:UNK:O	19:AY:22:UNK:C	2.68	0.41
2:BB:105:GLY:O	2:BB:108:PHE:HB3	2.20	0.41
2:BB:226:TYR:N	2:BB:231:MET:HE3	2.35	0.41
3:BC:29:GLU:OE2	3:BC:31:SER:N	2.31	0.41
3:BC:198:VAL:HG12	3:BC:200:THR:HG23	2.02	0.41
3:BC:250:TRP:HE1	22:BC:506:CLA:HED1	1.84	0.41
4:BD:79:SER:HA	4:BD:172:SER:HB3	2.02	0.41
4:BD:209:LEU:O	4:BD:213:ILE:HG22	2.20	0.41
4:BD:329:MET:O	4:BD:330:ALA:C	2.63	0.41
5:BE:30:LEU:HD11	6:BF:28:VAL:HG13	2.03	0.41
9:BJ:21:VAL:HA	9:BJ:24:ILE:HG22	2.03	0.41
10:BK:28:ILE:HA	10:BK:31:LEU:HD12	2.02	0.41
13:BO:81:GLU:HA	13:BO:82:PRO:HD3	1.89	0.41
13:BO:180:ALA:HB2	15:BU:120:ALA:O	2.19	0.41
15:BU:42:VAL:HG23	15:BU:43:VAL:N	2.33	0.41
15:BU:89:GLU:C	15:BU:91:VAL:H	2.29	0.41
19:BY:25:UNK:C	19:BY:27:UNK:N	2.82	0.41
1:AA:45:THR:HB	23:AA:405:PHO:H93	2.02	0.41
1:AA:206:PHE:HD2	1:AA:206:PHE:HA	1.76	0.41
1:AA:260:PHE:CD1	1:AA:260:PHE:C	2.98	0.41
2:AB:105:GLY:O	2:AB:108:PHE:HB3	2.19	0.41
2:AB:127:ARG:HD2	2:AB:127:ARG:C	2.45	0.41
3:AC:272:LEU:O	3:AC:273:SER:C	2.63	0.41
5:AE:78:THR:HA	5:AE:81:GLU:HG2	2.02	0.41
7:AH:10:ILE:H	7:AH:10:ILE:HG13	1.70	0.41
7:AH:53:LEU:HD21	7:AH:55:LEU:HD21	2.03	0.41
8:AI:7:THR:O	8:AI:8:VAL:C	2.63	0.41
2:BB:18:ARG:HD3	2:BB:118:TRP:HB3	2.01	0.41
2:BB:175:THR:O	2:BB:176:GLY:C	2.63	0.41
22:BB:604:CLA:HMB2	26:BX:101:BCR:H393	2.02	0.41
3:BC:42:LEU:HD11	22:BC:511:CLA:C1A	2.50	0.41
30:BC:519:LMG:H221	10:BK:30:VAL:CG1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BD:107:LEU:HD21	5:BE:76:VAL:HG21	2.01	0.41
5:BE:64:PRO:HB3	5:BE:84:LYS:CD	2.50	0.41
5:BE:64:PRO:CB	5:BE:84:LYS:HE2	2.50	0.41
7:BH:28:THR:O	7:BH:31:MET:HB3	2.20	0.41
13:BO:83:LYS:CG	13:BO:84:ASN:H	2.24	0.41
16:BV:128:PRO:C	16:BV:130:MET:N	2.78	0.41
1:AA:215:HIS:HA	24:AA:407:PL9:O1	2.21	0.41
2:AB:383:PHE:O	13:AO:192:SER:HA	2.20	0.41
3:AC:202:PRO:HB2	3:AC:235:GLY:HA2	2.01	0.41
5:AE:15:THR:O	9:AJ:8:ILE:CD1	2.69	0.41
5:AE:82:GLN:H	5:AE:82:GLN:HG3	1.54	0.41
7:AH:27:THR:O	7:AH:28:THR:C	2.63	0.41
10:AK:28:ILE:O	10:AK:31:LEU:HB2	2.20	0.41
11:AL:22:LEU:O	11:AL:26:VAL:HG13	2.21	0.41
30:AM:101:LMG:HC2	30:AM:101:LMG:HC72	1.96	0.41
2:BB:118:TRP:CH2	11:BL:5:PRO:HD2	2.56	0.41
28:BC:521:LHG:O9	28:BC:521:LHG:HC41	2.20	0.41
4:BD:56:THR:HB	5:BE:49:THR:HG23	2.02	0.41
4:BD:268:HIS:CE1	33:BD:401:BCT:O3	2.73	0.41
1:AA:292:THR:C	1:AA:294:ALA:H	2.28	0.41
2:AB:24:LEU:HD13	2:AB:111:ALA:N	2.36	0.41
2:AB:191:ASN:OD1	2:AB:193:TYR:N	2.52	0.41
3:AC:116:VAL:CG2	3:AC:117:VAL:N	2.84	0.41
27:AC:518:DGD:HG2	9:AJ:33:TYR:OH	2.21	0.41
4:AD:26:ARG:HD3	6:AF:18:VAL:CG1	2.32	0.41
4:AD:190:ASN:HB2	4:AD:296:TYR:CE1	2.56	0.41
5:AE:49:THR:HA	5:AE:50:PRO:HD3	1.86	0.41
10:AK:20:PRO:HB2	17:Ay:21:GLN:CB	2.51	0.41
10:AK:43:VAL:CG2	10:AK:46:ARG:HE	2.33	0.41
13:AO:120:THR:HA	13:AO:153:ALA:O	2.21	0.41
13:AO:135:GLN:HE21	13:AO:135:GLN:HB3	1.56	0.41
13:AO:192:SER:OG	13:AO:193:GLY:N	2.54	0.41
17:Ay:27:MET:C	17:Ay:29:GLY:N	2.79	0.41
1:BA:21:VAL:HG11	1:BA:32:TRP:CZ3	2.56	0.41
1:BA:249:VAL:HG11	2:BB:486:LEU:CD2	2.50	0.41
2:BB:187:PRO:C	2:BB:189:GLY:N	2.79	0.41
2:BB:191:ASN:ND2	7:BH:59:ASN:O	2.54	0.41
2:BB:377:VAL:HG11	4:BD:342:PRO:HG2	2.02	0.41
3:BC:141:GLU:HA	3:BC:148:GLY:HA3	2.03	0.41
3:BC:162:GLY:O	3:BC:166:ILE:HG13	2.21	0.41
5:BE:27:ILE:CB	5:BE:28:PRO:HD3	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:BK:20:PRO:HB2	17:By:21:GLN:CB	2.50	0.41
13:BO:136:MET:O	13:BO:137:ALA:C	2.62	0.41
13:BO:229:LYS:HB2	13:BO:238:ALA:HB3	2.02	0.41
16:BV:30:THR:HB	16:BV:31:PRO:HD2	2.02	0.41
16:BV:162:TYR:O	16:BV:163:TYR:C	2.63	0.41
1:AA:131:TRP:CE3	1:AA:132:GLU:CA	3.03	0.41
1:AA:277:ALA:O	1:AA:281:VAL:HG23	2.21	0.41
2:AB:479:PHE:O	2:AB:480:SER:CB	2.68	0.41
3:AC:101:PRO:O	3:AC:104:GLU:HB2	2.19	0.41
3:AC:203:THR:O	3:AC:235:GLY:HA3	2.20	0.41
26:AC:514:BCR:H341	26:AK:102:BCR:H322	2.02	0.41
4:AD:189:HIS:O	4:AD:190:ASN:C	2.63	0.41
12:AM:27:VAL:HG12	12:BM:28:GLN:CB	2.47	0.41
13:AO:73:PRO:HG2	13:AO:102:THR:HB	2.03	0.41
13:AO:136:MET:O	13:AO:137:ALA:C	2.63	0.41
1:BA:105:TRP:CZ3	1:BA:111:PRO:HG3	2.56	0.41
1:BA:202:VAL:O	1:BA:206:PHE:HB2	2.20	0.41
1:BA:296:ASN:HB3	3:BC:401:LEU:HA	2.02	0.41
22:BA:405:CLA:H202	30:BD:407:LMG:H401	2.03	0.41
2:BB:214:LEU:O	2:BB:218:LEU:HG	2.21	0.41
2:BB:331:ASN:HB3	2:BB:437:LEU:CD1	2.48	0.41
3:BC:63:TRP:O	3:BC:64:ALA:C	2.63	0.41
3:BC:441:HIS:O	3:BC:442:LEU:C	2.64	0.41
4:BD:199:MET:O	4:BD:200:GLY:C	2.61	0.41
15:BU:41:ASN:O	15:BU:42:VAL:C	2.64	0.41
17:By:20:ALA:HA	17:By:22:LEU:HD12	2.02	0.41
1:AA:136:ARG:HH22	8:AI:27:ASP:CG	2.29	0.41
1:AA:183:MET:HB3	22:AA:402:CLA:HBC2	2.02	0.41
1:AA:210:LEU:C	1:AA:210:LEU:HD23	2.46	0.41
1:AA:215:HIS:CD2	4:AD:268:HIS:CD2	3.08	0.41
1:AA:288:LEU:O	1:AA:292:THR:HB	2.21	0.41
2:AB:26:HIS:CE1	22:AB:612:CLA:HMA2	2.56	0.41
2:AB:91:TRP:HE1	32:AB:624:LMT:H12	1.86	0.41
2:AB:120:LEU:HD13	22:AB:616:CLA:HMD1	2.03	0.41
2:AB:393:GLU:HG2	15:AU:44:ASP:O	2.20	0.41
3:AC:165:LEU:HG	22:AC:507:CLA:HED1	2.03	0.41
3:AC:198:VAL:HG12	3:AC:200:THR:HG23	2.03	0.41
3:AC:267:SER:O	3:AC:271:TYR:CD2	2.74	0.41
3:AC:286:ALA:HB2	22:AC:502:CLA:HMD1	2.03	0.41
3:AC:307:PRO:HG3	3:AC:358:PHE:CD1	2.56	0.41
3:AC:308:GLU:HG3	3:AC:361:PHE:CZ	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:414:ILE:HG22	3:AC:415:ASN:N	2.35	0.41
4:AD:268:HIS:CE1	33:AD:401:BCT:O3	2.74	0.41
26:AJ:102:BCR:H15C	26:AJ:102:BCR:H351	1.91	0.41
10:AK:34:ALA:O	10:AK:37:PHE:HB2	2.20	0.41
13:AO:208:LEU:O	13:AO:209:ALA:C	2.63	0.41
14:AT:16:LEU:O	14:AT:17:PHE:C	2.63	0.41
15:AU:57:LEU:HD22	15:AU:79:ILE:CG2	2.51	0.41
16:AV:124:ALA:HB1	16:AV:131:ARG:CG	2.51	0.41
19:AY:23:UNK:O	19:AY:24:UNK:C	2.68	0.41
1:BA:22:THR:HG21	8:BI:30:ARG:CD	2.51	0.41
1:BA:24:THR:OG1	3:BC:469:MET:CE	2.68	0.41
1:BA:45:THR:HB	23:BA:406:PHO:H93	2.02	0.41
1:BA:110:GLY:O	1:BA:111:PRO:C	2.62	0.41
2:BB:30:VAL:HG11	22:BB:615:CLA:H112	2.03	0.41
2:BB:160:GLY:O	2:BB:161:LEU:C	2.64	0.41
2:BB:191:ASN:ND2	7:BH:59:ASN:C	2.79	0.41
2:BB:364:GLU:HG3	4:BD:296:TYR:CE2	2.56	0.41
3:BC:85:GLY:CA	27:BC:517:DGD:HE4	2.51	0.41
3:BC:116:VAL:CG2	3:BC:117:VAL:N	2.84	0.41
3:BC:141:GLU:CD	3:BC:141:GLU:N	2.76	0.41
3:BC:160:ILE:HA	3:BC:163:PHE:CD2	2.55	0.41
3:BC:242:LEU:O	3:BC:243:ILE:C	2.63	0.41
3:BC:414:ILE:HG22	3:BC:415:ASN:O	2.21	0.41
3:BC:449:ARG:NE	22:BC:505:CLA:HED1	2.21	0.41
3:BC:464:GLU:O	3:BC:467:LEU:HB2	2.20	0.41
27:BC:518:DGD:HG2	9:BJ:33:TYR:OH	2.21	0.41
12:BM:19:SER:O	12:BM:23:ILE:HG13	2.20	0.41
15:BU:54:LYS:CB	15:BU:113:THR:HG23	2.47	0.41
19:BY:21:UNK:HA	19:BY:24:UNK:CB	2.50	0.41
1:AA:10:SER:OG	1:AA:13:LEU:HD12	2.20	0.41
1:AA:114:LEU:HD23	1:AA:114:LEU:O	2.21	0.41
1:AA:334:ARG:NH1	13:AO:183:LEU:O	2.54	0.41
22:AA:403:CLA:H62	22:AA:403:CLA:H41	1.91	0.41
2:AB:113:TRP:CE2	2:AB:117:TYR:CD2	3.09	0.41
2:AB:137:LYS:NZ	7:AH:14:LEU:O	2.54	0.41
2:AB:168:VAL:O	2:AB:176:GLY:HA2	2.20	0.41
2:AB:331:ASN:HB3	2:AB:437:LEU:CD1	2.49	0.41
3:AC:80:PRO:HB3	3:AC:82:TYR:CE1	2.56	0.41
22:AC:512:CLA:HED2	22:AC:512:CLA:H2A	2.03	0.41
13:AO:49:ASP:CG	13:AO:50:ASP:N	2.79	0.41
15:AU:55:ILE:HG21	15:AU:65:PHE:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:AV:30:THR:OG1	16:AV:32:GLU:HB3	2.21	0.41
16:AV:81:ARG:CG	16:AV:157:GLY:HA3	2.51	0.41
17:Ay:22:LEU:H	17:Ay:22:LEU:HD12	1.86	0.41
1:BA:20:TRP:O	1:BA:23:SER:HB3	2.20	0.41
1:BA:183:MET:HB3	22:BA:403:CLA:HBC2	2.02	0.41
1:BA:215:HIS:CD2	4:BD:268:HIS:CD2	3.09	0.41
1:BA:247:ASN:HB3	1:BA:250:ALA:HB3	2.01	0.41
22:BA:404:CLA:H62	22:BA:404:CLA:H41	1.92	0.41
2:BB:348:ASN:O	2:BB:350:GLU:N	2.54	0.41
3:BC:80:PRO:HB3	3:BC:82:TYR:CE1	2.56	0.41
3:BC:261:ARG:HA	3:BC:266:TRP:HZ2	1.86	0.41
22:BC:511:CLA:HBA2	26:BC:514:BCR:H271	2.03	0.41
4:BD:53:THR:CB	4:BD:67:TYR:HD2	2.34	0.41
4:BD:263:ASN:O	4:BD:265:ARG:N	2.54	0.41
4:BD:283:ALA:HA	22:BD:402:CLA:HED2	2.03	0.41
8:BI:4:LEU:O	8:BI:8:VAL:HG23	2.20	0.41
12:BM:21:PHE:O	12:BM:22:LEU:C	2.63	0.41
15:BU:38:GLU:CG	15:BU:39:LEU:N	2.81	0.41
22:AA:403:CLA:HAA1	24:AD:405:PL9:C36	2.51	0.40
2:AB:170:ASP:HB2	2:AB:171:PRO:HD2	2.02	0.40
2:AB:280:PHE:O	2:AB:284:ILE:HG13	2.20	0.40
5:AE:64:PRO:HB3	5:AE:84:LYS:CD	2.50	0.40
16:AV:153:GLY:O	16:AV:154:ASP:C	2.62	0.40
19:AY:23:UNK:O	19:AY:25:UNK:N	2.54	0.40
1:BA:12:ASN:O	1:BA:13:LEU:C	2.63	0.40
1:BA:257:ARG:HG3	1:BA:257:ARG:NH1	2.33	0.40
2:BB:229:LEU:HD11	22:BB:612:CLA:O1A	2.21	0.40
4:BD:14:TRP:CD2	4:BD:15:PHE:N	2.89	0.40
4:BD:161:PRO:CB	4:BD:170:ALA:HB2	2.51	0.40
5:BE:14:ILE:O	5:BE:14:ILE:HG22	2.21	0.40
13:BO:44:LYS:HA	13:BO:72:GLN:OE1	2.21	0.40
1:AA:105:TRP:CZ3	1:AA:111:PRO:HG3	2.55	0.40
1:AA:339:PHE:HB3	1:AA:340:PRO:HD2	2.03	0.40
2:AB:16:PRO:HG3	2:AB:133:LEU:HD11	2.03	0.40
2:AB:103:LEU:HD21	22:AB:605:CLA:HMC2	2.02	0.40
3:AC:461:ARG:HG3	3:AC:461:ARG:NH1	2.33	0.40
15:AU:75:LEU:HD21	15:AU:101:GLN:HB3	2.03	0.40
16:AV:58:LEU:HD13	16:AV:137:ASP:HB3	2.02	0.40
17:Ay:20:ALA:O	17:Ay:23:THR:HG22	2.21	0.40
1:BA:126:TYR:O	1:BA:130:GLN:HG3	2.22	0.40
3:BC:155:ASN:O	3:BC:158:THR:CG2	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BC:272:LEU:O	3:BC:273:SER:C	2.64	0.40
3:BC:318:LEU:HG	3:BC:328:VAL:CG1	2.50	0.40
3:BC:350:ILE:CG2	3:BC:359:TRP:HB2	2.52	0.40
3:BC:394:GLU:OE2	3:BC:398:HIS:CD2	2.74	0.40
4:BD:205:LEU:HA	4:BD:205:LEU:HD12	1.72	0.40
30:BD:408:LMG:O6	11:BL:15:THR:HG21	2.21	0.40
12:BM:5:GLN:NE2	32:BM:101:LMT:O2B	2.55	0.40
18:BX:11:THR:O	18:BX:12:ILE:C	2.64	0.40
1:AA:257:ARG:HG3	1:AA:257:ARG:NH1	2.35	0.40
2:AB:289:GLN:OE1	2:AB:289:GLN:HA	2.21	0.40
3:AC:56:HIS:C	3:AC:58:GLY:H	2.27	0.40
32:AD:411:LMT:O3'	18:AX:21:ILE:HG21	2.21	0.40
5:AE:14:ILE:O	5:AE:14:ILE:HG22	2.20	0.40
17:Ay:20:ALA:C	17:Ay:22:LEU:N	2.79	0.40
30:BA:414:LMG:H292	11:BL:20:GLY:HA2	2.04	0.40
2:BB:54:PRO:HD2	2:BB:57:ARG:HG3	2.04	0.40
3:BC:338:GLY:O	3:BC:339:LYS:C	2.62	0.40
3:BC:362:ARG:H	27:BC:516:DGD:HE4	1.87	0.40
4:BD:48:TRP:CE2	23:BD:403:PHO:H161	2.56	0.40
5:BE:15:THR:CG2	9:BJ:7:ARG:HG3	2.51	0.40
7:BH:5:THR:O	7:BH:6:TRP:C	2.64	0.40
16:BV:128:PRO:O	16:BV:129:LYS:C	2.64	0.40
1:AA:16:ARG:O	1:AA:17:PHE:C	2.65	0.40
1:AA:24:THR:OG1	3:AC:469:MET:CE	2.70	0.40
3:AC:42:LEU:HD11	22:AC:511:CLA:C1A	2.51	0.40
3:AC:464:GLU:HA	3:AC:465:PRO:HD2	1.72	0.40
22:AC:502:CLA:HBD	22:AC:503:CLA:H43	2.03	0.40
26:AC:515:BCR:C33	8:AI:20:VAL:HG13	2.52	0.40
4:AD:43:LEU:HD12	4:AD:43:LEU:HA	1.94	0.40
4:AD:302:GLU:OE1	4:AD:302:GLU:HA	2.20	0.40
12:AM:21:PHE:O	12:AM:22:LEU:C	2.64	0.40
13:AO:120:THR:HG22	13:AO:154:SER:HG	1.83	0.40
15:AU:88:VAL:HG13	15:AU:109:LEU:HD22	2.03	0.40
15:AU:90:ASP:HA	15:AU:93:ASN:HD22	1.87	0.40
15:AU:94:ILE:HB	15:AU:97:LEU:HD11	2.03	0.40
16:AV:160:LYS:HA	16:AV:163:TYR:CD2	2.56	0.40
18:AX:43:ILE:O	18:AX:43:ILE:CG2	2.70	0.40
1:BA:30:VAL:O	1:BA:30:VAL:HG22	2.21	0.40
1:BA:271:LEU:HD21	24:BA:408:PL9:HC71	2.03	0.40
22:BA:404:CLA:HAA1	24:BD:405:PL9:C36	2.51	0.40
2:BB:12:LEU:O	2:BB:13:ILE:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BB:24:LEU:HD13	2:BB:111:ALA:N	2.37	0.40
2:BB:113:TRP:CD1	22:BB:619:CLA:HBA1	2.57	0.40
3:BC:109:PHE:CG	30:BC:520:LMG:HC61	2.56	0.40
3:BC:267:SER:O	3:BC:271:TYR:CD2	2.74	0.40
3:BC:461:ARG:HG3	3:BC:461:ARG:NH1	2.36	0.40
22:BC:511:CLA:HMB1	26:BC:514:BCR:H382	2.03	0.40
26:BC:515:BCR:H332	8:BI:20:VAL:HG13	2.02	0.40
10:BK:20:PRO:HB2	17:By:21:GLN:HB3	2.04	0.40
13:BO:116:ASP:OD2	13:BO:116:ASP:C	2.64	0.40
29:AA:412:SQD:H132	28:AC:521:LHG:H132	2.02	0.40
2:AB:233:ASN:O	2:AB:236:THR:HG22	2.22	0.40
22:AB:608:CLA:HMA1	4:AD:130:PHE:CE1	2.56	0.40
3:AC:94:THR:CG2	3:AC:298:PRO:HD2	2.51	0.40
3:AC:318:LEU:C	3:AC:318:LEU:CD2	2.94	0.40
3:AC:414:ILE:CG2	3:AC:415:ASN:N	2.84	0.40
28:AC:521:LHG:O9	28:AC:521:LHG:HC41	2.21	0.40
4:AD:205:LEU:HA	4:AD:205:LEU:HD12	1.71	0.40
4:AD:267:LEU:C	4:AD:267:LEU:CD2	2.90	0.40
9:AJ:9:PRO:HB2	9:AJ:12:ILE:HG13	2.03	0.40
13:AO:226:ASN:N	13:AO:226:ASN:ND2	2.69	0.40
26:AT:102:BCR:H393	22:BB:610:CLA:CAC	2.48	0.40
1:BA:116:ILE:HG13	1:BA:117:PHE:N	2.37	0.40
1:BA:129:ARG:C	1:BA:131:TRP:N	2.78	0.40
1:BA:184:ILE:HD11	4:BD:186:GLN:CD	2.47	0.40
1:BA:217:SER:O	1:BA:218:LEU:C	2.65	0.40
1:BA:291:SER:HB3	3:BC:431:PHE:CE2	2.57	0.40
2:BB:62:VAL:C	2:BB:64:PRO:HD2	2.47	0.40
2:BB:254:GLY:O	2:BB:258:TYR:HD2	2.05	0.40
2:BB:475:PHE:HB3	2:BB:478:VAL:CG2	2.52	0.40
3:BC:84:GLN:O	3:BC:86:LEU:HD13	2.22	0.40
3:BC:416:SER:OG	3:BC:417:VAL:N	2.54	0.40
4:BD:48:TRP:CD2	23:BD:403:PHO:H161	2.56	0.40
6:BF:25:THR:O	6:BF:29:PRO:HG2	2.21	0.40
8:BI:13:THR:O	8:BI:14:PHE:C	2.64	0.40
13:BO:49:ASP:CG	13:BO:50:ASP:N	2.79	0.40
13:BO:88:GLU:CD	13:BO:88:GLU:C	2.89	0.40
17:By:22:LEU:H	17:By:22:LEU:HD12	1.87	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	AA	333/344 (97%)	285 (86%)	41 (12%)	7 (2%)	5 21
1	BA	333/344 (97%)	285 (86%)	41 (12%)	7 (2%)	5 21
2	AB	488/510 (96%)	417 (86%)	57 (12%)	14 (3%)	3 15
2	BB	488/510 (96%)	422 (86%)	52 (11%)	14 (3%)	3 15
3	AC	445/473 (94%)	371 (83%)	58 (13%)	16 (4%)	2 11
3	BC	445/473 (94%)	372 (84%)	56 (13%)	17 (4%)	2 10
4	AD	338/352 (96%)	286 (85%)	43 (13%)	9 (3%)	4 16
4	BD	338/352 (96%)	288 (85%)	42 (12%)	8 (2%)	4 18
5	AE	80/84 (95%)	71 (89%)	5 (6%)	4 (5%)	1 6
5	BE	80/84 (95%)	70 (88%)	6 (8%)	4 (5%)	1 6
6	AF	33/45 (73%)	24 (73%)	8 (24%)	1 (3%)	3 14
6	BF	33/45 (73%)	24 (73%)	8 (24%)	1 (3%)	3 14
7	AH	63/66 (96%)	47 (75%)	10 (16%)	6 (10%)	0 1
7	BH	63/66 (96%)	48 (76%)	11 (18%)	4 (6%)	1 3
8	AI	33/38 (87%)	20 (61%)	11 (33%)	2 (6%)	1 4
8	BI	33/38 (87%)	21 (64%)	10 (30%)	2 (6%)	1 4
9	AJ	32/40 (80%)	26 (81%)	4 (12%)	2 (6%)	1 3
9	BJ	32/40 (80%)	26 (81%)	4 (12%)	2 (6%)	1 3
10	AK	35/37 (95%)	28 (80%)	5 (14%)	2 (6%)	1 4
10	BK	35/37 (95%)	28 (80%)	5 (14%)	2 (6%)	1 4
11	AL	35/37 (95%)	33 (94%)	2 (6%)	0	100 100
11	BL	35/37 (95%)	33 (94%)	2 (6%)	0	100 100
12	AM	32/36 (89%)	23 (72%)	9 (28%)	0	100 100
12	BM	32/36 (89%)	24 (75%)	8 (25%)	0	100 100
13	AO	241/247 (98%)	199 (83%)	30 (12%)	12 (5%)	1 6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
13	BO	241/247 (98%)	199 (83%)	31 (13%)	11 (5%)	2 7
14	AT	30/32 (94%)	25 (83%)	4 (13%)	1 (3%)	3 13
14	BT	30/32 (94%)	25 (83%)	4 (13%)	1 (3%)	3 13
15	AU	95/104 (91%)	79 (83%)	12 (13%)	4 (4%)	2 9
15	BU	95/104 (91%)	79 (83%)	12 (13%)	4 (4%)	2 9
16	AV	135/137 (98%)	111 (82%)	23 (17%)	1 (1%)	18 48
16	BV	135/137 (98%)	112 (83%)	22 (16%)	1 (1%)	18 48
17	Ay	26/46 (56%)	14 (54%)	8 (31%)	4 (15%)	0 0
17	By	26/46 (56%)	14 (54%)	8 (31%)	4 (15%)	0 0
18	AX	35/50 (70%)	26 (74%)	5 (14%)	4 (11%)	0 1
18	BX	35/50 (70%)	27 (77%)	4 (11%)	4 (11%)	0 1
20	AZ	60/62 (97%)	48 (80%)	9 (15%)	3 (5%)	1 6
20	BZ	60/62 (97%)	48 (80%)	9 (15%)	3 (5%)	1 6
All	All	5138/5480 (94%)	4278 (83%)	679 (13%)	181 (4%)	3 12

All (181) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AA	12	ASN
1	AA	141	PRO
1	AA	142	TRP
2	AB	176	GLY
2	AB	230	ARG
2	AB	484	PRO
2	AB	488	PRO
3	AC	144	SER
3	AC	257	PHE
3	AC	416	SER
3	AC	452	ALA
4	AD	239	GLN
4	AD	240	ALA
4	AD	262	SER
5	AE	82	GLN
7	AH	18	TYR
8	AI	25	SER
9	AJ	35	GLY
13	AO	52	ALA

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Mol	Chain	Res	Type
14	AT	30	THR
15	AU	72	TYR
15	AU	83	ALA
16	AV	75	ASN
17	Ay	43	ARG
18	AX	45	LYS
20	AZ	32	ASP
1	BA	12	ASN
1	BA	141	PRO
1	BA	142	TRP
2	BB	176	GLY
2	BB	230	ARG
2	BB	484	PRO
2	BB	488	PRO
3	BC	144	SER
3	BC	257	PHE
3	BC	416	SER
3	BC	452	ALA
4	BD	239	GLN
4	BD	240	ALA
4	BD	262	SER
7	BH	18	TYR
8	BI	25	SER
9	BJ	35	GLY
13	BO	52	ALA
14	BT	30	THR
15	BU	72	TYR
15	BU	83	ALA
17	By	43	ARG
18	BX	45	LYS
20	BZ	32	ASP
2	AB	349	LYS
3	AC	46	SER
3	AC	136	GLY
3	AC	194	GLY
3	AC	209	ILE
3	AC	456	GLU
4	AD	234	ALA
4	AD	264	LYS
7	AH	26	GLY
9	AJ	38	SER
13	AO	231	ASP

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Mol	Chain	Res	Type
15	AU	73	PRO
17	Ay	25	ILE
18	AX	43	ILE
2	BB	349	LYS
2	BB	436	THR
3	BC	136	GLY
3	BC	141	GLU
3	BC	194	GLY
4	BD	234	ALA
5	BE	82	GLN
7	BH	26	GLY
9	BJ	38	SER
13	BO	158	ASN
13	BO	231	ASP
15	BU	73	PRO
16	BV	75	ASN
18	BX	43	ILE
2	AB	127	ARG
2	AB	183	PRO
2	AB	414	PRO
2	AB	436	THR
3	AC	32	GLY
3	AC	141	GLU
3	AC	375	LEU
3	AC	453	ALA
4	AD	263	ASN
5	AE	9	PRO
7	AH	16	SER
10	AK	13	GLU
10	AK	45	PHE
13	AO	60	SER
13	AO	158	ASN
13	AO	165	SER
20	AZ	24	PRO
20	AZ	28	ALA
2	BB	13	ILE
2	BB	127	ARG
2	BB	183	PRO
2	BB	414	PRO
3	BC	32	GLY
3	BC	46	SER
3	BC	209	ILE

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Mol	Chain	Res	Type
3	BC	375	LEU
3	BC	411	ALA
3	BC	456	GLU
4	BD	263	ASN
4	BD	264	LYS
5	BE	9	PRO
7	BH	16	SER
10	BK	13	GLU
10	BK	45	PHE
13	BO	165	SER
17	By	25	ILE
20	BZ	24	PRO
20	BZ	28	ALA
2	AB	13	ILE
2	AB	173	GLY
2	AB	231	MET
2	AB	235	GLU
3	AC	154	LYS
4	AD	73	PHE
5	AE	10	PHE
13	AO	51	THR
13	AO	82	PRO
17	Ay	24	MET
18	AX	44	ASP
2	BB	235	GLU
5	BE	10	PHE
13	BO	60	SER
13	BO	82	PRO
1	AA	97	TRP
3	AC	462	GLU
6	AF	41	GLN
7	AH	6	TRP
15	AU	42	VAL
18	AX	12	ILE
2	BB	435	GLU
3	BC	453	ALA
3	BC	462	GLU
4	BD	252	PHE
6	BF	41	GLN
7	BH	6	TRP
13	BO	85	LYS
13	BO	88	GLU

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Mol	Chain	Res	Type
15	BU	42	VAL
17	By	24	MET
18	BX	44	ASP
1	AA	334	ARG
4	AD	351	ALA
7	AH	14	LEU
13	AO	88	GLU
1	BA	97	TRP
1	BA	334	ARG
2	BB	173	GLY
3	BC	382	ASN
4	BD	351	ALA
5	BE	52	PRO
13	BO	51	THR
13	BO	159	VAL
18	BX	12	ILE
1	AA	21	VAL
2	AB	16	PRO
13	AO	159	VAL
1	BA	21	VAL
17	By	35	ILE
3	AC	201	ASN
17	Ay	35	ILE
3	BC	201	ASN
5	AE	52	PRO
7	AH	60	VAL
8	AI	32	PRO
13	AO	232	GLY
2	BB	16	PRO
8	BI	32	PRO
1	AA	176	ILE
4	AD	160	TYR
13	AO	127	ILE
1	BA	39	PRO
13	AO	152	VAL
13	BO	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	AA	271/280 (97%)	256 (94%)	15 (6%)	19	50
1	BA	271/280 (97%)	257 (95%)	14 (5%)	21	52
2	AB	390/407 (96%)	373 (96%)	17 (4%)	25	59
2	BB	390/407 (96%)	372 (95%)	18 (5%)	24	57
3	AC	347/374 (93%)	334 (96%)	13 (4%)	30	64
3	BC	347/374 (93%)	332 (96%)	15 (4%)	26	60
4	AD	275/283 (97%)	257 (94%)	18 (6%)	15	44
4	BD	275/283 (97%)	256 (93%)	19 (7%)	14	41
5	AE	72/73 (99%)	65 (90%)	7 (10%)	8	25
5	BE	72/73 (99%)	65 (90%)	7 (10%)	8	25
6	AF	29/39 (74%)	29 (100%)	0	100	100
6	BF	29/39 (74%)	29 (100%)	0	100	100
7	AH	53/55 (96%)	50 (94%)	3 (6%)	18	49
7	BH	53/55 (96%)	50 (94%)	3 (6%)	18	49
8	AI	32/35 (91%)	30 (94%)	2 (6%)	16	45
8	BI	32/35 (91%)	30 (94%)	2 (6%)	16	45
9	AJ	24/28 (86%)	23 (96%)	1 (4%)	26	60
9	BJ	24/28 (86%)	23 (96%)	1 (4%)	26	60
10	AK	30/30 (100%)	27 (90%)	3 (10%)	7	24
10	BK	30/30 (100%)	28 (93%)	2 (7%)	15	43
11	AL	35/35 (100%)	32 (91%)	3 (9%)	10	30
11	BL	35/35 (100%)	32 (91%)	3 (9%)	10	30
12	AM	31/33 (94%)	30 (97%)	1 (3%)	34	68
12	BM	31/33 (94%)	29 (94%)	2 (6%)	15	44
13	AO	202/208 (97%)	196 (97%)	6 (3%)	36	70
13	BO	202/208 (97%)	196 (97%)	6 (3%)	36	70
14	AT	29/29 (100%)	28 (97%)	1 (3%)	32	66
14	BT	29/29 (100%)	28 (97%)	1 (3%)	32	66
15	AU	84/89 (94%)	80 (95%)	4 (5%)	23	55
15	BU	84/89 (94%)	80 (95%)	4 (5%)	23	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
16	AV	116/117 (99%)	112 (97%)	4 (3%)	32 66
16	BV	116/117 (99%)	112 (97%)	4 (3%)	32 66
17	Ay	20/37 (54%)	17 (85%)	3 (15%)	3 10
17	By	20/37 (54%)	17 (85%)	3 (15%)	3 10
18	AX	30/42 (71%)	24 (80%)	6 (20%)	1 4
18	BX	30/42 (71%)	24 (80%)	6 (20%)	1 4
20	AZ	52/52 (100%)	47 (90%)	5 (10%)	8 26
20	BZ	52/52 (100%)	47 (90%)	5 (10%)	8 26
All	All	4244/4492 (94%)	4017 (95%)	227 (5%)	20 52

All (227) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AA	30	VAL
1	AA	32	TRP
1	AA	157	VAL
1	AA	202	VAL
1	AA	206	PHE
1	AA	210	LEU
1	AA	214	MET
1	AA	218	LEU
1	AA	243	GLU
1	AA	271	LEU
1	AA	275	LEU
1	AA	286	THR
1	AA	292	THR
1	AA	306	VAL
1	AA	308	ASP
2	AB	11	VAL
2	AB	18	ARG
2	AB	84	THR
2	AB	116	VAL
2	AB	223	GLN
2	AB	262	THR
2	AB	271	THR
2	AB	308	LYS
2	AB	309	LEU
2	AB	362	PHE
2	AB	414	PRO

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Mol	Chain	Res	Type
2	AB	422	ARG
2	AB	433	ASP
2	AB	436	THR
2	AB	486	LEU
2	AB	488	PRO
2	AB	490	GLN
3	AC	29	GLU
3	AC	86	LEU
3	AC	165	LEU
3	AC	174	LEU
3	AC	244	CYS
3	AC	289	PHE
3	AC	305	THR
3	AC	355	THR
3	AC	391	ARG
3	AC	401	LEU
3	AC	417	VAL
3	AC	447	ARG
3	AC	472	LEU
4	AD	20	ASP
4	AD	43	LEU
4	AD	53	THR
4	AD	60	THR
4	AD	84	SER
4	AD	91	LEU
4	AD	130	PHE
4	AD	180	ARG
4	AD	201	VAL
4	AD	221	THR
4	AD	236	ASN
4	AD	241	GLU
4	AD	256	ILE
4	AD	259	ILE
4	AD	279	LEU
4	AD	291	LEU
4	AD	323	GLU
4	AD	346	LEU
5	AE	5	THR
5	AE	9	PRO
5	AE	18	ARG
5	AE	52	PRO
5	AE	77	GLU

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Mol	Chain	Res	Type
5	AE	82	GLN
5	AE	84	LYS
7	AH	21	VAL
7	AH	27	THR
7	AH	60	VAL
8	AI	32	PRO
8	AI	33	LYS
9	AJ	7	ARG
10	AK	12	PRO
10	AK	18	PHE
10	AK	19	ASP
11	AL	8	GLN
11	AL	11	GLU
11	AL	15	THR
12	AM	20	VAL
13	AO	31	LEU
13	AO	86	ARG
13	AO	97	VAL
13	AO	106	GLN
13	AO	178	ARG
13	AO	219	THR
14	AT	29	ILE
15	AU	61	ASN
15	AU	88	VAL
15	AU	114	VAL
15	AU	132	LEU
16	AV	35	THR
16	AV	45	ILE
16	AV	63	CYS
16	AV	116	GLU
17	Ay	25	ILE
17	Ay	28	ILE
17	Ay	46	LEU
18	AX	11	THR
18	AX	12	ILE
18	AX	32	LEU
18	AX	42	GLN
18	AX	45	LYS
18	AX	47	GLN
20	AZ	14	ILE
20	AZ	25	VAL
20	AZ	33	TRP

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Mol	Chain	Res	Type
20	AZ	58	ASN
20	AZ	62	VAL
1	BA	30	VAL
1	BA	32	TRP
1	BA	157	VAL
1	BA	202	VAL
1	BA	206	PHE
1	BA	210	LEU
1	BA	214	MET
1	BA	243	GLU
1	BA	271	LEU
1	BA	275	LEU
1	BA	286	THR
1	BA	292	THR
1	BA	306	VAL
1	BA	308	ASP
2	BB	11	VAL
2	BB	18	ARG
2	BB	84	THR
2	BB	116	VAL
2	BB	223	GLN
2	BB	262	THR
2	BB	271	THR
2	BB	308	LYS
2	BB	309	LEU
2	BB	362	PHE
2	BB	414	PRO
2	BB	422	ARG
2	BB	433	ASP
2	BB	436	THR
2	BB	483	ASP
2	BB	486	LEU
2	BB	488	PRO
2	BB	490	GLN
3	BC	29	GLU
3	BC	78	GLU
3	BC	86	LEU
3	BC	165	LEU
3	BC	174	LEU
3	BC	244	CYS
3	BC	289	PHE
3	BC	305	THR

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Mol	Chain	Res	Type
3	BC	330	SER
3	BC	355	THR
3	BC	391	ARG
3	BC	401	LEU
3	BC	417	VAL
3	BC	447	ARG
3	BC	472	LEU
4	BD	20	ASP
4	BD	43	LEU
4	BD	53	THR
4	BD	60	THR
4	BD	84	SER
4	BD	91	LEU
4	BD	130	PHE
4	BD	180	ARG
4	BD	201	VAL
4	BD	205	LEU
4	BD	221	THR
4	BD	236	ASN
4	BD	241	GLU
4	BD	256	ILE
4	BD	259	ILE
4	BD	279	LEU
4	BD	291	LEU
4	BD	323	GLU
4	BD	346	LEU
5	BE	5	THR
5	BE	9	PRO
5	BE	18	ARG
5	BE	52	PRO
5	BE	77	GLU
5	BE	82	GLN
5	BE	84	LYS
7	BH	21	VAL
7	BH	27	THR
7	BH	60	VAL
8	BI	32	PRO
8	BI	33	LYS
9	BJ	7	ARG
10	BK	18	PHE
10	BK	19	ASP
11	BL	8	GLN

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Mol	Chain	Res	Type
11	BL	11	GLU
11	BL	15	THR
12	BM	1	MET
12	BM	20	VAL
13	BO	31	LEU
13	BO	86	ARG
13	BO	97	VAL
13	BO	106	GLN
13	BO	178	ARG
13	BO	219	THR
14	BT	29	ILE
15	BU	61	ASN
15	BU	88	VAL
15	BU	114	VAL
15	BU	132	LEU
16	BV	35	THR
16	BV	45	ILE
16	BV	63	CYS
16	BV	116	GLU
17	By	25	ILE
17	By	28	ILE
17	By	46	LEU
18	BX	11	THR
18	BX	12	ILE
18	BX	32	LEU
18	BX	42	GLN
18	BX	45	LYS
18	BX	47	GLN
20	BZ	14	ILE
20	BZ	25	VAL
20	BZ	33	TRP
20	BZ	58	ASN
20	BZ	62	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81) such sidechains are listed below:

Mol	Chain	Res	Type
1	AA	12	ASN
1	AA	19	ASN
1	AA	165	GLN
1	AA	241	GLN
1	AA	247	ASN

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Mol	Chain	Res	Type
2	AB	26	HIS
2	AB	201	HIS
2	AB	216	HIS
2	AB	490	GLN
3	AC	44	ASN
3	AC	155	ASN
3	AC	398	HIS
3	AC	418	ASN
3	AC	444	HIS
4	AD	98	GLN
4	AD	117	HIS
4	AD	129	GLN
4	AD	224	GLN
4	AD	239	GLN
4	AD	250	ASN
4	AD	301	GLN
5	AE	75	GLN
7	AH	59	ASN
11	AL	8	GLN
12	AM	5	GLN
12	AM	32	GLN
12	AM	33	GLN
13	AO	87	GLN
13	AO	106	GLN
13	AO	135	GLN
13	AO	150	ASN
13	AO	173	ASN
13	AO	202	GLN
13	AO	222	GLN
13	AO	226	ASN
15	AU	82	ASN
15	AU	93	ASN
17	Ay	21	GLN
18	AX	42	GLN
20	AZ	6	GLN
1	BA	12	ASN
1	BA	19	ASN
1	BA	165	GLN
1	BA	241	GLN
1	BA	247	ASN
2	BB	26	HIS
2	BB	201	HIS

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Mol	Chain	Res	Type
2	BB	216	HIS
2	BB	282	GLN
2	BB	490	GLN
3	BC	44	ASN
3	BC	155	ASN
3	BC	251	HIS
3	BC	398	HIS
3	BC	418	ASN
3	BC	444	HIS
4	BD	98	GLN
4	BD	117	HIS
4	BD	129	GLN
4	BD	239	GLN
4	BD	250	ASN
7	BH	59	ASN
11	BL	8	GLN
12	BM	5	GLN
12	BM	32	GLN
12	BM	33	GLN
13	BO	87	GLN
13	BO	106	GLN
13	BO	135	GLN
13	BO	150	ASN
13	BO	173	ASN
13	BO	202	GLN
13	BO	222	GLN
13	BO	226	ASN
15	BU	82	ASN
15	BU	93	ASN
15	BU	108	ASN
15	BU	111	HIS
16	BV	104	ASN
18	BX	42	GLN
20	BZ	6	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 184 ligands modelled in this entry, 8 are monoatomic - leaving 176 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	$\#\|Z\| > 2$
30	LMG	AB	622	-	49,49,55	1.08	6 (12%)	57,57,63	1.02	3 (5%)
22	CLA	BA	407	1	69,73,73	1.23	6 (8%)	82,113,113	1.66	9 (10%)
26	BCR	AD	406	-	41,41,41	1.88	7 (17%)	56,56,56	2.35	22 (39%)
22	CLA	AB	614	2	69,73,73	1.42	9 (13%)	82,113,113	1.83	13 (15%)
22	CLA	AC	511	3	69,73,73	1.48	6 (8%)	82,113,113	1.84	10 (12%)
32	LMT	AT	101	-	36,36,36	1.36	5 (13%)	47,47,47	1.08	4 (8%)
22	CLA	BB	619	-	69,73,73	1.32	7 (10%)	82,113,113	1.83	11 (13%)
22	CLA	BC	510	-	69,73,73	1.20	8 (11%)	82,113,113	1.70	11 (13%)
27	DGD	AB	626	-	53,53,67	1.87	17 (32%)	67,67,81	1.58	9 (13%)
24	PL9	BD	405	-	55,55,55	0.55	0	68,69,69	1.73	18 (26%)
26	BCR	AH	101	-	41,41,41	1.89	7 (17%)	56,56,56	2.30	22 (39%)
22	CLA	BA	404	-	69,73,73	1.28	6 (8%)	82,113,113	1.85	15 (18%)
22	CLA	BD	404	-	69,73,73	1.41	11 (15%)	82,113,113	1.73	11 (13%)
26	BCR	AB	617	-	41,41,41	1.72	8 (19%)	56,56,56	2.04	15 (26%)
29	SQD	BB	601	-	45,47,54	2.69	23 (51%)	55,58,65	2.58	16 (29%)
26	BCR	AC	515	-	41,41,41	1.72	6 (14%)	56,56,56	2.22	19 (33%)
27	DGD	AD	410	-	64,64,67	1.84	16 (25%)	78,78,81	1.38	7 (8%)
30	LMG	BB	624	-	49,49,55	1.06	5 (10%)	57,57,63	1.01	3 (5%)
22	CLA	BC	511	3	69,73,73	1.50	8 (11%)	82,113,113	1.85	10 (12%)
22	CLA	AB	616	-	69,73,73	1.32	8 (11%)	82,113,113	1.77	11 (13%)
22	CLA	BC	502	3	69,73,73	1.31	6 (8%)	82,113,113	1.78	10 (12%)
22	CLA	AC	506	3	69,73,73	1.32	6 (8%)	82,113,113	1.78	10 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	DGD	BD	410	-	64,64,67	1.78	17 (26%)	78,78,81	1.38	7 (8%)
24	PL9	AA	407	-	45,45,55	0.94	2 (4%)	56,57,69	1.70	15 (26%)
22	CLA	BC	501	3	69,73,73	1.35	4 (5%)	82,113,113	1.78	12 (14%)
34	HEM	BV	201	16	50,50,50	1.98	16 (32%)	67,82,82	1.94	13 (19%)
27	DGD	AC	516	-	54,54,67	1.24	8 (14%)	68,68,81	1.51	7 (10%)
26	BCR	BX	101	-	41,41,41	1.88	7 (17%)	56,56,56	2.31	23 (41%)
29	SQD	BL	101	-	45,47,54	2.73	23 (51%)	55,58,65	2.58	15 (27%)
30	LMG	AB	621	-	49,49,55	1.04	5 (10%)	57,57,63	1.02	4 (7%)
22	CLA	BC	508	3	69,73,73	1.38	8 (11%)	82,113,113	1.80	11 (13%)
22	CLA	AC	507	-	69,73,73	1.26	5 (7%)	82,113,113	1.81	12 (14%)
22	CLA	BB	608	2	69,73,73	1.25	5 (7%)	82,113,113	1.70	10 (12%)
22	CLA	BB	615	-	69,73,73	1.35	9 (13%)	82,113,113	1.73	11 (13%)
29	SQD	AD	409	-	41,43,54	2.78	19 (46%)	51,54,65	2.82	15 (29%)
23	PHO	AA	405	-	58,69,69	1.71	8 (13%)	55,99,99	1.97	16 (29%)
22	CLA	BB	612	2	69,73,73	1.40	5 (7%)	82,113,113	1.72	12 (14%)
33	BCT	BD	401	21	3,3,3	0.53	0	2,3,3	0.36	0
26	BCR	BB	620	-	41,41,41	1.59	8 (19%)	56,56,56	2.04	15 (26%)
30	LMG	AI	101	-	43,43,55	1.50	8 (18%)	51,51,63	1.05	3 (5%)
22	CLA	BD	402	4	69,73,73	1.48	8 (11%)	82,113,113	1.81	10 (12%)
22	CLA	AC	512	-	69,73,73	1.43	10 (14%)	82,113,113	1.82	11 (13%)
32	LMT	AD	411	-	32,32,36	1.53	5 (15%)	43,43,47	1.01	2 (4%)
28	LHG	BC	521	-	36,36,48	1.08	2 (5%)	39,42,54	1.14	3 (7%)
27	DGD	AC	518	-	67,67,67	1.05	6 (8%)	81,81,81	1.27	4 (4%)
27	DGD	AC	517	-	63,63,67	1.07	5 (7%)	77,77,81	1.55	10 (12%)
28	LHG	AA	411	-	38,38,48	2.04	5 (13%)	41,44,54	1.40	4 (9%)
32	LMT	BB	626	-	36,36,36	1.37	5 (13%)	47,47,47	0.95	2 (4%)
34	HEM	AE	101	6,5	50,50,50	2.05	17 (34%)	67,82,82	2.08	12 (17%)
22	CLA	AC	508	3	69,73,73	1.39	7 (10%)	82,113,113	1.86	10 (12%)
22	CLA	AA	402	1	69,73,73	1.32	8 (11%)	82,113,113	1.72	9 (10%)
26	BCR	BB	621	-	41,41,41	1.89	6 (14%)	56,56,56	2.17	18 (32%)
22	CLA	AC	501	3	69,73,73	1.33	4 (5%)	82,113,113	1.76	11 (13%)
22	CLA	BB	614	2	69,73,73	1.15	5 (7%)	82,113,113	1.63	10 (12%)
22	CLA	BC	503	3	69,73,73	1.46	7 (10%)	82,113,113	1.81	10 (12%)
23	PHO	BA	406	-	58,69,69	1.59	7 (12%)	55,99,99	2.00	17 (30%)
32	LMT	BD	411	-	32,32,36	1.42	4 (12%)	43,43,47	0.96	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
34	HEM	AV	201	16	50,50,50	1.99	16 (32%)	67,82,82	1.93	11 (16%)
22	CLA	BB	605	2	69,73,73	1.25	6 (8%)	82,113,113	1.62	12 (14%)
30	LMG	AB	623	-	42,42,55	1.49	8 (19%)	50,50,63	0.99	3 (6%)
30	LMG	BC	520	-	45,45,55	1.55	10 (22%)	53,53,63	1.03	4 (7%)
22	CLA	BC	512	-	69,73,73	1.43	10 (14%)	82,113,113	1.83	11 (13%)
30	LMG	AA	413	-	51,51,55	0.91	3 (5%)	59,59,63	0.99	4 (6%)
22	CLA	AB	607	-	69,73,73	1.37	11 (15%)	82,113,113	1.76	9 (10%)
26	BCR	AK	102	-	41,41,41	1.87	6 (14%)	56,56,56	2.58	26 (46%)
30	LMG	BC	519	-	48,48,55	1.28	6 (12%)	56,56,63	0.84	2 (3%)
22	CLA	AD	404	-	69,73,73	1.41	8 (11%)	82,113,113	1.76	11 (13%)
32	LMT	AM	102	-	36,36,36	1.21	2 (5%)	47,47,47	0.96	2 (4%)
24	PL9	BJ	101	-	35,35,55	1.44	5 (14%)	44,45,69	1.70	13 (29%)
22	CLA	AB	601	-	69,73,73	1.43	8 (11%)	82,113,113	1.81	9 (10%)
30	LMG	AM	101	-	42,42,55	1.63	6 (14%)	50,50,63	1.16	5 (10%)
32	LMT	AB	625	-	36,36,36	1.39	7 (19%)	47,47,47	0.97	2 (4%)
27	DGD	AA	410	-	57,57,67	1.50	12 (21%)	71,71,81	1.42	8 (11%)
26	BCR	AB	619	-	41,41,41	1.96	7 (17%)	56,56,56	2.13	17 (30%)
26	BCR	BZ	101	-	41,41,41	2.03	9 (21%)	56,56,56	2.13	20 (35%)
26	BCR	BK	102	-	41,41,41	1.88	7 (17%)	56,56,56	2.58	27 (48%)
27	DGD	BA	411	-	57,57,67	1.63	13 (22%)	71,71,81	1.41	8 (11%)
29	SQD	AF	101	-	43,45,54	2.56	21 (48%)	53,56,65	2.74	20 (37%)
30	LMG	BM	102	-	42,42,55	1.66	8 (19%)	50,50,63	1.11	4 (8%)
23	PHO	AD	403	-	58,69,69	1.68	6 (10%)	55,99,99	1.99	14 (25%)
22	CLA	AB	603	2	69,73,73	1.35	8 (11%)	82,113,113	1.72	11 (13%)
22	CLA	BA	403	1	69,73,73	1.37	8 (11%)	82,113,113	1.70	9 (10%)
22	CLA	AB	608	2	69,73,73	1.32	7 (10%)	82,113,113	1.70	11 (13%)
22	CLA	AA	404	-	69,73,73	1.23	5 (7%)	82,113,113	1.70	10 (12%)
34	HEM	BE	101	6,5	50,50,50	2.10	17 (34%)	67,82,82	2.10	12 (17%)
26	BCR	BJ	102	-	41,41,41	2.18	8 (19%)	56,56,56	3.47	23 (41%)
29	SQD	AA	412	-	49,51,54	2.53	25 (51%)	59,62,65	2.66	19 (32%)
22	CLA	AB	610	-	69,73,73	1.28	9 (13%)	82,113,113	1.77	12 (14%)
26	BCR	AB	620	-	41,41,41	1.88	7 (17%)	56,56,56	2.10	19 (33%)
30	LMG	AE	102	-	44,44,55	1.34	6 (13%)	52,52,63	1.08	6 (11%)
23	PHO	BD	403	-	58,69,69	1.67	6 (10%)	55,99,99	2.01	15 (27%)
22	CLA	AC	513	3	69,73,73	1.53	8 (11%)	82,113,113	1.77	10 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	BB	617	2	69,73,73	1.39	8 (11%)	82,113,113	1.80	12 (14%)
24	PL9	AJ	101	-	35,35,55	1.40	4 (11%)	44,45,69	1.75	12 (27%)
33	BCT	AD	401	21	3,3,3	0.53	0	2,3,3	0.37	0
28	LHG	BA	412	-	38,38,48	1.99	6 (15%)	41,44,54	1.39	4 (9%)
30	LMG	AC	520	-	45,45,55	1.53	9 (20%)	53,53,63	1.01	3 (5%)
22	CLA	AC	505	3	69,73,73	1.49	10 (14%)	82,113,113	1.78	9 (10%)
27	DGD	BC	517	-	63,63,67	1.11	6 (9%)	77,77,81	1.56	8 (10%)
24	PL9	BA	408	-	45,45,55	0.97	2 (4%)	56,57,69	1.64	14 (25%)
26	BCR	AJ	102	-	41,41,41	2.07	9 (21%)	56,56,56	3.47	22 (39%)
22	CLA	AC	504	-	69,73,73	1.26	9 (13%)	82,113,113	1.67	11 (13%)
32	LMT	BT	101	-	36,36,36	1.31	5 (13%)	47,47,47	1.05	4 (8%)
26	BCR	AA	409	-	41,41,41	1.69	7 (17%)	56,56,56	2.13	21 (37%)
22	CLA	AB	615	-	69,73,73	1.28	9 (13%)	82,113,113	1.82	9 (10%)
22	CLA	BC	506	3	69,73,73	1.27	6 (8%)	82,113,113	1.75	9 (10%)
26	BCR	BB	622	-	41,41,41	1.86	7 (17%)	56,56,56	2.09	17 (30%)
32	LMT	BB	625	-	36,36,36	1.55	9 (25%)	47,47,47	1.24	3 (6%)
24	PL9	AD	405	-	55,55,55	0.57	0	68,69,69	1.72	18 (26%)
29	SQD	BA	401	-	52,54,54	2.69	31 (59%)	62,65,65	2.62	22 (35%)
22	CLA	AB	613	-	69,73,73	1.23	5 (7%)	82,113,113	1.72	10 (12%)
22	CLA	BC	513	3	69,73,73	1.47	8 (11%)	82,113,113	1.78	9 (10%)
22	CLA	AA	406	1	69,73,73	1.25	5 (7%)	82,113,113	1.66	10 (12%)
26	BCR	AC	514	-	41,41,41	1.82	8 (19%)	56,56,56	2.17	22 (39%)
22	CLA	AB	602	2	69,73,73	1.27	8 (11%)	82,113,113	1.62	11 (13%)
22	CLA	AB	609	2	69,73,73	1.38	6 (8%)	82,113,113	1.69	11 (13%)
22	CLA	AB	612	-	69,73,73	1.26	6 (8%)	82,113,113	1.71	10 (12%)
30	LMG	BA	414	-	51,51,55	0.93	4 (7%)	59,59,63	1.01	4 (6%)
22	CLA	BB	616	-	69,73,73	1.18	8 (11%)	82,113,113	1.69	9 (10%)
22	CLA	BB	618	-	69,73,73	1.22	8 (11%)	82,113,113	1.80	11 (13%)
28	LHG	AC	521	-	36,36,48	1.09	2 (5%)	39,42,54	1.14	3 (7%)
30	LMG	AD	408	-	48,48,55	1.07	3 (6%)	56,56,63	1.00	2 (3%)
32	LMT	AI	102	-	36,36,36	1.44	4 (11%)	47,47,47	0.95	2 (4%)
26	BCR	AB	618	-	41,41,41	1.74	6 (14%)	56,56,56	2.25	26 (46%)
30	LMG	AA	416	-	42,42,55	1.51	7 (16%)	50,50,63	0.97	3 (6%)
22	CLA	BC	507	-	69,73,73	1.28	6 (8%)	82,113,113	1.81	12 (14%)
22	CLA	AD	402	4	69,73,73	1.49	10 (14%)	82,113,113	1.81	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	DGD	BH	101	-	59,59,67	1.22	9 (15%)	73,73,81	1.43	6 (8%)
22	CLA	BB	613	-	69,73,73	1.31	7 (10%)	82,113,113	1.77	12 (14%)
30	LMG	BB	623	-	49,49,55	1.09	5 (10%)	57,57,63	1.04	4 (7%)
22	CLA	AB	606	2	69,73,73	1.34	4 (5%)	82,113,113	1.71	9 (10%)
26	BCR	AZ	101	-	41,41,41	1.91	7 (17%)	56,56,56	2.14	19 (33%)
22	CLA	BB	609	2	69,73,73	1.42	6 (8%)	82,113,113	1.74	9 (10%)
26	BCR	BD	406	-	41,41,41	1.97	8 (19%)	56,56,56	2.34	22 (39%)
22	CLA	BC	505	3	69,73,73	1.57	9 (13%)	82,113,113	1.83	10 (12%)
32	LMT	BM	101	-	36,36,36	1.21	3 (8%)	47,47,47	0.97	2 (4%)
22	CLA	AC	509	-	69,73,73	1.35	9 (13%)	82,113,113	1.74	11 (13%)
26	BCR	AT	102	-	41,41,41	1.66	6 (14%)	56,56,56	2.25	26 (46%)
32	LMT	AB	627	-	36,36,36	1.46	6 (16%)	47,47,47	1.04	3 (6%)
29	SQD	BD	409	-	41,43,54	2.76	20 (48%)	51,54,65	2.81	15 (29%)
22	CLA	BB	611	2	69,73,73	1.34	8 (11%)	82,113,113	1.68	13 (15%)
32	LMT	AB	624	-	36,36,36	1.45	7 (19%)	47,47,47	1.21	3 (6%)
32	LMT	BI	102	-	36,36,36	1.54	4 (11%)	47,47,47	0.97	2 (4%)
27	DGD	BC	516	-	54,54,67	1.36	9 (16%)	68,68,81	1.49	7 (10%)
29	SQD	BF	101	-	43,45,54	2.64	20 (46%)	53,56,65	2.72	19 (35%)
22	CLA	AC	510	-	69,73,73	1.22	10 (14%)	82,113,113	1.66	11 (13%)
22	CLA	BC	504	-	69,73,73	1.29	8 (11%)	82,113,113	1.68	8 (9%)
22	CLA	AC	502	3	69,73,73	1.32	8 (11%)	82,113,113	1.73	9 (10%)
29	SQD	AA	415	-	52,54,54	2.65	30 (57%)	62,65,65	2.60	21 (33%)
30	LMG	BD	408	-	48,48,55	1.16	4 (8%)	56,56,63	1.00	2 (3%)
22	CLA	AA	403	-	69,73,73	1.28	8 (11%)	82,113,113	1.78	14 (17%)
22	CLA	AC	503	3	69,73,73	1.50	8 (11%)	82,113,113	1.85	9 (10%)
27	DGD	AH	102	-	59,59,67	1.27	9 (15%)	73,73,81	1.44	7 (9%)
27	DGD	BB	602	-	53,53,67	1.87	17 (32%)	67,67,81	1.56	8 (11%)
30	LMG	BI	101	-	43,43,55	1.56	8 (18%)	51,51,63	1.07	4 (7%)
22	CLA	AB	604	2	69,73,73	1.45	10 (14%)	82,113,113	1.84	9 (10%)
26	BCR	BA	410	-	41,41,41	1.76	7 (17%)	56,56,56	2.12	24 (42%)
26	BCR	BC	514	-	41,41,41	1.97	8 (19%)	56,56,56	2.16	23 (41%)
22	CLA	BA	405	-	69,73,73	1.25	6 (8%)	82,113,113	1.74	11 (13%)
29	SQD	BA	413	-	49,51,54	2.56	25 (51%)	59,62,65	2.62	19 (32%)
30	LMG	AC	519	-	48,48,55	1.26	5 (10%)	56,56,63	0.84	2 (3%)
22	CLA	AB	611	2	69,73,73	1.21	7 (10%)	82,113,113	1.69	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	LMG	BD	407	-	46,46,55	1.04	4 (8%)	54,54,63	0.91	2 (3%)
30	LMG	AD	407	-	46,46,55	0.97	4 (8%)	54,54,63	0.90	2 (3%)
27	DGD	BC	518	-	67,67,67	1.18	6 (8%)	81,81,81	1.27	4 (4%)
30	LMG	BE	102	-	44,44,55	1.35	6 (13%)	52,52,63	1.08	5 (9%)
22	CLA	AB	605	-	69,73,73	1.32	6 (8%)	82,113,113	1.71	11 (13%)
22	CLA	BB	610	-	69,73,73	1.40	9 (13%)	82,113,113	1.78	10 (12%)
22	CLA	BB	604	-	69,73,73	1.50	11 (15%)	82,113,113	1.83	10 (12%)
26	BCR	BC	515	-	41,41,41	1.87	7 (17%)	56,56,56	2.20	20 (35%)
22	CLA	BC	509	-	69,73,73	1.37	8 (11%)	82,113,113	1.78	11 (13%)
22	CLA	BB	607	2	69,73,73	1.47	9 (13%)	82,113,113	1.81	9 (10%)
22	CLA	BB	606	2	69,73,73	1.28	6 (8%)	82,113,113	1.70	11 (13%)
32	LMT	BB	603	-	36,36,36	1.43	8 (22%)	47,47,47	1.06	3 (6%)

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
30	LMG	AB	622	-	2/2/8/8	19/44/64/70	0/1/1/1
22	CLA	BA	407	1	1/1/15/20	11/39/115/115	-
26	BCR	AD	406	-	-	3/29/63/63	0/2/2/2
22	CLA	AB	614	2	1/1/15/20	18/39/115/115	-
22	CLA	AC	511	3	1/1/15/20	14/39/115/115	-
32	LMT	AT	101	-	-	4/21/61/61	0/2/2/2
22	CLA	BB	619	-	1/1/15/20	16/39/115/115	-
22	CLA	BC	510	-	1/1/15/20	13/39/115/115	-
27	DGD	AB	626	-	3/3/13/13	25/41/81/95	0/2/2/2
24	PL9	BD	405	-	-	16/53/73/73	0/1/1/1
26	BCR	AH	101	-	-	2/29/63/63	0/2/2/2
22	CLA	BA	404	-	1/1/15/20	15/39/115/115	-
22	CLA	BD	404	-	1/1/15/20	9/39/115/115	-
26	BCR	AB	617	-	-	1/29/63/63	0/2/2/2
30	LMG	BB	624	-	2/2/8/8	17/44/64/70	0/1/1/1
27	DGD	AD	410	-	3/3/13/13	34/52/92/95	0/2/2/2
26	BCR	AC	515	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	SQD	BB	601	-	-	18/42/62/69	0/1/1/1
22	CLA	BC	511	3	1/1/15/20	14/39/115/115	-
22	CLA	AB	616	-	1/1/15/20	17/39/115/115	-
22	CLA	BC	502	3	1/1/15/20	11/39/115/115	-
22	CLA	AC	506	3	1/1/15/20	17/39/115/115	-
27	DGD	BD	410	-	3/3/13/13	34/52/92/95	0/2/2/2
24	PL9	AA	407	-	-	16/41/61/73	0/1/1/1
22	CLA	BC	501	3	1/1/15/20	11/39/115/115	-
34	HEM	BV	201	16	-	8/14/54/54	-
27	DGD	AC	516	-	3/3/13/13	17/42/82/95	0/2/2/2
26	BCR	BX	101	-	-	2/29/63/63	0/2/2/2
29	SQD	BL	101	-	-	18/42/62/69	0/1/1/1
30	LMG	AB	621	-	2/2/8/8	22/44/64/70	0/1/1/1
22	CLA	BC	508	3	1/1/15/20	14/39/115/115	-
22	CLA	AC	507	-	1/1/15/20	13/39/115/115	-
22	CLA	BB	608	2	1/1/15/20	18/39/115/115	-
22	CLA	BB	615	-	1/1/15/20	13/39/115/115	-
29	SQD	AD	409	-	-	11/38/58/69	0/1/1/1
23	PHO	AA	405	-	-	12/37/103/103	0/5/6/6
22	CLA	BB	612	2	1/1/15/20	10/39/115/115	-
30	LMG	AI	101	-	2/2/8/8	18/38/58/70	0/1/1/1
26	BCR	BB	620	-	-	1/29/63/63	0/2/2/2
22	CLA	BD	402	4	1/1/15/20	13/39/115/115	-
22	CLA	AC	512	-	1/1/15/20	23/39/115/115	-
32	LMT	AD	411	-	-	0/17/57/61	0/2/2/2
28	LHG	BC	521	-	-	15/41/41/53	-
27	DGD	AC	518	-	3/3/13/13	20/55/95/95	0/2/2/2
27	DGD	AC	517	-	3/3/13/13	29/51/91/95	0/2/2/2
28	LHG	AA	411	-	-	14/43/43/53	-
32	LMT	BB	626	-	-	2/21/61/61	0/2/2/2
34	HEM	AE	101	6,5	-	4/14/54/54	-
22	CLA	AC	508	3	1/1/15/20	14/39/115/115	-
22	CLA	AA	402	1	1/1/15/20	5/39/115/115	-
26	BCR	BB	621	-	-	0/29/63/63	0/2/2/2
22	CLA	AC	501	3	1/1/15/20	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	BB	614	2	1/1/15/20	16/39/115/115	-
22	CLA	BC	503	3	1/1/15/20	15/39/115/115	-
23	PHO	BA	406	-	-	12/37/103/103	0/5/6/6
32	LMT	BD	411	-	-	0/17/57/61	0/2/2/2
34	HEM	AV	201	16	-	7/14/54/54	-
22	CLA	BB	605	2	1/1/15/20	21/39/115/115	-
30	LMG	AB	623	-	2/2/8/8	17/37/57/70	0/1/1/1
30	LMG	BC	520	-	2/2/8/8	18/40/60/70	0/1/1/1
22	CLA	BC	512	-	1/1/15/20	23/39/115/115	-
30	LMG	AA	413	-	2/2/8/8	29/46/66/70	0/1/1/1
22	CLA	AB	607	-	1/1/15/20	13/39/115/115	-
26	BCR	AK	102	-	-	4/29/63/63	0/2/2/2
30	LMG	BC	519	-	2/2/8/8	24/43/63/70	0/1/1/1
22	CLA	AD	404	-	1/1/15/20	11/39/115/115	-
32	LMT	AM	102	-	-	1/21/61/61	0/2/2/2
24	PL9	BJ	101	-	-	10/29/49/73	0/1/1/1
22	CLA	AB	601	-	1/1/15/20	20/39/115/115	-
30	LMG	AM	101	-	2/2/8/8	16/37/57/70	0/1/1/1
32	LMT	AB	625	-	-	2/21/61/61	0/2/2/2
27	DGD	AA	410	-	3/3/13/13	18/45/85/95	0/2/2/2
27	DGD	BA	411	-	3/3/13/13	18/45/85/95	0/2/2/2
26	BCR	AB	619	-	-	0/29/63/63	0/2/2/2
26	BCR	BK	102	-	-	4/29/63/63	0/2/2/2
26	BCR	BZ	101	-	-	3/29/63/63	0/2/2/2
29	SQD	AF	101	-	-	14/40/60/69	0/1/1/1
30	LMG	BM	102	-	2/2/8/8	16/37/57/70	0/1/1/1
22	CLA	AB	603	2	1/1/15/20	11/39/115/115	-
22	CLA	BA	403	1	1/1/15/20	5/39/115/115	-
23	PHO	AD	403	-	-	12/37/103/103	0/5/6/6
22	CLA	AB	608	2	1/1/15/20	19/39/115/115	-
22	CLA	AA	404	-	1/1/15/20	13/39/115/115	-
34	HEM	BE	101	6,5	-	4/14/54/54	-
26	BCR	BJ	102	-	-	5/29/63/63	0/2/2/2
29	SQD	AA	412	-	-	17/46/66/69	0/1/1/1
22	CLA	AB	610	-	1/1/15/20	17/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	AB	620	-	-	2/29/63/63	0/2/2/2
30	LMG	AE	102	-	2/2/8/8	19/39/59/70	0/1/1/1
23	PHO	BD	403	-	-	12/37/103/103	0/5/6/6
22	CLA	AC	513	3	1/1/15/20	18/39/115/115	-
22	CLA	BB	617	2	1/1/15/20	17/39/115/115	-
24	PL9	AJ	101	-	-	10/29/49/73	0/1/1/1
28	LHG	BA	412	-	-	14/43/43/53	-
30	LMG	AC	520	-	2/2/8/8	18/40/60/70	0/1/1/1
22	CLA	AC	505	3	1/1/15/20	20/39/115/115	-
27	DGD	BC	517	-	3/3/13/13	30/51/91/95	0/2/2/2
24	PL9	BA	408	-	-	16/41/61/73	0/1/1/1
26	BCR	AJ	102	-	-	3/29/63/63	0/2/2/2
22	CLA	AC	504	-	1/1/15/20	10/39/115/115	-
32	LMT	BT	101	-	-	4/21/61/61	0/2/2/2
26	BCR	AA	409	-	-	5/29/63/63	0/2/2/2
22	CLA	AB	615	-	1/1/15/20	10/39/115/115	-
22	CLA	BC	506	3	1/1/15/20	17/39/115/115	-
26	BCR	BB	622	-	-	2/29/63/63	0/2/2/2
32	LMT	BB	625	-	-	4/21/61/61	0/2/2/2
24	PL9	AD	405	-	-	16/53/73/73	0/1/1/1
29	SQD	BA	401	-	-	21/49/69/69	0/1/1/1
22	CLA	AB	613	-	1/1/15/20	16/39/115/115	-
22	CLA	BC	513	3	1/1/15/20	18/39/115/115	-
22	CLA	AA	406	1	1/1/15/20	12/39/115/115	-
26	BCR	AC	514	-	-	5/29/63/63	0/2/2/2
22	CLA	AB	602	2	1/1/15/20	21/39/115/115	-
22	CLA	AB	609	2	1/1/15/20	9/39/115/115	-
22	CLA	AB	612	-	1/1/15/20	12/39/115/115	-
30	LMG	BA	414	-	2/2/8/8	27/46/66/70	0/1/1/1
22	CLA	BB	616	-	1/1/15/20	15/39/115/115	-
22	CLA	BB	618	-	1/1/15/20	10/39/115/115	-
30	LMG	AD	408	-	2/2/8/8	25/43/63/70	0/1/1/1
28	LHG	AC	521	-	-	16/41/41/53	-
32	LMT	AI	102	-	-	4/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	AB	618	-	-	3/29/63/63	0/2/2/2
30	LMG	AA	416	-	2/2/8/8	17/37/57/70	0/1/1/1
22	CLA	BC	507	-	1/1/15/20	13/39/115/115	-
22	CLA	AD	402	4	1/1/15/20	12/39/115/115	-
27	DGD	BH	101	-	3/3/13/13	18/47/87/95	0/2/2/2
22	CLA	BB	613	-	1/1/15/20	17/39/115/115	-
30	LMG	BB	623	-	2/2/8/8	22/44/64/70	0/1/1/1
22	CLA	AB	606	2	1/1/15/20	16/39/115/115	-
26	BCR	AZ	101	-	-	3/29/63/63	0/2/2/2
22	CLA	BB	609	2	1/1/15/20	16/39/115/115	-
26	BCR	BD	406	-	-	3/29/63/63	0/2/2/2
22	CLA	BC	505	3	1/1/15/20	20/39/115/115	-
32	LMT	BM	101	-	-	1/21/61/61	0/2/2/2
22	CLA	AC	509	-	1/1/15/20	13/39/115/115	-
26	BCR	AT	102	-	-	3/29/63/63	0/2/2/2
32	LMT	AB	627	-	-	4/21/61/61	0/2/2/2
29	SQD	BD	409	-	-	11/38/58/69	0/1/1/1
22	CLA	BB	611	2	1/1/15/20	19/39/115/115	-
32	LMT	AB	624	-	-	4/21/61/61	0/2/2/2
32	LMT	BI	102	-	-	4/21/61/61	0/2/2/2
27	DGD	BC	516	-	3/3/13/13	17/42/82/95	0/2/2/2
29	SQD	BF	101	-	-	14/40/60/69	0/1/1/1
22	CLA	AC	510	-	1/1/15/20	13/39/115/115	-
22	CLA	BC	504	-	1/1/15/20	10/39/115/115	-
22	CLA	AC	502	3	1/1/15/20	11/39/115/115	-
29	SQD	AA	415	-	-	22/49/69/69	0/1/1/1
30	LMG	BD	408	-	2/2/8/8	25/43/63/70	0/1/1/1
22	CLA	AA	403	-	1/1/15/20	15/39/115/115	-
22	CLA	AC	503	3	1/1/15/20	15/39/115/115	-
27	DGD	AH	102	-	3/3/13/13	18/47/87/95	0/2/2/2
27	DGD	BB	602	-	3/3/13/13	25/41/81/95	0/2/2/2
30	LMG	BI	101	-	2/2/8/8	19/38/58/70	0/1/1/1
22	CLA	AB	604	2	1/1/15/20	11/39/115/115	-
26	BCR	BA	410	-	-	5/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	BC	514	-	-	5/29/63/63	0/2/2/2
22	CLA	BA	405	-	1/1/15/20	13/39/115/115	-
29	SQD	BA	413	-	-	18/46/66/69	0/1/1/1
30	LMG	AC	519	-	2/2/8/8	24/43/63/70	0/1/1/1
22	CLA	AB	611	2	1/1/15/20	16/39/115/115	-
30	LMG	BD	407	-	2/2/8/8	16/41/61/70	0/1/1/1
30	LMG	AD	407	-	2/2/8/8	17/41/61/70	0/1/1/1
27	DGD	BC	518	-	3/3/13/13	19/55/95/95	0/2/2/2
30	LMG	BE	102	-	2/2/8/8	19/39/59/70	0/1/1/1
22	CLA	AB	605	-	1/1/15/20	17/39/115/115	-
22	CLA	BB	610	-	1/1/15/20	14/39/115/115	-
22	CLA	BB	604	-	1/1/15/20	21/39/115/115	-
26	BCR	BC	515	-	-	4/29/63/63	0/2/2/2
22	CLA	BC	509	-	1/1/15/20	14/39/115/115	-
22	CLA	BB	607	2	1/1/15/20	11/39/115/115	-
22	CLA	BB	606	2	1/1/15/20	11/39/115/115	-
32	LMT	BB	603	-	-	4/21/61/61	0/2/2/2

All (1408) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BC	505	CLA	MG-NA	8.49	2.26	2.06
29	BL	101	SQD	C4-C3	8.41	1.74	1.52
28	AA	411	LHG	P-O5	8.39	1.79	1.50
28	BA	412	LHG	P-O5	8.07	1.78	1.50
22	BC	511	CLA	MG-NA	7.96	2.25	2.06
22	AC	511	CLA	MG-NA	7.93	2.25	2.06
23	AD	403	PHO	C3B-C4B	7.90	1.49	1.41
29	BB	601	SQD	C4-C3	7.87	1.72	1.52
29	AA	412	SQD	C4-C3	7.82	1.72	1.52
29	BA	413	SQD	C4-C3	7.79	1.72	1.52
29	BA	401	SQD	C4-C3	7.77	1.72	1.52
29	AA	415	SQD	C4-C3	7.68	1.72	1.52
29	AD	409	SQD	C4-C3	7.59	1.72	1.52
22	AC	503	CLA	MG-NA	7.40	2.23	2.06
22	AC	513	CLA	MG-NA	7.37	2.23	2.06
29	BD	409	SQD	C4-C3	7.33	1.71	1.52
22	BD	402	CLA	MG-NA	7.30	2.23	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BB	609	CLA	MG-NA	7.30	2.23	2.06
22	AD	402	CLA	MG-NA	7.29	2.23	2.06
22	BC	503	CLA	MG-NA	7.25	2.23	2.06
23	BD	403	PHO	C3B-C4B	7.19	1.48	1.41
22	AC	505	CLA	MG-NA	7.19	2.23	2.06
23	AA	405	PHO	C1B-C2B	7.13	1.47	1.39
22	BB	607	CLA	MG-NA	7.11	2.23	2.06
29	BF	101	SQD	C4-C3	7.05	1.70	1.52
22	BC	513	CLA	MG-NA	7.04	2.23	2.06
23	AA	405	PHO	C3B-C4B	7.02	1.48	1.41
22	BB	604	CLA	MG-NA	7.00	2.22	2.06
29	AF	101	SQD	C4-C3	6.91	1.70	1.52
26	BC	514	BCR	C1-C6	6.86	1.62	1.53
22	AB	604	CLA	MG-NA	6.75	2.22	2.06
22	AC	508	CLA	MG-NA	6.72	2.22	2.06
22	BC	512	CLA	MG-NA	6.67	2.22	2.06
23	BA	406	PHO	C1B-C2B	6.53	1.46	1.39
26	BZ	101	BCR	C1-C6	6.51	1.62	1.53
22	BB	612	CLA	MG-NA	6.50	2.21	2.06
22	AB	606	CLA	MG-NA	6.41	2.21	2.06
27	BD	410	DGD	O3G-C1D	6.34	1.50	1.40
26	BJ	102	BCR	C30-C25	6.27	1.61	1.53
22	AC	512	CLA	MG-NA	6.25	2.21	2.06
22	AB	601	CLA	MG-NA	6.24	2.21	2.06
22	BC	508	CLA	MG-NA	6.20	2.21	2.06
26	BC	514	BCR	C30-C25	6.18	1.61	1.53
26	BB	622	BCR	C30-C25	6.16	1.61	1.53
22	BC	501	CLA	MG-NA	6.15	2.20	2.06
26	AB	619	BCR	C30-C25	6.12	1.61	1.53
22	AD	404	CLA	MG-NA	6.00	2.20	2.06
22	AB	609	CLA	MG-NA	5.94	2.20	2.06
26	BZ	101	BCR	C30-C25	5.94	1.61	1.53
27	AD	410	DGD	O3G-C1D	5.92	1.50	1.40
26	AC	514	BCR	C1-C6	5.91	1.61	1.53
26	AK	102	BCR	C30-C25	5.88	1.61	1.53
26	BK	102	BCR	C30-C25	5.86	1.61	1.53
22	AC	501	CLA	MG-NA	5.85	2.20	2.06
26	BB	621	BCR	C30-C25	5.84	1.61	1.53
26	AZ	101	BCR	C1-C6	5.79	1.61	1.53
26	BX	101	BCR	C26-C25	5.79	1.44	1.34
23	BD	403	PHO	C1B-C2B	5.76	1.45	1.39
22	AB	614	CLA	MG-NA	5.76	2.20	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	AB	620	BCR	C30-C25	5.68	1.61	1.53
22	AA	402	CLA	MG-NA	5.68	2.19	2.06
22	AC	506	CLA	MG-NA	5.68	2.19	2.06
26	BC	515	BCR	C1-C6	5.63	1.61	1.53
26	AJ	102	BCR	C5-C6	5.59	1.43	1.34
26	AC	514	BCR	C30-C25	5.59	1.60	1.53
26	AB	619	BCR	C1-C6	5.58	1.60	1.53
22	BD	404	CLA	MG-NA	5.56	2.19	2.06
26	AB	620	BCR	C1-C6	5.56	1.60	1.53
22	BC	509	CLA	MG-NA	5.55	2.19	2.06
22	BC	502	CLA	MG-NA	5.51	2.19	2.06
22	AB	605	CLA	MG-NA	5.50	2.19	2.06
26	AH	101	BCR	C26-C25	5.48	1.43	1.34
26	AZ	101	BCR	C30-C25	5.47	1.60	1.53
22	BB	615	CLA	MG-NA	5.46	2.19	2.06
22	BA	403	CLA	MG-NA	5.41	2.19	2.06
26	AJ	102	BCR	C30-C25	5.37	1.60	1.53
22	AC	502	CLA	MG-NA	5.35	2.19	2.06
26	BJ	102	BCR	C5-C6	5.34	1.43	1.34
23	BA	406	PHO	C3B-C4B	5.33	1.46	1.41
26	BD	406	BCR	C1-C6	5.32	1.60	1.53
22	BB	617	CLA	MG-NA	5.31	2.18	2.06
22	AB	607	CLA	MG-NA	5.30	2.18	2.06
22	AB	603	CLA	MG-NA	5.29	2.18	2.06
26	AA	409	BCR	C1-C6	5.24	1.60	1.53
26	BD	406	BCR	C26-C25	5.22	1.43	1.34
26	AD	406	BCR	C30-C25	5.22	1.60	1.53
23	AD	403	PHO	C1B-C2B	5.21	1.45	1.39
26	BX	101	BCR	C30-C25	5.20	1.60	1.53
26	BJ	102	BCR	C26-C25	5.17	1.43	1.34
29	BD	409	SQD	O7-S	5.15	1.59	1.45
26	BA	410	BCR	C1-C6	5.14	1.60	1.53
26	BA	410	BCR	C30-C25	5.12	1.60	1.53
26	BB	622	BCR	C1-C6	5.12	1.60	1.53
26	AJ	102	BCR	C1-C6	5.11	1.60	1.53
22	BB	610	CLA	MG-NA	5.10	2.18	2.06
28	BA	412	LHG	P-O3	5.08	1.79	1.59
26	AK	102	BCR	C5-C6	5.07	1.43	1.34
22	BB	608	CLA	MG-NA	5.07	2.18	2.06
26	BJ	102	BCR	C1-C6	5.06	1.60	1.53
27	BA	411	DGD	O5D-C1E	5.05	1.48	1.40
29	BB	601	SQD	O7-S	5.03	1.59	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BB	621	BCR	C1-C6	5.00	1.60	1.53
26	AB	618	BCR	C30-C25	4.99	1.60	1.53
26	AH	101	BCR	C30-C25	4.99	1.60	1.53
26	BC	515	BCR	C30-C25	4.97	1.60	1.53
22	AB	610	CLA	MG-NA	4.93	2.18	2.06
26	AC	515	BCR	C30-C25	4.93	1.60	1.53
29	AD	409	SQD	C1-C2	4.92	1.66	1.52
34	BV	201	HEM	CBC-CAC	4.91	1.54	1.30
29	BD	409	SQD	O5-C5	4.91	1.56	1.44
26	BK	102	BCR	C5-C6	4.91	1.42	1.34
34	AV	201	HEM	CBC-CAC	4.91	1.54	1.30
26	AH	101	BCR	C1-C6	4.90	1.60	1.53
30	AM	101	LMG	O1-C1	4.89	1.48	1.40
28	AA	411	LHG	P-O3	4.89	1.78	1.59
22	BC	507	CLA	MG-NA	4.89	2.17	2.06
26	AC	515	BCR	C1-C6	4.88	1.60	1.53
29	BL	101	SQD	O7-S	4.88	1.58	1.45
29	BA	413	SQD	O7-S	4.86	1.58	1.45
26	AT	102	BCR	C1-C6	4.86	1.60	1.53
30	BM	102	LMG	O1-C1	4.86	1.48	1.40
22	AC	509	CLA	MG-NA	4.84	2.17	2.06
26	BD	406	BCR	C30-C25	4.84	1.60	1.53
22	BA	405	CLA	MG-NA	4.83	2.17	2.06
34	BE	101	HEM	FE-NB	4.83	2.09	1.94
29	AD	409	SQD	O7-S	4.81	1.58	1.45
22	BB	606	CLA	MG-NA	4.78	2.17	2.06
34	BE	101	HEM	CBC-CAC	4.78	1.53	1.30
29	AD	409	SQD	O5-C5	4.74	1.56	1.44
22	AA	406	CLA	MG-NA	4.73	2.17	2.06
22	AC	507	CLA	MG-NA	4.71	2.17	2.06
29	AD	409	SQD	O48-C23	4.71	1.47	1.33
22	AB	615	CLA	MG-NA	4.71	2.17	2.06
26	AD	406	BCR	C26-C25	4.69	1.42	1.34
34	AE	101	HEM	FE-NB	4.68	2.09	1.94
26	BB	620	BCR	C30-C25	4.68	1.59	1.53
29	BF	101	SQD	O5-C5	4.62	1.55	1.44
26	AK	102	BCR	C1-C6	4.62	1.59	1.53
22	AB	612	CLA	MG-NA	4.61	2.17	2.06
22	AB	616	CLA	MG-NA	4.60	2.17	2.06
26	AA	409	BCR	C30-C25	4.60	1.59	1.53
29	BA	401	SQD	O47-C7	4.60	1.47	1.34
22	BB	611	CLA	MG-NA	4.60	2.17	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	AE	101	HEM	CBC-CAC	4.60	1.52	1.30
29	BF	101	SQD	O48-C23	4.59	1.46	1.33
26	AB	617	BCR	C30-C25	4.59	1.59	1.53
26	AB	618	BCR	C1-C6	4.58	1.59	1.53
34	AV	201	HEM	FE-NB	4.58	2.09	1.94
22	BB	613	CLA	MG-NA	4.57	2.17	2.06
29	BF	101	SQD	O47-C7	4.56	1.47	1.34
29	AF	101	SQD	O47-C7	4.56	1.47	1.34
26	BX	101	BCR	C1-C6	4.55	1.59	1.53
29	BL	101	SQD	O5-C5	4.55	1.55	1.44
26	BK	102	BCR	C1-C6	4.55	1.59	1.53
22	AA	404	CLA	MG-NA	4.53	2.17	2.06
29	BA	401	SQD	O7-S	4.51	1.57	1.45
29	BD	409	SQD	O47-C7	4.50	1.47	1.34
26	AJ	102	BCR	C26-C25	4.48	1.42	1.34
29	AF	101	SQD	O7-S	4.47	1.57	1.45
22	BB	619	CLA	MG-NA	4.47	2.16	2.06
29	BB	601	SQD	O5-C5	4.44	1.55	1.44
22	BA	404	CLA	MG-NA	4.44	2.16	2.06
29	BA	413	SQD	O47-C7	4.43	1.46	1.34
22	BA	404	CLA	CAA-C2A	4.42	1.62	1.54
26	AB	619	BCR	C26-C25	4.41	1.41	1.34
29	BF	101	SQD	O7-S	4.41	1.57	1.45
29	BD	409	SQD	C1-C2	4.41	1.65	1.52
29	AF	101	SQD	O48-C23	4.40	1.46	1.33
27	AD	410	DGD	O5D-C1E	4.39	1.47	1.40
29	AA	415	SQD	O7-S	4.38	1.57	1.45
22	BC	506	CLA	MG-NA	4.34	2.16	2.06
26	BB	621	BCR	C26-C25	4.33	1.41	1.34
26	AD	406	BCR	C1-C6	4.32	1.59	1.53
22	AB	613	CLA	MG-NA	4.31	2.16	2.06
29	AD	409	SQD	O6-C1	4.30	1.47	1.40
28	AC	521	LHG	O8-C23	4.30	1.45	1.33
29	AA	412	SQD	O47-C7	4.29	1.46	1.34
29	BA	401	SQD	O5-C5	4.28	1.54	1.44
29	BA	401	SQD	C1-C2	4.28	1.65	1.52
28	BC	521	LHG	O8-C23	4.27	1.45	1.33
27	AA	410	DGD	O5D-C1E	4.25	1.47	1.40
29	BL	101	SQD	C1-C2	4.25	1.65	1.52
27	AB	626	DGD	C4E-C3E	4.24	1.63	1.52
26	AB	617	BCR	C1-C6	4.19	1.59	1.53
26	AB	618	BCR	C5-C6	4.19	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	AD	409	SQD	O47-C7	4.16	1.46	1.34
22	AB	608	CLA	MG-NA	4.15	2.16	2.06
22	BA	407	CLA	MG-NA	4.15	2.16	2.06
22	AC	503	CLA	CAA-C2A	4.15	1.61	1.54
29	AA	415	SQD	O47-C7	4.14	1.46	1.34
32	AI	102	LMT	O1'-C1'	4.13	1.47	1.40
34	BV	201	HEM	FE-NC	4.13	2.08	1.95
28	AC	521	LHG	O7-C7	4.12	1.45	1.34
30	BD	408	LMG	O1-C1	4.11	1.47	1.40
29	BA	401	SQD	O48-C23	4.11	1.45	1.33
28	BC	521	LHG	O7-C7	4.10	1.45	1.34
29	BD	409	SQD	O48-C23	4.10	1.45	1.33
29	AF	101	SQD	O5-C5	4.10	1.54	1.44
22	BB	618	CLA	MG-NA	4.09	2.16	2.06
32	BI	102	LMT	O1'-C1'	4.09	1.47	1.40
26	BJ	102	BCR	C29-C30	4.09	1.63	1.54
26	AB	617	BCR	C26-C25	4.08	1.41	1.34
29	BB	601	SQD	C1-C2	4.05	1.64	1.52
22	BC	503	CLA	CAA-C2A	4.04	1.61	1.54
27	BB	602	DGD	C4E-C3E	4.03	1.62	1.52
34	AV	201	HEM	FE-NC	4.03	2.08	1.95
22	BB	610	CLA	CAA-C2A	4.02	1.61	1.54
26	AZ	101	BCR	C26-C25	4.02	1.41	1.34
26	AJ	102	BCR	C29-C30	4.01	1.63	1.54
26	BC	515	BCR	C5-C6	4.01	1.41	1.34
29	AA	415	SQD	O5-C5	4.00	1.54	1.44
29	BL	101	SQD	O47-C7	3.99	1.45	1.34
22	BC	510	CLA	MG-NA	3.99	2.15	2.06
26	AH	101	BCR	C29-C30	3.99	1.63	1.54
27	AH	102	DGD	O5D-C1E	3.98	1.46	1.40
34	AE	101	HEM	FE-NC	3.97	2.08	1.95
30	AM	101	LMG	O7-C10	3.97	1.45	1.34
23	BD	403	PHO	C3A-C2A	-3.96	1.51	1.54
28	AA	411	LHG	P-O6	3.96	1.74	1.59
22	AB	608	CLA	CAA-C2A	3.96	1.61	1.54
26	AD	406	BCR	C5-C6	3.96	1.41	1.34
30	BI	101	LMG	O6-C1	3.96	1.52	1.41
26	AT	102	BCR	C30-C25	3.96	1.58	1.53
34	BE	101	HEM	C4D-ND	-3.95	1.33	1.40
29	AA	412	SQD	O7-S	3.94	1.56	1.45
27	BC	516	DGD	O5D-C1E	3.94	1.46	1.40
26	BD	406	BCR	C29-C30	3.93	1.63	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BB	620	BCR	C1-C6	3.93	1.58	1.53
22	AC	513	CLA	CAA-C2A	3.93	1.61	1.54
27	AC	516	DGD	O5D-C1E	3.92	1.46	1.40
34	BE	101	HEM	FE-NA	3.92	2.08	1.95
30	AC	520	LMG	C4-C3	3.91	1.62	1.52
27	AD	410	DGD	O6D-C5D	3.91	1.53	1.44
32	AM	102	LMT	O1'-C1'	3.91	1.46	1.40
22	AB	602	CLA	MG-NA	3.90	2.15	2.06
26	BZ	101	BCR	C26-C25	3.89	1.41	1.34
29	BA	413	SQD	C1-C2	3.89	1.63	1.52
32	AD	411	LMT	O1'-C1'	3.86	1.46	1.40
30	BI	101	LMG	C4-C3	3.86	1.62	1.52
34	AE	101	HEM	C4D-ND	-3.85	1.33	1.40
29	BL	101	SQD	O48-C23	3.85	1.44	1.33
29	AA	415	SQD	C1-C2	3.84	1.63	1.52
27	BB	602	DGD	C4E-C5E	3.83	1.61	1.53
26	AD	406	BCR	C29-C30	3.82	1.62	1.54
29	BF	101	SQD	C1-C2	3.81	1.63	1.52
22	BB	611	CLA	CAA-C2A	3.81	1.61	1.54
30	BM	102	LMG	O7-C10	3.81	1.45	1.34
29	BB	601	SQD	O47-C7	3.81	1.45	1.34
26	AB	620	BCR	C5-C6	3.80	1.40	1.34
32	BB	625	LMT	O5'-C1'	3.80	1.51	1.41
29	BD	409	SQD	O6-C1	3.79	1.46	1.40
26	BZ	101	BCR	C2-C1	3.78	1.62	1.54
29	AA	412	SQD	C1-C2	3.78	1.63	1.52
32	BD	411	LMT	O1'-C1'	3.78	1.46	1.40
26	AT	102	BCR	C5-C6	3.78	1.40	1.34
34	BE	101	HEM	FE-NC	3.77	2.07	1.95
30	AD	408	LMG	O1-C1	3.77	1.46	1.40
22	AA	403	CLA	MG-NA	3.76	2.15	2.06
27	AB	626	DGD	O5D-C1E	3.75	1.46	1.40
30	AB	623	LMG	O6-C1	3.74	1.51	1.41
29	BB	601	SQD	O48-C23	3.74	1.44	1.33
22	AC	501	CLA	CAA-C2A	3.74	1.60	1.54
22	BC	501	CLA	CAA-C2A	3.74	1.60	1.54
34	BV	201	HEM	FE-NB	3.72	2.06	1.94
27	BH	101	DGD	O5D-C1E	3.72	1.46	1.40
28	AA	411	LHG	O7-C7	3.71	1.44	1.34
26	AB	619	BCR	C29-C30	3.71	1.62	1.54
23	AD	403	PHO	C3A-C2A	-3.71	1.51	1.54
26	AB	619	BCR	C5-C6	3.70	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	BA	413	SQD	O5-C5	3.69	1.53	1.44
22	BC	513	CLA	CAA-C2A	3.68	1.60	1.54
27	BA	411	DGD	C4D-C5D	3.68	1.60	1.53
22	AC	510	CLA	MG-NA	3.68	2.15	2.06
26	BX	101	BCR	C29-C30	3.68	1.62	1.54
27	AD	410	DGD	O6D-C1D	3.68	1.51	1.41
22	BC	502	CLA	CAA-C2A	3.67	1.60	1.54
26	AZ	101	BCR	C29-C30	3.67	1.62	1.54
29	AA	415	SQD	O6-C1	3.67	1.46	1.40
28	BA	412	LHG	P-O6	3.67	1.73	1.59
26	BZ	101	BCR	C29-C30	3.66	1.62	1.54
27	AD	410	DGD	O6E-C1E	3.66	1.51	1.41
30	AI	101	LMG	O6-C1	3.65	1.51	1.41
29	BF	101	SQD	O6-C1	3.65	1.46	1.40
32	AB	624	LMT	O5'-C1'	3.64	1.51	1.41
34	AE	101	HEM	FE-NA	3.64	2.07	1.95
29	AA	412	SQD	O48-C23	3.64	1.44	1.33
22	AA	403	CLA	CAA-C2A	3.64	1.60	1.54
32	BM	101	LMT	O1'-C1'	3.63	1.46	1.40
27	AB	626	DGD	C4D-C5D	3.63	1.60	1.53
22	AD	404	CLA	CAA-C2A	3.63	1.60	1.54
29	AF	101	SQD	O6-C1	3.63	1.46	1.40
30	BM	102	LMG	O6-C1	3.62	1.51	1.41
26	BD	406	BCR	C5-C6	3.62	1.40	1.34
22	BC	511	CLA	CAA-C2A	3.62	1.60	1.54
26	BB	621	BCR	C29-C30	3.61	1.62	1.54
26	AB	620	BCR	C29-C30	3.61	1.62	1.54
26	BB	622	BCR	C29-C30	3.59	1.62	1.54
30	AE	102	LMG	O6-C1	3.58	1.51	1.41
26	BC	515	BCR	C2-C1	3.58	1.62	1.54
27	BC	518	DGD	O5D-C1E	3.58	1.46	1.40
27	BB	602	DGD	O3G-C1D	3.58	1.46	1.40
26	AC	515	BCR	C5-C6	3.58	1.40	1.34
27	BC	518	DGD	O3G-C1D	3.57	1.46	1.40
22	AA	404	CLA	CAA-C2A	3.57	1.60	1.54
26	BC	514	BCR	C26-C25	3.57	1.40	1.34
26	BX	101	BCR	C2-C1	3.57	1.62	1.54
30	BC	520	LMG	C4-C3	3.56	1.61	1.52
26	BB	621	BCR	C5-C6	3.56	1.40	1.34
26	AA	409	BCR	C2-C1	3.56	1.62	1.54
27	AB	626	DGD	O6D-C5D	3.56	1.53	1.44
30	AA	416	LMG	O6-C1	3.56	1.51	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	AB	617	BCR	C5-C6	3.55	1.40	1.34
22	BB	605	CLA	MG-NA	3.55	2.14	2.06
29	BL	101	SQD	O8-S	3.55	1.60	1.47
30	BC	520	LMG	C4-C5	3.54	1.60	1.53
27	BD	410	DGD	O6D-C1D	3.54	1.50	1.41
27	BB	602	DGD	O6E-C1E	3.53	1.50	1.41
22	AB	614	CLA	CAA-C2A	3.53	1.60	1.54
29	AA	415	SQD	O48-C23	3.52	1.43	1.33
26	BB	622	BCR	C5-C6	3.52	1.40	1.34
26	AB	618	BCR	C2-C1	3.52	1.62	1.54
30	AI	101	LMG	C4-C3	3.51	1.61	1.52
26	AB	620	BCR	C2-C1	3.51	1.62	1.54
30	AC	519	LMG	O1-C1	3.50	1.46	1.40
24	AJ	101	PL9	C6-C1	3.49	1.54	1.48
26	AK	102	BCR	C29-C30	3.49	1.62	1.54
22	BC	504	CLA	MG-NA	3.49	2.14	2.06
30	AC	520	LMG	O6-C1	3.48	1.50	1.41
30	AM	101	LMG	O6-C1	3.48	1.50	1.41
24	BJ	101	PL9	C6-C1	3.48	1.54	1.48
26	BC	514	BCR	C29-C30	3.47	1.62	1.54
30	BC	520	LMG	O6-C1	3.47	1.50	1.41
26	AT	102	BCR	C2-C1	3.47	1.62	1.54
26	BC	514	BCR	C2-C1	3.47	1.62	1.54
27	BD	410	DGD	O5D-C1E	3.47	1.46	1.40
26	AC	514	BCR	C26-C25	3.46	1.40	1.34
22	BB	607	CLA	CAA-C2A	3.46	1.60	1.54
26	BB	622	BCR	C2-C1	3.46	1.62	1.54
27	BD	410	DGD	O6D-C5D	3.46	1.52	1.44
27	AB	626	DGD	O3G-C1D	3.45	1.46	1.40
34	BE	101	HEM	CBD-CAD	3.45	1.63	1.51
30	BD	408	LMG	O6-C1	3.44	1.50	1.41
22	AC	504	CLA	CAA-C2A	3.43	1.60	1.54
30	AB	623	LMG	C4-C5	3.43	1.60	1.53
27	BB	602	DGD	O5D-C1E	3.43	1.45	1.40
30	BM	102	LMG	O6-C5	3.43	1.52	1.44
22	BC	505	CLA	CAA-C2A	3.42	1.60	1.54
30	BC	519	LMG	O1-C1	3.42	1.45	1.40
22	AB	604	CLA	CAA-C2A	3.41	1.60	1.54
26	BA	410	BCR	C5-C6	3.40	1.40	1.34
26	BK	102	BCR	C29-C30	3.40	1.61	1.54
26	BD	406	BCR	C2-C1	3.40	1.61	1.54
28	BA	412	LHG	O7-C7	3.40	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	AB	617	BCR	C29-C30	3.39	1.61	1.54
27	AA	410	DGD	O3G-C1D	3.38	1.45	1.40
27	BC	517	DGD	O6D-C1D	3.38	1.50	1.41
26	BC	515	BCR	C26-C25	3.38	1.40	1.34
22	BC	506	CLA	CAA-C2A	3.38	1.60	1.54
27	BA	411	DGD	O3G-C1D	3.38	1.45	1.40
29	AD	409	SQD	O3-C3	3.38	1.51	1.43
30	BI	101	LMG	O6-C5	3.38	1.52	1.44
30	AB	623	LMG	O1-C1	3.38	1.45	1.40
22	BA	405	CLA	CAA-C2A	3.37	1.60	1.54
29	BB	601	SQD	O8-S	3.37	1.59	1.47
22	AD	402	CLA	CAA-C2A	3.37	1.60	1.54
29	BD	409	SQD	C12-C11	-3.36	1.35	1.51
30	BE	102	LMG	O1-C1	3.36	1.45	1.40
29	AF	101	SQD	C1-C2	3.36	1.62	1.52
29	BA	413	SQD	O48-C23	3.36	1.43	1.33
29	BD	409	SQD	C16-C15	-3.36	1.35	1.51
27	BB	602	DGD	C4D-C5D	3.35	1.60	1.53
22	BB	608	CLA	CAA-C2A	3.35	1.60	1.54
26	AC	514	BCR	C29-C30	3.35	1.61	1.54
29	AD	409	SQD	O8-S	3.35	1.59	1.47
22	AB	609	CLA	CAA-C2A	3.35	1.60	1.54
29	AA	412	SQD	C32-C31	-3.35	1.35	1.51
26	BJ	102	BCR	C2-C1	3.34	1.61	1.54
22	BA	403	CLA	CAA-C2A	3.33	1.60	1.54
26	AB	618	BCR	C29-C30	3.33	1.61	1.54
22	AB	605	CLA	CAA-C2A	3.33	1.60	1.54
29	BD	409	SQD	C15-C14	-3.32	1.35	1.51
29	BB	601	SQD	C17-C16	-3.32	1.35	1.51
29	AA	415	SQD	C17-C16	-3.32	1.35	1.51
22	BD	402	CLA	CAA-C2A	3.32	1.60	1.54
34	BV	201	HEM	FE-ND	3.32	2.05	1.94
26	BA	410	BCR	C2-C1	3.32	1.61	1.54
29	BA	401	SQD	C15-C14	-3.32	1.35	1.51
29	BA	401	SQD	O8-S	3.31	1.59	1.47
29	BD	409	SQD	O8-S	3.31	1.59	1.47
27	BA	411	DGD	O6D-C1D	3.31	1.50	1.41
34	AV	201	HEM	FE-NA	3.30	2.06	1.95
26	BC	515	BCR	C29-C30	3.30	1.61	1.54
22	BB	612	CLA	CAA-C2A	3.30	1.60	1.54
26	AB	617	BCR	C2-C1	3.30	1.61	1.54
30	AC	520	LMG	O6-C5	3.30	1.52	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	AA	415	SQD	C15-C14	-3.30	1.35	1.51
26	AC	515	BCR	C2-C1	3.30	1.61	1.54
22	AA	406	CLA	CHB-C1B	-3.29	1.32	1.39
26	AZ	101	BCR	C2-C1	3.29	1.61	1.54
29	AA	415	SQD	C11-C10	-3.29	1.35	1.51
29	AA	412	SQD	O5-C5	3.29	1.52	1.44
27	BC	518	DGD	O6D-C1D	3.29	1.50	1.41
30	AA	413	LMG	O6-C1	3.28	1.50	1.41
22	BB	619	CLA	CAA-C2A	3.28	1.60	1.54
34	AV	201	HEM	CMA-C3A	3.28	1.57	1.50
22	BB	605	CLA	CHB-C1B	-3.28	1.32	1.39
26	AB	620	BCR	C26-C25	3.27	1.40	1.34
26	BB	620	BCR	C29-C30	3.27	1.61	1.54
34	BV	201	HEM	CHB-C1B	-3.26	1.32	1.38
29	BA	401	SQD	C11-C10	-3.26	1.35	1.51
22	BC	504	CLA	CAA-C2A	3.26	1.60	1.54
22	BD	404	CLA	CAA-C2A	3.26	1.60	1.54
22	AB	616	CLA	CAA-C2A	3.26	1.60	1.54
29	AD	409	SQD	C11-C10	-3.26	1.35	1.51
29	BB	601	SQD	C19-C18	-3.26	1.35	1.51
27	BB	602	DGD	O2G-C1B	3.25	1.43	1.34
22	BC	507	CLA	MG-NC	3.25	2.14	2.06
27	AB	626	DGD	O6E-C1E	3.25	1.50	1.41
22	AB	607	CLA	CAA-C2A	3.25	1.60	1.54
30	AD	408	LMG	O6-C1	3.25	1.50	1.41
32	BB	626	LMT	O1'-C1'	3.25	1.45	1.40
30	AA	416	LMG	C4-C5	3.24	1.59	1.53
30	BA	414	LMG	O6-C1	3.24	1.50	1.41
29	AA	415	SQD	O8-S	3.24	1.59	1.47
22	BB	611	CLA	C1D-ND	-3.24	1.33	1.37
29	BA	401	SQD	C17-C16	-3.24	1.35	1.51
29	BL	101	SQD	C19-C18	-3.24	1.35	1.51
22	AC	505	CLA	CAA-C2A	3.24	1.60	1.54
22	BB	617	CLA	CAA-C2A	3.23	1.60	1.54
26	BA	410	BCR	C26-C25	3.23	1.39	1.34
29	AA	412	SQD	C33-C32	-3.23	1.35	1.51
22	AB	609	CLA	MG-NC	3.23	2.13	2.06
30	BC	519	LMG	O6-C1	3.23	1.50	1.41
26	BB	620	BCR	C2-C1	3.23	1.61	1.54
26	BB	621	BCR	C2-C1	3.23	1.61	1.54
26	AB	619	BCR	C2-C1	3.23	1.61	1.54
30	AE	102	LMG	O1-C1	3.23	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BD	410	DGD	O6E-C1E	3.22	1.50	1.41
32	AB	625	LMT	O1'-C1'	3.22	1.45	1.40
29	AA	415	SQD	C12-C11	-3.22	1.35	1.51
22	BB	614	CLA	MG-NC	3.22	2.13	2.06
29	BD	409	SQD	O3-C3	3.21	1.50	1.43
27	AD	410	DGD	C4E-C5E	3.21	1.59	1.53
29	AD	409	SQD	C12-C11	-3.21	1.35	1.51
27	AB	626	DGD	C4E-C5E	3.21	1.59	1.53
22	AC	507	CLA	MG-NC	3.21	2.13	2.06
34	AE	101	HEM	CMA-C3A	3.21	1.57	1.50
26	AK	102	BCR	C2-C1	3.21	1.61	1.54
26	AH	101	BCR	C2-C1	3.21	1.61	1.54
26	AA	409	BCR	C29-C30	3.20	1.61	1.54
34	BE	101	HEM	CHB-C1B	-3.20	1.32	1.38
22	AB	602	CLA	CHB-C1B	-3.19	1.32	1.39
30	AC	520	LMG	C4-C5	3.19	1.59	1.53
27	BB	602	DGD	O6D-C5D	3.18	1.52	1.44
29	AD	409	SQD	C15-C14	-3.18	1.35	1.51
29	BL	101	SQD	C17-C16	-3.18	1.36	1.51
29	BL	101	SQD	C11-C10	-3.18	1.36	1.51
32	AB	627	LMT	O1B-C1B	3.18	1.50	1.41
26	AD	406	BCR	C2-C1	3.17	1.61	1.54
34	AV	201	HEM	CHB-C1B	-3.17	1.32	1.38
29	BB	601	SQD	C16-C15	-3.17	1.36	1.51
29	AD	409	SQD	C16-C15	-3.16	1.36	1.51
29	BA	413	SQD	C12-C11	-3.16	1.36	1.51
29	BB	601	SQD	C20-C19	-3.16	1.36	1.51
26	BK	102	BCR	C2-C1	3.16	1.61	1.54
29	BD	409	SQD	C11-C10	-3.16	1.36	1.51
27	BC	516	DGD	O6D-C1D	3.15	1.50	1.41
27	AA	410	DGD	C4D-C5D	3.15	1.59	1.53
22	AC	506	CLA	CAA-C2A	3.15	1.59	1.54
29	AA	415	SQD	C16-C15	-3.15	1.36	1.51
29	BA	413	SQD	C32-C31	-3.15	1.36	1.51
30	AM	101	LMG	O6-C5	3.15	1.52	1.44
32	AT	101	LMT	O5B-C1B	3.14	1.49	1.41
22	BB	606	CLA	MG-NC	3.14	2.13	2.06
22	BB	605	CLA	MG-NC	3.14	2.13	2.06
30	BI	101	LMG	C4-C5	3.14	1.59	1.53
22	BB	614	CLA	CHB-C1B	-3.14	1.32	1.39
29	BB	601	SQD	C15-C14	-3.14	1.36	1.51
22	AB	611	CLA	CHB-C1B	-3.13	1.32	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	AA	409	BCR	C26-C25	3.13	1.39	1.34
29	BD	409	SQD	C14-C13	-3.13	1.36	1.51
30	AA	416	LMG	O1-C1	3.13	1.45	1.40
22	AC	511	CLA	CAA-C2A	3.13	1.59	1.54
29	BL	101	SQD	O3-C3	3.13	1.50	1.43
23	BA	406	PHO	C1D-C2D	3.13	1.43	1.39
29	BL	101	SQD	C12-C11	-3.13	1.36	1.51
29	AA	412	SQD	C12-C11	-3.12	1.36	1.51
29	BA	401	SQD	O6-C1	3.12	1.45	1.40
29	BL	101	SQD	C15-C14	-3.12	1.36	1.51
30	AI	101	LMG	O6-C5	3.12	1.52	1.44
27	BA	411	DGD	C4E-C3E	3.12	1.60	1.52
34	BE	101	HEM	CMA-C3A	3.12	1.57	1.50
30	BC	520	LMG	O6-C5	3.12	1.52	1.44
29	AA	412	SQD	C17-C16	-3.12	1.36	1.51
29	BD	409	SQD	C13-C12	-3.12	1.36	1.51
29	BB	601	SQD	C12-C11	-3.11	1.36	1.51
29	AD	409	SQD	O5-C1	3.11	1.49	1.41
30	AI	101	LMG	C4-C5	3.11	1.59	1.53
22	AA	402	CLA	CAA-C2A	3.11	1.59	1.54
26	BB	620	BCR	C26-C25	3.11	1.39	1.34
29	AA	415	SQD	C19-C18	-3.10	1.36	1.51
27	BA	411	DGD	C4E-C5E	3.10	1.59	1.53
29	BB	601	SQD	C11-C10	-3.10	1.36	1.51
29	BF	101	SQD	C17-C16	-3.10	1.36	1.51
34	AE	101	HEM	CHB-C1B	-3.10	1.32	1.38
29	BB	601	SQD	O5-C1	3.09	1.49	1.41
30	AC	519	LMG	O6-C1	3.09	1.49	1.41
29	AA	412	SQD	C16-C15	-3.09	1.36	1.51
29	AA	412	SQD	C15-C14	-3.08	1.36	1.51
22	AB	606	CLA	MG-NC	3.08	2.13	2.06
29	BF	101	SQD	O8-S	3.08	1.58	1.47
22	AC	512	CLA	MG-NC	3.08	2.13	2.06
29	BL	101	SQD	C20-C19	-3.08	1.36	1.51
22	BB	609	CLA	CAA-C2A	3.07	1.59	1.54
29	BF	101	SQD	C8-C7	3.07	1.59	1.50
29	BL	101	SQD	C14-C13	-3.07	1.36	1.51
22	BA	407	CLA	CHB-C1B	-3.06	1.32	1.39
29	BA	413	SQD	C33-C32	-3.06	1.36	1.51
29	BL	101	SQD	C16-C15	-3.06	1.36	1.51
27	AA	410	DGD	O6D-C1D	3.06	1.49	1.41
34	BE	101	HEM	CAA-C2A	3.06	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	AD	409	SQD	C14-C13	-3.06	1.36	1.51
29	AF	101	SQD	C17-C16	-3.05	1.36	1.51
29	BA	413	SQD	C16-C15	-3.05	1.36	1.51
22	BB	606	CLA	CHB-C1B	-3.05	1.32	1.39
22	AC	504	CLA	CHB-C1B	-3.05	1.32	1.39
29	BA	413	SQD	C11-C10	-3.05	1.36	1.51
22	AB	611	CLA	MG-NC	3.05	2.13	2.06
29	BA	413	SQD	C15-C14	-3.04	1.36	1.51
22	BA	404	CLA	CHB-C1B	-3.04	1.32	1.39
22	AB	611	CLA	CAA-C2A	3.04	1.59	1.54
27	AA	410	DGD	C4E-C3E	3.04	1.60	1.52
22	AC	502	CLA	CAA-C2A	3.04	1.59	1.54
29	BA	401	SQD	C12-C11	-3.04	1.36	1.51
29	AF	101	SQD	C15-C14	-3.04	1.36	1.51
29	BA	401	SQD	C19-C18	-3.03	1.36	1.51
32	BB	603	LMT	O1B-C1B	3.03	1.50	1.41
22	AB	603	CLA	CAA-C2A	3.03	1.59	1.54
30	BB	624	LMG	O1-C1	3.03	1.45	1.40
29	AA	412	SQD	C14-C13	-3.03	1.36	1.51
26	AT	102	BCR	C29-C30	3.03	1.61	1.54
29	AA	415	SQD	O3-C3	3.03	1.50	1.43
29	AA	412	SQD	C11-C10	-3.02	1.36	1.51
22	AB	601	CLA	MG-NC	3.02	2.13	2.06
22	AB	603	CLA	CHB-C1B	-3.02	1.32	1.39
29	BA	401	SQD	O3-C3	3.02	1.50	1.43
26	AC	515	BCR	C29-C30	3.02	1.61	1.54
22	AB	606	CLA	CAA-C2A	3.02	1.59	1.54
29	BA	413	SQD	C17-C16	-3.02	1.36	1.51
28	BA	412	LHG	O8-C23	3.01	1.42	1.33
32	BB	603	LMT	O5B-C1B	3.00	1.49	1.41
27	BC	517	DGD	O3G-C1D	3.00	1.45	1.40
27	BD	410	DGD	C4E-C3E	3.00	1.60	1.52
32	BT	101	LMT	O5B-C1B	3.00	1.49	1.41
34	BV	201	HEM	FE-NA	2.99	2.05	1.95
22	AC	507	CLA	CHB-C1B	-2.99	1.32	1.39
29	AD	409	SQD	C13-C12	-2.99	1.36	1.51
22	BC	504	CLA	MG-NB	2.99	2.11	2.05
29	BB	601	SQD	C18-C17	-2.99	1.36	1.51
29	BB	601	SQD	C14-C13	-2.98	1.36	1.51
29	BA	401	SQD	C16-C15	-2.98	1.36	1.51
30	AB	622	LMG	O6-C1	2.98	1.49	1.41
26	BA	410	BCR	C29-C30	2.98	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	BB	625	LMT	O5B-C1B	2.98	1.49	1.41
22	BB	610	CLA	CHB-C1B	-2.98	1.32	1.39
29	AF	101	SQD	C16-C15	-2.97	1.37	1.51
28	AA	411	LHG	O8-C23	2.97	1.42	1.33
22	BC	503	CLA	MG-NC	2.97	2.13	2.06
27	BC	516	DGD	O3G-C1D	2.97	1.45	1.40
29	BA	401	SQD	C14-C13	-2.97	1.37	1.51
34	AE	101	HEM	FE-ND	2.97	2.04	1.94
29	AF	101	SQD	C8-C7	2.96	1.59	1.50
22	BD	404	CLA	MG-NC	2.96	2.13	2.06
29	AA	412	SQD	O3-C3	2.96	1.50	1.43
34	BV	201	HEM	C4D-ND	-2.95	1.35	1.40
27	BD	410	DGD	C4E-C5E	2.95	1.59	1.53
22	BB	618	CLA	MG-NC	2.95	2.13	2.06
29	AA	412	SQD	O6-C44	-2.95	1.38	1.43
27	AC	517	DGD	O6D-C1D	2.95	1.49	1.41
29	BL	101	SQD	O5-C1	2.95	1.49	1.41
34	BV	201	HEM	C1A-NA	2.95	1.45	1.39
30	AI	101	LMG	C3-C2	2.95	1.60	1.52
30	AA	416	LMG	O6-C5	2.95	1.51	1.44
32	BD	411	LMT	O5'-C1'	2.94	1.49	1.41
26	AA	409	BCR	C5-C6	2.94	1.39	1.34
22	BB	612	CLA	MG-NC	2.94	2.13	2.06
29	BA	413	SQD	C19-C18	-2.93	1.37	1.51
27	BB	602	DGD	C4D-C3D	2.93	1.59	1.52
29	BA	401	SQD	C18-C17	-2.93	1.37	1.51
30	AM	101	LMG	C3-C2	2.93	1.59	1.52
30	BB	623	LMG	O6-C1	2.93	1.49	1.41
29	AA	415	SQD	C20-C19	-2.93	1.37	1.51
29	AA	415	SQD	C33-C32	-2.93	1.37	1.51
22	AB	612	CLA	MG-NC	2.93	2.13	2.06
29	AA	412	SQD	C20-C19	-2.92	1.37	1.51
34	AV	201	HEM	C1A-NA	2.92	1.45	1.39
29	BF	101	SQD	C15-C14	-2.92	1.37	1.51
29	AA	412	SQD	C19-C18	-2.92	1.37	1.51
30	BE	102	LMG	O6-C1	2.92	1.49	1.41
29	BF	101	SQD	C12-C11	-2.92	1.37	1.51
27	AD	410	DGD	C1D-C2D	2.91	1.61	1.52
29	BF	101	SQD	O5-C1	2.91	1.49	1.41
27	AB	626	DGD	O2G-C1B	2.91	1.42	1.34
22	AB	615	CLA	MG-NC	2.91	2.13	2.06
27	AB	626	DGD	O6D-C1D	2.91	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	AC	518	DGD	O3G-C1D	2.91	1.45	1.40
29	BL	101	SQD	C18-C17	-2.91	1.37	1.51
22	AB	602	CLA	MG-NC	2.90	2.13	2.06
29	BF	101	SQD	O3-C3	2.90	1.50	1.43
30	BB	624	LMG	O6-C1	2.90	1.49	1.41
29	AA	415	SQD	C18-C17	-2.90	1.37	1.51
22	BB	616	CLA	CHB-C1B	-2.90	1.32	1.39
32	BT	101	LMT	O1'-C1'	2.90	1.45	1.40
22	BC	509	CLA	CAA-C2A	2.90	1.59	1.54
27	AD	410	DGD	C4E-C3E	2.89	1.59	1.52
30	BB	623	LMG	O7-C10	2.89	1.42	1.34
22	AC	509	CLA	CAA-C2A	2.89	1.59	1.54
22	AC	505	CLA	MG-NC	2.89	2.13	2.06
30	BC	520	LMG	O7-C10	2.89	1.42	1.34
34	AE	101	HEM	CAA-C2A	2.89	1.58	1.51
29	BF	101	SQD	C11-C10	-2.89	1.37	1.51
29	BA	413	SQD	C14-C13	-2.88	1.37	1.51
29	AA	415	SQD	C32-C31	-2.88	1.37	1.51
27	AD	410	DGD	C3D-C2D	2.88	1.59	1.52
32	AB	627	LMT	O5B-C1B	2.88	1.49	1.41
29	BF	101	SQD	C16-C15	-2.88	1.37	1.51
29	BB	601	SQD	C13-C12	-2.88	1.37	1.51
22	BB	613	CLA	MG-NC	2.88	2.13	2.06
29	BA	413	SQD	C20-C19	-2.88	1.37	1.51
29	BA	413	SQD	O8-S	2.88	1.58	1.47
26	AJ	102	BCR	C2-C1	2.88	1.60	1.54
27	AA	410	DGD	O6E-C1E	2.88	1.49	1.41
22	AC	504	CLA	MG-NB	2.87	2.11	2.05
22	BB	617	CLA	MG-NC	2.87	2.13	2.06
22	BB	616	CLA	MG-NA	2.87	2.13	2.06
22	AB	607	CLA	CHB-C1B	-2.86	1.33	1.39
32	BI	102	LMT	O5'-C1'	2.86	1.49	1.41
30	AB	622	LMG	O1-C1	2.86	1.45	1.40
29	AA	415	SQD	O5-C1	2.86	1.49	1.41
22	BC	507	CLA	CHB-C1B	-2.86	1.33	1.39
22	AC	511	CLA	MG-NC	2.86	2.13	2.06
30	BM	102	LMG	C3-C2	2.86	1.59	1.52
22	AB	608	CLA	C1D-ND	-2.85	1.34	1.37
26	BZ	101	BCR	C5-C6	2.85	1.39	1.34
30	BI	101	LMG	C3-C2	2.85	1.59	1.52
29	BA	413	SQD	C13-C12	-2.85	1.37	1.51
32	BD	411	LMT	O5B-C1B	2.85	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	BD	407	LMG	C4-C3	2.85	1.59	1.52
27	AC	518	DGD	O6D-C1D	2.85	1.49	1.41
34	AE	101	HEM	CBD-CAD	2.85	1.61	1.51
32	AD	411	LMT	O5'-C1'	2.84	1.49	1.41
34	BE	101	HEM	FE-ND	2.84	2.03	1.94
29	AA	415	SQD	C14-C13	-2.84	1.37	1.51
23	BA	406	PHO	C3D-CAD	-2.84	1.42	1.47
22	AB	604	CLA	MG-NC	2.84	2.13	2.06
29	BA	401	SQD	C32-C31	-2.84	1.37	1.51
32	AB	624	LMT	O5B-C1B	2.84	1.49	1.41
22	BB	617	CLA	CHB-C1B	-2.84	1.33	1.39
26	BB	620	BCR	C5-C6	2.84	1.39	1.34
29	BB	601	SQD	O6-C1	2.84	1.44	1.40
22	BD	402	CLA	MG-NC	2.83	2.13	2.06
30	AC	519	LMG	O6-C5	2.83	1.51	1.44
29	BA	401	SQD	C33-C32	-2.83	1.37	1.51
26	AC	514	BCR	C2-C1	2.83	1.60	1.54
29	BL	101	SQD	C13-C12	-2.82	1.37	1.51
29	AF	101	SQD	C11-C10	-2.82	1.37	1.51
22	AB	613	CLA	CHB-C1B	-2.81	1.33	1.39
22	BA	403	CLA	CHB-C1B	-2.81	1.33	1.39
22	AC	505	CLA	CHC-C1C	2.81	1.44	1.38
22	AA	404	CLA	CHB-C1B	-2.81	1.33	1.39
32	AD	411	LMT	O5B-C1B	2.81	1.49	1.41
29	BB	601	SQD	O3-C3	2.80	1.49	1.43
22	BA	405	CLA	MG-NC	2.80	2.12	2.06
27	BD	410	DGD	O2G-C1B	2.80	1.42	1.34
22	AC	506	CLA	MG-NC	2.80	2.12	2.06
26	AZ	101	BCR	C5-C6	2.80	1.39	1.34
30	BC	519	LMG	O6-C5	2.80	1.51	1.44
32	AD	411	LMT	C4B-C5B	2.80	1.59	1.53
22	AD	402	CLA	MG-NC	2.79	2.12	2.06
24	BJ	101	PL9	C2-C1	2.79	1.52	1.44
27	AA	410	DGD	C4E-C5E	2.79	1.59	1.53
22	BC	506	CLA	MG-NC	2.79	2.12	2.06
22	AA	402	CLA	CHB-C1B	-2.79	1.33	1.39
22	BB	619	CLA	MG-NC	2.78	2.12	2.06
26	BC	514	BCR	C5-C6	2.78	1.39	1.34
29	AA	412	SQD	C13-C12	-2.78	1.37	1.51
29	AF	101	SQD	O3-C3	2.78	1.49	1.43
22	BC	502	CLA	MG-NC	2.78	2.12	2.06
30	AA	416	LMG	C3-C2	2.78	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	AH	102	DGD	C1E-C2E	2.78	1.60	1.52
26	AC	515	BCR	C26-C25	2.78	1.39	1.34
22	AC	505	CLA	C1D-C2D	-2.77	1.39	1.45
30	BD	407	LMG	O6-C1	2.77	1.49	1.41
29	BA	401	SQD	C13-C12	-2.77	1.38	1.51
29	AA	415	SQD	C13-C12	-2.77	1.38	1.51
29	AF	101	SQD	C12-C11	-2.77	1.38	1.51
22	BB	606	CLA	CAA-C2A	2.77	1.59	1.54
22	BC	512	CLA	MG-NC	2.77	2.12	2.06
22	BB	615	CLA	CHB-C1B	-2.76	1.33	1.39
30	BI	101	LMG	O7-C10	2.76	1.42	1.34
34	BV	201	HEM	CBD-CAD	2.76	1.61	1.51
32	BB	603	LMT	O5'-C1'	2.76	1.48	1.41
22	AB	614	CLA	CHB-C1B	-2.76	1.33	1.39
26	AH	101	BCR	C38-C26	2.76	1.55	1.50
22	AA	403	CLA	CHB-C1B	-2.76	1.33	1.39
22	AC	513	CLA	MG-NC	2.76	2.12	2.06
26	BK	102	BCR	C26-C25	2.76	1.39	1.34
32	BI	102	LMT	O5B-C1B	2.75	1.48	1.41
22	AC	504	CLA	MG-NA	2.75	2.12	2.06
29	BA	401	SQD	C20-C19	-2.75	1.38	1.51
32	AI	102	LMT	O5B-C1B	2.75	1.48	1.41
29	BA	401	SQD	C36-C35	-2.75	1.38	1.51
26	AB	618	BCR	C26-C25	2.75	1.39	1.34
26	BX	101	BCR	C38-C26	2.75	1.55	1.50
22	BC	504	CLA	CHB-C1B	-2.75	1.33	1.39
29	AF	101	SQD	O8-S	2.74	1.57	1.47
32	AT	101	LMT	O1'-C1'	2.74	1.44	1.40
22	BC	506	CLA	CHB-C1B	-2.74	1.33	1.39
23	BD	403	PHO	C4D-CHA	2.74	1.43	1.39
30	BB	623	LMG	C4-C3	2.74	1.59	1.52
26	BD	406	BCR	C38-C26	2.74	1.55	1.50
27	BC	516	DGD	C4E-C3E	2.74	1.59	1.52
27	AD	410	DGD	O2G-C1B	2.74	1.42	1.34
22	BC	513	CLA	MG-NC	2.74	2.12	2.06
30	AI	101	LMG	O7-C10	2.73	1.42	1.34
22	AC	503	CLA	MG-NC	2.73	2.12	2.06
22	AC	509	CLA	C1D-ND	-2.73	1.34	1.37
34	AE	101	HEM	C2A-C3A	2.73	1.46	1.38
27	AB	626	DGD	C3D-C2D	2.73	1.59	1.52
30	AM	101	LMG	C4-C5	2.73	1.58	1.53
29	BA	401	SQD	O5-C1	2.73	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	AB	625	LMT	O5'-C1'	2.73	1.48	1.41
22	BC	511	CLA	MG-NC	2.72	2.12	2.06
30	AB	622	LMG	C4-C5	2.72	1.58	1.53
27	AC	518	DGD	O6D-C5D	2.71	1.51	1.44
22	BB	619	CLA	CHB-C1B	-2.71	1.33	1.39
29	BF	101	SQD	C14-C13	-2.71	1.38	1.51
22	AC	508	CLA	CHC-C1C	2.71	1.43	1.38
22	BB	617	CLA	MG-NB	2.71	2.11	2.05
22	AB	616	CLA	CHB-C1B	-2.70	1.33	1.39
32	AB	627	LMT	O5'-C1'	2.69	1.48	1.41
22	BB	617	CLA	CHC-C1C	2.69	1.43	1.38
27	AA	410	DGD	C3E-C2E	2.69	1.59	1.52
22	BC	508	CLA	MG-NC	2.69	2.12	2.06
22	AC	504	CLA	MG-NC	2.69	2.12	2.06
22	AA	403	CLA	C5-C3	2.69	1.56	1.51
22	BB	615	CLA	C1D-ND	-2.69	1.34	1.37
22	AB	614	CLA	MG-NB	2.69	2.11	2.05
29	AF	101	SQD	C14-C13	-2.69	1.38	1.51
22	BB	613	CLA	CAA-C2A	2.68	1.59	1.54
30	AC	520	LMG	O7-C10	2.68	1.41	1.34
30	AC	519	LMG	C4-C5	2.68	1.58	1.53
30	AB	621	LMG	O1-C1	2.68	1.44	1.40
27	AH	102	DGD	C4E-C5E	2.67	1.58	1.53
27	BH	101	DGD	O3G-C1D	2.67	1.44	1.40
34	AV	201	HEM	FE-ND	2.67	2.03	1.94
30	BB	624	LMG	C4-C5	2.67	1.58	1.53
22	BB	616	CLA	MG-NC	2.66	2.12	2.06
30	BD	408	LMG	O6-C5	2.66	1.50	1.44
30	AB	623	LMG	C3-C2	2.66	1.59	1.52
29	AA	415	SQD	C36-C35	-2.66	1.38	1.51
29	BL	101	SQD	O6-C1	2.66	1.44	1.40
29	AF	101	SQD	O5-C1	2.66	1.48	1.41
26	AC	514	BCR	C5-C6	2.65	1.39	1.34
29	BA	413	SQD	O3-C3	2.65	1.49	1.43
22	AA	402	CLA	MG-NC	2.65	2.12	2.06
29	AA	415	SQD	C34-C33	-2.65	1.38	1.51
29	BD	409	SQD	C17-C16	-2.65	1.35	1.51
32	AB	627	LMT	O1'-C1'	2.65	1.44	1.40
27	AC	516	DGD	O6D-C5D	2.64	1.50	1.44
30	AB	621	LMG	O6-C1	2.64	1.48	1.41
30	AB	622	LMG	O6-C5	2.64	1.50	1.44
34	AV	201	HEM	CHA-C4D	2.64	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	AC	517	DGD	O6D-C5D	2.64	1.50	1.44
27	BA	411	DGD	O2G-C1B	2.64	1.41	1.34
32	AI	102	LMT	O5'-C1'	2.64	1.48	1.41
27	BC	516	DGD	O6D-C5D	2.63	1.50	1.44
22	BB	608	CLA	MG-NC	2.63	2.12	2.06
32	AT	101	LMT	O1B-C1B	2.63	1.49	1.41
29	AA	415	SQD	C35-C34	-2.63	1.38	1.51
22	AA	406	CLA	C4-C3	2.63	1.57	1.50
22	AA	404	CLA	MG-NC	2.63	2.12	2.06
22	BB	604	CLA	MG-NC	2.63	2.12	2.06
30	BI	101	LMG	C1-C2	2.63	1.60	1.52
27	AD	410	DGD	C4D-C3D	2.62	1.59	1.52
27	AH	102	DGD	O3G-C1D	2.62	1.44	1.40
22	BB	610	CLA	MG-NC	2.62	2.12	2.06
22	BC	501	CLA	MG-NC	2.61	2.12	2.06
22	AC	505	CLA	C1C-C2C	2.61	1.49	1.44
30	AA	413	LMG	O1-C1	2.61	1.44	1.40
23	BA	406	PHO	C4-C3	2.60	1.57	1.50
24	BJ	101	PL9	C7-C8	2.60	1.54	1.50
27	AC	518	DGD	C4E-C3E	2.60	1.59	1.52
27	BD	410	DGD	C1D-C2D	2.60	1.60	1.52
29	BA	401	SQD	C35-C34	-2.60	1.38	1.51
22	AB	616	CLA	MG-NC	2.60	2.12	2.06
32	BB	625	LMT	C4B-C5B	2.59	1.58	1.53
29	AA	412	SQD	O8-S	2.59	1.56	1.47
34	BE	101	HEM	C1A-NA	2.59	1.44	1.39
29	BF	101	SQD	C13-C12	-2.59	1.38	1.51
27	AC	518	DGD	O5D-C1E	2.59	1.44	1.40
30	AB	623	LMG	O6-C5	2.59	1.50	1.44
29	BD	409	SQD	O5-C1	2.59	1.48	1.41
22	BC	505	CLA	CHC-C1C	2.58	1.43	1.38
30	AD	408	LMG	O6-C5	2.58	1.50	1.44
27	BD	410	DGD	C4D-C3D	2.58	1.59	1.52
22	BB	618	CLA	CAA-C2A	2.58	1.58	1.54
22	BD	404	CLA	CHB-C1B	-2.57	1.33	1.39
22	BA	403	CLA	MG-NC	2.57	2.12	2.06
26	AT	102	BCR	C26-C25	2.57	1.38	1.34
24	AJ	101	PL9	C3-C4	2.57	1.53	1.49
22	AC	509	CLA	MG-NC	2.57	2.12	2.06
27	BA	411	DGD	O6E-C1E	2.57	1.48	1.41
27	AC	517	DGD	C4D-C5D	2.57	1.58	1.53
29	BA	413	SQD	C18-C17	-2.56	1.39	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BB	618	CLA	MG-NB	2.56	2.10	2.05
30	BE	102	LMG	O7-C10	2.56	1.41	1.34
24	BA	408	PL9	C7-C3	2.56	1.54	1.51
23	AA	405	PHO	C3A-C2A	-2.56	1.52	1.54
22	BC	505	CLA	MG-NC	2.56	2.12	2.06
22	AB	603	CLA	MG-NC	2.56	2.12	2.06
30	AB	623	LMG	C4-C3	2.56	1.59	1.52
23	AD	403	PHO	C1D-C2D	2.55	1.42	1.39
27	AC	516	DGD	C4E-C3E	2.55	1.59	1.52
30	BD	407	LMG	O1-C1	2.55	1.44	1.40
22	AC	501	CLA	MG-NC	2.55	2.12	2.06
22	AD	402	CLA	C4C-C3C	2.55	1.49	1.45
30	BA	414	LMG	O1-C1	2.55	1.44	1.40
27	AB	626	DGD	O6E-C5E	2.55	1.50	1.44
27	AD	410	DGD	C3E-C2E	2.55	1.59	1.52
30	AE	102	LMG	O6-C5	2.55	1.50	1.44
22	AA	403	CLA	MG-NB	2.55	2.10	2.05
22	AC	508	CLA	MG-NB	2.55	2.10	2.05
22	AD	404	CLA	MG-NC	2.55	2.12	2.06
30	AB	621	LMG	O7-C10	2.54	1.41	1.34
29	AF	101	SQD	C44-C45	2.54	1.58	1.50
30	BB	623	LMG	O6-C5	2.54	1.50	1.44
22	BB	613	CLA	CHB-C1B	-2.54	1.33	1.39
24	AJ	101	PL9	C2-C1	2.54	1.51	1.44
27	BC	517	DGD	O6D-C5D	2.54	1.50	1.44
30	AD	407	LMG	O1-C1	2.54	1.44	1.40
22	AC	508	CLA	MG-NC	2.54	2.12	2.06
27	BB	602	DGD	O6E-C5E	2.54	1.50	1.44
22	BB	611	CLA	C5-C3	2.54	1.56	1.51
27	AC	516	DGD	O6D-C1D	2.54	1.48	1.41
27	BC	518	DGD	O6D-C5D	2.54	1.50	1.44
26	AK	102	BCR	C26-C25	2.53	1.38	1.34
22	BA	403	CLA	CHC-C1C	2.53	1.43	1.38
22	AB	615	CLA	CAA-C2A	2.53	1.58	1.54
27	BB	602	DGD	C3E-C2E	2.53	1.58	1.52
32	AB	624	LMT	O1'-C1'	2.53	1.44	1.40
30	AC	520	LMG	O8-C28	2.53	1.40	1.33
30	BE	102	LMG	O6-C5	2.52	1.50	1.44
27	AD	410	DGD	C4D-C5D	2.52	1.58	1.53
30	AD	407	LMG	C4-C3	2.52	1.58	1.52
30	BC	520	LMG	O1-C1	2.52	1.44	1.40
22	AC	509	CLA	CHB-C1B	-2.52	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BC	516	DGD	C4D-C3D	2.52	1.58	1.52
27	BA	411	DGD	C1E-C2E	2.52	1.59	1.52
34	AV	201	HEM	CBD-CAD	2.52	1.60	1.51
22	AC	502	CLA	CHB-C1B	-2.51	1.33	1.39
27	BH	101	DGD	C4E-C3E	2.51	1.58	1.52
30	BC	519	LMG	C4-C5	2.51	1.58	1.53
22	BC	508	CLA	CAA-C2A	2.51	1.58	1.54
26	BB	622	BCR	C26-C25	2.51	1.38	1.34
22	BB	615	CLA	CAA-C2A	2.51	1.58	1.54
29	AD	409	SQD	C17-C16	-2.51	1.36	1.51
29	BA	413	SQD	O5-C1	2.51	1.48	1.41
22	AC	502	CLA	MG-NC	2.50	2.12	2.06
22	AA	402	CLA	CAA-CBA	-2.50	1.45	1.52
22	BC	505	CLA	C1D-C2D	-2.50	1.40	1.45
29	AA	412	SQD	C18-C17	-2.50	1.39	1.51
29	BA	401	SQD	C34-C33	-2.50	1.39	1.51
22	BA	403	CLA	CAA-CBA	-2.50	1.45	1.52
27	AD	410	DGD	O1G-C1A	2.49	1.40	1.33
22	AC	513	CLA	C4-C3	2.49	1.56	1.50
27	AB	626	DGD	C1D-C2D	2.49	1.59	1.52
22	AB	611	CLA	MG-NA	2.49	2.12	2.06
22	BA	407	CLA	C4-C3	2.49	1.56	1.50
29	BF	101	SQD	C44-C45	2.49	1.58	1.50
27	BB	602	DGD	O6D-C1D	2.49	1.48	1.41
30	AA	416	LMG	O8-C28	2.49	1.40	1.33
34	BE	101	HEM	C2A-C3A	2.49	1.45	1.38
30	BB	623	LMG	O1-C1	2.48	1.44	1.40
27	BH	101	DGD	C1E-C2E	2.48	1.59	1.52
22	AB	601	CLA	CHB-C4A	2.48	1.43	1.37
30	BM	102	LMG	C4-C5	2.48	1.58	1.53
32	BB	625	LMT	O1'-C1'	2.48	1.44	1.40
29	BL	101	SQD	C21-C20	-2.48	1.36	1.51
22	AB	614	CLA	CHC-C1C	2.48	1.43	1.38
22	BC	510	CLA	MG-NC	2.47	2.12	2.06
30	AC	520	LMG	C3-C2	2.47	1.58	1.52
27	BH	101	DGD	O6E-C1E	2.47	1.48	1.41
22	BA	405	CLA	CHB-C1B	-2.47	1.33	1.39
22	AB	602	CLA	CAA-CBA	-2.47	1.45	1.52
29	BB	601	SQD	C21-C20	-2.46	1.36	1.51
22	AC	505	CLA	C4C-C3C	2.46	1.49	1.45
22	BC	505	CLA	C1D-ND	-2.46	1.34	1.37
34	BV	201	HEM	CHA-C4D	2.46	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	AC	510	CLA	CHB-C1B	-2.46	1.33	1.39
22	AC	512	CLA	CMB-C2B	2.46	1.55	1.50
27	BD	410	DGD	C1E-C2E	2.46	1.59	1.52
30	AA	416	LMG	C4-C3	2.46	1.58	1.52
30	AD	407	LMG	O6-C1	2.46	1.48	1.41
22	AB	610	CLA	MG-NC	2.46	2.12	2.06
22	BB	607	CLA	MG-NC	2.46	2.12	2.06
22	BC	504	CLA	CHC-C1C	2.46	1.43	1.38
23	BA	406	PHO	CAA-CBA	-2.46	1.45	1.52
29	AF	101	SQD	C13-C12	-2.46	1.39	1.51
26	AA	409	BCR	C19-C18	-2.46	1.40	1.46
22	BC	510	CLA	CAA-C2A	2.46	1.58	1.54
27	BD	410	DGD	C3D-C2D	2.46	1.58	1.52
22	AB	603	CLA	C4-C3	2.46	1.56	1.50
22	AC	510	CLA	CAA-C2A	2.46	1.58	1.54
22	BB	619	CLA	C4-C3	2.46	1.56	1.50
29	BD	409	SQD	C8-C7	2.45	1.57	1.50
27	BC	517	DGD	C4D-C5D	2.45	1.58	1.53
30	BB	624	LMG	O6-C5	2.45	1.50	1.44
22	AB	605	CLA	CHB-C1B	-2.45	1.33	1.39
22	AB	614	CLA	MG-NC	2.45	2.12	2.06
30	AB	621	LMG	C4-C3	2.45	1.58	1.52
30	BE	102	LMG	C4-C5	2.44	1.58	1.53
22	BB	615	CLA	MG-NC	2.44	2.12	2.06
22	AC	510	CLA	C1D-ND	-2.44	1.34	1.37
32	BB	626	LMT	O5B-C1B	2.44	1.48	1.41
26	BZ	101	BCR	C23-C22	-2.44	1.40	1.46
22	BC	502	CLA	CHB-C1B	-2.44	1.33	1.39
30	BC	519	LMG	C4-C3	2.44	1.58	1.52
22	BC	504	CLA	C3B-C4B	2.43	1.49	1.42
22	BC	508	CLA	C4-C3	2.43	1.56	1.50
27	AH	102	DGD	C4E-C3E	2.43	1.58	1.52
22	AB	612	CLA	CAA-C2A	2.43	1.58	1.54
22	BC	508	CLA	MG-NB	2.43	2.10	2.05
30	AC	519	LMG	C4-C3	2.43	1.58	1.52
22	AB	604	CLA	MG-NB	2.42	2.10	2.05
22	BB	604	CLA	CHB-C4A	2.42	1.43	1.37
22	AC	502	CLA	C1D-ND	-2.42	1.34	1.37
30	BC	520	LMG	O8-C28	2.42	1.40	1.33
22	AB	610	CLA	C4-C3	2.42	1.56	1.50
34	BV	201	HEM	CMA-C3A	2.42	1.55	1.50
22	BB	616	CLA	CAA-C2A	2.42	1.58	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	AC	504	CLA	C3B-C4B	2.42	1.49	1.42
34	BE	101	HEM	C1A-C2A	2.42	1.49	1.44
30	BD	407	LMG	O6-C5	2.42	1.50	1.44
23	BA	406	PHO	C3A-C2A	-2.42	1.52	1.54
29	BA	401	SQD	C24-C23	2.42	1.57	1.50
22	BC	508	CLA	CHB-C1B	-2.41	1.34	1.39
22	AD	402	CLA	C1C-C2C	2.41	1.49	1.44
22	AB	610	CLA	CHB-C1B	-2.41	1.34	1.39
32	BB	626	LMT	O5'-C1'	2.41	1.48	1.41
23	AD	403	PHO	C4-C3	2.41	1.56	1.50
27	BD	410	DGD	O6E-C5E	2.41	1.50	1.44
22	AC	508	CLA	CHB-C1B	-2.41	1.34	1.39
22	BC	504	CLA	C4-C3	2.41	1.56	1.50
22	BB	618	CLA	CHB-C4A	2.41	1.43	1.37
30	BC	520	LMG	C3-C2	2.41	1.58	1.52
27	BA	411	DGD	O6E-C5E	2.41	1.50	1.44
22	BB	619	CLA	C2-C3	2.40	1.38	1.33
29	BA	413	SQD	O6-C44	-2.40	1.39	1.43
34	BV	201	HEM	CAA-C2A	2.40	1.57	1.51
22	AC	508	CLA	C4-C3	2.40	1.56	1.50
22	BB	611	CLA	C4-C3	2.40	1.56	1.50
27	BD	410	DGD	C4D-C5D	2.40	1.58	1.53
32	AB	625	LMT	O5B-C1B	2.40	1.48	1.41
24	BJ	101	PL9	C3-C4	2.40	1.53	1.49
22	AB	608	CLA	CHB-C1B	-2.40	1.34	1.39
22	BB	611	CLA	MG-NC	2.39	2.12	2.06
32	BB	625	LMT	C4B-C3B	2.39	1.58	1.52
22	BC	509	CLA	CHB-C1B	-2.39	1.34	1.39
24	BA	408	PL9	C2-C1	2.39	1.51	1.44
22	BB	606	CLA	C4-C3	2.39	1.56	1.50
32	BB	625	LMT	O5B-C5B	2.39	1.50	1.44
30	AE	102	LMG	O7-C10	2.39	1.41	1.34
22	AB	604	CLA	CHC-C1C	2.39	1.43	1.38
27	AC	517	DGD	C6D-C5D	2.38	1.58	1.51
27	AB	626	DGD	C4D-C3D	2.38	1.58	1.52
22	AB	605	CLA	MG-NB	2.38	2.10	2.05
32	BB	625	LMT	C1B-C2B	2.38	1.59	1.52
34	AV	201	HEM	C4D-ND	-2.38	1.36	1.40
22	BB	604	CLA	C1B-C2B	2.37	1.48	1.43
22	BB	607	CLA	CHC-C1C	2.37	1.43	1.38
22	BB	607	CLA	C1D-C2D	-2.37	1.40	1.45
22	AB	613	CLA	CAA-C2A	2.37	1.58	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	AC	504	CLA	CHC-C1C	2.37	1.43	1.38
22	BA	407	CLA	C1D-ND	-2.37	1.34	1.37
22	AB	610	CLA	C4C-C3C	2.37	1.49	1.45
26	BA	410	BCR	C19-C18	-2.37	1.40	1.46
26	AD	406	BCR	C38-C26	2.37	1.54	1.50
22	BC	501	CLA	CHB-C1B	-2.37	1.34	1.39
22	BB	608	CLA	CHB-C1B	-2.36	1.34	1.39
22	AB	601	CLA	C1B-C2B	2.36	1.48	1.43
34	AE	101	HEM	C1C-C2C	2.36	1.50	1.45
32	AB	625	LMT	C4B-C5B	2.36	1.58	1.53
22	AD	402	CLA	MG-NB	2.36	2.10	2.05
22	AC	501	CLA	CHB-C1B	-2.36	1.34	1.39
26	BB	620	BCR	C19-C18	-2.36	1.40	1.46
34	AV	201	HEM	CAA-C2A	2.36	1.57	1.51
27	AD	410	DGD	C1E-C2E	2.36	1.59	1.52
22	AB	605	CLA	C1D-ND	-2.36	1.34	1.37
22	BB	605	CLA	CAA-CBA	-2.36	1.45	1.52
22	AC	512	CLA	CHC-C1C	2.36	1.43	1.38
22	BB	605	CLA	CHC-C1C	2.35	1.43	1.38
22	BA	405	CLA	C1D-ND	-2.35	1.34	1.37
22	AC	508	CLA	CAA-C2A	2.35	1.58	1.54
22	AC	513	CLA	CHC-C1C	2.35	1.43	1.38
22	AC	512	CLA	MG-NB	2.35	2.10	2.05
23	AA	405	PHO	C1D-C2D	2.35	1.42	1.39
22	BC	508	CLA	CHC-C1C	2.35	1.43	1.38
34	AE	101	HEM	C1A-NA	2.34	1.44	1.39
22	BC	509	CLA	C5-C3	2.34	1.56	1.51
22	AB	602	CLA	CHC-C1C	2.34	1.43	1.38
34	AV	201	HEM	C2A-C3A	2.34	1.45	1.38
29	AA	412	SQD	C34-C33	-2.34	1.37	1.51
27	AB	626	DGD	O5D-C6D	2.34	1.47	1.43
22	BB	613	CLA	C4C-C3C	2.34	1.49	1.45
22	BC	509	CLA	MG-NC	2.33	2.11	2.06
34	AE	101	HEM	C3B-C4B	2.33	1.49	1.44
27	BC	517	DGD	C6D-C5D	2.33	1.58	1.51
22	BC	512	CLA	CMB-C2B	2.33	1.55	1.50
22	AB	608	CLA	C5-C3	2.33	1.56	1.51
22	BC	512	CLA	CHC-C1C	2.33	1.43	1.38
22	BC	509	CLA	C4C-C3C	2.33	1.49	1.45
22	AB	603	CLA	C1D-ND	-2.33	1.34	1.37
26	AH	101	BCR	C5-C6	2.33	1.38	1.34
22	AC	506	CLA	CHB-C1B	-2.32	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	AB	615	CLA	MG-NB	2.32	2.10	2.05
29	AA	412	SQD	O5-C1	2.32	1.47	1.41
27	BC	518	DGD	O6E-C1E	2.32	1.47	1.41
27	AH	102	DGD	O6D-C1D	2.32	1.47	1.41
22	BB	610	CLA	C1-C2	2.32	1.55	1.49
32	AB	627	LMT	O1B-C4'	2.32	1.49	1.43
22	AB	601	CLA	C4-C3	2.32	1.56	1.50
23	AA	405	PHO	CAA-CBA	-2.31	1.46	1.52
22	AC	510	CLA	C3B-C4B	2.31	1.49	1.42
22	AB	615	CLA	CHB-C4A	2.31	1.43	1.37
22	AD	402	CLA	CHC-C1C	2.31	1.43	1.38
22	BC	511	CLA	CHB-C4A	2.31	1.43	1.37
27	AD	410	DGD	O6E-C5E	2.31	1.50	1.44
22	AB	606	CLA	CHB-C1B	-2.31	1.34	1.39
32	BD	411	LMT	C4B-C5B	2.31	1.57	1.53
22	BC	513	CLA	C1C-C2C	2.31	1.49	1.44
22	BC	504	CLA	MG-NC	2.31	2.11	2.06
27	BA	411	DGD	C3E-C2E	2.31	1.58	1.52
27	AC	516	DGD	O3G-C1D	2.31	1.44	1.40
22	BB	614	CLA	CAA-C2A	2.31	1.58	1.54
30	BB	624	LMG	C4-C3	2.30	1.58	1.52
26	BZ	101	BCR	C35-C13	2.30	1.55	1.50
22	AC	512	CLA	CHB-C4A	2.30	1.43	1.37
27	BH	101	DGD	C3D-C2D	2.30	1.58	1.52
30	AI	101	LMG	O1-C1	2.29	1.44	1.40
26	BZ	101	BCR	C38-C26	2.29	1.54	1.50
22	BB	612	CLA	MG-NB	2.29	2.10	2.05
34	BE	101	HEM	C3B-C4B	2.29	1.49	1.44
22	AC	510	CLA	CAA-CBA	-2.29	1.46	1.52
29	AA	415	SQD	C37-C36	-2.29	1.37	1.51
22	AB	608	CLA	MG-NC	2.29	2.11	2.06
26	BC	514	BCR	C38-C26	2.29	1.54	1.50
26	BB	620	BCR	C23-C22	-2.29	1.41	1.46
22	BC	505	CLA	C4C-C3C	2.29	1.48	1.45
22	BB	607	CLA	C1D-ND	-2.29	1.34	1.37
22	AB	605	CLA	MG-NC	2.28	2.11	2.06
27	BC	516	DGD	O6E-C1E	2.28	1.47	1.41
27	AC	517	DGD	O3G-C1D	2.28	1.44	1.40
22	AB	615	CLA	CHB-C1B	-2.28	1.34	1.39
22	AB	610	CLA	C1D-ND	-2.28	1.34	1.37
22	AB	609	CLA	CHB-C4A	2.28	1.43	1.37
22	AB	613	CLA	C1D-ND	-2.28	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	AD	407	LMG	O6-C5	2.27	1.49	1.44
27	AH	102	DGD	O6E-C1E	2.27	1.47	1.41
27	AA	410	DGD	C1E-C2E	2.27	1.59	1.52
22	BC	512	CLA	CHB-C4A	2.27	1.43	1.37
22	BB	609	CLA	MG-NC	2.27	2.11	2.06
26	BJ	102	BCR	C3-C4	2.27	1.59	1.52
22	BB	611	CLA	CHB-C1B	-2.27	1.34	1.39
22	BB	618	CLA	CHB-C1B	-2.27	1.34	1.39
22	AC	511	CLA	CMB-C2B	2.27	1.55	1.50
22	AB	604	CLA	C1D-C2D	-2.27	1.40	1.45
27	AC	516	DGD	O6E-C1E	2.27	1.47	1.41
30	AC	520	LMG	C9-C8	2.27	1.57	1.50
27	BC	516	DGD	C4D-C5D	2.27	1.57	1.53
22	BB	608	CLA	MG-NB	2.26	2.10	2.05
22	AC	511	CLA	CHB-C4A	2.26	1.43	1.37
22	BB	614	CLA	MG-NA	2.26	2.11	2.06
22	AD	404	CLA	C4C-C3C	2.26	1.48	1.45
22	AD	404	CLA	CHB-C4A	2.26	1.43	1.37
27	BD	410	DGD	C3E-C2E	2.26	1.58	1.52
22	AC	513	CLA	CHB-C1B	-2.26	1.34	1.39
22	BB	604	CLA	C1-C2	2.26	1.55	1.49
30	AB	621	LMG	O6-C5	2.26	1.49	1.44
22	AB	610	CLA	CAA-C2A	2.26	1.58	1.54
27	AC	518	DGD	O6E-C1E	2.26	1.47	1.41
22	AB	613	CLA	MG-NC	2.25	2.11	2.06
26	AZ	101	BCR	C38-C26	2.25	1.54	1.50
30	BA	414	LMG	O6-C5	2.25	1.49	1.44
32	BB	625	LMT	C3B-C2B	2.25	1.58	1.52
34	AE	101	HEM	CAD-C3D	-2.25	1.45	1.51
27	BB	602	DGD	O5D-C6D	2.25	1.47	1.43
22	AB	612	CLA	CHC-C1C	2.25	1.43	1.38
22	AB	603	CLA	C1D-C2D	-2.24	1.40	1.45
22	AB	612	CLA	CHB-C1B	-2.24	1.34	1.39
27	AB	626	DGD	C3E-C2E	2.24	1.58	1.52
27	BB	602	DGD	O1G-C1A	2.24	1.39	1.33
22	AB	607	CLA	C1C-C2C	2.24	1.49	1.44
22	BC	513	CLA	C4-C3	2.24	1.56	1.50
22	BA	403	CLA	CMB-C2B	2.24	1.55	1.50
29	AA	415	SQD	C21-C20	-2.24	1.37	1.51
30	BC	520	LMG	C9-C8	2.24	1.57	1.50
30	AB	622	LMG	C4-C3	2.23	1.58	1.52
32	BB	626	LMT	C4B-C5B	2.23	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BD	404	CLA	CHC-C1C	2.23	1.43	1.38
22	BA	407	CLA	MG-NB	2.23	2.10	2.05
30	AI	101	LMG	C1-C2	2.23	1.59	1.52
27	AB	626	DGD	C1E-C2E	2.23	1.59	1.52
27	BD	410	DGD	O1G-C1A	2.23	1.39	1.33
32	AT	101	LMT	O1B-C4'	2.23	1.49	1.43
34	BV	201	HEM	CAD-C3D	-2.23	1.45	1.51
22	AB	601	CLA	CAA-C2A	2.22	1.58	1.54
26	AB	617	BCR	C23-C22	-2.22	1.41	1.46
22	BB	605	CLA	CMB-C2B	2.22	1.55	1.50
34	BV	201	HEM	CMB-C2B	2.22	1.55	1.50
29	BA	413	SQD	C34-C33	-2.22	1.37	1.51
22	AB	614	CLA	CMD-C2D	2.22	1.55	1.50
29	AD	409	SQD	C8-C7	2.22	1.57	1.50
22	BB	611	CLA	C1D-C2D	-2.22	1.40	1.45
29	BA	401	SQD	C21-C20	-2.22	1.37	1.51
32	BB	603	LMT	C4B-C5B	2.22	1.57	1.53
29	BA	413	SQD	C21-C20	-2.22	1.37	1.51
22	BB	607	CLA	C4-C3	2.22	1.56	1.50
30	BI	101	LMG	O1-C1	2.22	1.43	1.40
32	AB	624	LMT	C4B-C5B	2.22	1.57	1.53
22	AB	607	CLA	CMB-C2B	2.22	1.55	1.50
22	BB	618	CLA	CHC-C1C	2.22	1.42	1.38
27	AC	516	DGD	C4D-C5D	2.22	1.57	1.53
22	BB	607	CLA	MG-NB	2.21	2.10	2.05
22	AB	611	CLA	MG-NB	2.21	2.10	2.05
22	BC	510	CLA	C4-C3	2.21	1.56	1.50
32	AT	101	LMT	C3'-C4'	2.21	1.58	1.52
22	AB	603	CLA	C5-C3	2.21	1.55	1.51
22	BB	604	CLA	CMB-C2B	2.21	1.55	1.50
34	AV	201	HEM	CAC-C3C	2.21	1.53	1.47
22	AB	607	CLA	CHC-C1C	2.21	1.42	1.38
30	BA	414	LMG	C4-C3	2.21	1.58	1.52
22	AB	602	CLA	MG-NB	2.21	2.10	2.05
22	BB	612	CLA	CHC-C1C	2.21	1.42	1.38
22	BB	617	CLA	C1-C2	2.21	1.55	1.49
29	BA	401	SQD	C37-C36	-2.21	1.38	1.51
22	AC	510	CLA	MG-NC	2.21	2.11	2.06
22	BD	402	CLA	CHB-C1B	-2.20	1.34	1.39
22	BC	511	CLA	CMB-C2B	2.20	1.55	1.50
22	BD	404	CLA	C5-C3	2.20	1.55	1.51
22	AA	406	CLA	MG-NC	2.20	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	AB	614	CLA	C1-C2	2.20	1.55	1.49
22	BB	619	CLA	C1-C2	2.20	1.55	1.49
22	BB	604	CLA	C4-C3	2.20	1.56	1.50
26	AB	619	BCR	C24-C23	2.19	1.39	1.33
27	BH	101	DGD	O6D-C5D	2.19	1.49	1.44
34	AE	101	HEM	CHC-C1C	2.19	1.42	1.38
27	AA	410	DGD	O2G-C1B	2.19	1.40	1.34
23	BD	403	PHO	C1D-C2D	2.19	1.42	1.39
29	AF	101	SQD	C18-C17	-2.19	1.38	1.51
27	AC	516	DGD	C4D-C3D	2.19	1.58	1.52
22	BB	610	CLA	CHC-C1C	2.19	1.42	1.38
30	BE	102	LMG	C1-C2	2.19	1.58	1.52
29	AA	412	SQD	C21-C20	-2.19	1.38	1.51
22	BC	502	CLA	CHC-C1C	2.19	1.42	1.38
22	AB	607	CLA	MG-NC	2.19	2.11	2.06
29	BF	101	SQD	C18-C17	-2.19	1.38	1.51
22	AB	607	CLA	C1-C2	2.19	1.55	1.49
34	BE	101	HEM	CAD-C3D	-2.19	1.45	1.51
22	AB	604	CLA	CHB-C1B	-2.18	1.34	1.39
22	BC	510	CLA	CHB-C1B	-2.18	1.34	1.39
22	AB	616	CLA	C4-C3	2.18	1.56	1.50
22	AC	507	CLA	C4-C3	2.18	1.56	1.50
34	BV	201	HEM	C1A-C2A	2.18	1.49	1.44
22	AC	503	CLA	CHB-C4A	2.18	1.43	1.37
29	BL	101	SQD	C22-C21	-2.18	1.34	1.50
22	AA	402	CLA	CMB-C2B	2.18	1.55	1.50
22	BC	512	CLA	C4-C3	2.18	1.56	1.50
23	BD	403	PHO	C4-C3	2.18	1.56	1.50
22	BC	512	CLA	MG-NB	2.17	2.10	2.05
22	AC	513	CLA	C1C-C2C	2.17	1.48	1.44
22	AB	616	CLA	C1-C2	2.17	1.55	1.49
22	AD	404	CLA	CHB-C1B	-2.17	1.34	1.39
32	AM	102	LMT	O5'-C1'	2.17	1.47	1.41
30	BM	102	LMG	C4-C3	2.17	1.58	1.52
22	BD	402	CLA	CAA-CBA	-2.17	1.46	1.52
22	AB	602	CLA	CMB-C2B	2.17	1.55	1.50
29	AD	409	SQD	C44-C45	2.17	1.57	1.50
32	BM	101	LMT	O5'-C1'	2.16	1.47	1.41
27	BC	518	DGD	C4E-C3E	2.16	1.58	1.52
22	BB	615	CLA	CHC-C1C	2.16	1.42	1.38
22	AB	615	CLA	C3B-C4B	2.16	1.49	1.42
22	AB	607	CLA	MG-NB	2.16	2.10	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BB	602	DGD	C1D-C2D	2.16	1.58	1.52
32	BT	101	LMT	O1B-C1B	2.16	1.47	1.41
26	BC	515	BCR	C19-C18	-2.16	1.41	1.46
32	AB	624	LMT	C6'-C5'	2.16	1.59	1.51
22	BC	509	CLA	C4-C3	2.16	1.56	1.50
29	AA	415	SQD	C38-C37	-2.16	1.34	1.50
29	BA	401	SQD	C8-C7	2.16	1.57	1.50
28	BA	412	LHG	O8-C6	-2.15	1.40	1.45
32	AB	625	LMT	O5B-C5B	2.15	1.49	1.44
32	BT	101	LMT	O1B-C4'	2.15	1.49	1.43
32	BI	102	LMT	C4B-C5B	2.15	1.57	1.53
22	BB	613	CLA	CAA-CBA	-2.15	1.46	1.52
22	BB	610	CLA	C1C-C2C	2.15	1.48	1.44
22	BD	404	CLA	CHB-C4A	2.15	1.43	1.37
22	BA	407	CLA	CAA-C2A	2.15	1.58	1.54
22	AB	611	CLA	CMD-C2D	2.15	1.55	1.50
30	BC	519	LMG	O7-C10	2.15	1.40	1.34
26	AJ	102	BCR	C32-C1	2.15	1.57	1.53
32	BB	603	LMT	C3'-C4'	2.14	1.58	1.52
23	AA	405	PHO	CMC-C2C	2.14	1.53	1.50
22	BC	507	CLA	C4C-C3C	2.14	1.48	1.45
30	AB	623	LMG	C1-C2	2.14	1.58	1.52
26	AC	514	BCR	C38-C26	2.14	1.54	1.50
22	BB	615	CLA	C4-C3	2.14	1.55	1.50
32	AI	102	LMT	C4B-C5B	2.14	1.57	1.53
22	AB	604	CLA	CHB-C4A	2.14	1.43	1.37
23	AA	405	PHO	C3D-CAD	-2.13	1.43	1.47
22	BD	404	CLA	C3B-C4B	2.13	1.48	1.42
22	BB	613	CLA	C4-C3	2.13	1.55	1.50
22	AC	510	CLA	C1B-C2B	2.13	1.48	1.43
22	BC	502	CLA	MG-NB	2.13	2.10	2.05
32	BB	625	LMT	C6'-C5'	2.13	1.58	1.51
26	BX	101	BCR	C5-C6	2.13	1.38	1.34
22	AB	616	CLA	C2-C3	2.12	1.38	1.33
22	BD	402	CLA	CHC-C1C	2.12	1.42	1.38
22	AB	609	CLA	C1C-C2C	2.12	1.48	1.44
22	AC	511	CLA	C4-C3	2.12	1.55	1.50
22	AC	512	CLA	CHB-C1B	-2.12	1.34	1.39
22	AC	510	CLA	C1C-C2C	2.12	1.48	1.44
22	AA	406	CLA	C1D-ND	-2.12	1.35	1.37
22	BB	615	CLA	CHB-C4A	2.12	1.43	1.37
22	BA	404	CLA	C5-C3	2.12	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	AD	402	CLA	CHB-C1B	-2.12	1.34	1.39
22	BC	506	CLA	C4-C3	2.12	1.55	1.50
22	BB	606	CLA	C5-C3	2.12	1.55	1.51
22	BB	604	CLA	C5-C3	2.12	1.55	1.51
22	BC	513	CLA	CMB-C2B	2.12	1.55	1.50
22	AB	610	CLA	CMB-C2B	2.12	1.55	1.50
32	AB	625	LMT	C4'-C5'	2.12	1.58	1.52
27	BC	516	DGD	C4E-C5E	2.12	1.57	1.53
27	AA	410	DGD	O6E-C5E	2.12	1.49	1.44
26	BD	406	BCR	C19-C18	-2.12	1.41	1.46
22	AC	505	CLA	CHB-C4A	2.11	1.43	1.37
27	BH	101	DGD	C4E-C5E	2.11	1.57	1.53
22	BA	404	CLA	C1D-ND	-2.11	1.35	1.37
22	BC	508	CLA	C3B-C4B	2.11	1.48	1.42
29	BD	409	SQD	C44-C45	2.11	1.57	1.50
22	AC	506	CLA	MG-NB	2.11	2.10	2.05
22	AC	504	CLA	C4-C3	2.11	1.55	1.50
22	BB	609	CLA	CMD-C2D	2.11	1.55	1.50
34	BV	201	HEM	C1C-C2C	2.10	1.49	1.45
22	AC	503	CLA	CHB-C1B	-2.10	1.34	1.39
22	AD	402	CLA	CAA-CBA	-2.10	1.46	1.52
22	BC	503	CLA	CHB-C4A	2.10	1.43	1.37
26	BB	622	BCR	C33-C5	2.10	1.54	1.50
32	BB	603	LMT	C1B-C2B	2.10	1.58	1.52
22	AB	601	CLA	CMB-C2B	2.10	1.55	1.50
29	AF	101	SQD	C24-C23	2.10	1.56	1.50
22	AC	503	CLA	CMB-C2B	2.10	1.55	1.50
22	BB	610	CLA	CMB-C2B	2.10	1.55	1.50
24	AA	407	PL9	C7-C3	2.10	1.54	1.51
22	BC	512	CLA	C3B-C4B	2.10	1.48	1.42
22	BC	512	CLA	CMD-C2D	2.10	1.55	1.50
29	BA	401	SQD	C22-C21	-2.10	1.35	1.50
22	AA	404	CLA	C4-C3	2.10	1.55	1.50
22	BC	511	CLA	C1C-C2C	2.09	1.48	1.44
22	BB	616	CLA	C1D-ND	-2.09	1.35	1.37
32	BB	603	LMT	O1B-C4'	2.09	1.49	1.43
29	BB	601	SQD	C8-C7	2.09	1.56	1.50
22	AC	513	CLA	CMB-C2B	2.09	1.55	1.50
22	BC	510	CLA	CHB-C4A	2.09	1.42	1.37
22	AB	607	CLA	C5-C3	2.09	1.55	1.51
22	AC	509	CLA	C4-C3	2.09	1.55	1.50
22	BB	614	CLA	CMD-C2D	2.09	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BB	602	DGD	C3D-C2D	2.09	1.57	1.52
27	BA	411	DGD	O1G-C1A	2.09	1.39	1.33
22	BC	511	CLA	C4-C3	2.09	1.55	1.50
22	AC	505	CLA	CHB-C1B	-2.09	1.34	1.39
22	BB	609	CLA	CHB-C1B	-2.09	1.34	1.39
29	BB	601	SQD	C22-C21	-2.09	1.35	1.50
22	AA	403	CLA	MG-NC	2.08	2.11	2.06
22	AC	503	CLA	C4C-C3C	2.08	1.48	1.45
22	BC	509	CLA	C3B-C4B	2.08	1.48	1.42
22	BC	503	CLA	CMB-C2B	2.08	1.55	1.50
27	BH	101	DGD	O6D-C1D	2.08	1.47	1.41
23	AD	403	PHO	C3D-CAD	-2.08	1.43	1.47
22	BC	510	CLA	C1D-ND	-2.08	1.35	1.37
29	AA	415	SQD	C24-C23	2.08	1.56	1.50
22	AB	615	CLA	C4-C3	2.08	1.55	1.50
30	AC	520	LMG	O1-C1	2.07	1.43	1.40
32	AB	624	LMT	C3B-C2B	2.07	1.57	1.52
26	BC	514	BCR	C19-C18	-2.07	1.41	1.46
22	AB	604	CLA	C4-C3	2.07	1.55	1.50
22	AC	509	CLA	C4C-C3C	2.07	1.48	1.45
34	AV	201	HEM	C1C-C2C	2.07	1.49	1.45
22	BB	610	CLA	MG-NB	2.07	2.09	2.05
27	BC	517	DGD	C4E-C3E	2.07	1.57	1.52
26	AB	617	BCR	C38-C26	2.07	1.54	1.50
22	AC	505	CLA	C1D-ND	-2.07	1.35	1.37
22	AD	404	CLA	CHC-C1C	2.07	1.42	1.38
22	BB	615	CLA	MG-NB	2.07	2.09	2.05
26	BJ	102	BCR	C33-C5	2.07	1.54	1.50
22	AB	610	CLA	CAA-CBA	-2.07	1.46	1.52
27	AH	102	DGD	C3D-C2D	2.07	1.57	1.52
22	AA	402	CLA	CHC-C1C	2.06	1.42	1.38
22	BA	404	CLA	C3B-C4B	2.06	1.48	1.42
30	BM	102	LMG	C11-C10	2.06	1.56	1.50
22	BC	505	CLA	C1C-C2C	2.06	1.48	1.44
22	AC	510	CLA	CMD-C2D	2.06	1.55	1.50
29	AA	412	SQD	C8-C7	2.06	1.56	1.50
22	AB	614	CLA	C1C-C2C	2.06	1.48	1.44
22	AD	402	CLA	CHB-C4A	2.06	1.42	1.37
22	AC	503	CLA	C1C-C2C	2.06	1.48	1.44
34	AE	101	HEM	C1A-C2A	2.06	1.48	1.44
22	BD	402	CLA	C1C-C2C	2.06	1.48	1.44
22	BC	513	CLA	CHB-C1B	-2.06	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	BC	520	LMG	C29-C28	2.06	1.56	1.50
22	AC	512	CLA	CAA-C2A	2.06	1.57	1.54
22	BC	506	CLA	CMB-C2B	2.05	1.55	1.50
22	BB	604	CLA	CAA-C2A	2.05	1.57	1.54
22	BA	405	CLA	MG-NB	2.05	2.09	2.05
22	AA	402	CLA	MG-NB	2.05	2.09	2.05
22	BB	617	CLA	C1D-ND	-2.05	1.35	1.37
29	BA	401	SQD	O6-C44	-2.05	1.40	1.43
22	BB	607	CLA	CHB-C1B	-2.05	1.34	1.39
22	AC	502	CLA	CHC-C1C	2.05	1.42	1.38
22	BC	505	CLA	CHB-C4A	2.05	1.42	1.37
23	AA	405	PHO	C4D-CHA	2.05	1.42	1.39
22	BC	507	CLA	MG-NB	2.05	2.09	2.05
27	BB	602	DGD	C1E-C2E	2.05	1.58	1.52
22	AB	604	CLA	C1D-ND	-2.05	1.35	1.37
22	BC	511	CLA	CMD-C2D	2.05	1.55	1.50
22	BB	616	CLA	CBA-CGA	-2.05	1.44	1.50
22	AB	611	CLA	C4-C3	2.05	1.55	1.50
22	BB	616	CLA	CAA-CBA	-2.05	1.46	1.52
26	BK	102	BCR	C7-C6	2.05	1.52	1.45
26	AJ	102	BCR	C3-C4	2.04	1.58	1.52
32	AB	624	LMT	O5B-C5B	2.04	1.49	1.44
32	AD	411	LMT	C4B-C3B	2.04	1.57	1.52
22	BC	510	CLA	CHC-C1C	2.04	1.42	1.38
22	AB	615	CLA	CMB-C2B	2.04	1.55	1.50
22	AB	616	CLA	C5-C3	2.04	1.55	1.51
27	BA	411	DGD	O6D-C5D	2.04	1.49	1.44
22	AC	507	CLA	CHD-C1D	2.04	1.42	1.38
22	BD	404	CLA	MG-NB	2.04	2.09	2.05
30	AB	623	LMG	O8-C28	2.04	1.39	1.33
34	BE	101	HEM	C4A-C3A	2.04	1.47	1.43
22	AC	512	CLA	C1C-C2C	2.04	1.48	1.44
30	AE	102	LMG	C4-C5	2.04	1.57	1.53
22	AC	502	CLA	C1D-C2D	-2.04	1.41	1.45
22	AB	607	CLA	C2-C3	2.04	1.37	1.33
27	AB	626	DGD	O1G-C1A	2.03	1.39	1.33
27	AH	102	DGD	O6D-C5D	2.03	1.49	1.44
34	BE	101	HEM	CHC-C1C	2.03	1.42	1.38
29	AA	415	SQD	C22-C21	-2.03	1.35	1.50
22	BB	604	CLA	CAA-CBA	-2.03	1.46	1.52
22	BD	402	CLA	C4C-C3C	2.03	1.48	1.45
27	AA	410	DGD	O1G-C1A	2.03	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	AB	625	LMT	O1B-C1B	2.03	1.47	1.41
22	BC	513	CLA	CHC-C1C	2.03	1.42	1.38
22	AA	403	CLA	CHB-C4A	2.03	1.42	1.37
29	BD	409	SQD	O6-C44	-2.03	1.40	1.43
26	AC	514	BCR	C19-C18	-2.03	1.41	1.46
22	BB	604	CLA	C3C-C2C	2.03	1.41	1.36
26	AB	620	BCR	C23-C22	-2.02	1.41	1.46
24	BJ	101	PL9	C7-C3	2.02	1.53	1.51
22	BC	512	CLA	CHB-C1B	-2.02	1.34	1.39
22	AC	504	CLA	CMD-C2D	2.02	1.54	1.50
32	BB	603	LMT	O1'-C1'	2.02	1.43	1.40
22	AC	509	CLA	CHC-C1C	2.02	1.42	1.38
22	BD	404	CLA	CHD-C1D	2.02	1.42	1.38
30	AB	622	LMG	O7-C10	2.02	1.40	1.34
32	BM	101	LMT	O5B-C1B	2.02	1.47	1.41
32	BT	101	LMT	O5B-C5B	2.02	1.49	1.44
22	AC	509	CLA	CHB-C4A	2.02	1.42	1.37
22	AB	602	CLA	C3B-C4B	2.02	1.48	1.42
30	BD	408	LMG	O7-C10	2.02	1.40	1.34
22	AB	609	CLA	C3B-C4B	2.02	1.48	1.42
32	AB	627	LMT	C4B-C5B	2.02	1.57	1.53
27	BD	410	DGD	O3G-C3G	2.02	1.47	1.43
29	BL	101	SQD	C24-C23	2.01	1.56	1.50
30	AA	413	LMG	C4-C3	2.01	1.57	1.52
26	AJ	102	BCR	C37-C22	2.01	1.54	1.50
22	AB	612	CLA	CHB-C4A	2.01	1.42	1.37
24	AA	407	PL9	C6-C1	2.01	1.52	1.48
22	AA	403	CLA	C1D-ND	-2.01	1.35	1.37
30	AE	102	LMG	C4-C3	2.01	1.57	1.52
32	BB	626	LMT	O1B-C1B	2.01	1.47	1.41
22	BC	503	CLA	CHD-C1D	2.01	1.42	1.38
22	BB	616	CLA	C1B-NB	-2.01	1.35	1.37
22	AC	502	CLA	CMB-C2B	2.01	1.54	1.50
22	BC	507	CLA	CMB-C2B	2.01	1.54	1.50
22	BB	609	CLA	C4C-C3C	2.01	1.48	1.45
34	AV	201	HEM	CAD-C3D	-2.01	1.46	1.51
22	BC	503	CLA	CHB-C1B	-2.01	1.34	1.39
29	BA	413	SQD	C22-C21	-2.01	1.36	1.50
22	AB	608	CLA	C4-C3	2.01	1.55	1.50
22	BB	618	CLA	C3B-C4B	2.01	1.48	1.42
22	AC	512	CLA	CAA-CBA	-2.01	1.46	1.52
22	AD	404	CLA	MG-NB	2.01	2.09	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BD	404	CLA	C4-C3	2.00	1.55	1.50
22	AC	506	CLA	C4-C3	2.00	1.55	1.50
22	BA	403	CLA	C4-C3	2.00	1.55	1.50
22	AB	601	CLA	C1D-C2D	-2.00	1.41	1.45
24	AJ	101	PL9	C7-C3	2.00	1.53	1.51

All (1845) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	AB	604	CLA	C4A-NA-C1A	13.13	112.67	106.68
22	BB	607	CLA	C4A-NA-C1A	12.99	112.61	106.68
22	AC	508	CLA	C4A-NA-C1A	12.89	112.56	106.68
22	BC	511	CLA	C4A-NA-C1A	12.77	112.50	106.68
22	AC	503	CLA	C4A-NA-C1A	12.70	112.47	106.68
22	AC	511	CLA	C4A-NA-C1A	12.60	112.43	106.68
22	AB	615	CLA	C4A-NA-C1A	12.32	112.30	106.68
22	AB	601	CLA	C4A-NA-C1A	12.31	112.30	106.68
22	BB	604	CLA	C4A-NA-C1A	12.30	112.29	106.68
22	BB	618	CLA	C4A-NA-C1A	12.30	112.29	106.68
22	BC	505	CLA	C4A-NA-C1A	12.27	112.28	106.68
22	BC	508	CLA	C4A-NA-C1A	12.24	112.26	106.68
22	BC	503	CLA	C4A-NA-C1A	12.22	112.26	106.68
22	BC	512	CLA	C4A-NA-C1A	12.05	112.18	106.68
22	BC	502	CLA	C4A-NA-C1A	12.00	112.15	106.68
22	BC	513	CLA	C4A-NA-C1A	11.96	112.14	106.68
22	AD	402	CLA	C4A-NA-C1A	11.95	112.13	106.68
22	BB	610	CLA	C4A-NA-C1A	11.95	112.13	106.68
22	BD	402	CLA	C4A-NA-C1A	11.90	112.11	106.68
22	AC	513	CLA	C4A-NA-C1A	11.85	112.09	106.68
22	AC	506	CLA	C4A-NA-C1A	11.84	112.08	106.68
22	AB	614	CLA	C4A-NA-C1A	11.79	112.06	106.68
22	AC	512	CLA	C4A-NA-C1A	11.77	112.05	106.68
22	BB	619	CLA	C4A-NA-C1A	11.72	112.03	106.68
22	AC	507	CLA	C4A-NA-C1A	11.71	112.02	106.68
22	BC	501	CLA	C4A-NA-C1A	11.70	112.02	106.68
22	BB	609	CLA	C4A-NA-C1A	11.67	112.00	106.68
22	BD	404	CLA	C4A-NA-C1A	11.67	112.00	106.68
22	AC	505	CLA	C4A-NA-C1A	11.67	112.00	106.68
22	AD	404	CLA	C4A-NA-C1A	11.62	111.98	106.68
22	AB	607	CLA	C4A-NA-C1A	11.60	111.97	106.68
22	BC	506	CLA	C4A-NA-C1A	11.60	111.97	106.68
22	BC	507	CLA	C4A-NA-C1A	11.58	111.96	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	AC	501	CLA	C4A-NA-C1A	11.49	111.92	106.68
22	BB	617	CLA	C4A-NA-C1A	11.49	111.92	106.68
22	AB	610	CLA	C4A-NA-C1A	11.44	111.90	106.68
22	BA	405	CLA	C4A-NA-C1A	11.42	111.89	106.68
22	AC	502	CLA	C4A-NA-C1A	11.42	111.89	106.68
22	BB	615	CLA	C4A-NA-C1A	11.38	111.87	106.68
22	BC	509	CLA	C4A-NA-C1A	11.38	111.87	106.68
22	AB	613	CLA	C4A-NA-C1A	11.36	111.86	106.68
22	AB	606	CLA	C4A-NA-C1A	11.33	111.85	106.68
22	BB	613	CLA	C4A-NA-C1A	11.30	111.83	106.68
22	BB	612	CLA	C4A-NA-C1A	11.19	111.78	106.68
22	BC	504	CLA	C4A-NA-C1A	11.14	111.76	106.68
22	AB	616	CLA	C4A-NA-C1A	11.11	111.75	106.68
22	AA	402	CLA	C4A-NA-C1A	11.10	111.74	106.68
22	BB	608	CLA	C4A-NA-C1A	11.07	111.73	106.68
22	AB	612	CLA	C4A-NA-C1A	11.04	111.72	106.68
22	BA	403	CLA	C4A-NA-C1A	11.04	111.71	106.68
22	AA	404	CLA	C4A-NA-C1A	11.02	111.71	106.68
22	AC	509	CLA	C4A-NA-C1A	10.99	111.69	106.68
22	BB	616	CLA	C4A-NA-C1A	10.98	111.69	106.68
22	AB	605	CLA	C4A-NA-C1A	10.96	111.68	106.68
22	AB	611	CLA	C4A-NA-C1A	10.93	111.66	106.68
22	AC	504	CLA	C4A-NA-C1A	10.91	111.66	106.68
22	AB	603	CLA	C4A-NA-C1A	10.89	111.65	106.68
22	BC	510	CLA	C4A-NA-C1A	10.88	111.64	106.68
22	AB	608	CLA	C4A-NA-C1A	10.87	111.64	106.68
22	AB	609	CLA	C4A-NA-C1A	10.75	111.58	106.68
22	BB	606	CLA	C4A-NA-C1A	10.68	111.55	106.68
22	AA	406	CLA	C4A-NA-C1A	10.68	111.55	106.68
22	BA	404	CLA	C4A-NA-C1A	10.66	111.54	106.68
22	BB	611	CLA	C4A-NA-C1A	10.64	111.53	106.68
22	AC	510	CLA	C4A-NA-C1A	10.46	111.45	106.68
22	BA	407	CLA	C4A-NA-C1A	10.37	111.41	106.68
26	BJ	102	BCR	C32-C1-C31	-10.36	78.96	108.63
22	BB	614	CLA	C4A-NA-C1A	10.35	111.40	106.68
26	AJ	102	BCR	C32-C1-C6	-10.31	94.07	110.24
26	BJ	102	BCR	C32-C1-C6	-10.15	94.32	110.24
26	AJ	102	BCR	C32-C1-C31	-10.02	79.94	108.63
22	AB	602	CLA	C4A-NA-C1A	9.82	111.16	106.68
22	AA	403	CLA	C4A-NA-C1A	9.79	111.14	106.68
22	BB	605	CLA	C4A-NA-C1A	9.63	111.07	106.68
29	AF	101	SQD	O5-C1-O6	9.20	131.79	110.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	BF	101	SQD	O5-C1-O6	9.13	131.61	110.04
23	BA	406	PHO	C4D-CHA-CBD	-8.82	104.22	108.45
23	BD	403	PHO	C4D-CHA-CBD	-8.66	104.30	108.45
34	BE	101	HEM	CAD-C3D-C2D	8.60	143.98	127.87
29	AA	415	SQD	O5-C1-O6	8.55	130.25	110.04
29	AD	409	SQD	O5-C1-O6	8.52	130.18	110.04
34	AE	101	HEM	CAD-C3D-C2D	8.52	143.81	127.87
29	BD	409	SQD	O5-C1-O6	8.44	129.98	110.04
29	AA	412	SQD	O5-C1-O6	8.42	129.94	110.04
29	BA	413	SQD	O5-C1-O6	8.36	129.80	110.04
29	BA	401	SQD	O5-C1-O6	8.35	129.78	110.04
23	AD	403	PHO	C4D-CHA-CBD	-8.26	104.49	108.45
23	AA	405	PHO	C4D-CHA-CBD	-8.15	104.54	108.45
29	AD	409	SQD	O6-C1-C2	8.00	120.42	108.27
29	BB	601	SQD	O5-C1-O6	7.94	128.79	110.04
29	BL	101	SQD	O5-C1-O6	7.89	128.68	110.04
34	BE	101	HEM	CAD-C3D-C4D	-7.88	110.97	124.70
29	BD	409	SQD	O6-C1-C2	7.88	120.24	108.27
29	BB	601	SQD	O6-C1-C2	7.86	120.21	108.27
34	AE	101	HEM	CAD-C3D-C4D	-7.74	111.20	124.70
29	BL	101	SQD	O6-C1-C2	7.59	119.80	108.27
27	BC	517	DGD	O6E-C5E-C4E	7.57	123.34	109.70
27	AC	517	DGD	O6E-C5E-C4E	7.57	123.33	109.70
27	BA	411	DGD	O6E-C5E-C4E	7.52	123.25	109.70
27	AA	410	DGD	O6E-C5E-C4E	7.51	123.23	109.70
26	AJ	102	BCR	C2-C1-C6	7.49	121.32	110.44
27	AH	102	DGD	O6E-C5E-C4E	7.48	123.17	109.70
34	AV	201	HEM	CAD-C3D-C2D	7.46	141.84	127.87
29	AD	409	SQD	O7-S-C6	7.39	117.79	106.76
34	BV	201	HEM	CAD-C3D-C2D	7.38	141.69	127.87
26	AJ	102	BCR	C32-C1-C2	-7.36	80.67	108.95
29	BA	401	SQD	O6-C1-C2	7.32	119.39	108.27
27	BH	101	DGD	O6E-C5E-C4E	7.31	122.88	109.70
26	BJ	102	BCR	C32-C1-C2	-7.29	80.97	108.95
29	BD	409	SQD	O7-S-C6	7.28	117.63	106.76
26	BJ	102	BCR	C2-C1-C6	7.27	120.99	110.44
27	BC	516	DGD	O6E-C5E-C4E	7.20	122.67	109.70
27	BD	410	DGD	O6E-C5E-C4E	7.19	122.66	109.70
27	BC	518	DGD	O6E-C5E-C4E	7.19	122.65	109.70
26	BX	101	BCR	C38-C26-C25	7.18	132.32	124.48
27	AB	626	DGD	O6E-C5E-C4E	7.17	122.61	109.70
27	AD	410	DGD	O6E-C5E-C4E	7.15	122.59	109.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	AA	415	SQD	O6-C1-C2	7.14	119.12	108.27
29	BA	413	SQD	O6-C1-C2	7.12	119.08	108.27
29	AA	412	SQD	O6-C1-C2	7.11	119.08	108.27
27	BB	602	DGD	O6E-C5E-C4E	7.07	122.44	109.70
26	AJ	102	BCR	C38-C26-C25	7.03	132.16	124.48
27	AC	518	DGD	O6E-C5E-C4E	7.02	122.36	109.70
26	BJ	102	BCR	C38-C26-C25	7.01	132.13	124.48
26	BJ	102	BCR	C33-C5-C6	6.99	132.11	124.48
26	AH	101	BCR	C38-C26-C25	6.93	132.05	124.48
27	AC	516	DGD	O6E-C5E-C4E	6.89	122.12	109.70
26	BD	406	BCR	C38-C26-C25	6.88	132.00	124.48
26	AJ	102	BCR	C33-C5-C6	6.86	131.97	124.48
26	AK	102	BCR	C33-C5-C6	6.83	131.94	124.48
29	AA	412	SQD	O7-S-C6	6.81	116.93	106.76
26	AD	406	BCR	C38-C26-C25	6.78	131.88	124.48
29	AF	101	SQD	O6-C1-C2	6.77	118.56	108.27
34	AV	201	HEM	CAD-C3D-C4D	-6.69	113.05	124.70
29	BF	101	SQD	O6-C1-C2	6.68	118.42	108.27
34	BV	201	HEM	CAD-C3D-C4D	-6.64	113.13	124.70
26	BB	621	BCR	C38-C26-C25	6.61	131.69	124.48
26	AD	406	BCR	C33-C5-C6	6.52	131.60	124.48
26	BK	102	BCR	C33-C5-C6	6.48	131.55	124.48
29	BA	413	SQD	O7-S-C6	6.46	116.40	106.76
29	BL	101	SQD	O7-S-C6	6.44	116.37	106.76
29	BF	101	SQD	C10-C9-C8	6.31	136.31	113.13
26	AB	619	BCR	C38-C26-C25	6.30	131.36	124.48
29	AF	101	SQD	C10-C9-C8	6.30	136.26	113.13
29	AA	412	SQD	C10-C9-C8	6.28	136.20	113.13
29	BA	413	SQD	C10-C9-C8	6.24	136.06	113.13
29	BB	601	SQD	O7-S-C6	6.19	116.00	106.76
28	BA	412	LHG	C25-C24-C23	6.18	136.36	113.69
28	AA	411	LHG	C25-C24-C23	6.18	136.33	113.69
26	AZ	101	BCR	C38-C26-C25	6.14	131.18	124.48
29	AF	101	SQD	O7-S-C6	6.13	115.91	106.76
29	BB	601	SQD	C10-C9-C8	6.12	135.62	113.13
26	AT	102	BCR	C38-C26-C25	6.09	131.13	124.48
26	BD	406	BCR	C33-C5-C6	6.09	131.13	124.48
26	AB	617	BCR	C38-C26-C25	6.07	131.10	124.48
26	BC	515	BCR	C33-C5-C6	6.03	131.06	124.48
29	AD	409	SQD	C10-C9-C8	5.98	135.12	113.13
26	BZ	101	BCR	C38-C26-C25	5.98	131.01	124.48
29	BL	101	SQD	C10-C9-C8	5.98	135.09	113.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	BA	401	SQD	O7-S-C6	5.98	115.68	106.76
26	AT	102	BCR	C33-C5-C6	5.97	131.00	124.48
29	AA	415	SQD	C10-C9-C8	5.95	134.98	113.13
29	BD	409	SQD	C10-C9-C8	5.94	134.96	113.13
26	AB	620	BCR	C38-C26-C25	5.92	130.95	124.48
29	BF	101	SQD	O7-S-C6	5.92	115.60	106.76
26	AC	515	BCR	C33-C5-C6	5.89	130.91	124.48
26	AB	618	BCR	C33-C5-C6	5.85	130.87	124.48
26	AC	515	BCR	C38-C26-C25	5.84	130.86	124.48
29	BA	401	SQD	C10-C9-C8	5.84	134.57	113.13
29	BA	401	SQD	C25-C24-C23	5.82	135.03	113.69
26	AB	618	BCR	C38-C26-C25	5.81	130.82	124.48
29	AA	415	SQD	C25-C24-C23	5.78	134.88	113.69
29	AA	415	SQD	O7-S-C6	5.78	115.38	106.76
26	BB	620	BCR	C33-C5-C6	5.77	130.78	124.48
26	BC	515	BCR	C38-C26-C25	5.76	130.77	124.48
29	BF	101	SQD	C25-C24-C23	5.74	134.74	113.69
29	BA	413	SQD	C25-C24-C23	5.74	134.72	113.69
26	BB	620	BCR	C38-C26-C25	5.74	130.74	124.48
26	BC	514	BCR	C38-C26-C25	5.70	130.71	124.48
26	AJ	102	BCR	C23-C24-C25	5.68	142.16	127.00
29	AA	412	SQD	C25-C24-C23	5.67	134.46	113.69
26	AB	617	BCR	C33-C5-C6	5.66	130.66	124.48
26	AC	514	BCR	C38-C26-C25	5.61	130.61	124.48
29	BL	101	SQD	C25-C24-C23	5.58	134.16	113.69
26	BJ	102	BCR	C23-C24-C25	5.58	141.90	127.00
26	AB	619	BCR	C33-C5-C6	5.57	130.57	124.48
24	BD	405	PL9	C7-C3-C4	5.57	121.50	116.91
32	BB	625	LMT	C1-O1'-C1'	-5.57	104.17	113.68
26	AB	620	BCR	C33-C5-C6	5.57	130.56	124.48
26	AK	102	BCR	C7-C8-C9	5.56	134.46	126.23
29	BB	601	SQD	C25-C24-C23	5.55	134.05	113.69
26	BB	622	BCR	C33-C5-C6	5.55	130.54	124.48
29	AF	101	SQD	C25-C24-C23	5.55	134.03	113.69
26	BK	102	BCR	C7-C8-C9	5.53	134.41	126.23
26	BB	622	BCR	C38-C26-C25	5.53	130.51	124.48
26	BB	621	BCR	C33-C5-C6	5.48	130.47	124.48
29	AD	409	SQD	C25-C24-C23	5.48	133.76	113.69
24	AD	405	PL9	C7-C3-C4	5.47	121.41	116.91
26	AC	514	BCR	C33-C5-C6	5.46	130.44	124.48
26	AA	409	BCR	C33-C5-C6	5.45	130.43	124.48
32	AB	624	LMT	C1-O1'-C1'	-5.45	104.38	113.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	BD	409	SQD	C25-C24-C23	5.43	133.58	113.69
26	BA	410	BCR	C33-C5-C6	5.37	130.34	124.48
26	BA	410	BCR	C38-C26-C25	5.37	130.34	124.48
26	AA	409	BCR	C38-C26-C25	5.26	130.23	124.48
26	AK	102	BCR	C11-C10-C9	5.26	134.66	127.28
26	AZ	101	BCR	C33-C5-C6	5.26	130.22	124.48
26	AJ	102	BCR	C8-C7-C6	5.25	141.01	127.00
26	BK	102	BCR	C11-C10-C9	5.24	134.63	127.28
26	BC	514	BCR	C33-C5-C6	5.23	130.20	124.48
29	AD	409	SQD	O8-S-C6	-5.19	95.95	105.97
34	BE	101	HEM	CHA-C4D-ND	5.17	130.76	124.37
26	BJ	102	BCR	C8-C7-C6	5.14	140.74	127.00
26	BJ	102	BCR	C31-C1-C6	5.13	118.29	110.24
26	BK	102	BCR	C38-C26-C25	5.11	130.06	124.48
34	AE	101	HEM	CHA-C4D-ND	5.04	130.60	124.37
26	AJ	102	BCR	C31-C1-C6	5.03	118.14	110.24
26	BZ	101	BCR	C33-C5-C6	5.01	129.95	124.48
34	AV	201	HEM	CHA-C4D-ND	4.96	130.51	124.37
27	AD	410	DGD	O3G-C1D-C2D	4.88	115.68	108.27
27	BD	410	DGD	O3G-C1D-C2D	4.88	115.68	108.27
27	AB	626	DGD	O5D-C1E-C2E	4.87	115.68	108.27
29	BD	409	SQD	O8-S-C6	-4.85	96.62	105.97
34	BV	201	HEM	CHA-C4D-ND	4.80	130.31	124.37
26	AK	102	BCR	C38-C26-C25	4.80	129.72	124.48
26	BX	101	BCR	C33-C5-C6	4.78	129.70	124.48
26	AK	102	BCR	C2-C1-C6	4.78	117.38	110.44
26	AH	101	BCR	C33-C5-C6	4.77	129.69	124.48
29	BF	101	SQD	C44-O6-C1	4.76	124.00	113.80
29	AA	412	SQD	O8-S-C6	-4.75	96.80	105.97
24	AJ	101	PL9	C7-C3-C4	4.74	120.81	116.91
29	AF	101	SQD	C44-O6-C1	4.68	123.83	113.80
23	AA	405	PHO	O2D-CGD-CBD	4.65	116.06	110.95
27	AC	517	DGD	O5D-C6D-C5D	4.65	119.90	109.42
27	BC	517	DGD	O5D-C6D-C5D	4.57	119.71	109.42
27	AC	516	DGD	O5D-C1E-C2E	4.56	115.20	108.27
22	AA	403	CLA	CAA-C2A-C3A	-4.53	100.76	113.00
26	BK	102	BCR	C2-C1-C6	4.52	117.01	110.44
23	AD	403	PHO	O2D-CGD-CBD	4.44	115.82	110.95
24	BJ	101	PL9	C7-C3-C4	4.44	120.56	116.91
29	BA	413	SQD	O8-S-C6	-4.40	97.48	105.97
27	BB	602	DGD	O5D-C1E-C2E	4.40	114.95	108.27
27	BC	517	DGD	C3G-O3G-C1D	-4.37	104.44	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	404	CLA	CAA-C2A-C3A	-4.36	101.22	113.00
27	AC	517	DGD	C3G-O3G-C1D	-4.35	104.47	113.80
26	AJ	102	BCR	C1-C6-C5	-4.34	116.71	122.64
26	AT	102	BCR	C29-C30-C25	4.33	116.73	110.44
23	BD	403	PHO	O2D-CGD-CBD	4.30	115.67	110.95
26	BC	515	BCR	C29-C30-C25	4.29	116.67	110.44
29	BD	409	SQD	C44-O6-C1	4.26	122.92	113.80
26	AZ	101	BCR	C23-C24-C25	4.25	138.34	127.00
26	BD	406	BCR	C29-C30-C25	4.24	116.60	110.44
26	AC	515	BCR	C29-C30-C25	4.21	116.56	110.44
26	AB	618	BCR	C29-C30-C25	4.20	116.53	110.44
23	BA	406	PHO	O2D-CGD-CBD	4.19	115.55	110.95
26	AD	406	BCR	C29-C30-C25	4.18	116.50	110.44
24	BD	405	PL9	C7-C3-C2	-4.17	118.48	123.39
26	AJ	102	BCR	C38-C26-C27	-4.16	104.74	113.60
26	BB	622	BCR	C29-C30-C25	4.15	116.47	110.44
29	AF	101	SQD	O8-S-C6	-4.15	97.96	105.97
27	BC	517	DGD	O2G-C1B-C2B	4.15	120.46	111.48
26	AJ	102	BCR	C29-C30-C25	4.15	116.47	110.44
26	BJ	102	BCR	C38-C26-C27	-4.15	104.75	113.60
24	AA	407	PL9	C7-C8-C9	-4.13	119.71	126.83
26	BZ	101	BCR	C23-C24-C25	4.13	138.02	127.00
26	BD	406	BCR	C24-C23-C22	4.12	132.34	126.23
29	BF	101	SQD	O8-S-C6	-4.08	98.09	105.97
26	BJ	102	BCR	C1-C6-C5	-4.07	117.07	122.64
30	AM	101	LMG	O7-C10-C11	4.07	120.28	111.48
24	AD	405	PL9	C7-C3-C2	-4.07	118.59	123.39
26	AC	515	BCR	C2-C1-C6	4.06	116.34	110.44
29	BA	401	SQD	O8-S-C6	-4.06	98.14	105.97
34	BV	201	HEM	C2A-C1A-NA	-4.05	105.66	110.15
29	BA	401	SQD	O48-C23-C24	4.04	124.16	111.83
28	BC	521	LHG	O7-C7-C8	4.03	120.21	111.48
26	BX	101	BCR	C24-C23-C22	4.03	132.19	126.23
29	BB	601	SQD	O48-C23-C24	4.02	124.10	111.83
22	BC	503	CLA	C1-C2-C3	4.02	132.78	126.20
29	AA	415	SQD	O8-S-C6	-4.02	98.21	105.97
28	AC	521	LHG	O7-C7-C8	4.02	120.17	111.48
27	BC	516	DGD	O5D-C1E-C2E	4.02	114.37	108.27
30	BM	102	LMG	O7-C10-C11	4.01	120.15	111.48
27	AC	517	DGD	O2G-C1B-C2B	4.01	120.15	111.48
34	BE	101	HEM	CBD-CAD-C3D	-3.99	101.50	112.53
29	AA	415	SQD	O48-C23-C24	3.99	124.00	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BK	102	BCR	C8-C9-C10	-3.98	112.74	119.01
27	AC	518	DGD	O6D-C5D-C6D	3.97	114.57	106.69
26	BK	102	BCR	C29-C30-C25	3.96	116.19	110.44
22	AC	503	CLA	C1-C2-C3	3.95	132.67	126.20
27	AB	626	DGD	O2G-C1B-C2B	3.95	120.02	111.48
29	BA	401	SQD	C44-O6-C1	3.94	122.25	113.80
29	AD	409	SQD	C44-O6-C1	3.94	122.25	113.80
26	BJ	102	BCR	C29-C30-C25	3.94	116.16	110.44
26	AH	101	BCR	C29-C30-C25	3.94	116.16	110.44
29	BL	101	SQD	O48-C23-C24	3.94	123.84	111.83
26	BX	101	BCR	C29-C30-C25	3.94	116.16	110.44
29	BB	601	SQD	O8-S-C6	-3.93	98.38	105.97
26	AH	101	BCR	C24-C23-C22	3.93	132.04	126.23
29	AA	415	SQD	C44-O6-C1	3.91	122.17	113.80
26	AK	102	BCR	C33-C5-C4	-3.90	105.28	113.60
26	AB	619	BCR	C30-C25-C26	-3.90	117.31	122.64
26	AK	102	BCR	C29-C30-C25	3.89	116.09	110.44
26	BZ	101	BCR	C29-C30-C25	3.88	116.08	110.44
26	BJ	102	BCR	C16-C15-C14	3.88	131.46	123.52
26	AD	406	BCR	C38-C26-C27	-3.88	105.32	113.60
29	BL	101	SQD	O8-S-C6	-3.88	98.48	105.97
26	AK	102	BCR	C8-C9-C10	-3.86	112.93	119.01
34	AE	101	HEM	CBD-CAD-C3D	-3.86	101.85	112.53
26	AB	620	BCR	C29-C30-C25	3.85	116.04	110.44
26	BD	406	BCR	C38-C26-C27	-3.85	105.38	113.60
26	AZ	101	BCR	C29-C30-C25	3.85	116.03	110.44
27	AH	102	DGD	O5D-C1E-C2E	3.85	114.11	108.27
29	AA	412	SQD	C11-C10-C9	3.84	133.75	114.37
24	BA	408	PL9	C7-C8-C9	-3.81	120.26	126.83
26	BB	622	BCR	C2-C1-C6	3.81	115.97	110.44
26	BK	102	BCR	C33-C5-C4	-3.81	105.48	113.60
29	BA	413	SQD	C11-C10-C9	3.81	133.61	114.37
27	BB	602	DGD	O2G-C1B-C2B	3.80	119.71	111.48
26	BB	621	BCR	C29-C30-C25	3.80	115.96	110.44
27	BC	518	DGD	O6D-C5D-C6D	3.80	114.23	106.69
26	AJ	102	BCR	C16-C15-C14	3.79	131.28	123.52
26	BB	621	BCR	C30-C25-C26	-3.79	117.45	122.64
26	AD	406	BCR	C24-C23-C22	3.79	131.84	126.23
22	AA	403	CLA	CBA-CAA-C2A	3.78	125.05	113.79
23	AD	403	PHO	C7-C6-C5	-3.78	103.19	113.26
26	BB	621	BCR	C38-C26-C27	-3.78	105.54	113.60
26	AC	515	BCR	C23-C24-C25	3.77	137.08	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	AK	102	BCR	C1-C6-C5	-3.76	117.49	122.64
26	BC	515	BCR	C2-C1-C6	3.76	115.90	110.44
29	BA	413	SQD	C31-C30-C29	3.75	133.32	114.37
27	BH	101	DGD	O5D-C1E-C2E	3.74	113.96	108.27
26	BX	101	BCR	C38-C26-C27	-3.74	105.61	113.60
26	AD	406	BCR	C33-C5-C4	-3.74	105.62	113.60
26	BK	102	BCR	C1-C6-C5	-3.74	117.53	122.64
29	AA	412	SQD	C31-C30-C29	3.74	133.27	114.37
26	AH	101	BCR	C38-C26-C27	-3.74	105.63	113.60
26	AB	619	BCR	C38-C26-C27	-3.73	105.63	113.60
27	BB	602	DGD	C1E-O6E-C5E	3.72	120.99	113.72
26	AC	515	BCR	C8-C7-C6	3.72	136.95	127.00
22	BB	612	CLA	CED-O2D-CGD	3.72	124.36	115.92
29	AA	415	SQD	C31-C30-C29	3.72	133.18	114.37
27	AB	626	DGD	C1E-O6E-C5E	3.72	120.98	113.72
26	BB	620	BCR	C2-C1-C6	3.72	115.84	110.44
29	BD	409	SQD	C11-C10-C9	3.72	133.17	114.37
26	BD	406	BCR	C30-C25-C26	-3.71	117.56	122.64
26	BK	102	BCR	C23-C24-C25	3.71	136.92	127.00
26	AT	102	BCR	C38-C26-C27	-3.71	105.68	113.60
26	BC	515	BCR	C23-C24-C25	3.70	136.88	127.00
26	AK	102	BCR	C23-C24-C25	3.70	136.88	127.00
26	AB	618	BCR	C8-C7-C6	3.70	136.87	127.00
26	AD	406	BCR	C30-C25-C26	-3.69	117.60	122.64
26	AH	101	BCR	C30-C25-C26	-3.69	117.60	122.64
29	AD	409	SQD	O48-C23-C24	3.69	123.07	111.83
22	BB	619	CLA	CAA-C2A-C3A	-3.68	103.04	113.00
26	AD	406	BCR	C8-C7-C6	3.68	136.83	127.00
27	AC	516	DGD	C1E-O6E-C5E	3.68	120.91	113.72
26	BC	514	BCR	C2-C1-C6	3.67	115.78	110.44
26	BC	515	BCR	C30-C25-C26	-3.67	117.62	122.64
26	AT	102	BCR	C8-C7-C6	3.67	136.80	127.00
22	BA	404	CLA	O2A-CGA-CBA	3.67	123.02	111.83
26	AZ	101	BCR	C2-C1-C6	3.67	115.76	110.44
26	BC	515	BCR	C8-C7-C6	3.66	136.78	127.00
34	AV	201	HEM	C2A-C1A-NA	-3.66	106.09	110.15
26	BX	101	BCR	C30-C25-C26	-3.66	117.64	122.64
26	BD	406	BCR	C8-C7-C6	3.66	136.77	127.00
29	AD	409	SQD	C11-C10-C9	3.66	132.86	114.37
29	BA	401	SQD	C11-C10-C9	3.66	132.86	114.37
29	AF	101	SQD	C11-C10-C9	3.66	132.85	114.37
26	AA	409	BCR	C24-C23-C22	3.65	131.63	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	BB	601	SQD	C11-C10-C9	3.65	132.81	114.37
32	AT	101	LMT	C1-O1'-C1'	-3.64	107.45	113.68
30	AD	408	LMG	O6-C5-C6	3.64	115.47	106.44
22	AB	616	CLA	CAA-C2A-C3A	-3.63	103.18	113.00
22	BB	611	CLA	O2A-CGA-CBA	3.63	122.90	111.83
24	AJ	101	PL9	C7-C3-C2	-3.63	119.11	123.39
32	AI	102	LMT	C1-O1'-C1'	-3.63	107.49	113.68
29	AA	415	SQD	C11-C10-C9	3.63	132.69	114.37
22	BA	404	CLA	CBA-CAA-C2A	3.62	124.57	113.79
27	BH	101	DGD	O6D-C5D-C6D	3.62	113.87	106.69
29	BL	101	SQD	C11-C10-C9	3.62	132.66	114.37
26	AB	619	BCR	C24-C23-C22	3.62	131.58	126.23
26	BK	102	BCR	C16-C17-C18	3.61	132.34	127.28
22	BB	613	CLA	C1-C2-C3	3.61	132.11	126.20
26	AA	409	BCR	C29-C30-C25	3.61	115.68	110.44
29	BA	401	SQD	C31-C30-C29	3.60	132.58	114.37
24	AJ	101	PL9	C7-C8-C9	-3.60	120.63	126.83
26	BA	410	BCR	C29-C30-C25	3.60	115.67	110.44
26	AD	406	BCR	C2-C1-C6	3.59	115.66	110.44
29	BD	409	SQD	O48-C23-C24	3.59	122.80	111.83
26	AC	515	BCR	C30-C25-C26	-3.59	117.73	122.64
29	BF	101	SQD	C11-C10-C9	3.59	132.49	114.37
26	BB	622	BCR	C30-C25-C26	-3.58	117.74	122.64
26	AK	102	BCR	C30-C25-C26	-3.58	117.74	122.64
26	AB	618	BCR	C33-C5-C4	-3.58	105.97	113.60
26	AC	515	BCR	C38-C26-C27	-3.58	105.97	113.60
22	AA	403	CLA	O2A-CGA-CBA	3.57	122.73	111.83
23	BD	403	PHO	C7-C6-C5	-3.57	103.74	113.26
26	BJ	102	BCR	C33-C5-C4	-3.57	105.99	113.60
32	BI	102	LMT	C1-O1'-C1'	-3.56	107.59	113.68
22	AC	507	CLA	C7-C6-C5	-3.56	103.76	113.26
26	BD	406	BCR	C2-C1-C6	3.56	115.61	110.44
27	AC	518	DGD	C1E-O6E-C5E	3.56	120.68	113.72
26	AB	619	BCR	C29-C30-C25	3.56	115.61	110.44
26	AC	514	BCR	C33-C5-C4	-3.56	106.00	113.60
26	AB	617	BCR	C29-C30-C25	3.56	115.61	110.44
22	AB	609	CLA	CED-O2D-CGD	3.56	123.99	115.92
26	AD	406	BCR	C1-C6-C5	-3.55	117.78	122.64
22	BB	605	CLA	C7-C6-C5	-3.54	103.82	113.26
26	AB	620	BCR	C38-C26-C27	-3.54	106.05	113.60
27	BH	101	DGD	O2G-C1B-C2B	3.54	119.14	111.48
22	BB	604	CLA	C1-C2-C3	3.54	131.99	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BX	101	BCR	C2-C1-C6	3.54	115.58	110.44
34	BV	201	HEM	CBD-CAD-C3D	-3.54	102.76	112.53
22	AC	512	CLA	O2A-CGA-CBA	3.53	122.60	111.83
22	AB	611	CLA	C7-C6-C5	-3.53	103.86	113.26
26	AA	409	BCR	C7-C8-C9	3.53	131.46	126.23
26	AZ	101	BCR	C16-C17-C18	3.52	132.22	127.28
26	AB	618	BCR	C30-C25-C26	-3.52	117.82	122.64
26	AB	618	BCR	C38-C26-C27	-3.52	106.09	113.60
22	AB	608	CLA	O2A-CGA-CBA	3.52	122.56	111.83
26	AA	409	BCR	C30-C25-C26	-3.52	117.83	122.64
26	AH	101	BCR	C2-C1-C6	3.51	115.54	110.44
26	BC	515	BCR	C38-C26-C27	-3.50	106.12	113.60
26	BB	621	BCR	C24-C23-C22	3.50	131.42	126.23
26	BX	101	BCR	C8-C7-C6	3.50	136.36	127.00
34	BE	101	HEM	CHA-C4D-C3D	-3.50	118.77	125.23
26	AB	620	BCR	C30-C25-C26	-3.50	117.85	122.64
22	BC	512	CLA	O2A-CGA-CBA	3.50	122.51	111.83
22	BC	506	CLA	CED-O2D-CGD	3.50	123.85	115.92
24	AJ	101	PL9	C10-C9-C11	3.50	121.30	115.23
26	AT	102	BCR	C33-C5-C4	-3.50	106.14	113.60
22	BC	507	CLA	O2A-CGA-CBA	3.50	122.50	111.83
26	BD	406	BCR	C1-C6-C5	-3.49	117.86	122.64
26	AH	101	BCR	C8-C7-C6	3.49	136.33	127.00
30	BA	414	LMG	O6-C5-C6	3.49	115.10	106.44
26	AC	514	BCR	C2-C1-C6	3.49	115.51	110.44
30	AD	408	LMG	O7-C10-C11	3.49	119.03	111.48
26	AT	102	BCR	C30-C25-C26	-3.49	117.87	122.64
22	AB	603	CLA	CAA-C2A-C3A	-3.49	103.58	113.00
34	AE	101	HEM	CHA-C4D-C3D	-3.48	118.81	125.23
26	BD	406	BCR	C33-C5-C4	-3.48	106.18	113.60
22	BB	614	CLA	C7-C6-C5	-3.48	104.00	113.26
22	AB	614	CLA	C1-C2-C3	3.47	131.88	126.20
27	AH	102	DGD	O6D-C5D-C6D	3.47	113.58	106.69
26	BB	620	BCR	C38-C26-C27	-3.47	106.21	113.60
26	BA	410	BCR	C24-C23-C22	3.46	131.36	126.23
26	BZ	101	BCR	C2-C1-C6	3.46	115.47	110.44
30	BB	623	LMG	O6-C5-C6	3.46	115.01	106.44
26	AB	617	BCR	C8-C7-C6	3.46	136.23	127.00
22	AC	506	CLA	CED-O2D-CGD	3.46	123.75	115.92
22	AB	601	CLA	C1-C2-C3	3.45	131.86	126.20
30	BD	408	LMG	O6-C5-C6	3.45	114.99	106.44
22	AC	507	CLA	O2A-CGA-CBA	3.45	122.36	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	AJ	102	BCR	C30-C25-C26	-3.44	117.93	122.64
22	BB	617	CLA	C1-C2-C3	3.44	131.84	126.20
26	BB	620	BCR	C8-C7-C6	3.44	136.19	127.00
22	BB	606	CLA	CAA-C2A-C3A	-3.44	103.71	113.00
26	AB	619	BCR	C33-C5-C4	-3.44	106.27	113.60
30	BD	408	LMG	O7-C10-C11	3.44	118.91	111.48
22	BC	509	CLA	C1-C2-C3	3.44	131.83	126.20
27	AH	102	DGD	O2G-C1B-C2B	3.44	118.91	111.48
29	AF	101	SQD	O48-C23-C24	3.43	122.31	111.83
26	BC	515	BCR	C33-C5-C4	-3.43	106.29	113.60
27	AC	516	DGD	O6D-C5D-C6D	3.43	113.49	106.69
28	AA	411	LHG	O8-C23-C24	3.43	122.28	111.83
30	AC	520	LMG	O7-C10-C11	3.42	118.89	111.48
26	BB	620	BCR	C33-C5-C4	-3.42	106.30	113.60
26	AB	617	BCR	C23-C24-C25	3.42	136.14	127.00
26	BB	621	BCR	C33-C5-C4	-3.42	106.31	113.60
34	AE	101	HEM	CAB-C3B-C2B	-3.41	117.33	128.43
26	AJ	102	BCR	C21-C20-C19	3.41	133.08	123.20
26	AB	620	BCR	C33-C5-C4	-3.41	106.33	113.60
26	BK	102	BCR	C30-C25-C26	-3.41	117.98	122.64
30	BC	520	LMG	O7-C10-C11	3.41	118.85	111.48
22	BA	403	CLA	O2A-CGA-CBA	3.40	122.22	111.83
26	BB	620	BCR	C23-C24-C25	3.40	136.08	127.00
27	BD	410	DGD	C1E-O6E-C5E	3.40	120.36	113.72
30	AB	621	LMG	O6-C5-C6	3.40	114.86	106.44
26	BB	621	BCR	C23-C24-C25	3.39	136.07	127.00
26	AC	515	BCR	C33-C5-C4	-3.39	106.36	113.60
26	BC	514	BCR	C38-C26-C27	-3.39	106.36	113.60
22	BC	507	CLA	C7-C6-C5	-3.39	104.22	113.26
30	AA	413	LMG	O6-C5-C6	3.39	114.84	106.44
34	BE	101	HEM	CAB-C3B-C2B	-3.39	117.41	128.43
26	BB	620	BCR	C29-C30-C25	3.39	115.36	110.44
27	BC	516	DGD	O6D-C5D-C6D	3.39	113.41	106.69
27	BC	518	DGD	C1E-O6E-C5E	3.39	120.33	113.72
34	AV	201	HEM	CBD-CAD-C3D	-3.38	103.18	112.53
26	BC	514	BCR	C33-C5-C4	-3.38	106.39	113.60
22	AB	616	CLA	CED-O2D-CGD	3.38	123.58	115.92
26	AC	514	BCR	C29-C30-C25	3.37	115.34	110.44
22	AA	406	CLA	C7-C6-C5	-3.37	104.27	113.26
26	AZ	101	BCR	C38-C26-C27	-3.37	106.41	113.60
22	BC	511	CLA	CED-O2D-CGD	3.37	123.56	115.92
26	AC	514	BCR	C38-C26-C27	-3.37	106.41	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BD	402	CLA	O2A-CGA-CBA	3.36	122.09	111.83
29	BF	101	SQD	O48-C23-C24	3.36	122.09	111.83
26	BJ	102	BCR	C30-C25-C26	-3.36	118.04	122.64
27	BA	411	DGD	O5D-C6D-C5D	3.36	117.00	109.42
22	AB	602	CLA	C7-C6-C5	-3.36	104.30	113.26
26	AA	409	BCR	C38-C26-C27	-3.36	106.43	113.60
26	AB	618	BCR	C2-C1-C6	3.36	115.31	110.44
32	BT	101	LMT	C1-O1'-C1'	-3.36	107.95	113.68
29	BA	413	SQD	O48-C23-C24	3.35	122.05	111.83
26	BZ	101	BCR	C16-C17-C18	3.35	131.98	127.28
26	BJ	102	BCR	C21-C20-C19	3.35	132.89	123.20
26	BA	410	BCR	C7-C8-C9	3.34	131.18	126.23
24	AA	407	PL9	C27-C28-C29	-3.34	119.97	127.62
26	AT	102	BCR	C23-C24-C25	3.34	135.92	127.00
26	BB	621	BCR	C8-C7-C6	3.34	135.92	127.00
22	AC	505	CLA	CAA-C2A-C3A	-3.34	103.98	113.00
24	BJ	101	PL9	C10-C9-C11	3.34	121.02	115.23
27	BH	101	DGD	C1E-O6E-C5E	3.34	120.23	113.72
26	AB	617	BCR	C38-C26-C27	-3.33	106.49	113.60
26	BC	514	BCR	C24-C23-C22	3.33	131.16	126.23
26	BB	622	BCR	C24-C23-C22	3.33	131.16	126.23
22	AA	402	CLA	O2A-CGA-CBA	3.33	121.97	111.83
24	BA	408	PL9	C27-C28-C29	-3.32	120.01	127.62
22	AB	603	CLA	O2A-CGA-CBA	3.32	121.97	111.83
26	BA	410	BCR	C30-C25-C26	-3.32	118.10	122.64
26	AA	409	BCR	C33-C5-C4	-3.32	106.52	113.60
22	BB	606	CLA	O2A-CGA-CBA	3.32	121.95	111.83
29	AA	412	SQD	O48-C23-C24	3.32	121.95	111.83
24	AA	407	PL9	C17-C18-C19	-3.32	120.03	127.62
26	BB	621	BCR	C2-C1-C6	3.31	115.25	110.44
30	BI	101	LMG	O7-C10-C11	3.31	118.65	111.48
26	AJ	102	BCR	C33-C5-C4	-3.31	106.53	113.60
26	AC	514	BCR	C1-C6-C5	-3.31	118.11	122.64
27	BC	516	DGD	C1E-O6E-C5E	3.31	120.18	113.72
26	BK	102	BCR	C38-C26-C27	-3.31	106.54	113.60
26	AB	617	BCR	C2-C1-C6	3.31	115.24	110.44
27	AD	410	DGD	C1E-O6E-C5E	3.30	120.17	113.72
32	AM	102	LMT	C1B-O1B-C4'	-3.30	110.15	117.98
23	AD	403	PHO	CED-O2D-CGD	3.30	123.40	115.92
26	AH	101	BCR	C15-C14-C13	3.30	131.90	127.28
26	BB	622	BCR	C33-C5-C4	-3.30	106.57	113.60
24	BJ	101	PL9	C7-C3-C2	-3.29	119.51	123.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	AC	514	BCR	C24-C23-C22	3.29	131.11	126.23
27	AA	410	DGD	C1E-O6E-C5E	3.29	120.15	113.72
22	AD	402	CLA	O2A-CGA-CBA	3.29	121.87	111.83
22	BC	513	CLA	CED-O2D-CGD	3.29	123.37	115.92
26	BZ	101	BCR	C38-C26-C27	-3.28	106.59	113.60
22	AA	404	CLA	CAA-C2A-C3A	-3.28	104.12	113.00
26	AB	617	BCR	C33-C5-C4	-3.28	106.60	113.60
22	AB	610	CLA	C1-C2-C3	3.28	131.57	126.20
30	AB	623	LMG	O7-C10-C11	3.28	118.58	111.48
22	BC	509	CLA	CED-O2D-CGD	3.28	123.35	115.92
26	BC	514	BCR	C29-C30-C25	3.28	115.20	110.44
26	AK	102	BCR	C16-C17-C18	3.28	131.87	127.28
26	BB	622	BCR	C38-C26-C27	-3.27	106.61	113.60
26	AK	102	BCR	C24-C23-C22	3.27	131.08	126.23
22	AC	505	CLA	O2A-CGA-CBA	3.27	121.81	111.83
26	AB	618	BCR	C23-C24-C25	3.27	135.74	127.00
26	BC	514	BCR	C1-C6-C5	-3.27	118.17	122.64
26	AT	102	BCR	C2-C1-C6	3.27	115.19	110.44
22	BA	407	CLA	CED-O2D-CGD	3.26	123.32	115.92
22	BC	505	CLA	CAA-C2A-C3A	-3.26	104.18	113.00
26	AB	619	BCR	C8-C7-C6	3.26	135.71	127.00
26	AB	619	BCR	C23-C24-C25	3.26	135.71	127.00
22	AC	513	CLA	CED-O2D-CGD	3.26	123.31	115.92
26	AB	620	BCR	C2-C1-C6	3.26	115.17	110.44
22	BB	617	CLA	O2D-CGD-CBD	3.26	116.92	111.23
30	AI	101	LMG	O7-C10-C11	3.25	118.52	111.48
22	BC	502	CLA	CED-O2D-CGD	3.25	123.30	115.92
22	BB	619	CLA	C1-C2-C3	3.25	131.52	126.20
26	AB	620	BCR	C24-C23-C22	3.24	131.03	126.23
22	BB	618	CLA	C1-C2-C3	3.24	131.51	126.20
26	BA	410	BCR	C38-C26-C27	-3.24	106.68	113.60
30	BD	407	LMG	O7-C10-C11	3.24	118.49	111.48
26	BK	102	BCR	C24-C23-C22	3.24	131.03	126.23
22	BC	501	CLA	O2A-CGA-CBA	3.24	121.72	111.83
22	AC	512	CLA	C1-C2-C3	3.24	131.50	126.20
22	BC	507	CLA	C1-C2-C3	3.24	131.50	126.20
24	AA	407	PL9	C22-C23-C24	-3.24	120.22	127.62
26	AA	409	BCR	C2-C1-C6	3.23	115.14	110.44
22	AD	402	CLA	CBA-CAA-C2A	3.23	123.42	113.79
22	AB	602	CLA	CED-O2D-CGD	3.23	123.25	115.92
22	AC	509	CLA	C1-C2-C3	3.23	131.49	126.20
27	AH	102	DGD	C1E-O6E-C5E	3.23	120.02	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	AH	101	BCR	C12-C13-C14	-3.23	113.94	119.01
30	AB	621	LMG	O7-C10-C11	3.22	118.46	111.48
27	AA	410	DGD	O5D-C6D-C5D	3.22	116.69	109.42
27	BA	411	DGD	C1E-O6E-C5E	3.22	120.01	113.72
22	BA	407	CLA	C7-C6-C5	-3.22	104.68	113.26
26	AB	619	BCR	C2-C1-C6	3.22	115.11	110.44
29	AA	415	SQD	C3-C4-C5	-3.21	104.41	110.23
23	AA	405	PHO	C1-C2-C3	3.21	131.46	126.20
26	BB	621	BCR	C1-C6-C5	-3.21	118.25	122.64
22	BA	405	CLA	CAA-C2A-C3A	-3.21	104.33	113.00
23	BA	406	PHO	C7-C6-C5	-3.21	104.71	113.26
28	BA	412	LHG	O8-C23-C24	3.21	121.61	111.83
32	BM	101	LMT	C1B-O1B-C4'	-3.21	110.38	117.98
22	BC	512	CLA	C1-C2-C3	3.20	131.44	126.20
26	BX	101	BCR	C12-C13-C14	-3.20	113.97	119.01
22	BC	507	CLA	CED-O2D-CGD	3.20	123.18	115.92
22	BA	405	CLA	C7-C6-C5	-3.19	104.75	113.26
22	BB	608	CLA	CED-O2D-CGD	3.19	123.15	115.92
26	AB	617	BCR	C30-C25-C26	-3.19	118.28	122.64
22	AB	615	CLA	C7-C6-C5	-3.19	104.76	113.26
26	AK	102	BCR	C38-C26-C27	-3.18	106.81	113.60
22	AC	501	CLA	O2A-CGA-CBA	3.18	121.53	111.83
27	AC	518	DGD	O2G-C1B-C2B	3.18	118.36	111.48
22	AB	605	CLA	C1-C2-C3	3.18	131.41	126.20
22	AB	616	CLA	C7-C6-C5	-3.18	104.80	113.26
26	BA	410	BCR	C33-C5-C4	-3.17	106.83	113.60
26	BK	102	BCR	C34-C9-C8	3.17	122.94	118.09
34	BV	201	HEM	CBC-CAC-C3C	-3.17	111.69	127.53
27	AA	410	DGD	O2G-C1B-C2B	3.17	118.34	111.48
29	BL	101	SQD	O9-S-C6	-3.17	102.02	106.76
26	AC	515	BCR	C1-C6-C5	-3.17	118.31	122.64
22	AB	615	CLA	C1-C2-C3	3.17	131.38	126.20
27	BC	518	DGD	O2G-C1B-C2B	3.16	118.32	111.48
29	BA	401	SQD	C3-C4-C5	-3.16	104.50	110.23
22	AC	502	CLA	CED-O2D-CGD	3.16	123.08	115.92
22	BB	619	CLA	CED-O2D-CGD	3.16	123.08	115.92
26	AC	514	BCR	C32-C1-C6	3.15	115.19	110.24
26	BC	514	BCR	C35-C13-C12	3.15	122.91	118.09
26	BB	620	BCR	C30-C25-C26	-3.15	118.33	122.64
22	BB	615	CLA	CED-O2D-CGD	3.15	123.06	115.92
24	BJ	101	PL9	C7-C8-C9	-3.15	121.40	126.83
24	BA	408	PL9	C22-C23-C24	-3.15	120.42	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	AA	407	PL9	C35-C34-C36	3.15	120.69	115.23
30	BB	623	LMG	O7-C10-C11	3.15	118.29	111.48
24	AA	407	PL9	C12-C13-C14	-3.15	120.42	127.62
22	BB	618	CLA	C7-C6-C5	-3.14	104.89	113.26
29	BA	413	SQD	C32-C31-C30	3.14	130.25	114.37
26	BA	410	BCR	C23-C24-C25	3.14	135.38	127.00
24	BA	408	PL9	C17-C18-C19	-3.14	120.44	127.62
22	BB	619	CLA	C7-C6-C5	-3.14	104.91	113.26
26	AH	101	BCR	C11-C10-C9	3.13	131.67	127.28
22	BB	609	CLA	C1-C2-C3	3.13	131.32	126.20
22	AC	501	CLA	CAA-C2A-C3A	-3.13	104.55	113.00
26	AC	514	BCR	C35-C13-C12	3.12	122.86	118.09
24	BD	405	PL9	C20-C19-C21	3.12	120.65	115.23
22	BB	605	CLA	CAA-C2A-C3A	-3.12	104.56	113.00
22	BC	505	CLA	CED-O2D-CGD	3.12	122.99	115.92
29	AA	412	SQD	C32-C31-C30	3.12	130.13	114.37
30	AB	622	LMG	O7-C10-C11	3.12	118.22	111.48
22	AB	614	CLA	O2D-CGD-CBD	3.12	116.68	111.23
26	AH	101	BCR	C33-C5-C4	-3.11	106.96	113.60
22	BC	512	CLA	C7-C6-C5	-3.11	104.96	113.26
32	BB	626	LMT	C1B-O1B-C4'	-3.11	110.60	117.98
22	BC	506	CLA	C7-C6-C5	-3.11	104.96	113.26
30	AD	407	LMG	O7-C10-C11	3.11	118.22	111.48
30	AE	102	LMG	O7-C10-C11	3.11	118.21	111.48
26	AA	409	BCR	C23-C24-C25	3.11	135.30	127.00
30	BI	101	LMG	C7-O1-C1	-3.11	107.14	113.80
22	AB	611	CLA	CED-O2D-CGD	3.11	122.96	115.92
22	AB	609	CLA	C7-C6-C5	-3.10	104.99	113.26
22	AC	507	CLA	C1-C2-C3	3.10	131.28	126.20
22	BC	509	CLA	O2A-CGA-CBA	3.10	121.29	111.83
22	AC	509	CLA	CED-O2D-CGD	3.10	122.94	115.92
22	BB	610	CLA	O2A-CGA-CBA	3.10	121.28	111.83
22	BC	505	CLA	O2A-CGA-CBA	3.10	121.28	111.83
22	BC	510	CLA	C7-C6-C5	-3.09	105.03	113.26
22	AC	509	CLA	O2A-CGA-CBA	3.09	121.26	111.83
26	BX	101	BCR	C33-C5-C4	-3.09	107.01	113.60
22	AC	504	CLA	C1-C2-C3	3.09	131.26	126.20
27	BA	411	DGD	O2G-C1B-C2B	3.09	118.16	111.48
26	BA	410	BCR	C2-C1-C6	3.09	114.92	110.44
26	AD	406	BCR	C23-C24-C25	3.09	135.24	127.00
22	BC	501	CLA	C7-C6-C5	-3.08	105.04	113.26
24	BJ	101	PL9	C25-C24-C26	3.08	120.58	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	BD	409	SQD	O9-S-C6	-3.08	102.15	106.76
27	BC	516	DGD	O2G-C1B-C2B	3.08	118.15	111.48
22	AB	602	CLA	CAA-C2A-C3A	-3.08	104.67	113.00
22	AB	607	CLA	O2A-CGA-CBA	3.08	121.22	111.83
22	AD	404	CLA	CAA-C2A-C3A	-3.08	104.68	113.00
26	AK	102	BCR	C34-C9-C8	3.08	122.79	118.09
26	BX	101	BCR	C15-C14-C13	3.08	131.59	127.28
26	BZ	101	BCR	C33-C5-C4	-3.08	107.03	113.60
22	AC	505	CLA	CED-O2D-CGD	3.08	122.89	115.92
22	BC	511	CLA	C7-C6-C5	-3.08	105.07	113.26
26	AC	514	BCR	C30-C25-C26	-3.07	118.43	122.64
22	AB	613	CLA	C7-C6-C5	-3.07	105.08	113.26
26	AC	514	BCR	C23-C24-C25	3.07	135.20	127.00
24	BD	405	PL9	C17-C18-C19	-3.07	120.60	127.62
34	BV	201	HEM	C4A-NA-C1A	3.07	110.82	105.82
23	AD	403	PHO	OBD-CAD-CBD	-3.07	121.32	125.82
22	AA	404	CLA	C7-C6-C5	-3.07	105.09	113.26
29	BA	413	SQD	O9-S-C6	-3.06	102.18	106.76
23	AD	403	PHO	CAA-C2A-C3A	-3.06	104.72	113.00
24	BA	408	PL9	C12-C13-C14	-3.06	120.62	127.62
22	AB	601	CLA	CED-O2D-CGD	3.06	122.86	115.92
26	BC	514	BCR	C23-C24-C25	3.06	135.17	127.00
22	AB	606	CLA	C1-C2-C3	3.06	131.21	126.20
22	AC	512	CLA	C7-C6-C5	-3.06	105.12	113.26
22	AB	603	CLA	CED-O2D-CGD	3.06	122.85	115.92
22	AB	605	CLA	CED-O2D-CGD	3.05	122.84	115.92
23	BD	403	PHO	CED-O2D-CGD	3.05	122.84	115.92
34	AV	201	HEM	CBC-CAC-C3C	-3.05	112.27	127.53
29	AA	415	SQD	C32-C31-C30	3.05	129.80	114.37
22	BB	605	CLA	CED-O2D-CGD	3.05	122.83	115.92
23	AA	405	PHO	CED-O2D-CGD	3.05	122.83	115.92
26	AH	101	BCR	C16-C17-C18	3.05	131.55	127.28
22	AC	510	CLA	C7-C6-C5	-3.05	105.14	113.26
26	BB	622	BCR	C1-C6-C5	-3.05	118.47	122.64
23	BD	403	PHO	OBD-CAD-CBD	-3.05	121.35	125.82
22	AC	510	CLA	C1-C2-C3	3.05	131.19	126.20
23	BD	403	PHO	CAA-C2A-C3A	-3.04	104.78	113.00
26	BC	514	BCR	C30-C25-C26	-3.04	118.48	122.64
22	BB	612	CLA	C7-C6-C5	-3.04	105.16	113.26
22	BB	605	CLA	O2A-CGA-CBA	3.04	121.11	111.83
22	AC	510	CLA	O2A-CGA-CBA	3.04	121.10	111.83
22	AA	402	CLA	CED-O2D-CGD	3.04	122.81	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	AA	407	PL9	C30-C29-C31	3.04	120.50	115.23
22	BB	609	CLA	O2A-CGA-CBA	3.04	121.09	111.83
22	BC	504	CLA	C1-C2-C3	3.03	131.17	126.20
30	AB	622	LMG	C7-O1-C1	-3.03	107.29	113.80
26	BC	515	BCR	C1-C6-C5	-3.03	118.50	122.64
22	AB	615	CLA	CED-O2D-CGD	3.03	122.79	115.92
34	AE	101	HEM	C4A-NA-C1A	3.03	110.76	105.82
32	BB	603	LMT	C1B-O1B-C4'	-3.03	110.80	117.98
29	BA	401	SQD	C32-C31-C30	3.03	129.66	114.37
26	BB	620	BCR	C1-C6-C5	-3.03	118.50	122.64
32	AB	625	LMT	C1B-O1B-C4'	-3.02	110.81	117.98
22	BD	402	CLA	CBA-CAA-C2A	3.02	122.79	113.79
30	AA	416	LMG	O7-C10-C11	3.02	118.02	111.48
23	BA	406	PHO	C1-C2-C3	3.02	131.15	126.20
24	AD	405	PL9	C7-C8-C9	-3.02	121.62	126.83
34	AE	101	HEM	CBC-CAC-C3C	-3.02	112.42	127.53
22	BB	613	CLA	O2D-CGD-CBD	3.02	116.52	111.23
22	BA	403	CLA	CED-O2D-CGD	3.02	122.77	115.92
22	AA	404	CLA	CED-O2D-CGD	3.02	122.77	115.92
26	BX	101	BCR	C23-C24-C25	3.02	135.07	127.00
22	AC	511	CLA	CED-O2D-CGD	3.02	122.77	115.92
22	AB	614	CLA	CED-O2D-CGD	3.02	122.76	115.92
34	AV	201	HEM	C4A-NA-C1A	3.02	110.74	105.82
26	AT	102	BCR	C24-C23-C22	3.02	130.70	126.23
26	BZ	101	BCR	C8-C7-C6	3.02	135.05	127.00
26	AA	409	BCR	C1-C6-C5	-3.01	118.52	122.64
26	BD	406	BCR	C37-C22-C23	3.01	122.69	118.09
22	AB	602	CLA	O2A-CGA-CBA	3.01	121.01	111.83
22	AB	601	CLA	O2A-CGA-CBA	3.01	121.01	111.83
26	AZ	101	BCR	C33-C5-C4	-3.01	107.18	113.60
22	BC	502	CLA	C7-C6-C5	-3.01	105.25	113.26
30	BB	624	LMG	O7-C10-C11	3.01	117.98	111.48
26	AB	618	BCR	C24-C23-C22	3.01	130.68	126.23
22	BC	513	CLA	C7-C6-C5	-3.00	105.26	113.26
22	AB	606	CLA	O2A-CGA-CBA	3.00	120.98	111.83
30	BB	623	LMG	C7-O1-C1	-3.00	107.36	113.80
22	BB	617	CLA	CED-O2D-CGD	3.00	122.72	115.92
30	AE	102	LMG	O6-C5-C6	3.00	113.87	106.44
22	AC	506	CLA	C7-C6-C5	-3.00	105.28	113.26
22	AC	502	CLA	C1-C2-C3	3.00	131.10	126.20
32	AB	627	LMT	C1B-O1B-C4'	-2.99	110.88	117.98
22	AB	616	CLA	C1-C2-C3	2.99	131.10	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	AJ	101	PL9	C25-C24-C26	2.99	120.42	115.23
27	AD	410	DGD	O2G-C1B-C2B	2.99	117.95	111.48
24	BA	408	PL9	C30-C29-C31	2.99	120.41	115.23
27	BD	410	DGD	O2G-C1B-C2B	2.99	117.94	111.48
24	AD	405	PL9	C17-C18-C19	-2.99	120.79	127.62
26	BZ	101	BCR	C35-C13-C12	2.98	122.65	118.09
22	AD	404	CLA	CED-O2D-CGD	2.98	122.68	115.92
26	AB	619	BCR	C1-C6-C5	-2.98	118.56	122.64
22	BB	604	CLA	O2A-CGA-CBA	2.98	120.93	111.83
26	AH	101	BCR	C23-C24-C25	2.98	134.96	127.00
26	BA	410	BCR	C37-C22-C23	2.98	122.64	118.09
32	BD	411	LMT	C1-O1'-C1'	-2.98	108.59	113.68
30	BB	624	LMG	C7-O1-C1	-2.98	107.41	113.80
22	AA	406	CLA	CAA-C2A-C3A	-2.98	104.96	113.00
30	BA	414	LMG	O7-C10-C11	2.97	117.91	111.48
26	AZ	101	BCR	C8-C7-C6	2.97	134.94	127.00
26	BJ	102	BCR	C16-C17-C18	2.97	131.45	127.28
30	BM	102	LMG	O6-C5-C6	2.97	113.81	106.44
23	AA	405	PHO	OBD-CAD-CBD	-2.97	121.46	125.82
22	AB	601	CLA	C7-C6-C5	-2.97	105.34	113.26
22	AC	511	CLA	C7-C6-C5	-2.97	105.35	113.26
32	AD	411	LMT	C1-O1'-C1'	-2.97	108.61	113.68
22	AB	612	CLA	C1-C2-C3	2.96	131.05	126.20
30	BE	102	LMG	O6-C5-C6	2.96	113.78	106.44
22	AA	406	CLA	CED-O2D-CGD	2.96	122.63	115.92
22	BA	407	CLA	CAA-C2A-C3A	-2.96	105.00	113.00
30	BE	102	LMG	O7-C10-C11	2.96	117.88	111.48
22	BB	616	CLA	C7-C6-C5	-2.96	105.37	113.26
29	BA	401	SQD	O9-S-C6	-2.96	102.34	106.76
22	BC	510	CLA	C1-C2-C3	2.96	131.04	126.20
26	AD	406	BCR	C37-C22-C23	2.96	122.61	118.09
22	AC	505	CLA	C7-C6-C5	-2.96	105.38	113.26
24	BD	405	PL9	C7-C8-C9	-2.95	121.74	126.83
23	AA	405	PHO	C7-C6-C5	-2.95	105.40	113.26
34	BE	101	HEM	CBC-CAC-C3C	-2.95	112.79	127.53
26	BD	406	BCR	C23-C24-C25	2.95	134.88	127.00
26	BX	101	BCR	C16-C17-C18	2.94	131.41	127.28
22	BC	501	CLA	CAA-C2A-C3A	-2.94	105.05	113.00
22	BB	604	CLA	CED-O2D-CGD	2.94	122.59	115.92
22	BB	606	CLA	CED-O2D-CGD	2.94	122.58	115.92
22	BB	614	CLA	CED-O2D-CGD	2.94	122.58	115.92
29	AF	101	SQD	C3-C4-C5	-2.94	104.91	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	AB	620	BCR	C23-C24-C25	2.94	134.84	127.00
22	AB	608	CLA	CAA-C2A-C3A	-2.93	105.07	113.00
22	AA	402	CLA	C3B-C4B-NB	-2.93	107.91	110.53
22	AB	608	CLA	CED-O2D-CGD	2.93	122.56	115.92
22	AB	615	CLA	O2A-CGA-CBA	2.93	120.77	111.83
22	AC	507	CLA	CED-O2D-CGD	2.93	122.56	115.92
34	BE	101	HEM	C4A-NA-C1A	2.93	110.60	105.82
30	AM	101	LMG	O6-C5-C6	2.93	113.70	106.44
22	AB	605	CLA	C7-C6-C5	-2.93	105.46	113.26
22	AC	502	CLA	C7-C6-C5	-2.93	105.46	113.26
22	BC	508	CLA	CED-O2D-CGD	2.93	122.56	115.92
22	BC	501	CLA	CED-O2D-CGD	2.93	122.56	115.92
26	BK	102	BCR	C12-C13-C14	-2.93	114.41	119.01
22	AC	506	CLA	C1-C2-C3	2.92	130.99	126.20
22	AC	513	CLA	C1-C2-C3	2.92	130.99	126.20
34	BE	101	HEM	C2A-C1A-NA	-2.92	106.91	110.15
22	BB	604	CLA	C7-C6-C5	-2.92	105.48	113.26
26	BX	101	BCR	C35-C13-C12	2.91	122.54	118.09
22	AC	508	CLA	C7-C6-C5	-2.91	105.50	113.26
22	AA	403	CLA	O2D-CGD-CBD	2.91	116.32	111.23
22	AB	605	CLA	O2A-CGA-CBA	2.91	120.71	111.83
22	BB	611	CLA	CED-O2D-CGD	2.91	122.52	115.92
22	BD	402	CLA	C7-C6-C5	-2.91	105.51	113.26
22	BB	610	CLA	C1-C2-C3	2.91	130.96	126.20
26	AB	618	BCR	C1-C6-C5	-2.91	118.66	122.64
30	AC	520	LMG	O6-C5-C6	2.91	113.64	106.44
24	BA	408	PL9	C35-C34-C36	2.90	120.27	115.23
29	AD	409	SQD	C31-C30-C29	2.90	132.96	113.36
22	BB	619	CLA	O2A-CGA-CBA	2.90	120.68	111.83
27	AC	516	DGD	O2G-C1B-C2B	2.90	117.75	111.48
26	AT	102	BCR	C1-C6-C5	-2.90	118.67	122.64
26	BX	101	BCR	C1-C6-C5	-2.90	118.67	122.64
32	AD	411	LMT	C1B-O1B-C4'	-2.90	111.11	117.98
22	AC	511	CLA	C1-C2-C3	2.90	130.94	126.20
34	AV	201	HEM	CAB-C3B-C2B	-2.90	119.01	128.43
24	AJ	101	PL9	C22-C23-C24	-2.90	120.99	127.62
22	AC	511	CLA	O2A-CGA-CBA	2.90	120.66	111.83
24	AD	405	PL9	C20-C19-C21	2.89	120.25	115.23
26	AB	617	BCR	C1-C6-C5	-2.89	118.69	122.64
22	AC	501	CLA	C7-C6-C5	-2.89	105.56	113.26
22	AB	607	CLA	C1-C2-C3	2.89	130.93	126.20
22	BB	618	CLA	O2A-CGA-CBA	2.89	120.64	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BD	402	CLA	CED-O2D-CGD	2.89	122.47	115.92
22	BC	505	CLA	CBA-CAA-C2A	2.89	122.38	113.79
22	BC	510	CLA	O2A-CGA-CBA	2.89	120.64	111.83
22	AC	510	CLA	CED-O2D-CGD	2.89	122.46	115.92
26	BK	102	BCR	C35-C13-C12	2.88	122.50	118.09
22	AC	508	CLA	O2A-CGA-CBA	2.88	120.62	111.83
22	BB	608	CLA	CAA-C2A-C3A	-2.88	105.22	113.00
30	AC	519	LMG	O7-C10-C11	2.88	117.71	111.48
22	BB	618	CLA	CED-O2D-CGD	2.88	122.45	115.92
22	BC	508	CLA	O2A-CGA-CBA	2.88	120.61	111.83
22	AB	604	CLA	O2A-CGA-CBA	2.88	120.61	111.83
24	AD	405	PL9	C37-C38-C39	-2.88	121.04	127.62
29	AA	412	SQD	C44-O6-C1	2.87	119.95	113.80
22	BC	505	CLA	C7-C6-C5	-2.87	105.61	113.26
32	BM	101	LMT	C1-O1'-C1'	-2.87	108.78	113.68
34	AE	101	HEM	C2A-C1A-NA	-2.87	106.97	110.15
22	BC	502	CLA	C1-C2-C3	2.87	130.90	126.20
27	BC	517	DGD	C1E-O6E-C5E	2.87	119.32	113.72
22	BB	614	CLA	O2A-CGA-CBA	2.87	120.57	111.83
22	BB	615	CLA	O2A-CGA-CBA	2.87	120.57	111.83
22	BA	404	CLA	C1-C2-C3	2.86	130.89	126.20
22	AD	404	CLA	O2D-CGD-CBD	2.86	116.23	111.23
26	BD	406	BCR	C12-C13-C14	-2.86	114.51	119.01
22	BB	613	CLA	O2A-CGA-CBA	2.86	120.56	111.83
22	AC	513	CLA	C7-C6-C5	-2.86	105.64	113.26
29	BF	101	SQD	O9-S-C6	-2.86	102.48	106.76
26	BB	622	BCR	C23-C24-C25	2.86	134.64	127.00
34	AV	201	HEM	CHA-C4D-C3D	-2.86	119.96	125.23
26	BA	410	BCR	C1-C6-C5	-2.86	118.73	122.64
24	AD	405	PL9	C42-C43-C44	-2.85	121.09	127.62
22	AC	508	CLA	O2D-CGD-CBD	2.85	116.22	111.23
29	BD	409	SQD	C31-C30-C29	2.85	132.63	113.36
29	BD	409	SQD	C3-C4-C5	-2.85	105.06	110.23
29	BB	601	SQD	C31-C30-C29	2.85	132.62	113.36
26	AB	620	BCR	C1-C6-C5	-2.85	118.74	122.64
29	AD	409	SQD	O47-C7-C8	2.85	117.65	111.48
22	AD	404	CLA	O2A-CGA-CBA	2.85	120.52	111.83
26	BC	514	BCR	C32-C1-C6	2.85	114.71	110.24
22	AC	501	CLA	CED-O2D-CGD	2.85	122.37	115.92
22	BB	607	CLA	O2A-CGA-CBA	2.85	120.51	111.83
22	BC	508	CLA	C7-C6-C5	-2.85	105.68	113.26
22	AC	503	CLA	CED-O2D-CGD	2.85	122.37	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BD	406	BCR	C23-C22-C21	-2.84	114.54	119.01
22	AB	616	CLA	O2A-CGA-CBA	2.84	120.50	111.83
30	AB	621	LMG	C7-O1-C1	-2.84	107.71	113.80
22	BD	404	CLA	O2A-CGA-CBA	2.84	120.49	111.83
34	AV	201	HEM	O2A-CGA-CBA	2.84	122.97	114.00
22	BD	404	CLA	CED-O2D-CGD	2.84	122.35	115.92
24	BJ	101	PL9	C22-C23-C24	-2.84	121.13	127.62
22	AB	605	CLA	CAA-C2A-C3A	-2.84	105.34	113.00
22	AB	606	CLA	C7-C6-C5	-2.84	105.71	113.26
24	AA	407	PL9	C25-C24-C26	2.83	120.14	115.23
22	BA	407	CLA	O2A-CGA-CBA	2.83	120.47	111.83
30	AI	101	LMG	C7-O1-C1	-2.83	107.72	113.80
22	BA	405	CLA	CED-O2D-CGD	2.83	122.34	115.92
29	BL	101	SQD	C31-C30-C29	2.83	132.47	113.36
30	AD	407	LMG	O6-C5-C6	2.83	113.45	106.44
29	BD	409	SQD	O47-C7-C8	2.83	117.59	111.48
22	AB	612	CLA	O2A-CGA-CBA	2.83	120.45	111.83
22	BC	508	CLA	CAA-C2A-C3A	-2.82	105.37	113.00
26	AK	102	BCR	C30-C25-C24	2.82	123.31	115.65
22	AA	406	CLA	O2A-CGA-CBA	2.82	120.44	111.83
22	AC	503	CLA	C7-C6-C5	-2.82	105.75	113.26
34	BV	201	HEM	CAB-C3B-C2B	-2.82	119.27	128.43
22	AB	614	CLA	O2A-CGA-CBA	2.82	120.42	111.83
22	BC	506	CLA	C1-C2-C3	2.82	130.81	126.20
30	BC	519	LMG	O6-C5-C6	2.82	113.42	106.44
24	AD	405	PL9	C25-C24-C26	2.81	120.11	115.23
22	BB	617	CLA	O2A-CGA-CBA	2.81	120.41	111.83
22	BC	503	CLA	C7-C6-C5	-2.81	105.77	113.26
22	BC	513	CLA	C1-C2-C3	2.81	130.80	126.20
23	BD	403	PHO	C1-C2-C3	2.81	130.79	126.20
22	AB	612	CLA	C6-C5-C3	2.80	120.29	113.47
26	AZ	101	BCR	C1-C6-C5	-2.80	118.81	122.64
29	BB	601	SQD	O9-S-C6	-2.80	102.58	106.76
22	BB	610	CLA	CAA-C2A-C3A	-2.80	105.44	113.00
26	BC	515	BCR	C40-C30-C29	-2.80	98.20	108.95
22	AB	612	CLA	CED-O2D-CGD	2.80	122.26	115.92
22	AB	607	CLA	CAA-C2A-C3A	-2.80	105.44	113.00
26	BC	514	BCR	C40-C30-C25	2.80	114.63	110.24
22	BD	404	CLA	CAA-C2A-C3A	-2.80	105.45	113.00
22	AB	612	CLA	O2D-CGD-CBD	2.79	116.11	111.23
22	AC	506	CLA	CAA-C2A-C3A	-2.79	105.45	113.00
22	AC	512	CLA	CED-O2D-CGD	2.79	122.25	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BB	608	CLA	C1-C2-C3	2.79	130.77	126.20
26	AK	102	BCR	C35-C13-C12	2.79	122.35	118.09
23	AD	403	PHO	C2D-C1D-ND	2.79	111.44	109.43
22	AC	513	CLA	O2A-CGA-CBA	2.79	120.33	111.83
24	BD	405	PL9	C37-C38-C39	-2.79	121.25	127.62
22	BB	608	CLA	C7-C6-C5	-2.79	105.84	113.26
24	BD	405	PL9	C42-C43-C44	-2.78	121.25	127.62
22	BC	512	CLA	O2D-CGD-CBD	2.78	116.10	111.23
22	AC	503	CLA	O2A-CGA-CBA	2.78	120.33	111.83
22	AC	505	CLA	CBA-CAA-C2A	2.78	122.08	113.79
26	BX	101	BCR	C11-C10-C9	2.78	131.18	127.28
22	AD	402	CLA	CED-O2D-CGD	2.78	122.23	115.92
22	AB	604	CLA	C7-C6-C5	-2.78	105.85	113.26
34	BV	201	HEM	O2A-CGA-CBA	2.78	122.78	114.00
26	AC	515	BCR	C40-C30-C29	-2.78	98.28	108.95
26	AH	101	BCR	C1-C6-C5	-2.78	118.84	122.64
22	BB	609	CLA	C7-C6-C5	-2.78	105.86	113.26
34	BV	201	HEM	CHA-C4D-C3D	-2.78	120.11	125.23
24	BA	408	PL9	C25-C24-C26	2.78	120.05	115.23
22	BA	404	CLA	O2D-CGD-CBD	2.78	116.08	111.23
24	BD	405	PL9	C15-C14-C16	2.77	120.04	115.23
27	AC	517	DGD	C1E-O6E-C5E	2.77	119.14	113.72
24	BA	408	PL9	C15-C14-C16	2.77	120.04	115.23
26	AK	102	BCR	C12-C13-C14	-2.77	114.65	119.01
22	BB	619	CLA	C2A-C3A-C4A	2.77	106.34	101.87
22	BC	503	CLA	CED-O2D-CGD	2.77	122.19	115.92
22	BA	404	CLA	CMD-C2D-C1D	2.76	129.60	124.73
22	AA	403	CLA	C2A-C3A-C4A	2.76	106.33	101.87
26	AJ	102	BCR	C15-C16-C17	-2.76	117.87	123.52
26	BB	622	BCR	C7-C8-C9	2.76	130.32	126.23
23	BA	406	PHO	CED-O2D-CGD	2.76	122.18	115.92
22	BC	510	CLA	CED-O2D-CGD	2.76	122.17	115.92
30	BE	102	LMG	O1-C1-C2	2.75	112.45	108.27
22	BA	404	CLA	CED-O2D-CGD	2.75	122.16	115.92
24	AD	405	PL9	C15-C14-C16	2.75	120.01	115.23
34	AE	101	HEM	O2A-CGA-CBA	2.75	122.69	114.00
27	BC	517	DGD	C3G-C2G-C1G	-2.75	105.37	111.78
29	BF	101	SQD	C3-C4-C5	-2.75	105.25	110.23
26	BZ	101	BCR	C1-C6-C5	-2.74	118.89	122.64
22	BB	606	CLA	C3B-C4B-NB	-2.74	108.08	110.53
23	BA	406	PHO	C4A-C3A-C2A	2.74	105.45	102.84
22	BC	513	CLA	O2A-CGA-CBA	2.74	120.19	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BB	608	CLA	O2A-CGA-CBA	2.74	120.19	111.83
22	AC	508	CLA	CAA-C2A-C3A	-2.74	105.60	113.00
22	AB	608	CLA	C7-C6-C5	-2.74	105.97	113.26
22	AC	508	CLA	CED-O2D-CGD	2.74	122.12	115.92
22	AC	510	CLA	C2A-C3A-C4A	2.74	106.29	101.87
26	AD	406	BCR	C23-C22-C21	-2.74	114.71	119.01
26	AA	409	BCR	C37-C22-C23	2.73	122.27	118.09
22	BB	615	CLA	C6-C5-C3	2.73	120.13	113.47
27	AC	517	DGD	C3G-C2G-C1G	-2.73	105.41	111.78
23	AD	403	PHO	C4A-C3A-C2A	2.73	105.44	102.84
28	AC	521	LHG	O8-C23-C24	2.73	120.17	111.83
26	BC	515	BCR	C16-C17-C18	2.73	131.11	127.28
22	BA	403	CLA	C7-C6-C5	-2.73	105.98	113.26
23	BD	403	PHO	O2A-CGA-CBA	2.73	120.16	111.83
28	BC	521	LHG	O8-C23-C24	2.73	120.16	111.83
24	AA	407	PL9	C10-C9-C11	2.73	119.97	115.23
29	AA	412	SQD	C3-C4-C5	-2.73	105.28	110.23
30	AA	416	LMG	C7-O1-C1	-2.73	107.94	113.80
26	AC	515	BCR	C16-C17-C18	2.73	131.10	127.28
26	AD	406	BCR	C12-C13-C14	-2.73	114.72	119.01
26	BZ	101	BCR	C30-C25-C26	-2.73	118.91	122.64
26	AH	101	BCR	C35-C13-C12	2.73	122.25	118.09
34	BE	101	HEM	O2A-CGA-CBA	2.72	122.61	114.00
32	AT	101	LMT	O1B-C1B-C2B	2.72	114.79	108.09
22	BC	511	CLA	O2A-CGA-CBA	2.72	120.13	111.83
22	AB	607	CLA	C3B-C4B-NB	-2.72	108.10	110.53
30	BC	520	LMG	O6-C5-C6	2.72	113.17	106.44
22	BC	503	CLA	O2A-CGA-CBA	2.72	120.11	111.83
26	AB	617	BCR	C35-C13-C12	2.71	122.23	118.09
23	AD	403	PHO	O2A-CGA-CBA	2.71	120.11	111.83
22	AD	402	CLA	C7-C6-C5	-2.71	106.04	113.26
24	AD	405	PL9	C45-C44-C46	2.71	119.93	115.23
22	AA	402	CLA	C7-C6-C5	-2.71	106.04	113.26
22	AB	613	CLA	O2A-CGA-CBA	2.71	120.09	111.83
29	AD	409	SQD	O9-S-C6	-2.71	102.72	106.76
26	AZ	101	BCR	C30-C25-C26	-2.70	118.94	122.64
22	BC	504	CLA	CAA-C2A-C3A	-2.70	105.71	113.00
22	BC	501	CLA	O2D-CGD-CBD	2.70	115.95	111.23
22	AB	611	CLA	O2A-CGA-CBA	2.70	120.06	111.83
22	AB	610	CLA	O2A-CGA-CBA	2.70	120.06	111.83
22	AB	610	CLA	O2D-CGD-CBD	2.69	115.94	111.23
29	BA	401	SQD	C45-O47-C7	2.69	124.24	117.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	AD	402	CLA	C1-C2-C3	2.69	130.61	126.20
23	BD	403	PHO	C2D-C1D-ND	2.69	111.38	109.43
26	AZ	101	BCR	C35-C13-C12	2.69	122.19	118.09
22	BC	513	CLA	C3B-C4B-NB	-2.69	108.13	110.53
26	BC	515	BCR	C30-C25-C24	2.69	122.94	115.65
22	AC	510	CLA	C3B-C4B-NB	-2.68	108.13	110.53
30	BC	519	LMG	O7-C10-C11	2.68	117.28	111.48
26	BK	102	BCR	C30-C25-C24	2.68	122.92	115.65
23	BA	406	PHO	C2D-C1D-ND	2.68	111.37	109.43
30	AC	519	LMG	O6-C5-C6	2.68	113.08	106.44
23	AA	405	PHO	C2D-C1D-ND	2.68	111.36	109.43
30	BD	407	LMG	O6-C5-C6	2.68	113.07	106.44
30	AA	413	LMG	O7-C10-C11	2.67	117.26	111.48
22	BB	616	CLA	O2A-CGA-CBA	2.67	119.98	111.83
30	BI	101	LMG	O6-C5-C6	2.67	113.06	106.44
22	BC	512	CLA	CAA-C2A-C3A	-2.67	105.79	113.00
34	AE	101	HEM	CAB-C3B-C4B	2.67	136.17	124.39
27	AA	410	DGD	O6D-C5D-C6D	2.66	111.98	106.69
24	BJ	101	PL9	C17-C18-C19	-2.66	121.53	127.62
22	BA	405	CLA	CAA-CBA-CGA	2.66	120.77	113.21
22	AC	509	CLA	C7-C6-C5	-2.66	106.17	113.26
22	AC	504	CLA	O2A-CGA-CBA	2.66	119.95	111.83
26	AK	102	BCR	C32-C1-C2	-2.66	98.74	108.95
22	AB	606	CLA	CED-O2D-CGD	2.66	121.95	115.92
22	AC	504	CLA	C7-C6-C5	-2.66	106.17	113.26
22	BB	611	CLA	CAA-C2A-C3A	-2.66	105.82	113.00
26	AB	620	BCR	C8-C7-C6	2.66	134.10	127.00
22	AC	502	CLA	O2A-CGA-CBA	2.66	119.94	111.83
24	AD	405	PL9	C12-C13-C14	-2.65	121.55	127.62
24	BD	405	PL9	C25-C24-C26	2.65	119.83	115.23
29	AF	101	SQD	O9-S-C6	-2.65	102.80	106.76
22	BC	504	CLA	C7-C6-C5	-2.65	106.20	113.26
24	AA	407	PL9	C15-C14-C16	2.65	119.83	115.23
24	AA	407	PL9	C20-C19-C21	2.65	119.83	115.23
24	AJ	101	PL9	C20-C19-C21	2.65	119.82	115.23
22	AC	501	CLA	O2D-CGD-CBD	2.64	115.85	111.23
22	BC	504	CLA	O2A-CGA-CBA	2.64	119.89	111.83
34	BE	101	HEM	CAB-C3B-C4B	2.64	136.05	124.39
22	AC	506	CLA	O2A-CGA-CBA	2.64	119.88	111.83
22	AA	403	CLA	CED-O2D-CGD	2.64	121.90	115.92
26	BA	410	BCR	C30-C25-C24	2.64	122.80	115.65
23	BA	406	PHO	OBD-CAD-CBD	-2.64	121.95	125.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	BA	413	SQD	C3-C4-C5	-2.64	105.45	110.23
22	BB	613	CLA	C7-C6-C5	-2.64	106.23	113.26
32	BD	411	LMT	C1B-O1B-C4'	-2.64	111.73	117.98
22	BC	506	CLA	CAA-C2A-C3A	-2.64	105.88	113.00
22	AC	508	CLA	C3B-C4B-NB	-2.64	108.18	110.53
26	AC	515	BCR	C30-C25-C24	2.63	122.78	115.65
27	BB	602	DGD	O6D-C5D-C6D	2.63	111.90	106.69
22	BC	511	CLA	C1-C2-C3	2.62	130.50	126.20
29	AA	412	SQD	O47-C7-C8	2.62	117.16	111.48
26	AJ	102	BCR	C20-C21-C22	-2.62	123.60	127.28
22	AB	614	CLA	C1-O2A-CGA	2.62	122.99	116.65
22	AB	609	CLA	CAA-C2A-C3A	-2.62	105.92	113.00
22	AB	610	CLA	CAA-C2A-C3A	-2.62	105.93	113.00
22	AC	504	CLA	CAA-C2A-C3A	-2.62	105.93	113.00
22	BB	607	CLA	C7-C6-C5	-2.62	106.29	113.26
22	BB	611	CLA	C7-C6-C5	-2.61	106.29	113.26
22	BC	508	CLA	C3B-C4B-NB	-2.61	108.20	110.53
32	AM	102	LMT	C1-O1'-C1'	-2.61	109.21	113.68
32	BB	603	LMT	C1-O1'-C1'	-2.61	109.22	113.68
22	AA	404	CLA	CAA-CBA-CGA	2.61	120.62	113.21
22	AA	403	CLA	CMD-C2D-C1D	2.61	129.33	124.73
27	BA	411	DGD	O6D-C5D-C6D	2.61	111.87	106.69
26	AB	620	BCR	C7-C8-C9	2.61	130.09	126.23
26	AC	515	BCR	C24-C23-C22	2.61	130.09	126.23
24	AD	405	PL9	C40-C39-C41	2.61	119.75	115.23
26	AC	515	BCR	C35-C13-C12	2.60	122.07	118.09
29	AA	412	SQD	O9-S-C6	-2.60	102.87	106.76
22	BB	615	CLA	O2D-CGD-CBD	2.60	115.78	111.23
24	BD	405	PL9	C45-C44-C46	2.60	119.74	115.23
22	AC	504	CLA	C3B-C4B-NB	-2.60	108.21	110.53
22	BB	618	CLA	O2D-CGD-CBD	2.60	115.77	111.23
22	BC	505	CLA	C3B-C4B-NB	-2.60	108.21	110.53
26	BB	621	BCR	C32-C1-C6	2.60	114.31	110.24
22	AB	610	CLA	C7-C6-C5	-2.60	106.34	113.26
22	BC	502	CLA	O2A-CGA-CBA	2.59	119.75	111.83
22	AC	507	CLA	C2A-C1A-CHA	2.59	128.37	123.87
24	BD	405	PL9	C30-C29-C31	2.59	119.73	115.23
26	AD	406	BCR	C35-C13-C12	2.59	122.05	118.09
26	AJ	102	BCR	C16-C17-C18	2.59	130.91	127.28
22	BC	508	CLA	O2D-CGD-CBD	2.59	115.76	111.23
22	BC	507	CLA	C2A-C1A-CHA	2.59	128.36	123.87
22	BB	612	CLA	C1-C2-C3	2.59	130.44	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	AD	403	PHO	O1D-CGD-CBD	-2.58	120.80	124.72
24	BD	405	PL9	C35-C34-C36	2.58	119.71	115.23
22	BB	612	CLA	CAA-C2A-C3A	-2.58	106.02	113.00
26	AD	406	BCR	C15-C14-C13	2.58	130.90	127.28
22	BC	509	CLA	C2A-C3A-C4A	2.58	106.04	101.87
22	BC	506	CLA	O2A-CGA-CBA	2.58	119.70	111.83
22	BB	617	CLA	C1-O2A-CGA	2.58	122.89	116.65
22	AB	616	CLA	C2A-C3A-C4A	2.58	106.03	101.87
22	AB	615	CLA	O2D-CGD-CBD	2.57	115.73	111.23
26	BJ	102	BCR	C15-C16-C17	-2.57	118.25	123.52
26	AA	409	BCR	C16-C17-C18	2.57	130.89	127.28
22	AB	604	CLA	C1-C2-C3	2.57	130.41	126.20
22	AC	510	CLA	O2D-CGD-CBD	2.57	115.73	111.23
30	AB	623	LMG	C7-O1-C1	-2.57	108.28	113.80
22	BB	609	CLA	CED-O2D-CGD	2.57	121.74	115.92
26	BB	622	BCR	C8-C7-C6	2.57	133.86	127.00
22	BC	512	CLA	CED-O2D-CGD	2.57	121.74	115.92
22	BA	404	CLA	C2A-C3A-C4A	2.56	106.01	101.87
24	BA	408	PL9	C10-C9-C11	2.56	119.68	115.23
30	AI	101	LMG	O6-C5-C6	2.56	112.79	106.44
24	BD	405	PL9	C27-C28-C29	-2.56	121.76	127.62
23	BA	406	PHO	CBC-CAC-C3C	-2.56	109.21	112.87
29	BA	413	SQD	C15-C14-C13	2.56	127.30	114.37
29	BF	101	SQD	C45-O47-C7	2.56	123.92	117.80
22	BA	403	CLA	C3B-C4B-NB	-2.56	108.25	110.53
23	AA	405	PHO	O1D-CGD-CBD	-2.56	120.85	124.72
22	AC	512	CLA	O2D-CGD-CBD	2.55	115.69	111.23
27	AD	410	DGD	O6D-C5D-C4D	2.55	114.30	109.70
26	BZ	101	BCR	C36-C18-C19	2.55	121.98	118.09
26	BD	406	BCR	C15-C14-C13	2.55	130.85	127.28
26	AC	514	BCR	C7-C8-C9	2.55	130.01	126.23
22	AC	505	CLA	C3B-C4B-NB	-2.55	108.26	110.53
26	AB	619	BCR	C32-C1-C6	2.55	114.24	110.24
22	AC	507	CLA	O2D-CGD-CBD	2.55	115.68	111.23
22	BB	616	CLA	CED-O2D-CGD	2.55	121.69	115.92
26	AB	618	BCR	C32-C1-C6	2.54	114.23	110.24
28	BA	412	LHG	O7-C7-C8	2.54	116.98	111.48
29	AF	101	SQD	C45-O47-C7	2.54	123.88	117.80
23	AD	403	PHO	OBD-CAD-C3D	2.54	131.86	127.89
26	BK	102	BCR	C32-C1-C2	-2.54	99.20	108.95
26	BB	620	BCR	C35-C13-C12	2.54	121.96	118.09
26	BC	514	BCR	C37-C22-C23	2.54	121.96	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BJ	102	BCR	C20-C21-C22	-2.54	123.72	127.28
29	AA	415	SQD	C36-C35-C34	2.53	127.18	114.37
22	BB	616	CLA	C2A-C3A-C4A	2.53	105.96	101.87
22	BC	511	CLA	C2A-C1A-CHA	2.53	128.26	123.87
28	BA	412	LHG	P-O6-C4	-2.53	106.83	121.35
28	AA	411	LHG	P-O6-C4	-2.53	106.84	121.35
26	AH	101	BCR	C1-C6-C7	2.53	122.52	115.65
22	AC	512	CLA	CAA-C2A-C3A	-2.53	106.17	113.00
30	AE	102	LMG	O7-C8-C7	2.53	117.42	108.34
32	BT	101	LMT	O1B-C1B-C2B	2.53	114.31	108.09
29	AA	412	SQD	C15-C14-C13	2.53	127.14	114.37
22	AC	512	CLA	C3B-C4B-NB	-2.53	108.27	110.53
22	BC	510	CLA	O2D-CGD-CBD	2.53	115.65	111.23
27	AC	516	DGD	O5D-C6D-C5D	2.53	115.11	109.42
22	BC	504	CLA	C3B-C4B-NB	-2.52	108.28	110.53
30	BC	520	LMG	O8-C28-C29	2.52	119.53	111.83
26	BC	514	BCR	C1-C6-C7	2.52	122.50	115.65
22	BC	510	CLA	C3B-C4B-NB	-2.52	108.28	110.53
22	BC	509	CLA	O2D-CGD-CBD	2.52	115.64	111.23
26	BK	102	BCR	C8-C7-C6	2.52	133.74	127.00
22	AB	611	CLA	O2D-CGD-CBD	2.52	115.64	111.23
28	AA	411	LHG	O7-C7-C8	2.52	116.93	111.48
30	AB	622	LMG	O6-C5-C6	2.52	112.69	106.44
29	BL	101	SQD	C44-O6-C1	2.52	119.20	113.80
26	AK	102	BCR	C8-C7-C6	2.52	133.72	127.00
26	AT	102	BCR	C23-C22-C21	-2.51	115.06	119.01
29	BB	601	SQD	O47-C7-C8	2.51	116.92	111.48
28	BC	521	LHG	C5-O7-C7	-2.51	111.79	117.80
22	AA	403	CLA	C3B-C4B-NB	-2.51	108.29	110.53
22	BB	614	CLA	O2D-CGD-CBD	2.51	115.62	111.23
28	AC	521	LHG	C5-O7-C7	-2.51	111.79	117.80
24	BD	405	PL9	C12-C13-C14	-2.51	121.88	127.62
26	AZ	101	BCR	C19-C18-C17	-2.51	115.07	119.01
22	AC	511	CLA	C2A-C1A-CHA	2.51	128.22	123.87
26	BC	515	BCR	C24-C23-C22	2.51	129.94	126.23
26	AB	618	BCR	C36-C18-C19	2.50	121.91	118.09
22	AB	613	CLA	CED-O2D-CGD	2.50	121.59	115.92
24	AD	405	PL9	C30-C29-C31	2.50	119.57	115.23
26	AB	618	BCR	C7-C8-C9	2.50	129.93	126.23
22	AB	610	CLA	CED-O2D-CGD	2.50	121.58	115.92
22	BC	502	CLA	CAA-C2A-C3A	-2.50	106.25	113.00
26	AB	618	BCR	C23-C22-C21	-2.49	115.08	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BC	515	BCR	C37-C22-C23	2.49	121.90	118.09
29	AD	409	SQD	C3-C4-C5	-2.49	105.71	110.23
26	AC	514	BCR	C12-C13-C14	-2.49	115.09	119.01
22	BA	403	CLA	C6-C5-C3	2.49	119.53	113.47
24	BA	408	PL9	C20-C19-C21	2.49	119.55	115.23
27	BD	410	DGD	O6D-C5D-C6D	2.49	111.63	106.69
26	BD	406	BCR	C35-C13-C12	2.49	121.89	118.09
22	AB	612	CLA	C7-C6-C5	-2.49	106.64	113.26
22	BB	615	CLA	C3B-C4B-NB	-2.48	108.31	110.53
26	AA	409	BCR	C30-C25-C24	2.48	122.39	115.65
29	AA	415	SQD	C34-C33-C32	2.48	126.93	114.37
26	BK	102	BCR	C37-C22-C23	2.48	121.88	118.09
24	AD	405	PL9	C27-C28-C29	-2.48	121.94	127.62
22	AC	509	CLA	C2A-C3A-C4A	2.48	105.88	101.87
26	AZ	101	BCR	C36-C18-C19	2.48	121.88	118.09
26	BZ	101	BCR	C12-C13-C14	-2.48	115.11	119.01
22	BC	503	CLA	O2D-CGD-CBD	2.48	115.56	111.23
29	BA	401	SQD	C36-C35-C34	2.48	126.90	114.37
30	BB	624	LMG	O6-C5-C6	2.48	112.58	106.44
22	AB	603	CLA	C7-C6-C5	-2.48	106.66	113.26
22	AB	603	CLA	O2D-CGD-CBD	2.47	115.56	111.23
26	AB	618	BCR	C30-C25-C24	2.47	122.36	115.65
24	BJ	101	PL9	C20-C19-C21	2.47	119.52	115.23
22	BC	505	CLA	C2A-C1A-CHA	2.47	128.16	123.87
26	AT	102	BCR	C40-C30-C29	-2.47	99.47	108.95
22	AB	611	CLA	C3B-C4B-NB	-2.47	108.33	110.53
22	AA	402	CLA	C6-C5-C3	2.47	119.48	113.47
24	BD	405	PL9	C40-C39-C41	2.47	119.51	115.23
26	AB	618	BCR	C8-C9-C10	-2.47	115.13	119.01
22	BD	402	CLA	C2A-C1A-CHA	2.46	128.14	123.87
26	AA	409	BCR	C35-C13-C12	2.46	121.85	118.09
26	AC	514	BCR	C23-C22-C21	-2.46	115.14	119.01
22	BC	510	CLA	C2A-C3A-C4A	2.46	105.85	101.87
22	BB	616	CLA	C1-C2-C3	2.46	130.23	126.20
22	BB	604	CLA	CAA-C2A-C3A	-2.46	106.35	113.00
26	BA	410	BCR	C8-C9-C10	-2.46	115.14	119.01
22	AC	513	CLA	C3B-C4B-NB	-2.46	108.33	110.53
26	AK	102	BCR	C37-C22-C23	2.46	121.84	118.09
22	AB	602	CLA	C1-C2-C3	2.46	130.23	126.20
26	AB	618	BCR	C11-C10-C9	2.46	130.72	127.28
22	BB	607	CLA	C2A-C3A-C4A	2.46	105.84	101.87
29	BA	413	SQD	O47-C7-C8	2.46	116.79	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	AT	102	BCR	C36-C18-C19	2.46	121.84	118.09
26	AC	514	BCR	C1-C6-C7	2.46	122.31	115.65
22	BB	614	CLA	CAA-C2A-C3A	-2.45	106.37	113.00
22	BB	613	CLA	C2A-C3A-C4A	2.45	105.83	101.87
22	AD	404	CLA	C2A-C3A-C4A	2.45	105.83	101.87
22	BC	509	CLA	C7-C6-C5	-2.45	106.73	113.26
22	BB	613	CLA	CED-O2D-CGD	2.45	121.47	115.92
23	BD	403	PHO	C4A-C3A-C2A	2.45	105.17	102.84
22	BB	615	CLA	C1-C2-C3	2.45	130.21	126.20
22	BC	511	CLA	C3B-C4B-NB	-2.45	108.35	110.53
22	AA	404	CLA	O2A-CGA-CBA	2.45	119.29	111.83
29	AF	101	SQD	C32-C31-C30	2.44	129.86	113.36
22	BC	512	CLA	C2A-C1A-CHA	2.44	128.10	123.87
22	AB	608	CLA	C6-C5-C3	2.44	119.42	113.47
26	BC	514	BCR	C12-C13-C14	-2.44	115.17	119.01
29	AA	415	SQD	C45-O47-C7	2.44	123.64	117.80
22	BC	512	CLA	C3B-C4B-NB	-2.44	108.35	110.53
23	AA	405	PHO	C4A-C3A-C2A	2.44	105.16	102.84
22	AA	404	CLA	C1-C2-C3	2.44	130.19	126.20
32	AB	627	LMT	C1-O1'-C1'	-2.44	109.52	113.68
26	BX	101	BCR	C1-C6-C7	2.44	122.26	115.65
22	BB	613	CLA	CAA-C2A-C3A	-2.44	106.41	113.00
26	BC	514	BCR	C30-C25-C24	2.43	122.25	115.65
27	AD	410	DGD	O6D-C5D-C6D	2.43	111.52	106.69
22	BB	612	CLA	O2A-CGA-CBA	2.43	119.25	111.83
22	BB	608	CLA	C3B-C4B-NB	-2.43	108.36	110.53
26	AC	514	BCR	C37-C22-C23	2.43	121.80	118.09
30	AC	520	LMG	O8-C28-C29	2.43	119.24	111.83
30	AA	416	LMG	O6-C5-C6	2.43	112.46	106.44
26	BB	620	BCR	C16-C17-C18	2.43	130.68	127.28
22	BA	405	CLA	O2A-CGA-CBA	2.43	119.23	111.83
27	AD	410	DGD	C2G-O2G-C1B	2.43	123.60	117.80
27	BB	602	DGD	C3G-O3G-C1D	-2.42	108.60	113.80
26	BA	410	BCR	C34-C9-C8	2.42	121.79	118.09
27	BB	602	DGD	O3G-C1D-C2D	2.42	111.95	108.27
22	AB	609	CLA	O2A-CGA-CBA	2.42	119.22	111.83
22	BA	405	CLA	C1-C2-C3	2.42	130.16	126.20
29	BF	101	SQD	C32-C31-C30	2.42	129.71	113.36
29	AA	412	SQD	O8-S-O7	2.42	117.45	111.40
27	AB	626	DGD	O3G-C1D-C2D	2.42	111.95	108.27
26	BJ	102	BCR	C31-C1-C2	2.42	118.23	108.95
30	BA	414	LMG	C7-O1-C1	-2.42	108.61	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BB	618	CLA	C3B-C4B-NB	-2.42	108.37	110.53
26	BX	101	BCR	C36-C18-C19	2.41	121.78	118.09
26	BJ	102	BCR	C8-C9-C10	-2.41	115.21	119.01
22	AB	614	CLA	CAA-C2A-C3A	-2.41	106.48	113.00
22	AB	609	CLA	C1-C2-C3	2.41	130.15	126.20
32	BB	603	LMT	O1B-C1B-C2B	2.41	114.02	108.09
22	AC	509	CLA	O2D-CGD-CBD	2.41	115.45	111.23
22	BD	404	CLA	O2D-CGD-CBD	2.41	115.44	111.23
29	BA	401	SQD	C15-C14-C13	2.41	126.55	114.37
29	BB	601	SQD	C3-C4-C5	-2.41	105.86	110.23
26	AJ	102	BCR	C31-C1-C2	2.41	118.20	108.95
22	AB	605	CLA	O2D-CGD-CBD	2.41	115.44	111.23
22	AB	615	CLA	C3B-C4B-NB	-2.41	108.38	110.53
22	BA	403	CLA	CBA-CAA-C2A	2.41	120.95	113.79
26	AT	102	BCR	C35-C13-C12	2.41	121.76	118.09
29	BB	601	SQD	C15-C14-C13	2.40	126.52	114.37
22	BC	509	CLA	C6-C5-C3	2.40	119.32	113.47
22	BA	405	CLA	CMD-C2D-C1D	2.40	128.96	124.73
22	BC	509	CLA	C3B-C4B-NB	-2.40	108.39	110.53
26	AB	617	BCR	C12-C13-C14	-2.40	115.23	119.01
26	BA	410	BCR	C16-C17-C18	2.40	130.64	127.28
22	AA	404	CLA	C2A-C3A-C4A	2.40	105.75	101.87
22	AD	402	CLA	C2A-C1A-CHA	2.40	128.03	123.87
26	AZ	101	BCR	C12-C13-C14	-2.40	115.24	119.01
26	AT	102	BCR	C7-C8-C9	2.40	129.78	126.23
26	BX	101	BCR	C37-C22-C23	2.40	121.75	118.09
22	BB	611	CLA	C6-C5-C3	2.40	119.31	113.47
22	BD	404	CLA	C2A-C3A-C4A	2.40	105.74	101.87
26	AB	620	BCR	C32-C1-C6	2.40	114.00	110.24
22	AC	509	CLA	C6-C5-C3	2.39	119.30	113.47
22	AB	607	CLA	C7-C6-C5	-2.39	106.88	113.26
22	AB	612	CLA	C3B-C4B-NB	-2.39	108.39	110.53
32	AT	101	LMT	O1B-C4'-C3'	2.39	113.31	107.23
22	AB	615	CLA	C2A-C3A-C4A	2.39	105.73	101.87
30	AM	101	LMG	O1-C1-C2	2.39	111.90	108.27
22	AA	402	CLA	CBA-CAA-C2A	2.39	120.90	113.79
22	BC	510	CLA	CAA-C2A-C3A	-2.39	106.55	113.00
23	BD	403	PHO	O1D-CGD-CBD	-2.39	121.10	124.72
26	AT	102	BCR	C11-C10-C9	2.39	130.62	127.28
30	AE	102	LMG	O1-C1-C2	2.38	111.89	108.27
22	BB	606	CLA	C7-C6-C5	-2.38	106.91	113.26
22	AC	502	CLA	O2D-CGD-CBD	2.38	115.40	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	BB	623	LMG	C9-C8-C7	-2.38	106.23	111.78
26	BC	514	BCR	C23-C22-C21	-2.38	115.26	119.01
29	AA	415	SQD	C15-C14-C13	2.38	126.39	114.37
24	BD	405	PL9	C10-C9-C11	2.38	119.36	115.23
22	BD	402	CLA	C1-C2-C3	2.38	130.09	126.20
26	BB	622	BCR	C32-C1-C6	2.38	113.97	110.24
22	AB	613	CLA	C2A-C3A-C4A	2.38	105.71	101.87
26	AB	618	BCR	C37-C22-C23	2.38	121.72	118.09
29	AA	415	SQD	O9-S-C6	-2.37	103.21	106.76
26	AZ	101	BCR	C1-C6-C7	2.37	122.09	115.65
22	BB	613	CLA	C3B-C4B-NB	-2.37	108.41	110.53
22	AC	505	CLA	C2A-C1A-CHA	2.37	127.99	123.87
29	BL	101	SQD	O47-C7-C8	2.37	116.62	111.48
26	AB	618	BCR	C40-C30-C29	-2.37	99.85	108.95
24	AD	405	PL9	C35-C34-C36	2.37	119.34	115.23
23	AA	405	PHO	C6-C5-C3	2.37	119.24	113.47
22	BB	614	CLA	C3B-C4B-NB	-2.37	108.42	110.53
22	AC	502	CLA	CAA-C2A-C3A	-2.37	106.60	113.00
22	BB	610	CLA	C7-C6-C5	-2.37	106.95	113.26
23	AA	405	PHO	O2A-CGA-CBA	2.37	119.05	111.83
27	AC	517	DGD	O6D-C5D-C6D	2.37	111.38	106.69
22	AC	505	CLA	C2A-C3A-C4A	2.36	105.69	101.87
22	BA	405	CLA	O2D-CGD-CBD	2.36	115.36	111.23
27	AB	626	DGD	O6D-C5D-C6D	2.36	111.38	106.69
26	AH	101	BCR	C32-C1-C6	2.36	113.95	110.24
29	BB	601	SQD	C44-O6-C1	2.36	118.86	113.80
22	BB	607	CLA	CED-O2D-CGD	2.36	121.27	115.92
26	AH	101	BCR	C37-C22-C23	2.36	121.69	118.09
22	BB	617	CLA	C7-C6-C5	-2.36	106.97	113.26
29	BA	401	SQD	C34-C33-C32	2.36	126.30	114.37
22	AB	608	CLA	C3B-C4B-NB	-2.36	108.43	110.53
22	BB	606	CLA	O2D-CGD-CBD	2.36	115.35	111.23
22	AB	614	CLA	C7-C6-C5	-2.36	106.98	113.26
26	BC	514	BCR	C7-C8-C9	2.35	129.72	126.23
24	AJ	101	PL9	C17-C18-C19	-2.35	122.24	127.62
29	BA	413	SQD	C44-O6-C1	2.35	118.84	113.80
26	BB	620	BCR	C12-C13-C14	-2.35	115.31	119.01
22	AB	601	CLA	O2D-CGD-CBD	2.35	115.34	111.23
22	BA	405	CLA	C2A-C3A-C4A	2.35	105.67	101.87
26	AB	618	BCR	C35-C13-C12	2.35	121.68	118.09
22	BC	502	CLA	O2D-CGD-CBD	2.35	115.34	111.23
22	AC	507	CLA	C3B-C4B-NB	-2.35	108.43	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	AB	605	CLA	C3B-C4B-NB	-2.35	108.43	110.53
27	BD	410	DGD	O6D-C5D-C4D	2.35	113.93	109.70
26	AB	617	BCR	C36-C18-C19	2.35	121.67	118.09
29	BA	413	SQD	O8-S-O7	2.35	117.27	111.40
26	BB	622	BCR	C30-C25-C24	2.35	122.01	115.65
22	BC	507	CLA	O2D-CGD-CBD	2.34	115.33	111.23
22	BB	611	CLA	C1-C2-C3	2.34	130.04	126.20
29	BF	101	SQD	C15-C14-C13	2.34	126.21	114.37
26	BC	515	BCR	C35-C13-C12	2.34	121.67	118.09
22	AB	601	CLA	CAA-C2A-C3A	-2.34	106.68	113.00
29	BL	101	SQD	C3-C4-C5	-2.34	106.00	110.23
30	AA	413	LMG	C7-O1-C1	-2.34	108.79	113.80
27	BD	410	DGD	C2G-O2G-C1B	2.33	123.38	117.80
22	AC	512	CLA	C2A-C1A-CHA	2.33	127.92	123.87
22	BB	605	CLA	C3B-C4B-NB	-2.33	108.45	110.53
26	AB	618	BCR	C20-C21-C22	2.33	130.55	127.28
22	BB	615	CLA	C7-C6-C5	-2.33	107.05	113.26
24	AD	405	PL9	C10-C9-C11	2.33	119.27	115.23
26	BA	410	BCR	C35-C13-C12	2.33	121.65	118.09
30	BE	102	LMG	O7-C8-C7	2.33	116.70	108.34
24	BJ	101	PL9	C12-C13-C14	-2.33	122.29	127.62
29	BA	401	SQD	O5-C5-C4	2.33	113.90	109.70
22	AC	503	CLA	O2D-CGD-CBD	2.33	115.30	111.23
22	AB	611	CLA	C6-C5-C3	2.33	119.14	113.47
22	BC	502	CLA	C3B-C4B-NB	-2.33	108.45	110.53
22	BC	507	CLA	C3B-C4B-NB	-2.33	108.45	110.53
22	AD	404	CLA	C1-C2-C3	2.33	130.01	126.20
26	AT	102	BCR	C30-C25-C24	2.33	121.96	115.65
22	BB	611	CLA	CBA-CAA-C2A	2.33	120.71	113.79
22	BD	404	CLA	C3B-C4B-NB	-2.32	108.45	110.53
27	BC	516	DGD	O5D-C6D-C5D	2.32	114.66	109.42
26	AC	514	BCR	C30-C25-C24	2.32	121.95	115.65
22	BB	613	CLA	C6-C5-C3	2.32	119.12	113.47
26	AA	409	BCR	C34-C9-C8	2.32	121.63	118.09
22	AA	404	CLA	CMD-C2D-C1D	2.32	128.81	124.73
26	BZ	101	BCR	C19-C18-C17	-2.32	115.36	119.01
26	BK	102	BCR	C40-C30-C25	2.32	113.88	110.24
22	BA	404	CLA	C6-C5-C3	2.32	119.11	113.47
22	AB	609	CLA	C3B-C4B-NB	-2.32	108.46	110.53
22	BA	404	CLA	C3B-C4B-NB	-2.31	108.46	110.53
24	BD	405	PL9	C22-C23-C24	-2.31	122.33	127.62
26	AC	515	BCR	C37-C22-C23	2.31	121.62	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	AD	405	PL9	C22-C23-C24	-2.31	122.33	127.62
26	AH	101	BCR	C23-C22-C21	-2.31	115.38	119.01
22	BB	604	CLA	O2D-CGD-CBD	2.31	115.27	111.23
29	AA	412	SQD	C17-C16-C15	2.31	126.04	114.37
29	AF	101	SQD	C15-C14-C13	2.31	126.04	114.37
27	BB	602	DGD	O5D-C6D-C5D	2.31	114.62	109.42
22	AB	603	CLA	C3B-C4B-NB	-2.31	108.47	110.53
22	AA	404	CLA	O2D-CGD-CBD	2.30	115.26	111.23
23	AA	405	PHO	C1-O2A-CGA	2.30	122.23	116.65
22	AB	613	CLA	CAA-C2A-C3A	-2.30	106.78	113.00
22	BB	613	CLA	C12-C11-C10	-2.30	102.98	113.28
26	BB	622	BCR	C1-C6-C7	2.30	121.89	115.65
26	BZ	101	BCR	C1-C6-C7	2.30	121.89	115.65
34	AV	201	HEM	CAB-C3B-C4B	2.30	134.54	124.39
22	BB	610	CLA	C3B-C4B-NB	-2.30	108.48	110.53
29	AA	412	SQD	O8-S-O9	-2.30	105.66	111.40
23	AA	405	PHO	CMA-C3A-C4A	-2.29	109.67	114.61
22	AB	604	CLA	CAA-C2A-C3A	-2.29	106.80	113.00
26	AH	101	BCR	C36-C18-C19	2.29	121.59	118.09
22	BA	405	CLA	C3B-C4B-NB	-2.29	108.48	110.53
22	BC	509	CLA	C12-C11-C10	-2.29	103.01	113.28
22	AB	611	CLA	C2A-C3A-C4A	2.29	105.57	101.87
22	BC	502	CLA	C2A-C3A-C4A	2.29	105.57	101.87
22	BB	617	CLA	C3B-C4B-NB	-2.29	108.49	110.53
22	BC	507	CLA	CAA-C2A-C3A	-2.29	106.81	113.00
26	AT	102	BCR	C32-C1-C6	2.29	113.83	110.24
22	BB	618	CLA	C2A-C3A-C4A	2.29	105.57	101.87
26	AB	619	BCR	C1-C6-C7	2.29	121.86	115.65
22	AC	509	CLA	C3B-C4B-NB	-2.29	108.49	110.53
26	BZ	101	BCR	C34-C9-C8	2.29	121.58	118.09
26	AB	618	BCR	C12-C13-C14	-2.28	115.42	119.01
22	AB	615	CLA	C2A-C1A-CHA	2.28	127.83	123.87
26	AA	409	BCR	C1-C6-C7	2.28	121.84	115.65
22	AB	612	CLA	C2A-C3A-C4A	2.28	105.56	101.87
22	AB	611	CLA	CAA-C2A-C3A	-2.28	106.84	113.00
22	AB	608	CLA	C2A-C3A-C4A	2.28	105.55	101.87
30	BC	520	LMG	C7-O1-C1	-2.28	108.92	113.80
22	AB	606	CLA	CBA-CAA-C2A	2.28	120.56	113.79
22	AB	610	CLA	C12-C11-C10	-2.28	103.08	113.28
22	BB	607	CLA	C3B-C4B-NB	-2.27	108.50	110.53
29	BA	413	SQD	C17-C16-C15	2.27	125.86	114.37
26	BX	101	BCR	C23-C22-C21	-2.27	115.44	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	BD	403	PHO	OBD-CAD-C3D	2.27	131.44	127.89
23	BA	406	PHO	O2A-CGA-CBA	2.27	118.76	111.83
29	BL	101	SQD	C15-C14-C13	2.27	125.84	114.37
22	BB	607	CLA	C1-C2-C3	2.27	129.91	126.20
22	BB	609	CLA	CBA-CAA-C2A	2.27	120.54	113.79
22	AB	604	CLA	C2A-C3A-C4A	2.27	105.53	101.87
26	AC	514	BCR	C40-C30-C25	2.27	113.80	110.24
22	BB	604	CLA	C2A-C1A-CHA	2.27	127.80	123.87
22	AB	604	CLA	C3B-C4B-NB	-2.27	108.51	110.53
22	AB	610	CLA	C2A-C3A-C4A	2.27	105.53	101.87
26	BJ	102	BCR	C34-C9-C8	2.27	121.55	118.09
30	AB	621	LMG	C9-C8-C7	-2.26	106.51	111.78
22	BC	503	CLA	C3B-C4B-NB	-2.26	108.51	110.53
27	BC	517	DGD	O6D-C5D-C6D	2.26	111.18	106.69
22	AB	604	CLA	CED-O2D-CGD	2.26	121.05	115.92
22	AC	506	CLA	C3B-C4B-NB	-2.26	108.51	110.53
22	AB	609	CLA	C2A-C3A-C4A	2.26	105.52	101.87
26	BC	515	BCR	C36-C18-C19	2.26	121.54	118.09
22	AB	601	CLA	C2A-C1A-CHA	2.26	127.79	123.87
22	AC	512	CLA	C12-C11-C10	-2.26	103.16	113.28
23	BA	406	PHO	C1-O2A-CGA	2.26	122.11	116.65
26	AB	620	BCR	C30-C25-C24	2.26	121.77	115.65
23	BD	403	PHO	CMB-C2B-C3B	2.26	129.19	124.68
26	AT	102	BCR	C8-C9-C10	-2.26	115.46	119.01
22	AC	512	CLA	C2A-C3A-C4A	2.25	105.51	101.87
22	AC	509	CLA	C12-C11-C10	-2.25	103.18	113.28
32	BT	101	LMT	O1B-C4'-C3'	2.25	112.96	107.23
26	AT	102	BCR	C37-C22-C23	2.25	121.53	118.09
26	AC	515	BCR	C12-C13-C14	-2.25	115.47	119.01
30	BE	102	LMG	C8-O7-C10	2.25	123.18	117.80
26	BB	621	BCR	C1-C6-C7	2.25	121.75	115.65
22	AC	510	CLA	CMA-C3A-C2A	-2.25	105.29	113.98
22	BB	615	CLA	C2A-C3A-C4A	2.25	105.50	101.87
26	BK	102	BCR	C36-C18-C19	2.25	121.52	118.09
26	BB	621	BCR	C35-C13-C12	2.25	121.52	118.09
22	BC	503	CLA	C1-O2A-CGA	2.25	122.09	116.65
29	BD	409	SQD	C15-C14-C13	2.24	125.71	114.37
27	AB	626	DGD	C3G-O3G-C1D	-2.24	108.98	113.80
22	AB	608	CLA	CBA-CAA-C2A	2.24	120.47	113.79
22	BB	611	CLA	C2A-C3A-C4A	2.24	105.49	101.87
22	BD	402	CLA	C12-C11-C10	-2.24	103.22	113.28
22	AB	606	CLA	C2A-C3A-C4A	2.24	105.49	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BB	617	CLA	CAA-C2A-C3A	-2.24	106.95	113.00
23	BA	406	PHO	C3D-C4D-ND	2.24	110.57	107.71
26	BK	102	BCR	C23-C22-C21	-2.23	115.49	119.01
22	AB	614	CLA	C6-C5-C3	2.23	118.91	113.47
22	AB	616	CLA	C6-C5-C3	2.23	118.91	113.47
22	AA	403	CLA	C6-C5-C3	2.23	118.91	113.47
26	AK	102	BCR	C40-C30-C25	2.23	113.74	110.24
22	AC	504	CLA	CED-O2D-CGD	2.23	120.97	115.92
22	BB	609	CLA	C2A-C1A-CHA	2.23	127.74	123.87
22	BA	407	CLA	O2D-CGD-CBD	2.23	115.13	111.23
26	AC	515	BCR	C36-C18-C19	2.23	121.49	118.09
22	BC	505	CLA	C2A-C3A-C4A	2.23	105.47	101.87
22	AB	606	CLA	C3B-C4B-NB	-2.23	108.54	110.53
24	AJ	101	PL9	C12-C13-C14	-2.23	122.52	127.62
22	BB	605	CLA	C1-C2-C3	2.23	129.85	126.20
22	AC	501	CLA	C12-C11-C10	-2.23	103.30	113.28
22	BC	501	CLA	C12-C11-C10	-2.22	103.31	113.28
22	BB	605	CLA	C12-C11-C10	-2.22	103.31	113.28
22	AC	502	CLA	C3B-C4B-NB	-2.22	108.55	110.53
26	AB	618	BCR	C34-C9-C8	2.22	121.48	118.09
22	BB	618	CLA	C2A-C1A-CHA	2.22	127.72	123.87
26	AB	620	BCR	C1-C6-C7	2.22	121.67	115.65
26	AT	102	BCR	C12-C13-C14	-2.22	115.52	119.01
22	AC	511	CLA	C12-C11-C10	-2.22	103.34	113.28
29	AD	409	SQD	O8-S-O7	2.22	116.95	111.40
22	BA	407	CLA	C3B-C4B-NB	-2.22	108.55	110.53
22	AB	604	CLA	C2A-C1A-CHA	2.22	127.71	123.87
22	AC	506	CLA	O2D-CGD-CBD	2.21	115.10	111.23
22	BB	612	CLA	C3B-C4B-NB	-2.21	108.55	110.53
22	BC	504	CLA	C2A-C3A-C4A	2.21	105.44	101.87
26	BA	410	BCR	C36-C18-C19	2.21	121.47	118.09
32	AB	627	LMT	O1B-C1B-C2B	2.21	113.53	108.09
34	BV	201	HEM	CAB-C3B-C4B	2.21	134.16	124.39
32	AT	101	LMT	C1B-O1B-C4'	-2.21	112.74	117.98
30	AE	102	LMG	C9-C8-C7	-2.21	106.63	111.78
32	BB	625	LMT	C6'-C5'-C4'	-2.21	107.17	113.38
27	AA	410	DGD	C3G-C2G-C1G	-2.21	106.64	111.78
22	AB	608	CLA	C6-C7-C8	2.20	123.29	115.97
22	AB	612	CLA	CAA-C2A-C3A	-2.20	107.05	113.00
22	BB	608	CLA	CMD-C2D-C1D	2.20	128.60	124.73
22	BB	617	CLA	C6-C5-C3	2.20	118.83	113.47
26	AT	102	BCR	C19-C18-C17	-2.20	115.55	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	AB	620	BCR	C16-C17-C18	2.20	130.36	127.28
22	AB	610	CLA	C6-C5-C3	2.20	118.83	113.47
24	BD	405	PL9	C32-C33-C34	-2.20	122.59	127.62
22	AB	605	CLA	C2A-C3A-C4A	2.20	105.42	101.87
22	AC	504	CLA	C2A-C3A-C4A	2.20	105.42	101.87
26	BX	101	BCR	C32-C1-C6	2.20	113.69	110.24
29	AD	409	SQD	C15-C14-C13	2.20	125.48	114.37
22	AB	610	CLA	C3B-C4B-NB	-2.20	108.57	110.53
22	AB	609	CLA	CMA-C3A-C2A	-2.20	105.48	113.98
24	BJ	101	PL9	C31-C29-C30	2.20	119.65	114.59
26	BC	514	BCR	C11-C10-C9	2.20	130.36	127.28
22	BB	616	CLA	C3B-C4B-NB	-2.20	108.57	110.53
22	AC	508	CLA	C1-C2-C3	2.20	129.79	126.20
26	BA	410	BCR	C23-C22-C21	-2.19	115.56	119.01
22	AC	502	CLA	C2A-C3A-C4A	2.19	105.41	101.87
24	AJ	101	PL9	C31-C29-C30	2.19	119.63	114.59
29	BD	409	SQD	O8-S-O7	2.19	116.88	111.40
26	BD	406	BCR	C32-C1-C6	2.19	113.68	110.24
22	AB	609	CLA	C6-C5-C3	2.19	118.80	113.47
22	BC	511	CLA	C12-C11-C10	-2.19	103.47	113.28
26	BX	101	BCR	C34-C9-C8	2.19	121.43	118.09
26	AB	618	BCR	C16-C17-C18	2.19	130.35	127.28
24	AJ	101	PL9	C15-C14-C16	2.19	119.02	115.23
22	BB	606	CLA	C1-C2-C3	2.19	129.78	126.20
22	BC	506	CLA	C2A-C3A-C4A	2.19	105.40	101.87
22	BD	404	CLA	CMD-C2D-C1D	2.19	128.58	124.73
22	BB	607	CLA	CAA-C2A-C3A	-2.19	107.09	113.00
22	AA	406	CLA	C2A-C3A-C4A	2.19	105.40	101.87
22	AD	402	CLA	C12-C11-C10	-2.18	103.49	113.28
22	AB	602	CLA	C3B-C4B-NB	-2.18	108.58	110.53
22	BB	619	CLA	CBA-CAA-C2A	2.18	120.29	113.79
30	AM	101	LMG	C7-O1-C1	-2.18	109.12	113.80
23	BA	406	PHO	O1D-CGD-CBD	-2.18	121.41	124.72
22	BA	407	CLA	CMD-C2D-C1D	2.18	128.57	124.73
22	AC	504	CLA	CMD-C2D-C1D	2.18	128.57	124.73
22	AC	503	CLA	C3B-C4B-NB	-2.18	108.58	110.53
22	AB	602	CLA	C2A-C3A-C4A	2.18	105.39	101.87
22	BD	404	CLA	C7-C6-C5	-2.18	107.46	113.26
22	BB	618	CLA	CMD-C2D-C1D	2.18	128.56	124.73
26	BB	622	BCR	C37-C22-C23	2.18	121.41	118.09
22	AB	609	CLA	C1-O2A-CGA	2.18	121.92	116.65
22	AB	601	CLA	C2A-C3A-C4A	2.18	105.38	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	AB	607	CLA	CMD-C2D-C1D	2.18	128.56	124.73
22	BC	507	CLA	CMD-C2D-C1D	2.18	128.56	124.73
22	BB	611	CLA	O2D-CGD-CBD	2.18	115.03	111.23
26	AK	102	BCR	C36-C18-C19	2.17	121.41	118.09
26	BK	102	BCR	C19-C18-C17	-2.17	115.59	119.01
26	BC	515	BCR	C12-C13-C14	-2.17	115.59	119.01
22	AC	501	CLA	C1-C2-C3	2.17	129.75	126.20
29	BA	401	SQD	O48-C23-O10	-2.17	118.20	123.63
32	AB	624	LMT	C6'-C5'-C4'	-2.17	107.28	113.38
22	BB	607	CLA	C2A-C1A-CHA	2.17	127.63	123.87
26	AT	102	BCR	C20-C21-C22	2.17	130.32	127.28
22	AC	508	CLA	C2A-C3A-C4A	2.17	105.37	101.87
22	BA	407	CLA	C2A-C3A-C4A	2.17	105.37	101.87
24	AA	407	PL9	C53-C6-C1	2.17	119.72	115.28
26	BA	410	BCR	C8-C7-C6	2.17	132.79	127.00
26	BB	621	BCR	C7-C8-C9	2.17	129.44	126.23
22	AC	511	CLA	C3B-C4B-NB	-2.17	108.60	110.53
26	AA	409	BCR	C8-C9-C10	-2.16	115.60	119.01
22	BC	508	CLA	C2A-C3A-C4A	2.16	105.36	101.87
22	AB	613	CLA	C3B-C4B-NB	-2.16	108.60	110.53
22	AC	506	CLA	C2A-C3A-C4A	2.16	105.36	101.87
22	BD	402	CLA	O2D-CGD-CBD	2.16	115.01	111.23
30	AB	623	LMG	O6-C5-C6	2.16	111.80	106.44
22	BC	512	CLA	C2A-C3A-C4A	2.16	105.36	101.87
22	BB	604	CLA	C1-O2A-CGA	2.16	121.88	116.65
26	AJ	102	BCR	C3-C4-C5	2.16	117.91	114.06
22	BB	610	CLA	C2A-C3A-C4A	2.16	105.36	101.87
24	AA	407	PL9	C32-C33-C34	-2.16	122.68	127.62
26	AB	620	BCR	C40-C30-C25	2.16	113.63	110.24
30	BI	101	LMG	O6-C1-C2	2.16	114.81	110.37
26	BD	406	BCR	C16-C17-C18	2.16	130.31	127.28
22	AB	613	CLA	C1-C2-C3	2.16	129.73	126.20
27	AA	410	DGD	C6D-C5D-C4D	2.16	116.60	112.07
32	BT	101	LMT	C1B-O1B-C4'	-2.16	112.86	117.98
24	BA	408	PL9	C32-C33-C34	-2.16	122.69	127.62
22	AD	404	CLA	CMD-C2D-C1D	2.16	128.53	124.73
22	BB	612	CLA	C2A-C3A-C4A	2.16	105.35	101.87
22	BB	619	CLA	C2A-C1A-CHA	2.16	127.61	123.87
22	BC	501	CLA	C2A-C3A-C4A	2.16	105.35	101.87
22	AB	606	CLA	C2A-C1A-CHA	2.16	127.61	123.87
22	BB	610	CLA	CMD-C2D-C1D	2.16	128.52	124.73
22	BB	611	CLA	C3B-C4B-NB	-2.15	108.61	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	AB	619	BCR	C37-C22-C23	2.15	121.38	118.09
22	BB	612	CLA	C1-O2A-CGA	2.15	121.86	116.65
22	BB	605	CLA	C2A-C3A-C4A	2.15	105.35	101.87
22	BB	615	CLA	CAA-C2A-C3A	-2.15	107.18	113.00
26	AC	515	BCR	C32-C1-C6	2.15	113.62	110.24
29	BA	413	SQD	O8-S-O9	-2.15	106.02	111.40
22	AB	613	CLA	CMD-C2D-C1D	2.15	128.52	124.73
22	BC	503	CLA	CMD-C2D-C1D	2.15	128.51	124.73
22	AC	507	CLA	C12-C11-C10	-2.15	103.65	113.28
22	AB	602	CLA	C12-C11-C10	-2.15	103.65	113.28
26	AC	514	BCR	C11-C10-C9	2.15	130.29	127.28
22	AC	501	CLA	C2A-C1A-CHA	2.15	127.59	123.87
22	BC	501	CLA	C1-C2-C3	2.15	129.72	126.20
32	BI	102	LMT	C1B-O1B-C4'	-2.15	112.89	117.98
23	AA	405	PHO	CBC-CAC-C3C	-2.14	109.80	112.87
26	BA	410	BCR	C1-C6-C7	2.14	121.47	115.65
22	BB	612	CLA	CMA-C3A-C2A	-2.14	105.69	113.98
23	AA	405	PHO	OBD-CAD-C3D	2.14	131.23	127.89
26	AC	514	BCR	C32-C1-C2	-2.14	100.73	108.95
22	AB	603	CLA	C2A-C3A-C4A	2.14	105.33	101.87
22	AC	507	CLA	CAA-C2A-C3A	-2.14	107.21	113.00
22	BB	614	CLA	C2A-C3A-C4A	2.14	105.33	101.87
22	BC	502	CLA	C1-O2A-CGA	2.14	121.83	116.65
26	AD	406	BCR	C36-C18-C19	2.14	121.36	118.09
24	AD	405	PL9	C32-C33-C34	-2.14	122.73	127.62
26	BD	406	BCR	C7-C8-C9	2.14	129.40	126.23
26	AK	102	BCR	C19-C18-C17	-2.14	115.65	119.01
26	BZ	101	BCR	C15-C16-C17	-2.14	119.15	123.52
26	BB	621	BCR	C37-C22-C23	2.14	121.35	118.09
22	BA	403	CLA	C2A-C3A-C4A	2.14	105.32	101.87
26	AA	409	BCR	C36-C18-C19	2.13	121.35	118.09
22	AD	404	CLA	C2A-C1A-CHA	2.13	127.57	123.87
29	AA	415	SQD	O8-S-O7	2.13	116.73	111.40
23	BA	406	PHO	CMA-C3A-C4A	-2.13	110.02	114.61
22	BB	614	CLA	C6-C5-C3	2.13	118.66	113.47
27	BA	411	DGD	C6D-C5D-C4D	2.13	116.53	112.07
22	AB	616	CLA	C2A-C1A-CHA	2.13	127.56	123.87
22	AC	511	CLA	C1-O2A-CGA	2.13	121.80	116.65
24	AA	407	PL9	C41-C39-C40	2.13	119.48	114.59
26	AC	514	BCR	C36-C18-C19	2.13	121.34	118.09
23	BD	403	PHO	C1-O2A-CGA	2.13	121.80	116.65
29	BF	101	SQD	C17-C16-C15	2.13	125.12	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	AJ	101	PL9	C53-C6-C1	2.13	119.64	115.28
22	AB	608	CLA	C1-C2-C3	2.12	129.68	126.20
23	AD	403	PHO	CMB-C2B-C3B	2.12	128.93	124.68
22	BB	612	CLA	C6-C5-C3	2.12	118.64	113.47
22	BB	619	CLA	C3B-C4B-NB	-2.12	108.64	110.53
22	BD	402	CLA	CMD-C2D-C1D	2.12	128.46	124.73
22	BB	613	CLA	C1-O2A-CGA	2.12	121.78	116.65
23	BD	403	PHO	CMA-C3A-C2A	-2.12	105.94	114.13
22	AA	403	CLA	C1-C2-C3	2.12	129.67	126.20
29	BL	101	SQD	C17-C16-C15	2.12	125.08	114.37
26	AJ	102	BCR	C28-C27-C26	2.12	117.83	114.06
22	AA	406	CLA	C3B-C4B-NB	-2.12	108.64	110.53
29	BF	101	SQD	O48-C46-C45	2.12	114.50	108.40
32	BB	625	LMT	C1'-O5'-C5'	-2.12	109.58	113.72
22	BC	508	CLA	C2A-C1A-CHA	2.12	127.54	123.87
30	BM	102	LMG	O1-C1-C2	2.12	111.49	108.27
24	BA	408	PL9	C37-C38-C39	-2.12	120.58	127.64
22	AB	614	CLA	C3B-C4B-NB	-2.12	108.64	110.53
27	AH	102	DGD	O3G-C1D-C2D	2.12	111.48	108.27
22	AB	603	CLA	C1-C2-C3	2.11	129.66	126.20
22	AC	503	CLA	CMD-C2D-C1D	2.11	128.45	124.73
22	AC	508	CLA	C2A-C1A-CHA	2.11	127.54	123.87
26	BA	410	BCR	C40-C30-C25	2.11	113.56	110.24
26	BD	406	BCR	C36-C18-C19	2.11	121.32	118.09
22	AD	404	CLA	C3B-C4B-NB	-2.11	108.64	110.53
22	AC	513	CLA	CBA-CAA-C2A	2.11	120.08	113.79
24	AA	407	PL9	C37-C38-C39	-2.11	120.60	127.64
22	BC	501	CLA	CBA-CAA-C2A	2.11	120.08	113.79
22	AC	501	CLA	C2A-C3A-C4A	2.11	105.28	101.87
22	AC	506	CLA	CMD-C2D-C1D	2.11	128.44	124.73
26	AT	102	BCR	C34-C9-C8	2.11	121.31	118.09
23	AA	405	PHO	C3D-C4D-ND	2.11	110.41	107.71
22	BB	609	CLA	C2A-C3A-C4A	2.11	105.27	101.87
22	AB	602	CLA	CMD-C2D-C1D	2.11	128.44	124.73
26	AB	619	BCR	C21-C20-C19	2.11	129.31	123.20
32	AB	624	LMT	C1'-O5'-C5'	-2.11	109.60	113.72
22	BC	505	CLA	C1-C2-C3	2.11	129.65	126.20
26	BA	410	BCR	C32-C1-C6	2.11	113.55	110.24
29	AF	101	SQD	C13-C12-C11	2.11	125.02	114.37
29	AA	415	SQD	O48-C23-O10	-2.11	118.36	123.63
26	AZ	101	BCR	C34-C9-C8	2.11	121.31	118.09
26	AD	406	BCR	C16-C17-C18	2.10	130.23	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BC	512	CLA	C12-C11-C10	-2.10	103.85	113.28
22	BB	618	CLA	C12-C11-C10	-2.10	103.85	113.28
22	AC	504	CLA	C12-C11-C10	-2.10	103.86	113.28
22	BC	507	CLA	C2A-C3A-C4A	2.10	105.26	101.87
22	BB	616	CLA	CAA-C2A-C3A	-2.10	107.32	113.00
22	AC	507	CLA	C2A-C3A-C4A	2.10	105.26	101.87
22	BA	403	CLA	CMD-C2D-C1D	2.10	128.43	124.73
27	AC	517	DGD	C6D-C5D-C4D	2.10	116.48	112.07
22	BC	510	CLA	CMA-C3A-C2A	-2.10	105.86	113.98
22	AC	513	CLA	C12-C11-C10	-2.10	103.87	113.28
26	BA	410	BCR	C12-C13-C14	-2.10	115.71	119.01
26	BC	515	BCR	C32-C1-C6	2.10	113.53	110.24
22	AC	513	CLA	O2D-CGD-CBD	2.10	114.89	111.23
22	BC	501	CLA	C2A-C1A-CHA	2.10	127.50	123.87
23	BA	406	PHO	CMA-C3A-C2A	-2.10	106.03	114.13
29	AF	101	SQD	O48-C46-C45	2.10	114.44	108.40
34	AE	101	HEM	CMD-C2D-C1D	2.10	128.31	125.03
29	AF	101	SQD	O47-C7-C8	2.09	116.01	111.48
26	AD	406	BCR	C34-C9-C8	2.09	121.29	118.09
22	BB	604	CLA	C2A-C3A-C4A	2.09	105.25	101.87
26	AB	617	BCR	C16-C17-C18	2.09	130.21	127.28
22	AD	404	CLA	C7-C6-C5	-2.09	107.69	113.26
32	AI	102	LMT	C1B-O1B-C4'	-2.09	113.03	117.98
26	BB	621	BCR	C21-C20-C19	2.09	129.25	123.20
26	BC	514	BCR	C32-C1-C2	-2.09	100.93	108.95
22	BB	608	CLA	O2D-CGD-CBD	2.09	114.88	111.23
27	BH	101	DGD	C3G-O3G-C1D	-2.09	109.33	113.80
22	BC	506	CLA	CMD-C2D-C1D	2.09	128.40	124.73
22	AA	403	CLA	CMA-C3A-C2A	-2.08	105.92	113.98
29	BB	601	SQD	C17-C16-C15	2.08	124.91	114.37
34	BE	101	HEM	CMD-C2D-C1D	2.08	128.29	125.03
22	BC	508	CLA	CMD-C2D-C1D	2.08	128.40	124.73
29	BA	401	SQD	C13-C12-C11	2.08	124.90	114.37
22	BA	404	CLA	CMA-C3A-C2A	-2.08	105.93	113.98
26	BB	620	BCR	C36-C18-C19	2.08	121.27	118.09
32	BB	626	LMT	O1B-C1B-C2B	2.08	113.21	108.09
24	BJ	101	PL9	C53-C6-C1	2.08	119.54	115.28
24	BJ	101	PL9	C15-C14-C16	2.08	118.84	115.23
22	BC	508	CLA	C1-C2-C3	2.08	129.61	126.20
22	AA	403	CLA	C2A-C1A-CHA	2.08	127.48	123.87
22	AB	616	CLA	C3B-C4B-NB	-2.08	108.67	110.53
26	AA	409	BCR	C32-C1-C6	2.08	113.50	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	AA	415	SQD	O5-C5-C4	2.08	113.44	109.70
26	BC	515	BCR	C23-C22-C21	-2.08	115.74	119.01
29	AF	101	SQD	O5-C5-C4	2.08	113.44	109.70
22	BC	504	CLA	C12-C11-C10	-2.08	103.97	113.28
26	BB	622	BCR	C16-C17-C18	2.07	130.19	127.28
22	BB	612	CLA	C2A-C1A-CHA	2.07	127.47	123.87
26	AB	618	BCR	C19-C18-C17	-2.07	115.75	119.01
23	AD	403	PHO	C3D-C4D-ND	2.07	110.36	107.71
26	BB	620	BCR	C19-C18-C17	-2.07	115.75	119.01
22	AB	616	CLA	CBA-CAA-C2A	2.07	119.95	113.79
22	AB	605	CLA	CMD-C2D-C1D	2.07	128.37	124.73
22	AC	504	CLA	C1-O2A-CGA	2.07	121.66	116.65
22	AB	603	CLA	C2A-C1A-CHA	2.07	127.46	123.87
22	AB	602	CLA	C2A-C1A-CHA	2.07	127.46	123.87
26	BZ	101	BCR	C32-C1-C6	2.07	113.49	110.24
24	BA	408	PL9	C41-C39-C40	2.07	119.35	114.59
22	AA	406	CLA	CMD-C2D-C1D	2.07	128.37	124.73
26	BK	102	BCR	C40-C30-C29	-2.07	101.01	108.95
22	BC	503	CLA	C2A-C3A-C4A	2.07	105.21	101.87
26	BZ	101	BCR	C7-C8-C9	2.07	129.29	126.23
26	AD	406	BCR	C40-C30-C25	2.07	113.48	110.24
22	AA	403	CLA	C7-C6-C5	-2.07	107.75	113.26
22	AB	607	CLA	C2A-C3A-C4A	2.07	105.21	101.87
22	BB	611	CLA	C6-C7-C8	2.07	122.83	115.97
30	AM	101	LMG	O8-C9-C8	-2.07	102.44	108.40
34	BV	201	HEM	CAA-C2A-C1A	2.07	128.97	124.94
22	AB	614	CLA	C16-C15-C13	2.07	122.83	115.97
27	BA	411	DGD	C3G-C2G-C1G	-2.07	106.97	111.78
26	AH	101	BCR	C34-C9-C8	2.06	121.24	118.09
22	AB	614	CLA	C2A-C3A-C4A	2.06	105.20	101.87
26	AD	406	BCR	C20-C21-C22	2.06	130.17	127.28
26	AZ	101	BCR	C7-C8-C9	2.06	129.29	126.23
29	BF	101	SQD	C13-C12-C11	2.06	124.79	114.37
22	BB	611	CLA	CMA-C3A-C2A	-2.06	106.01	113.98
22	BB	608	CLA	CMA-C3A-C2A	-2.06	106.01	113.98
22	BA	404	CLA	C2A-C1A-CHA	2.06	127.44	123.87
30	BA	414	LMG	C9-C8-C7	-2.06	106.98	111.78
26	AK	102	BCR	C11-C12-C13	2.06	132.00	126.36
22	BC	506	CLA	C3B-C4B-NB	-2.06	108.69	110.53
29	AF	101	SQD	C17-C16-C15	2.05	124.75	114.37
22	AA	402	CLA	C2A-C3A-C4A	2.05	105.19	101.87
22	BC	513	CLA	O2D-CGD-CBD	2.05	114.82	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	AB	605	CLA	CMA-C3A-C2A	-2.05	106.05	113.98
23	BA	406	PHO	C6-C5-C3	2.05	118.46	113.47
22	BC	513	CLA	C12-C11-C10	-2.05	104.09	113.28
22	BC	501	CLA	C3B-C4B-NB	-2.05	108.70	110.53
22	AB	610	CLA	C1-O2A-CGA	2.05	121.61	116.65
22	BD	404	CLA	C1-C2-C3	2.05	129.55	126.20
22	AC	511	CLA	C2A-C3A-C4A	2.05	105.18	101.87
26	AT	102	BCR	C16-C17-C18	2.05	130.15	127.28
27	AH	102	DGD	C3G-O3G-C1D	-2.05	109.41	113.80
22	BB	605	CLA	C2A-C1A-CHA	2.04	127.42	123.87
22	BB	610	CLA	CED-O2D-CGD	2.04	120.55	115.92
27	BA	411	DGD	C3G-O3G-C1D	-2.04	109.42	113.80
26	AB	619	BCR	C7-C8-C9	2.04	129.25	126.23
22	BB	606	CLA	CMA-C3A-C2A	-2.04	106.10	113.98
34	BV	201	HEM	C2D-C1D-ND	2.04	112.26	109.90
29	BF	101	SQD	O47-C7-C8	2.04	115.89	111.48
22	BA	404	CLA	CHD-C1D-ND	-2.04	121.94	124.80
22	AB	613	CLA	CMA-C3A-C2A	-2.04	106.10	113.98
27	AB	626	DGD	O5D-C6D-C5D	2.04	114.01	109.42
29	BB	601	SQD	O48-C23-O10	-2.04	118.53	123.63
26	BD	406	BCR	C8-C9-C10	-2.04	115.81	119.01
22	AB	603	CLA	C6-C5-C3	2.04	118.43	113.47
22	BC	511	CLA	CAA-C2A-C3A	-2.04	107.50	113.00
22	BC	507	CLA	C12-C11-C10	-2.03	104.16	113.28
26	AD	406	BCR	C32-C1-C6	2.03	113.43	110.24
29	AA	412	SQD	C20-C19-C18	2.03	124.65	114.37
26	AB	619	BCR	C32-C1-C2	-2.03	101.14	108.95
26	AK	102	BCR	C40-C30-C29	-2.03	101.15	108.95
26	AB	620	BCR	C12-C13-C14	-2.03	115.81	119.01
22	AB	607	CLA	CED-O2D-CGD	2.03	120.52	115.92
22	AC	509	CLA	C2A-C1A-CHA	2.03	127.39	123.87
22	AC	510	CLA	CAA-C2A-C3A	-2.03	107.51	113.00
24	BJ	101	PL9	C27-C28-C29	-2.03	120.87	127.64
22	BB	614	CLA	CMD-C2D-C1D	2.03	128.30	124.73
30	AA	413	LMG	C9-C8-C7	-2.03	107.05	111.78
22	BB	606	CLA	C2A-C3A-C4A	2.03	105.15	101.87
27	BC	517	DGD	C6E-C5E-C4E	-2.03	108.04	113.02
22	AC	501	CLA	CBA-CAA-C2A	2.03	119.83	113.79
26	BC	514	BCR	C34-C9-C8	2.03	121.19	118.09
22	BB	610	CLA	C1-O2A-CGA	2.03	121.56	116.65
29	BA	401	SQD	C17-C16-C15	2.03	124.61	114.37
22	AA	406	CLA	C12-C11-C10	-2.03	104.20	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	AC	510	CLA	C12-C11-C10	-2.03	104.20	113.28
30	AE	102	LMG	C8-O7-C10	2.03	122.64	117.80
27	AC	517	DGD	O3G-C3G-C2G	2.02	115.74	110.82
26	BC	514	BCR	C8-C7-C6	2.02	132.41	127.00
29	BA	401	SQD	O47-C45-C44	2.02	115.60	108.34
22	AC	503	CLA	C1-O2A-CGA	2.02	121.55	116.65
26	AA	409	BCR	C12-C13-C14	-2.02	115.83	119.01
22	AC	513	CLA	C2A-C3A-C4A	2.02	105.14	101.87
26	BJ	102	BCR	C28-C27-C26	2.02	117.66	114.06
27	AC	516	DGD	O3E-C3E-C2E	-2.02	105.62	110.38
32	AB	625	LMT	O1B-C1B-C2B	2.02	113.06	108.09
22	BB	617	CLA	CMD-C2D-C1D	2.02	128.28	124.73
22	BB	605	CLA	O2D-CGD-CBD	2.02	114.76	111.23
22	BD	404	CLA	C2A-C1A-CHA	2.02	127.37	123.87
22	BC	509	CLA	C1-O2A-CGA	2.02	121.54	116.65
22	BB	605	CLA	CMD-C2D-C1D	2.02	128.28	124.73
27	BC	516	DGD	C3G-C2G-C1G	-2.02	107.08	111.78
29	AA	415	SQD	C13-C12-C11	2.02	124.57	114.37
26	BK	102	BCR	C11-C12-C13	2.02	131.90	126.36
22	BC	510	CLA	C12-C11-C10	-2.02	104.24	113.28
22	AA	402	CLA	C1-C2-C3	2.02	129.50	126.20
22	AC	507	CLA	CMD-C2D-C1D	2.02	128.28	124.73
22	BB	609	CLA	O2D-CGD-CBD	2.02	114.75	111.23
29	BF	101	SQD	C31-C30-C29	2.02	132.93	115.25
27	AC	517	DGD	C6E-C5E-C4E	-2.01	108.07	113.02
30	BM	102	LMG	O8-C9-C8	-2.01	102.59	108.40
27	AA	410	DGD	C3G-O3G-C1D	-2.01	109.48	113.80
22	BB	615	CLA	CBA-CAA-C2A	2.01	119.78	113.79
22	AA	406	CLA	CMA-C3A-C2A	-2.01	106.20	113.98
22	BB	619	CLA	C6-C5-C3	2.01	118.36	113.47
23	BA	406	PHO	OBD-CAD-C3D	2.01	131.03	127.89
29	AF	101	SQD	C31-C30-C29	2.01	132.88	115.25
26	BX	101	BCR	C11-C12-C13	2.01	131.87	126.36
23	AD	403	PHO	C4D-ND-C1D	-2.01	106.47	108.87
29	BA	413	SQD	O3-C3-C2	-2.01	105.64	110.38
22	BA	404	CLA	O1D-CGD-CBD	-2.01	120.56	124.52
26	AB	617	BCR	C24-C23-C22	2.01	129.20	126.23
26	BD	406	BCR	C34-C9-C8	2.01	121.15	118.09
22	BC	513	CLA	CMD-C2D-C1D	2.01	128.26	124.73
22	AB	614	CLA	CBA-CAA-C2A	2.01	119.76	113.79
26	BB	621	BCR	C32-C1-C2	-2.00	101.25	108.95
22	BB	616	CLA	C1-O2A-CGA	2.00	121.50	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	AB	620	BCR	C37-C22-C23	2.00	121.15	118.09
22	BC	511	CLA	C2A-C3A-C4A	2.00	105.11	101.87
26	AZ	101	BCR	C37-C22-C23	2.00	121.15	118.09
27	AB	626	DGD	O6D-C5D-C4D	2.00	113.31	109.70
22	BB	617	CLA	C16-C15-C13	2.00	122.62	115.97
22	BB	606	CLA	C2A-C1A-CHA	2.00	127.34	123.87

All (156) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	AA	402	CLA	ND
22	AA	403	CLA	ND
22	AA	404	CLA	ND
22	AA	406	CLA	ND
22	AB	601	CLA	ND
22	AB	602	CLA	ND
22	AB	603	CLA	ND
22	AB	604	CLA	ND
22	AB	605	CLA	ND
22	AB	606	CLA	ND
22	AB	607	CLA	ND
22	AB	608	CLA	ND
22	AB	609	CLA	ND
22	AB	610	CLA	ND
22	AB	611	CLA	ND
22	AB	612	CLA	ND
22	AB	613	CLA	ND
22	AB	614	CLA	ND
22	AB	615	CLA	ND
22	AB	616	CLA	ND
22	AC	501	CLA	ND
22	AC	502	CLA	ND
22	AC	503	CLA	ND
22	AC	504	CLA	ND
22	AC	505	CLA	ND
22	AC	506	CLA	ND
22	AC	507	CLA	ND
22	AC	508	CLA	ND
22	AC	509	CLA	ND
22	AC	510	CLA	ND
22	AC	511	CLA	ND
22	AC	512	CLA	ND

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Mol	Chain	Res	Type	Atom
22	AC	513	CLA	ND
22	AD	402	CLA	ND
22	AD	404	CLA	ND
22	BA	403	CLA	ND
22	BA	404	CLA	ND
22	BA	405	CLA	ND
22	BA	407	CLA	ND
22	BB	604	CLA	ND
22	BB	605	CLA	ND
22	BB	606	CLA	ND
22	BB	607	CLA	ND
22	BB	608	CLA	ND
22	BB	609	CLA	ND
22	BB	610	CLA	ND
22	BB	611	CLA	ND
22	BB	612	CLA	ND
22	BB	613	CLA	ND
22	BB	614	CLA	ND
22	BB	615	CLA	ND
22	BB	616	CLA	ND
22	BB	617	CLA	ND
22	BB	618	CLA	ND
22	BB	619	CLA	ND
22	BC	501	CLA	ND
22	BC	502	CLA	ND
22	BC	503	CLA	ND
22	BC	504	CLA	ND
22	BC	505	CLA	ND
22	BC	506	CLA	ND
22	BC	507	CLA	ND
22	BC	508	CLA	ND
22	BC	509	CLA	ND
22	BC	510	CLA	ND
22	BC	511	CLA	ND
22	BC	512	CLA	ND
22	BC	513	CLA	ND
22	BD	402	CLA	ND
22	BD	404	CLA	ND
27	AA	410	DGD	C5D
27	AA	410	DGD	C2D
27	AA	410	DGD	C5E
27	AB	626	DGD	C5D

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Mol	Chain	Res	Type	Atom
27	AB	626	DGD	C2D
27	AB	626	DGD	C5E
27	AC	516	DGD	C5D
27	AC	516	DGD	C2D
27	AC	516	DGD	C5E
27	AC	517	DGD	C5D
27	AC	517	DGD	C2D
27	AC	517	DGD	C5E
27	AC	518	DGD	C5D
27	AC	518	DGD	C2D
27	AC	518	DGD	C5E
27	AD	410	DGD	C5D
27	AD	410	DGD	C2D
27	AD	410	DGD	C5E
27	AH	102	DGD	C5D
27	AH	102	DGD	C2D
27	AH	102	DGD	C5E
27	BA	411	DGD	C5D
27	BA	411	DGD	C2D
27	BA	411	DGD	C5E
27	BB	602	DGD	C5D
27	BB	602	DGD	C2D
27	BB	602	DGD	C5E
27	BC	516	DGD	C5D
27	BC	516	DGD	C2D
27	BC	516	DGD	C5E
27	BC	517	DGD	C5D
27	BC	517	DGD	C2D
27	BC	517	DGD	C5E
27	BC	518	DGD	C5D
27	BC	518	DGD	C2D
27	BC	518	DGD	C5E
27	BD	410	DGD	C5D
27	BD	410	DGD	C2D
27	BD	410	DGD	C5E
27	BH	101	DGD	C5D
27	BH	101	DGD	C2D
27	BH	101	DGD	C5E
30	AA	413	LMG	C5
30	AA	413	LMG	C2
30	AA	416	LMG	C5
30	AA	416	LMG	C2

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Mol	Chain	Res	Type	Atom
30	AB	621	LMG	C5
30	AB	621	LMG	C2
30	AB	622	LMG	C5
30	AB	622	LMG	C2
30	AB	623	LMG	C5
30	AB	623	LMG	C2
30	AC	519	LMG	C5
30	AC	519	LMG	C2
30	AC	520	LMG	C5
30	AC	520	LMG	C2
30	AD	407	LMG	C5
30	AD	407	LMG	C2
30	AD	408	LMG	C5
30	AD	408	LMG	C2
30	AE	102	LMG	C5
30	AE	102	LMG	C2
30	AI	101	LMG	C5
30	AI	101	LMG	C2
30	AM	101	LMG	C5
30	AM	101	LMG	C2
30	BA	414	LMG	C5
30	BA	414	LMG	C2
30	BB	623	LMG	C5
30	BB	623	LMG	C2
30	BB	624	LMG	C5
30	BB	624	LMG	C2
30	BC	519	LMG	C5
30	BC	519	LMG	C2
30	BC	520	LMG	C5
30	BC	520	LMG	C2
30	BD	407	LMG	C5
30	BD	407	LMG	C2
30	BD	408	LMG	C5
30	BD	408	LMG	C2
30	BE	102	LMG	C5
30	BE	102	LMG	C2
30	BI	101	LMG	C5
30	BI	101	LMG	C2
30	BM	102	LMG	C5
30	BM	102	LMG	C2

All (2261) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	AA	403	CLA	C1A-C2A-CAA-CBA
22	AA	403	CLA	C3A-C2A-CAA-CBA
22	AA	403	CLA	C1-C2-C3-C4
22	AA	403	CLA	C1-C2-C3-C5
22	AA	403	CLA	C4-C3-C5-C6
22	AA	404	CLA	C2B-C3B-CAB-CBB
22	AA	404	CLA	C4B-C3B-CAB-CBB
22	AA	404	CLA	C1-C2-C3-C5
22	AA	406	CLA	C2B-C3B-CAB-CBB
22	AA	406	CLA	C4B-C3B-CAB-CBB
22	AB	601	CLA	CBD-CGD-O2D-CED
22	AB	601	CLA	C1-C2-C3-C4
22	AB	602	CLA	C1A-C2A-CAA-CBA
22	AB	602	CLA	C1-C2-C3-C4
22	AB	602	CLA	C1-C2-C3-C5
22	AB	603	CLA	C2B-C3B-CAB-CBB
22	AB	603	CLA	C4B-C3B-CAB-CBB
22	AB	604	CLA	C2B-C3B-CAB-CBB
22	AB	604	CLA	C4B-C3B-CAB-CBB
22	AB	604	CLA	CBD-CGD-O2D-CED
22	AB	605	CLA	C2B-C3B-CAB-CBB
22	AB	605	CLA	C4B-C3B-CAB-CBB
22	AB	605	CLA	CBD-CGD-O2D-CED
22	AB	605	CLA	C1-C2-C3-C5
22	AB	606	CLA	C1A-C2A-CAA-CBA
22	AB	606	CLA	C3A-C2A-CAA-CBA
22	AB	606	CLA	C2B-C3B-CAB-CBB
22	AB	606	CLA	C4B-C3B-CAB-CBB
22	AB	606	CLA	C1-C2-C3-C4
22	AB	606	CLA	C1-C2-C3-C5
22	AB	607	CLA	C1A-C2A-CAA-CBA
22	AB	607	CLA	C3A-C2A-CAA-CBA
22	AB	607	CLA	C2B-C3B-CAB-CBB
22	AB	607	CLA	C4B-C3B-CAB-CBB
22	AB	608	CLA	C1A-C2A-CAA-CBA
22	AB	608	CLA	C3A-C2A-CAA-CBA
22	AB	608	CLA	C2B-C3B-CAB-CBB
22	AB	608	CLA	C4B-C3B-CAB-CBB
22	AB	608	CLA	C1-C2-C3-C4
22	AB	608	CLA	C4-C3-C5-C6
22	AB	608	CLA	C6-C7-C8-C9
22	AB	610	CLA	CBD-CGD-O2D-CED
22	AB	610	CLA	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
22	AB	610	CLA	C1-C2-C3-C5
22	AB	611	CLA	C1-C2-C3-C4
22	AB	612	CLA	C2B-C3B-CAB-CBB
22	AB	612	CLA	C4B-C3B-CAB-CBB
22	AB	613	CLA	C4-C3-C5-C6
22	AB	614	CLA	C4B-C3B-CAB-CBB
22	AB	615	CLA	C2B-C3B-CAB-CBB
22	AB	615	CLA	C4B-C3B-CAB-CBB
22	AB	615	CLA	C1-C2-C3-C4
22	AB	615	CLA	C1-C2-C3-C5
22	AB	616	CLA	C1A-C2A-CAA-CBA
22	AB	616	CLA	CBD-CGD-O2D-CED
22	AB	616	CLA	C1-C2-C3-C4
22	AB	616	CLA	C1-C2-C3-C5
22	AC	501	CLA	C4B-C3B-CAB-CBB
22	AC	502	CLA	C2B-C3B-CAB-CBB
22	AC	502	CLA	C4B-C3B-CAB-CBB
22	AC	502	CLA	C1-C2-C3-C5
22	AC	503	CLA	C2B-C3B-CAB-CBB
22	AC	503	CLA	C4B-C3B-CAB-CBB
22	AC	503	CLA	CBD-CGD-O2D-CED
22	AC	504	CLA	CBD-CGD-O2D-CED
22	AC	505	CLA	C1A-C2A-CAA-CBA
22	AC	505	CLA	C2B-C3B-CAB-CBB
22	AC	505	CLA	C4B-C3B-CAB-CBB
22	AC	505	CLA	CBD-CGD-O2D-CED
22	AC	505	CLA	C1-C2-C3-C4
22	AC	506	CLA	C2B-C3B-CAB-CBB
22	AC	506	CLA	C4B-C3B-CAB-CBB
22	AC	506	CLA	C1-C2-C3-C5
22	AC	507	CLA	C2B-C3B-CAB-CBB
22	AC	507	CLA	C4B-C3B-CAB-CBB
22	AC	508	CLA	C2B-C3B-CAB-CBB
22	AC	508	CLA	C4B-C3B-CAB-CBB
22	AC	508	CLA	CBD-CGD-O2D-CED
22	AC	509	CLA	CHA-CBD-CGD-O2D
22	AC	509	CLA	C1-C2-C3-C4
22	AC	509	CLA	C1-C2-C3-C5
22	AC	510	CLA	C1-C2-C3-C5
22	AC	511	CLA	C2B-C3B-CAB-CBB
22	AC	511	CLA	C4B-C3B-CAB-CBB
22	AC	511	CLA	C1-C2-C3-C5

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Mol	Chain	Res	Type	Atoms
22	AC	512	CLA	C2B-C3B-CAB-CBB
22	AC	512	CLA	C4B-C3B-CAB-CBB
22	AC	513	CLA	C2B-C3B-CAB-CBB
22	AC	513	CLA	C4B-C3B-CAB-CBB
22	AC	513	CLA	C1-C2-C3-C4
22	AC	513	CLA	C1-C2-C3-C5
22	AD	402	CLA	C1-C2-C3-C4
22	AD	402	CLA	C1-C2-C3-C5
22	AD	404	CLA	C1A-C2A-CAA-CBA
22	AD	404	CLA	C2B-C3B-CAB-CBB
22	AD	404	CLA	C4B-C3B-CAB-CBB
22	BA	404	CLA	C1A-C2A-CAA-CBA
22	BA	404	CLA	C3A-C2A-CAA-CBA
22	BA	404	CLA	C1-C2-C3-C4
22	BA	404	CLA	C1-C2-C3-C5
22	BA	405	CLA	C2B-C3B-CAB-CBB
22	BA	405	CLA	C4B-C3B-CAB-CBB
22	BA	405	CLA	C1-C2-C3-C5
22	BA	407	CLA	C2B-C3B-CAB-CBB
22	BA	407	CLA	C4B-C3B-CAB-CBB
22	BB	604	CLA	CBD-CGD-O2D-CED
22	BB	605	CLA	C1A-C2A-CAA-CBA
22	BB	605	CLA	C1-C2-C3-C4
22	BB	605	CLA	C1-C2-C3-C5
22	BB	606	CLA	C2B-C3B-CAB-CBB
22	BB	606	CLA	C4B-C3B-CAB-CBB
22	BB	607	CLA	C2B-C3B-CAB-CBB
22	BB	607	CLA	C4B-C3B-CAB-CBB
22	BB	607	CLA	CBD-CGD-O2D-CED
22	BB	608	CLA	C2B-C3B-CAB-CBB
22	BB	608	CLA	C4B-C3B-CAB-CBB
22	BB	608	CLA	CBD-CGD-O2D-CED
22	BB	608	CLA	C1-C2-C3-C5
22	BB	609	CLA	C1A-C2A-CAA-CBA
22	BB	609	CLA	C3A-C2A-CAA-CBA
22	BB	609	CLA	C2B-C3B-CAB-CBB
22	BB	609	CLA	C4B-C3B-CAB-CBB
22	BB	609	CLA	CBD-CGD-O2D-CED
22	BB	609	CLA	C1-C2-C3-C4
22	BB	609	CLA	C1-C2-C3-C5
22	BB	610	CLA	C1A-C2A-CAA-CBA
22	BB	610	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	BB	610	CLA	C2B-C3B-CAB-CBB
22	BB	610	CLA	C4B-C3B-CAB-CBB
22	BB	611	CLA	C1A-C2A-CAA-CBA
22	BB	611	CLA	C2B-C3B-CAB-CBB
22	BB	611	CLA	C4B-C3B-CAB-CBB
22	BB	611	CLA	C1-C2-C3-C4
22	BB	611	CLA	C4-C3-C5-C6
22	BB	611	CLA	C6-C7-C8-C9
22	BB	613	CLA	CBD-CGD-O2D-CED
22	BB	613	CLA	C1-C2-C3-C4
22	BB	613	CLA	C1-C2-C3-C5
22	BB	614	CLA	C1-C2-C3-C4
22	BB	615	CLA	C2B-C3B-CAB-CBB
22	BB	615	CLA	C4B-C3B-CAB-CBB
22	BB	616	CLA	C4-C3-C5-C6
22	BB	617	CLA	C4B-C3B-CAB-CBB
22	BB	618	CLA	C2B-C3B-CAB-CBB
22	BB	618	CLA	C4B-C3B-CAB-CBB
22	BB	618	CLA	C1-C2-C3-C4
22	BB	618	CLA	C1-C2-C3-C5
22	BB	619	CLA	C1A-C2A-CAA-CBA
22	BB	619	CLA	CBD-CGD-O2D-CED
22	BB	619	CLA	C1-C2-C3-C4
22	BB	619	CLA	C1-C2-C3-C5
22	BC	502	CLA	C2B-C3B-CAB-CBB
22	BC	502	CLA	C4B-C3B-CAB-CBB
22	BC	502	CLA	C1-C2-C3-C5
22	BC	503	CLA	C2B-C3B-CAB-CBB
22	BC	503	CLA	C4B-C3B-CAB-CBB
22	BC	503	CLA	CBD-CGD-O2D-CED
22	BC	504	CLA	CBD-CGD-O2D-CED
22	BC	505	CLA	C1A-C2A-CAA-CBA
22	BC	505	CLA	C2B-C3B-CAB-CBB
22	BC	505	CLA	C4B-C3B-CAB-CBB
22	BC	505	CLA	CBD-CGD-O2D-CED
22	BC	505	CLA	C1-C2-C3-C4
22	BC	506	CLA	C2B-C3B-CAB-CBB
22	BC	506	CLA	C4B-C3B-CAB-CBB
22	BC	506	CLA	C1-C2-C3-C5
22	BC	507	CLA	C2B-C3B-CAB-CBB
22	BC	507	CLA	C4B-C3B-CAB-CBB
22	BC	508	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
22	BC	508	CLA	C4B-C3B-CAB-CBB
22	BC	508	CLA	CBD-CGD-O2D-CED
22	BC	509	CLA	C1-C2-C3-C4
22	BC	509	CLA	C1-C2-C3-C5
22	BC	510	CLA	C1-C2-C3-C5
22	BC	511	CLA	C2B-C3B-CAB-CBB
22	BC	511	CLA	C4B-C3B-CAB-CBB
22	BC	511	CLA	C1-C2-C3-C5
22	BC	512	CLA	C2B-C3B-CAB-CBB
22	BC	512	CLA	C4B-C3B-CAB-CBB
22	BC	513	CLA	C2B-C3B-CAB-CBB
22	BC	513	CLA	C4B-C3B-CAB-CBB
22	BC	513	CLA	C1-C2-C3-C4
22	BC	513	CLA	C1-C2-C3-C5
22	BD	402	CLA	C1-C2-C3-C4
22	BD	402	CLA	C1-C2-C3-C5
22	BD	404	CLA	C1A-C2A-CAA-CBA
22	BD	404	CLA	C2B-C3B-CAB-CBB
22	BD	404	CLA	C4B-C3B-CAB-CBB
23	AA	405	PHO	C1-C2-C3-C4
23	AA	405	PHO	C1-C2-C3-C5
23	BA	406	PHO	C1-C2-C3-C4
23	BA	406	PHO	C1-C2-C3-C5
23	BA	406	PHO	C6-C7-C8-C9
24	AA	407	PL9	C7-C8-C9-C11
24	AA	407	PL9	C12-C13-C14-C15
24	AA	407	PL9	C12-C13-C14-C16
24	AA	407	PL9	C17-C18-C19-C20
24	AA	407	PL9	C17-C18-C19-C21
24	AA	407	PL9	C27-C28-C29-C30
24	AA	407	PL9	C27-C28-C29-C31
24	AA	407	PL9	C32-C33-C34-C36
24	AA	407	PL9	C37-C38-C39-C40
24	AA	407	PL9	C37-C38-C39-C41
24	AD	405	PL9	C18-C19-C21-C22
24	AD	405	PL9	C20-C19-C21-C22
24	AD	405	PL9	C22-C23-C24-C25
24	AD	405	PL9	C42-C43-C44-C45
24	AD	405	PL9	C42-C43-C44-C46
24	AJ	101	PL9	C7-C8-C9-C10
24	AJ	101	PL9	C7-C8-C9-C11
24	AJ	101	PL9	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
24	AJ	101	PL9	C12-C13-C14-C16
24	AJ	101	PL9	C17-C18-C19-C21
24	AJ	101	PL9	C22-C23-C24-C25
24	AJ	101	PL9	C22-C23-C24-C26
24	BA	408	PL9	C7-C8-C9-C11
24	BA	408	PL9	C12-C13-C14-C15
24	BA	408	PL9	C12-C13-C14-C16
24	BA	408	PL9	C17-C18-C19-C20
24	BA	408	PL9	C17-C18-C19-C21
24	BA	408	PL9	C27-C28-C29-C30
24	BA	408	PL9	C27-C28-C29-C31
24	BA	408	PL9	C32-C33-C34-C36
24	BA	408	PL9	C37-C38-C39-C40
24	BA	408	PL9	C37-C38-C39-C41
24	BD	405	PL9	C18-C19-C21-C22
24	BD	405	PL9	C20-C19-C21-C22
24	BD	405	PL9	C22-C23-C24-C25
24	BD	405	PL9	C42-C43-C44-C45
24	BD	405	PL9	C42-C43-C44-C46
24	BJ	101	PL9	C7-C8-C9-C10
24	BJ	101	PL9	C7-C8-C9-C11
24	BJ	101	PL9	C12-C13-C14-C15
24	BJ	101	PL9	C12-C13-C14-C16
24	BJ	101	PL9	C17-C18-C19-C21
24	BJ	101	PL9	C22-C23-C24-C25
24	BJ	101	PL9	C22-C23-C24-C26
26	AB	618	BCR	C6-C7-C8-C9
26	AB	620	BCR	C23-C24-C25-C26
26	AB	620	BCR	C23-C24-C25-C30
26	AC	514	BCR	C1-C6-C7-C8
26	AC	514	BCR	C5-C6-C7-C8
26	AC	514	BCR	C6-C7-C8-C9
26	AC	515	BCR	C23-C24-C25-C26
26	AD	406	BCR	C6-C7-C8-C9
26	AT	102	BCR	C6-C7-C8-C9
26	AZ	101	BCR	C1-C6-C7-C8
26	AZ	101	BCR	C5-C6-C7-C8
26	BB	622	BCR	C23-C24-C25-C26
26	BB	622	BCR	C23-C24-C25-C30
26	BC	514	BCR	C1-C6-C7-C8
26	BC	514	BCR	C5-C6-C7-C8
26	BC	514	BCR	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
26	BC	515	BCR	C23-C24-C25-C26
26	BD	406	BCR	C6-C7-C8-C9
26	BZ	101	BCR	C1-C6-C7-C8
26	BZ	101	BCR	C5-C6-C7-C8
27	AA	410	DGD	O6D-C1D-O3G-C3G
27	AB	626	DGD	O1B-C1B-O2G-C2G
27	AB	626	DGD	C2D-C1D-O3G-C3G
27	AB	626	DGD	C5D-C6D-O5D-C1E
27	AB	626	DGD	C2E-C1E-O5D-C6D
27	AC	516	DGD	C2D-C1D-O3G-C3G
27	AC	517	DGD	C2B-C1B-O2G-C2G
27	AC	517	DGD	C4D-C5D-C6D-O5D
27	AC	518	DGD	O6D-C1D-O3G-C3G
27	AD	410	DGD	C2B-C1B-O2G-C2G
27	AD	410	DGD	C1G-C2G-O2G-C1B
27	AD	410	DGD	C2D-C1D-O3G-C3G
27	AD	410	DGD	O6D-C1D-O3G-C3G
27	AD	410	DGD	O6E-C1E-O5D-C6D
27	AH	102	DGD	O6E-C1E-O5D-C6D
27	BA	411	DGD	O6D-C1D-O3G-C3G
27	BB	602	DGD	O1B-C1B-O2G-C2G
27	BB	602	DGD	C2D-C1D-O3G-C3G
27	BB	602	DGD	C5D-C6D-O5D-C1E
27	BB	602	DGD	C2E-C1E-O5D-C6D
27	BC	516	DGD	C2D-C1D-O3G-C3G
27	BC	517	DGD	C2B-C1B-O2G-C2G
27	BC	517	DGD	C4D-C5D-C6D-O5D
27	BC	518	DGD	O6D-C1D-O3G-C3G
27	BD	410	DGD	C2B-C1B-O2G-C2G
27	BD	410	DGD	C1G-C2G-O2G-C1B
27	BD	410	DGD	C2D-C1D-O3G-C3G
27	BD	410	DGD	O6D-C1D-O3G-C3G
27	BD	410	DGD	O6E-C1E-O5D-C6D
27	BH	101	DGD	O6E-C1E-O5D-C6D
28	AA	411	LHG	C1-C2-C3-O3
28	AC	521	LHG	O1-C1-C2-C3
28	AC	521	LHG	C1-C2-C3-O3
28	AC	521	LHG	C3-O3-P-O4
28	BA	412	LHG	C1-C2-C3-O3
28	BC	521	LHG	O1-C1-C2-C3
29	AA	412	SQD	C2-C1-O6-C44
29	AA	412	SQD	O5-C5-C6-S

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Mol	Chain	Res	Type	Atoms
29	AA	412	SQD	C5-C6-S-O7
29	AA	412	SQD	C5-C6-S-O8
29	AA	415	SQD	O5-C1-O6-C44
29	AA	415	SQD	O6-C44-C45-O47
29	AA	415	SQD	O10-C23-O48-C46
29	AD	409	SQD	O49-C7-O47-C45
29	AD	409	SQD	C8-C7-O47-C45
29	AD	409	SQD	O5-C5-C6-S
29	AF	101	SQD	O5-C1-O6-C44
29	BA	401	SQD	O5-C1-O6-C44
29	BA	401	SQD	O6-C44-C45-O47
29	BA	413	SQD	C2-C1-O6-C44
29	BA	413	SQD	O5-C5-C6-S
29	BA	413	SQD	C5-C6-S-O7
29	BA	413	SQD	C5-C6-S-O8
29	BB	601	SQD	O5-C1-O6-C44
29	BB	601	SQD	O5-C5-C6-S
29	BD	409	SQD	O49-C7-O47-C45
29	BD	409	SQD	C8-C7-O47-C45
29	BD	409	SQD	O5-C5-C6-S
29	BF	101	SQD	O5-C1-O6-C44
29	BL	101	SQD	O5-C1-O6-C44
29	BL	101	SQD	O5-C5-C6-S
30	AB	621	LMG	C11-C10-O7-C8
30	AB	622	LMG	C11-C10-O7-C8
30	AC	520	LMG	C11-C10-O7-C8
30	AD	407	LMG	C11-C10-O7-C8
30	AD	408	LMG	O6-C1-O1-C7
30	AE	102	LMG	O6-C1-O1-C7
30	AM	101	LMG	O6-C1-O1-C7
30	AM	101	LMG	O9-C10-O7-C8
30	BB	623	LMG	C11-C10-O7-C8
30	BB	624	LMG	C11-C10-O7-C8
30	BC	520	LMG	C11-C10-O7-C8
30	BD	407	LMG	C11-C10-O7-C8
30	BD	408	LMG	O6-C1-O1-C7
30	BE	102	LMG	O6-C1-O1-C7
30	BM	102	LMG	O6-C1-O1-C7
30	BM	102	LMG	O9-C10-O7-C8
34	AE	101	HEM	C2C-C3C-CAC-CBC
34	AE	101	HEM	C4C-C3C-CAC-CBC
34	AV	201	HEM	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
34	AV	201	HEM	C4B-C3B-CAB-CBB
34	AV	201	HEM	C2C-C3C-CAC-CBC
34	AV	201	HEM	C4C-C3C-CAC-CBC
34	BE	101	HEM	C2C-C3C-CAC-CBC
34	BE	101	HEM	C4C-C3C-CAC-CBC
34	BV	201	HEM	C2B-C3B-CAB-CBB
34	BV	201	HEM	C4B-C3B-CAB-CBB
34	BV	201	HEM	C2C-C3C-CAC-CBC
34	BV	201	HEM	C4C-C3C-CAC-CBC
32	AT	101	LMT	C3'-C4'-O1B-C1B
32	BT	101	LMT	C3'-C4'-O1B-C1B
22	AC	505	CLA	O1D-CGD-O2D-CED
22	BC	505	CLA	O1D-CGD-O2D-CED
22	AA	402	CLA	O1D-CGD-O2D-CED
22	AB	604	CLA	O1D-CGD-O2D-CED
22	AB	616	CLA	O1D-CGD-O2D-CED
22	BA	403	CLA	O1D-CGD-O2D-CED
22	BB	607	CLA	O1D-CGD-O2D-CED
22	BB	619	CLA	O1D-CGD-O2D-CED
22	AA	402	CLA	CBD-CGD-O2D-CED
22	AB	603	CLA	CBD-CGD-O2D-CED
22	AB	606	CLA	CBD-CGD-O2D-CED
22	AB	607	CLA	CBD-CGD-O2D-CED
22	AB	613	CLA	CBD-CGD-O2D-CED
22	AC	507	CLA	CBD-CGD-O2D-CED
22	AC	511	CLA	CBD-CGD-O2D-CED
22	AC	512	CLA	CBD-CGD-O2D-CED
22	AC	513	CLA	CBD-CGD-O2D-CED
22	BA	403	CLA	CBD-CGD-O2D-CED
22	BB	606	CLA	CBD-CGD-O2D-CED
22	BB	610	CLA	CBD-CGD-O2D-CED
22	BB	611	CLA	CBD-CGD-O2D-CED
22	BB	616	CLA	CBD-CGD-O2D-CED
22	BC	507	CLA	CBD-CGD-O2D-CED
22	BC	510	CLA	CBD-CGD-O2D-CED
22	BC	511	CLA	CBD-CGD-O2D-CED
22	BC	512	CLA	CBD-CGD-O2D-CED
22	BC	513	CLA	CBD-CGD-O2D-CED
23	AD	403	PHO	CBD-CGD-O2D-CED
23	BD	403	PHO	CBD-CGD-O2D-CED
29	BA	401	SQD	O10-C23-O48-C46
30	AA	413	LMG	O10-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
30	AC	520	LMG	O10-C28-O8-C9
30	BA	414	LMG	O10-C28-O8-C9
30	BC	520	LMG	O10-C28-O8-C9
24	AJ	101	PL9	C27-C28-C29-C30
24	AJ	101	PL9	C27-C28-C29-C31
24	BJ	101	PL9	C27-C28-C29-C31
30	AC	520	LMG	C8-C9-O8-C28
30	BC	520	LMG	C8-C9-O8-C28
22	AC	511	CLA	O1D-CGD-O2D-CED
22	BC	511	CLA	O1D-CGD-O2D-CED
29	BA	401	SQD	C24-C23-O48-C46
30	AA	413	LMG	C29-C28-O8-C9
30	AC	520	LMG	C29-C28-O8-C9
30	BC	520	LMG	C29-C28-O8-C9
22	AB	608	CLA	CBD-CGD-O2D-CED
22	AC	510	CLA	CBD-CGD-O2D-CED
27	AD	410	DGD	O1A-C1A-O1G-C1G
27	BD	410	DGD	O1A-C1A-O1G-C1G
29	AF	101	SQD	O10-C23-O48-C46
29	BF	101	SQD	O10-C23-O48-C46
30	AB	621	LMG	O10-C28-O8-C9
30	AD	408	LMG	O10-C28-O8-C9
30	AE	102	LMG	O10-C28-O8-C9
30	BB	623	LMG	O10-C28-O8-C9
30	BD	408	LMG	O10-C28-O8-C9
30	BE	102	LMG	O10-C28-O8-C9
22	AC	504	CLA	O1D-CGD-O2D-CED
22	AC	508	CLA	O1D-CGD-O2D-CED
22	BB	613	CLA	O1D-CGD-O2D-CED
22	BC	503	CLA	O1D-CGD-O2D-CED
22	BC	504	CLA	O1D-CGD-O2D-CED
22	BC	508	CLA	O1D-CGD-O2D-CED
22	AB	601	CLA	O1D-CGD-O2D-CED
22	AB	610	CLA	O1D-CGD-O2D-CED
22	AC	503	CLA	O1D-CGD-O2D-CED
22	BB	604	CLA	O1D-CGD-O2D-CED
22	BB	614	CLA	CBD-CGD-O2D-CED
22	BC	509	CLA	CBD-CGD-O2D-CED
27	AD	410	DGD	O1B-C1B-O2G-C2G
27	BC	517	DGD	O1B-C1B-O2G-C2G
27	BD	410	DGD	O1B-C1B-O2G-C2G
30	AB	622	LMG	O9-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
30	AC	520	LMG	O9-C10-O7-C8
30	AD	407	LMG	O9-C10-O7-C8
30	BB	624	LMG	O9-C10-O7-C8
30	BC	520	LMG	O9-C10-O7-C8
30	BD	407	LMG	O9-C10-O7-C8
22	AB	605	CLA	O1D-CGD-O2D-CED
24	BJ	101	PL9	C27-C28-C29-C30
22	AB	608	CLA	C3-C5-C6-C7
22	BB	611	CLA	C3-C5-C6-C7
22	AB	603	CLA	O1D-CGD-O2D-CED
28	AA	411	LHG	C24-C23-O8-C6
28	BA	412	LHG	C24-C23-O8-C6
29	AA	415	SQD	C24-C23-O48-C46
29	AF	101	SQD	C24-C23-O48-C46
29	BF	101	SQD	C24-C23-O48-C46
30	AB	621	LMG	C29-C28-O8-C9
30	AD	408	LMG	C29-C28-O8-C9
30	AI	101	LMG	C29-C28-O8-C9
30	BA	414	LMG	C29-C28-O8-C9
30	BB	623	LMG	C29-C28-O8-C9
30	BD	408	LMG	C29-C28-O8-C9
30	BI	101	LMG	C29-C28-O8-C9
22	AA	404	CLA	CBD-CGD-O2D-CED
22	AB	611	CLA	CBD-CGD-O2D-CED
22	AB	614	CLA	CBD-CGD-O2D-CED
22	AC	501	CLA	CBD-CGD-O2D-CED
22	AC	509	CLA	CBD-CGD-O2D-CED
22	BA	405	CLA	CBD-CGD-O2D-CED
22	BB	605	CLA	CBD-CGD-O2D-CED
22	BB	617	CLA	CBD-CGD-O2D-CED
22	BC	501	CLA	CBD-CGD-O2D-CED
27	AB	626	DGD	C2B-C1B-O2G-C2G
27	BB	602	DGD	C2B-C1B-O2G-C2G
30	AM	101	LMG	C11-C10-O7-C8
30	BM	102	LMG	C11-C10-O7-C8
22	BB	606	CLA	O1D-CGD-O2D-CED
22	BB	608	CLA	O1D-CGD-O2D-CED
22	BB	609	CLA	O1D-CGD-O2D-CED
22	AB	606	CLA	O1D-CGD-O2D-CED
22	AB	603	CLA	C4-C3-C5-C6
22	BA	404	CLA	C4-C3-C5-C6
22	BB	606	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	AA	403	CLA	C2-C3-C5-C6
22	AB	603	CLA	C2-C3-C5-C6
22	AB	608	CLA	C2-C3-C5-C6
22	AB	613	CLA	C2-C3-C5-C6
22	BB	606	CLA	C2-C3-C5-C6
22	BB	611	CLA	C2-C3-C5-C6
22	BB	616	CLA	C2-C3-C5-C6
22	AB	613	CLA	O1D-CGD-O2D-CED
22	BB	616	CLA	O1D-CGD-O2D-CED
23	AD	403	PHO	O1D-CGD-O2D-CED
22	AC	508	CLA	C2A-CAA-CBA-CGA
22	AC	511	CLA	C2A-CAA-CBA-CGA
22	BC	508	CLA	C2A-CAA-CBA-CGA
22	BC	511	CLA	C2A-CAA-CBA-CGA
27	AD	410	DGD	C2A-C1A-O1G-C1G
27	BD	410	DGD	C2A-C1A-O1G-C1G
30	AC	519	LMG	C29-C28-O8-C9
30	AE	102	LMG	C29-C28-O8-C9
30	BE	102	LMG	C29-C28-O8-C9
24	AA	407	PL9	C7-C8-C9-C10
24	AA	407	PL9	C22-C23-C24-C25
24	AA	407	PL9	C32-C33-C34-C35
24	AD	405	PL9	C12-C13-C14-C15
24	AD	405	PL9	C27-C28-C29-C30
24	AJ	101	PL9	C17-C18-C19-C20
24	BA	408	PL9	C7-C8-C9-C10
24	BA	408	PL9	C22-C23-C24-C25
24	BA	408	PL9	C32-C33-C34-C35
24	BD	405	PL9	C12-C13-C14-C15
24	BD	405	PL9	C27-C28-C29-C30
24	BJ	101	PL9	C17-C18-C19-C20
27	AA	410	DGD	C4D-C5D-C6D-O5D
27	BA	411	DGD	C4D-C5D-C6D-O5D
24	AA	407	PL9	C22-C23-C24-C26
24	AD	405	PL9	C12-C13-C14-C16
24	AD	405	PL9	C27-C28-C29-C31
24	BA	408	PL9	C22-C23-C24-C26
24	BD	405	PL9	C12-C13-C14-C16
24	BD	405	PL9	C27-C28-C29-C31
28	AA	411	LHG	O10-C23-O8-C6
28	BA	412	LHG	O10-C23-O8-C6
30	AC	519	LMG	O10-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
30	BC	519	LMG	O10-C28-O8-C9
27	AC	517	DGD	O1B-C1B-O2G-C2G
30	AB	621	LMG	O9-C10-O7-C8
30	BB	623	LMG	O9-C10-O7-C8
30	BD	408	LMG	O6-C5-C6-O5
30	BC	520	LMG	C4-C5-C6-O5
22	AB	607	CLA	O1D-CGD-O2D-CED
22	AC	512	CLA	O1D-CGD-O2D-CED
23	BD	403	PHO	O1D-CGD-O2D-CED
22	AC	506	CLA	CBD-CGD-O2D-CED
23	AA	405	PHO	CBD-CGD-O2D-CED
28	AA	411	LHG	O2-C2-C3-O3
28	BA	412	LHG	O2-C2-C3-O3
22	AC	507	CLA	O1D-CGD-O2D-CED
22	AC	513	CLA	O1D-CGD-O2D-CED
22	BC	507	CLA	O1D-CGD-O2D-CED
22	BC	512	CLA	O1D-CGD-O2D-CED
22	BC	513	CLA	O1D-CGD-O2D-CED
30	BC	519	LMG	C29-C28-O8-C9
27	AB	626	DGD	O6E-C5E-C6E-O5E
27	BB	602	DGD	O6E-C5E-C6E-O5E
30	AD	408	LMG	O6-C5-C6-O5
30	AI	101	LMG	O10-C28-O8-C9
30	BI	101	LMG	O10-C28-O8-C9
30	AC	520	LMG	C4-C5-C6-O5
30	AC	520	LMG	O6-C5-C6-O5
30	AM	101	LMG	O6-C5-C6-O5
30	BM	102	LMG	O6-C5-C6-O5
32	AB	627	LMT	C3'-C4'-O1B-C1B
22	AB	602	CLA	CBD-CGD-O2D-CED
22	BC	506	CLA	CBD-CGD-O2D-CED
27	AC	516	DGD	C2B-C1B-O2G-C2G
27	BC	516	DGD	C2B-C1B-O2G-C2G
32	BB	603	LMT	C3'-C4'-O1B-C1B
30	BC	519	LMG	C4-C5-C6-O5
30	BM	102	LMG	C4-C5-C6-O5
22	BB	610	CLA	O1D-CGD-O2D-CED
23	BA	406	PHO	CBD-CGD-O2D-CED
30	BC	520	LMG	O6-C5-C6-O5
30	AA	413	LMG	C4-C5-C6-O5
30	AM	101	LMG	C4-C5-C6-O5
22	BC	510	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
27	BC	516	DGD	O1B-C1B-O2G-C2G
30	AD	407	LMG	O6-C5-C6-O5
24	AD	405	PL9	C24-C26-C27-C28
24	BD	405	PL9	C24-C26-C27-C28
30	AC	519	LMG	C4-C5-C6-O5
27	BD	410	DGD	O6E-C5E-C6E-O5E
30	BD	407	LMG	O6-C5-C6-O5
30	BA	414	LMG	C4-C5-C6-O5
30	BI	101	LMG	C4-C5-C6-O5
27	AB	626	DGD	O6D-C1D-O3G-C3G
27	AC	516	DGD	O6D-C1D-O3G-C3G
27	BB	602	DGD	O6D-C1D-O3G-C3G
27	BC	516	DGD	O6D-C1D-O3G-C3G
29	AD	409	SQD	O5-C1-O6-C44
29	BD	409	SQD	O5-C1-O6-C44
30	AB	622	LMG	O6-C1-O1-C7
30	AC	519	LMG	O6-C1-O1-C7
30	AC	520	LMG	O6-C1-O1-C7
30	BB	624	LMG	O6-C1-O1-C7
30	BC	519	LMG	O6-C1-O1-C7
30	BC	520	LMG	O6-C1-O1-C7
22	AB	612	CLA	CBD-CGD-O2D-CED
27	AD	410	DGD	O6E-C5E-C6E-O5E
30	AB	621	LMG	O6-C5-C6-O5
30	AI	101	LMG	C4-C5-C6-O5
30	BB	623	LMG	O6-C5-C6-O5
22	BC	509	CLA	O1D-CGD-O2D-CED
27	BA	411	DGD	C4E-C5E-C6E-O5E
30	AB	623	LMG	C11-C10-O7-C8
32	AI	102	LMT	C3'-C4'-O1B-C1B
32	BI	102	LMT	C3'-C4'-O1B-C1B
27	AA	410	DGD	C4E-C5E-C6E-O5E
27	AC	516	DGD	O1B-C1B-O2G-C2G
28	BC	521	LHG	C1-C2-C3-O3
28	AC	521	LHG	C24-C23-O8-C6
28	BC	521	LHG	C24-C23-O8-C6
29	BB	601	SQD	C24-C23-O48-C46
29	BL	101	SQD	C24-C23-O48-C46
30	AB	622	LMG	C29-C28-O8-C9
30	BB	624	LMG	C29-C28-O8-C9
22	BB	615	CLA	CBD-CGD-O2D-CED
29	AF	101	SQD	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
29	BF	101	SQD	C24-C25-C26-C27
22	AB	608	CLA	O1D-CGD-O2D-CED
22	AC	509	CLA	O1D-CGD-O2D-CED
22	AC	510	CLA	O1D-CGD-O2D-CED
22	BB	611	CLA	O1D-CGD-O2D-CED
22	BB	614	CLA	O1D-CGD-O2D-CED
22	BC	501	CLA	O1D-CGD-O2D-CED
22	BA	404	CLA	C2-C3-C5-C6
22	BB	604	CLA	C2C-C3C-CAC-CBC
22	AA	403	CLA	C6-C7-C8-C9
22	AB	602	CLA	C6-C7-C8-C9
22	AC	511	CLA	C6-C7-C8-C9
22	BA	404	CLA	C6-C7-C8-C9
22	BB	605	CLA	C6-C7-C8-C9
22	BC	511	CLA	C6-C7-C8-C9
23	AA	405	PHO	C6-C7-C8-C9
30	AB	621	LMG	C4-C5-C6-O5
30	AD	408	LMG	C4-C5-C6-O5
30	BD	408	LMG	C4-C5-C6-O5
22	AC	501	CLA	O1D-CGD-O2D-CED
22	BA	405	CLA	O1D-CGD-O2D-CED
27	AA	410	DGD	C2D-C1D-O3G-C3G
27	BA	411	DGD	C2D-C1D-O3G-C3G
30	AB	622	LMG	C2-C1-O1-C7
30	AC	519	LMG	C2-C1-O1-C7
30	AC	520	LMG	C2-C1-O1-C7
30	BB	624	LMG	C2-C1-O1-C7
30	BC	519	LMG	C2-C1-O1-C7
30	BC	520	LMG	C2-C1-O1-C7
22	BB	617	CLA	C2C-C3C-CAC-CBC
22	AB	611	CLA	O1D-CGD-O2D-CED
30	BC	519	LMG	O6-C5-C6-O5
29	BA	413	SQD	C11-C10-C9-C8
30	AA	413	LMG	O6-C5-C6-O5
30	AC	519	LMG	O6-C5-C6-O5
27	BD	410	DGD	C4E-C5E-C6E-O5E
29	AA	412	SQD	C11-C10-C9-C8
22	BB	604	CLA	C2A-CAA-CBA-CGA
22	AB	614	CLA	C2C-C3C-CAC-CBC
27	BH	101	DGD	C1B-C2B-C3B-C4B
30	BB	623	LMG	C10-C11-C12-C13
22	AA	404	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
29	BB	601	SQD	O10-C23-O48-C46
29	BL	101	SQD	O10-C23-O48-C46
30	AB	622	LMG	O10-C28-O8-C9
30	BB	624	LMG	O10-C28-O8-C9
30	BA	414	LMG	O6-C5-C6-O5
30	AA	416	LMG	C11-C10-O7-C8
27	BB	602	DGD	O2G-C2G-C3G-O3G
22	AA	403	CLA	C15-C16-C17-C18
27	AC	516	DGD	C1B-C2B-C3B-C4B
30	AB	621	LMG	C10-C11-C12-C13
22	AB	601	CLA	C2C-C3C-CAC-CBC
22	AB	604	CLA	C8-C10-C11-C12
22	AC	510	CLA	C15-C16-C17-C18
22	BC	505	CLA	C10-C11-C12-C13
22	BC	508	CLA	C10-C11-C12-C13
22	BC	510	CLA	C15-C16-C17-C18
27	AD	410	DGD	C4E-C5E-C6E-O5E
30	BB	623	LMG	C4-C5-C6-O5
27	BC	516	DGD	C1B-C2B-C3B-C4B
24	BD	405	PL9	C22-C23-C24-C26
30	BI	101	LMG	O6-C5-C6-O5
22	BB	604	CLA	C10-C11-C12-C13
22	BB	617	CLA	O1D-CGD-O2D-CED
30	AD	407	LMG	C10-C11-C12-C13
30	BC	520	LMG	C28-C29-C30-C31
30	BD	407	LMG	C10-C11-C12-C13
30	AA	416	LMG	O9-C10-O7-C8
30	AB	623	LMG	O9-C10-O7-C8
24	AD	405	PL9	C34-C36-C37-C38
24	BD	405	PL9	C34-C36-C37-C38
22	AB	614	CLA	C3-C5-C6-C7
22	AC	503	CLA	C10-C11-C12-C13
22	AC	505	CLA	C10-C11-C12-C13
22	BB	617	CLA	C5-C6-C7-C8
22	BC	501	CLA	C15-C16-C17-C18
27	BC	517	DGD	O6E-C5E-C6E-O5E
27	AH	102	DGD	C1B-C2B-C3B-C4B
27	BC	516	DGD	C1A-C2A-C3A-C4A
30	AA	416	LMG	C28-C29-C30-C31
30	AD	408	LMG	C10-C11-C12-C13
30	BD	408	LMG	C10-C11-C12-C13
30	BE	102	LMG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
28	AC	521	LHG	O10-C23-O8-C6
28	BC	521	LHG	O10-C23-O8-C6
22	AA	406	CLA	C13-C15-C16-C17
22	AB	601	CLA	C13-C15-C16-C17
22	AB	602	CLA	C13-C15-C16-C17
22	AB	608	CLA	C15-C16-C17-C18
22	AB	616	CLA	C15-C16-C17-C18
22	AC	504	CLA	C10-C11-C12-C13
22	AC	508	CLA	C10-C11-C12-C13
22	BA	404	CLA	C15-C16-C17-C18
22	BA	407	CLA	C13-C15-C16-C17
22	BB	604	CLA	C13-C15-C16-C17
22	BB	607	CLA	C8-C10-C11-C12
22	BB	614	CLA	C15-C16-C17-C18
22	BB	616	CLA	C5-C6-C7-C8
22	BB	616	CLA	C13-C15-C16-C17
22	BB	619	CLA	C15-C16-C17-C18
22	BC	503	CLA	C10-C11-C12-C13
22	BC	504	CLA	C10-C11-C12-C13
22	BC	507	CLA	C5-C6-C7-C8
22	BC	512	CLA	C13-C15-C16-C17
23	BD	403	PHO	C15-C16-C17-C18
27	AC	517	DGD	O6E-C5E-C6E-O5E
30	AI	101	LMG	O6-C5-C6-O5
27	BC	517	DGD	O6D-C5D-C6D-O5D
30	BD	407	LMG	C4-C5-C6-O5
22	AB	601	CLA	C2A-CAA-CBA-CGA
22	AB	607	CLA	C2A-CAA-CBA-CGA
22	AB	610	CLA	C2A-CAA-CBA-CGA
22	BB	610	CLA	C2A-CAA-CBA-CGA
22	BB	613	CLA	C2A-CAA-CBA-CGA
22	AB	601	CLA	C10-C11-C12-C13
22	AB	614	CLA	C15-C16-C17-C18
22	AC	501	CLA	C15-C16-C17-C18
22	AC	506	CLA	C13-C15-C16-C17
22	AD	404	CLA	C15-C16-C17-C18
22	BB	617	CLA	C15-C16-C17-C18
22	BC	506	CLA	C13-C15-C16-C17
22	BC	509	CLA	C15-C16-C17-C18
24	AD	405	PL9	C47-C48-C49-C51
24	BD	405	PL9	C47-C48-C49-C51
27	AA	410	DGD	C1B-C2B-C3B-C4B

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Mol	Chain	Res	Type	Atoms
27	AC	516	DGD	C1A-C2A-C3A-C4A
27	BA	411	DGD	C1B-C2B-C3B-C4B
30	AB	622	LMG	C10-C11-C12-C13
30	AB	623	LMG	C28-C29-C30-C31
30	AC	520	LMG	C28-C29-C30-C31
30	AE	102	LMG	C28-C29-C30-C31
30	BB	624	LMG	C10-C11-C12-C13
22	AB	614	CLA	O1D-CGD-O2D-CED
22	BB	605	CLA	O1D-CGD-O2D-CED
22	BB	617	CLA	C3-C5-C6-C7
30	AD	407	LMG	C4-C5-C6-O5
22	AB	609	CLA	C5-C6-C7-C8
22	AB	611	CLA	C15-C16-C17-C18
22	AB	613	CLA	C5-C6-C7-C8
22	AB	613	CLA	C13-C15-C16-C17
22	AB	614	CLA	C5-C6-C7-C8
22	AC	507	CLA	C5-C6-C7-C8
22	AC	509	CLA	C15-C16-C17-C18
22	AC	512	CLA	C13-C15-C16-C17
22	BB	605	CLA	C13-C15-C16-C17
22	BB	611	CLA	C15-C16-C17-C18
22	BC	504	CLA	C13-C15-C16-C17
22	BD	404	CLA	C15-C16-C17-C18
23	AD	403	PHO	C15-C16-C17-C18
29	AA	412	SQD	C29-C30-C31-C32
29	BA	413	SQD	C29-C30-C31-C32
27	AC	516	DGD	O6D-C5D-C6D-O5D
27	AC	517	DGD	O6D-C5D-C6D-O5D
27	BC	516	DGD	O6D-C5D-C6D-O5D
28	AC	521	LHG	O2-C2-C3-O3
28	BC	521	LHG	O2-C2-C3-O3
27	AB	626	DGD	C1A-C2A-C3A-C4A
27	BB	602	DGD	C1A-C2A-C3A-C4A
30	AC	519	LMG	C10-C11-C12-C13
30	BC	519	LMG	C10-C11-C12-C13
22	AB	603	CLA	C5-C6-C7-C8
22	AB	607	CLA	C13-C15-C16-C17
22	AC	504	CLA	C13-C15-C16-C17
22	BB	606	CLA	C5-C6-C7-C8
22	BB	610	CLA	C13-C15-C16-C17
22	BC	506	CLA	C5-C6-C7-C8
24	AD	405	PL9	C47-C48-C49-C50

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Mol	Chain	Res	Type	Atoms
24	BD	405	PL9	C47-C48-C49-C50
22	AD	402	CLA	C15-C16-C17-C18
22	BB	610	CLA	C5-C6-C7-C8
22	BD	402	CLA	C15-C16-C17-C18
27	AD	410	DGD	C1B-C2B-C3B-C4B
27	BD	410	DGD	C1B-C2B-C3B-C4B
30	AB	623	LMG	C10-C11-C12-C13
22	AB	607	CLA	C5-C6-C7-C8
22	AB	615	CLA	C5-C6-C7-C8
22	BB	612	CLA	C5-C6-C7-C8
22	BB	615	CLA	C13-C15-C16-C17
22	BB	618	CLA	C5-C6-C7-C8
29	AF	101	SQD	C8-C7-O47-C45
30	BI	101	LMG	C11-C10-O7-C8
30	AA	416	LMG	C10-C11-C12-C13
22	AB	605	CLA	C5-C6-C7-C8
22	AB	612	CLA	C13-C15-C16-C17
29	AF	101	SQD	O49-C7-O47-C45
30	BI	101	LMG	O9-C10-O7-C8
22	AB	604	CLA	C13-C15-C16-C17
22	AB	606	CLA	C10-C11-C12-C13
22	AB	612	CLA	C5-C6-C7-C8
22	AB	615	CLA	C13-C15-C16-C17
22	AC	506	CLA	C5-C6-C7-C8
22	AC	508	CLA	C15-C16-C17-C18
22	BA	407	CLA	C10-C11-C12-C13
22	BB	605	CLA	C5-C6-C7-C8
22	BB	607	CLA	C13-C15-C16-C17
22	BB	609	CLA	C10-C11-C12-C13
22	BB	615	CLA	C5-C6-C7-C8
22	BB	618	CLA	C13-C15-C16-C17
22	BC	508	CLA	C15-C16-C17-C18
22	AA	406	CLA	C5-C6-C7-C8
22	BB	608	CLA	C5-C6-C7-C8
27	BB	602	DGD	C4E-C5E-C6E-O5E
22	AC	506	CLA	O1D-CGD-O2D-CED
22	AB	602	CLA	C5-C6-C7-C8
22	AC	508	CLA	C5-C6-C7-C8
22	BB	619	CLA	C13-C15-C16-C17
23	AA	405	PHO	O1D-CGD-O2D-CED
23	AA	405	PHO	C4-C3-C5-C6
22	AB	616	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
29	BF	101	SQD	C8-C7-O47-C45
30	AD	408	LMG	C11-C10-O7-C8
30	AI	101	LMG	C11-C10-O7-C8
30	BD	408	LMG	C11-C10-O7-C8
22	AB	602	CLA	O1D-CGD-O2D-CED
29	BF	101	SQD	O49-C7-O47-C45
30	AD	408	LMG	O9-C10-O7-C8
30	AI	101	LMG	O9-C10-O7-C8
30	BD	408	LMG	O9-C10-O7-C8
27	AC	517	DGD	C2D-C1D-O3G-C3G
27	BC	517	DGD	C2D-C1D-O3G-C3G
22	AD	402	CLA	C13-C15-C16-C17
22	BC	506	CLA	O1D-CGD-O2D-CED
22	BC	508	CLA	C5-C6-C7-C8
22	AB	602	CLA	C2A-CAA-CBA-CGA
22	AC	504	CLA	C2A-CAA-CBA-CGA
22	AC	512	CLA	C2A-CAA-CBA-CGA
22	BB	605	CLA	C2A-CAA-CBA-CGA
22	BC	504	CLA	C2A-CAA-CBA-CGA
22	BC	512	CLA	C2A-CAA-CBA-CGA
22	AA	404	CLA	C10-C11-C12-C13
22	AA	406	CLA	C10-C11-C12-C13
22	AB	616	CLA	C10-C11-C12-C13
22	BA	405	CLA	C10-C11-C12-C13
22	BB	619	CLA	C10-C11-C12-C13
30	BI	101	LMG	C10-C11-C12-C13
22	AA	403	CLA	O2A-C1-C2-C3
22	AC	509	CLA	O2A-C1-C2-C3
22	BA	404	CLA	O2A-C1-C2-C3
22	BC	509	CLA	O2A-C1-C2-C3
23	AA	405	PHO	O2A-C1-C2-C3
23	BA	406	PHO	O2A-C1-C2-C3
30	AE	102	LMG	C7-C8-O7-C10
30	BE	102	LMG	C7-C8-O7-C10
22	BB	610	CLA	C3-C5-C6-C7
30	AC	519	LMG	O9-C10-O7-C8
27	AB	626	DGD	O6E-C1E-O5D-C6D
27	AC	517	DGD	O6D-C1D-O3G-C3G
27	BB	602	DGD	O6E-C1E-O5D-C6D
27	BC	517	DGD	O6D-C1D-O3G-C3G
30	AC	519	LMG	C11-C10-O7-C8
30	BC	519	LMG	C11-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
22	AC	513	CLA	C15-C16-C17-C18
27	AC	516	DGD	C4D-C5D-C6D-O5D
27	BC	516	DGD	C4D-C5D-C6D-O5D
30	BE	102	LMG	O6-C5-C6-O5
27	AB	626	DGD	O2G-C2G-C3G-O3G
32	AB	624	LMT	C1-C2-C3-C4
22	BC	503	CLA	C5-C6-C7-C8
27	AC	516	DGD	C3A-C4A-C5A-C6A
27	AC	517	DGD	C2A-C3A-C4A-C5A
27	BC	516	DGD	C3A-C4A-C5A-C6A
27	BD	410	DGD	CAB-CBB-CCB-CDB
28	AA	411	LHG	C25-C26-C27-C28
27	AC	516	DGD	C3B-C4B-C5B-C6B
27	AC	517	DGD	CAB-CBB-CCB-CDB
27	AD	410	DGD	CAB-CBB-CCB-CDB
27	BC	517	DGD	C2A-C3A-C4A-C5A
28	BA	412	LHG	C25-C26-C27-C28
29	BB	601	SQD	C11-C10-C9-C8
29	BL	101	SQD	C11-C10-C9-C8
30	AA	416	LMG	C18-C19-C20-C21
30	AI	101	LMG	C14-C15-C16-C17
30	BI	101	LMG	C14-C15-C16-C17
23	BA	406	PHO	O1D-CGD-O2D-CED
22	AC	503	CLA	C5-C6-C7-C8
22	BB	619	CLA	C5-C6-C7-C8
27	AC	518	DGD	C9B-CAB-CBB-CCB
27	AD	410	DGD	C2A-C3A-C4A-C5A
27	AH	102	DGD	C6B-C7B-C8B-C9B
27	BC	516	DGD	C3B-C4B-C5B-C6B
27	BD	410	DGD	C2A-C3A-C4A-C5A
27	AA	410	DGD	O6D-C5D-C6D-O5D
27	AH	102	DGD	O6D-C5D-C6D-O5D
27	BA	411	DGD	O6D-C5D-C6D-O5D
27	BH	101	DGD	O6D-C5D-C6D-O5D
27	BB	602	DGD	C9B-CAB-CBB-CCB
27	BC	517	DGD	CAB-CBB-CCB-CDB
27	BD	410	DGD	C3B-C4B-C5B-C6B
27	BD	410	DGD	CDB-CEB-CFB-CGB
27	BH	101	DGD	C6B-C7B-C8B-C9B
29	AA	412	SQD	C27-C28-C29-C30
30	AA	413	LMG	C14-C15-C16-C17
30	AB	623	LMG	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
30	AD	408	LMG	C19-C20-C21-C22
30	BA	414	LMG	C14-C15-C16-C17
27	BC	518	DGD	O1B-C1B-O2G-C2G
28	AC	521	LHG	O1-C1-C2-O2
28	BC	521	LHG	O1-C1-C2-O2
27	AB	626	DGD	C9B-CAB-CBB-CCB
27	AD	410	DGD	C3B-C4B-C5B-C6B
27	BC	518	DGD	C9B-CAB-CBB-CCB
27	BD	410	DGD	C3A-C4A-C5A-C6A
27	BD	410	DGD	C5A-C6A-C7A-C8A
30	AC	520	LMG	C12-C13-C14-C15
30	BC	520	LMG	C12-C13-C14-C15
22	BC	513	CLA	C15-C16-C17-C18
22	BB	617	CLA	C4C-C3C-CAC-CBC
22	AB	602	CLA	C4B-C3B-CAB-CBB
22	AB	609	CLA	C4B-C3B-CAB-CBB
22	AB	613	CLA	C4B-C3B-CAB-CBB
22	AC	510	CLA	C4B-C3B-CAB-CBB
22	BB	605	CLA	C4B-C3B-CAB-CBB
22	BB	612	CLA	C4B-C3B-CAB-CBB
22	BB	616	CLA	C4B-C3B-CAB-CBB
22	BC	501	CLA	C4B-C3B-CAB-CBB
22	BC	510	CLA	C4B-C3B-CAB-CBB
27	AD	410	DGD	C5A-C6A-C7A-C8A
27	AD	410	DGD	CDB-CEB-CFB-CGB
29	AF	101	SQD	C27-C28-C29-C30
29	BF	101	SQD	C27-C28-C29-C30
24	AD	405	PL9	C22-C23-C24-C26
29	BA	413	SQD	C27-C28-C29-C30
30	AA	416	LMG	C32-C33-C34-C35
22	AB	609	CLA	C13-C15-C16-C17
22	AB	616	CLA	C5-C6-C7-C8
22	BB	612	CLA	C13-C15-C16-C17
32	BB	625	LMT	C1-C2-C3-C4
27	AC	518	DGD	C2B-C1B-O2G-C2G
27	BC	518	DGD	C2B-C1B-O2G-C2G
28	AA	411	LHG	C8-C7-O7-C5
28	BA	412	LHG	C8-C7-O7-C5
28	AA	411	LHG	C30-C31-C32-C33
22	BC	511	CLA	C11-C10-C8-C7
27	AC	517	DGD	C9A-CAA-CBA-CCA
27	AD	410	DGD	C3A-C4A-C5A-C6A

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Mol	Chain	Res	Type	Atoms
28	BA	412	LHG	C30-C31-C32-C33
30	AE	102	LMG	C15-C16-C17-C18
30	BB	623	LMG	C31-C32-C33-C34
32	BI	102	LMT	C6-C7-C8-C9
30	AI	101	LMG	C10-C11-C12-C13
22	BA	407	CLA	C5-C6-C7-C8
22	BD	402	CLA	C13-C15-C16-C17
27	AD	410	DGD	C7B-C8B-C9B-CAB
29	AD	409	SQD	C11-C10-C9-C8
30	AB	621	LMG	C31-C32-C33-C34
30	AB	622	LMG	C15-C16-C17-C18
30	AB	623	LMG	C32-C33-C34-C35
30	AM	101	LMG	C29-C30-C31-C32
30	BD	408	LMG	C19-C20-C21-C22
30	BE	102	LMG	C15-C16-C17-C18
30	BM	102	LMG	C29-C30-C31-C32
27	AB	626	DGD	C4E-C5E-C6E-O5E
22	AB	602	CLA	C3A-C2A-CAA-CBA
22	AC	505	CLA	C3A-C2A-CAA-CBA
22	AC	507	CLA	C3A-C2A-CAA-CBA
22	AC	512	CLA	C3A-C2A-CAA-CBA
22	BB	605	CLA	C3A-C2A-CAA-CBA
22	BB	611	CLA	C3A-C2A-CAA-CBA
22	BC	505	CLA	C3A-C2A-CAA-CBA
22	BC	507	CLA	C3A-C2A-CAA-CBA
22	BC	512	CLA	C3A-C2A-CAA-CBA
28	BC	521	LHG	C25-C26-C27-C28
29	BB	601	SQD	C11-C12-C13-C14
32	AI	102	LMT	C6-C7-C8-C9
22	AB	614	CLA	C4C-C3C-CAC-CBC
28	AC	521	LHG	C25-C26-C27-C28
22	AB	612	CLA	O1D-CGD-O2D-CED
27	BB	602	DGD	C5A-C6A-C7A-C8A
27	BD	410	DGD	C7B-C8B-C9B-CAB
30	BC	519	LMG	O9-C10-O7-C8
30	AD	408	LMG	C32-C33-C34-C35
27	AC	517	DGD	C1G-C2G-C3G-O3G
27	AA	410	DGD	C8B-C9B-CAB-CBB
27	BA	411	DGD	C8B-C9B-CAB-CBB
27	BH	101	DGD	C5B-C6B-C7B-C8B
30	AA	416	LMG	C11-C12-C13-C14
30	AB	623	LMG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
30	AI	101	LMG	C16-C17-C18-C19
30	BB	624	LMG	C13-C14-C15-C16
30	BD	408	LMG	C29-C30-C31-C32
30	BD	408	LMG	C32-C33-C34-C35
30	BI	101	LMG	C16-C17-C18-C19
22	AB	607	CLA	C3-C5-C6-C7
22	AB	616	CLA	C3-C5-C6-C7
22	AC	512	CLA	C3-C5-C6-C7
22	BB	619	CLA	C3-C5-C6-C7
30	AC	520	LMG	C10-C11-C12-C13
27	AC	516	DGD	C4B-C5B-C6B-C7B
27	AD	410	DGD	CEB-CFB-CGB-CHB
27	AH	102	DGD	C5B-C6B-C7B-C8B
27	BC	517	DGD	C9A-CAA-CBA-CCA
27	BD	410	DGD	C6B-C7B-C8B-C9B
28	BC	521	LHG	C24-C25-C26-C27
30	AA	413	LMG	C31-C32-C33-C34
30	AB	623	LMG	C31-C32-C33-C34
30	AD	407	LMG	C17-C18-C19-C20
30	AI	101	LMG	C12-C13-C14-C15
30	BB	624	LMG	C15-C16-C17-C18
30	BD	407	LMG	C17-C18-C19-C20
27	AB	626	DGD	C5A-C6A-C7A-C8A
27	BC	516	DGD	C4B-C5B-C6B-C7B
27	BD	410	DGD	C7A-C8A-C9A-CAA
29	BL	101	SQD	C11-C12-C13-C14
30	BA	414	LMG	C31-C32-C33-C34
27	BD	410	DGD	CEB-CFB-CGB-CHB
28	AC	521	LHG	C24-C25-C26-C27
29	BD	409	SQD	C11-C10-C9-C8
30	BI	101	LMG	C12-C13-C14-C15
22	BB	615	CLA	O1D-CGD-O2D-CED
30	AA	413	LMG	C34-C35-C36-C37
30	AB	622	LMG	C13-C14-C15-C16
30	AB	622	LMG	C31-C32-C33-C34
30	AD	408	LMG	C29-C30-C31-C32
30	BA	414	LMG	C34-C35-C36-C37
30	BD	408	LMG	C15-C16-C17-C18
27	AD	410	DGD	C1A-C2A-C3A-C4A
27	BD	410	DGD	C1A-C2A-C3A-C4A
22	AB	609	CLA	C2B-C3B-CAB-CBB
22	AB	611	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
22	AB	614	CLA	C2B-C3B-CAB-CBB
22	AC	501	CLA	C2B-C3B-CAB-CBB
22	AC	510	CLA	C2B-C3B-CAB-CBB
22	BB	612	CLA	C2B-C3B-CAB-CBB
22	BB	617	CLA	C2B-C3B-CAB-CBB
22	BC	501	CLA	C2B-C3B-CAB-CBB
22	BC	510	CLA	C2B-C3B-CAB-CBB
26	AA	409	BCR	C1-C6-C7-C8
26	AA	409	BCR	C5-C6-C7-C8
26	AA	409	BCR	C23-C24-C25-C26
26	AA	409	BCR	C23-C24-C25-C30
26	AC	515	BCR	C23-C24-C25-C30
26	AD	406	BCR	C1-C6-C7-C8
26	AD	406	BCR	C5-C6-C7-C8
26	AH	101	BCR	C1-C6-C7-C8
26	AH	101	BCR	C5-C6-C7-C8
26	AJ	102	BCR	C23-C24-C25-C26
26	AK	102	BCR	C1-C6-C7-C8
26	AK	102	BCR	C5-C6-C7-C8
26	AK	102	BCR	C23-C24-C25-C26
26	AK	102	BCR	C23-C24-C25-C30
26	BA	410	BCR	C1-C6-C7-C8
26	BA	410	BCR	C5-C6-C7-C8
26	BA	410	BCR	C23-C24-C25-C26
26	BA	410	BCR	C23-C24-C25-C30
26	BC	514	BCR	C23-C24-C25-C30
26	BC	515	BCR	C23-C24-C25-C30
26	BD	406	BCR	C1-C6-C7-C8
26	BD	406	BCR	C5-C6-C7-C8
26	BK	102	BCR	C1-C6-C7-C8
26	BK	102	BCR	C5-C6-C7-C8
26	BK	102	BCR	C23-C24-C25-C26
26	BK	102	BCR	C23-C24-C25-C30
26	BX	101	BCR	C1-C6-C7-C8
26	BX	101	BCR	C5-C6-C7-C8
27	AD	410	DGD	C6B-C7B-C8B-C9B
27	AD	410	DGD	CCB-CDB-CEB-CFB
30	AA	416	LMG	C31-C32-C33-C34
30	AC	519	LMG	C34-C35-C36-C37
30	BA	414	LMG	C30-C31-C32-C33
30	BB	624	LMG	C31-C32-C33-C34
22	AC	506	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
27	BD	410	DGD	C4B-C5B-C6B-C7B
27	BD	410	DGD	CCB-CDB-CEB-CFB
30	BI	101	LMG	C13-C14-C15-C16
30	AB	621	LMG	C15-C16-C17-C18
30	AD	408	LMG	C15-C16-C17-C18
30	AI	101	LMG	C13-C14-C15-C16
30	BC	520	LMG	C10-C11-C12-C13
27	AC	518	DGD	C3B-C4B-C5B-C6B
27	AD	410	DGD	C4B-C5B-C6B-C7B
30	AA	413	LMG	C30-C31-C32-C33
30	AB	623	LMG	C30-C31-C32-C33
27	BC	517	DGD	C4B-C5B-C6B-C7B
30	BC	519	LMG	C34-C35-C36-C37
32	BT	101	LMT	C7-C8-C9-C10
27	AC	518	DGD	O1B-C1B-O2G-C2G
28	AA	411	LHG	O9-C7-O7-C5
28	BA	412	LHG	O9-C7-O7-C5
23	BA	406	PHO	C4-C3-C5-C6
27	AH	102	DGD	C3B-C4B-C5B-C6B
30	BB	623	LMG	C20-C21-C22-C23
22	AB	610	CLA	C2-C3-C5-C6
22	BB	613	CLA	C2-C3-C5-C6
23	AA	405	PHO	C2-C3-C5-C6
23	BA	406	PHO	C2-C3-C5-C6
27	AC	517	DGD	C4A-C5A-C6A-C7A
27	AD	410	DGD	C7A-C8A-C9A-CAA
27	BH	101	DGD	C3B-C4B-C5B-C6B
30	AA	416	LMG	C30-C31-C32-C33
30	BB	623	LMG	C15-C16-C17-C18
30	BE	102	LMG	C17-C18-C19-C20
27	AC	517	DGD	C4B-C5B-C6B-C7B
27	BC	518	DGD	C3B-C4B-C5B-C6B
30	AB	621	LMG	C17-C18-C19-C20
30	AE	102	LMG	C17-C18-C19-C20
32	AT	101	LMT	C7-C8-C9-C10
26	AJ	102	BCR	C6-C7-C8-C9
26	BJ	102	BCR	C6-C7-C8-C9
30	AB	621	LMG	C20-C21-C22-C23
27	AH	102	DGD	C2E-C1E-O5D-C6D
27	BH	101	DGD	C2E-C1E-O5D-C6D
30	AE	102	LMG	C2-C1-O1-C7
27	AB	626	DGD	C8B-C9B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
27	AC	516	DGD	C2A-C3A-C4A-C5A
27	AC	518	DGD	C1A-C2A-C3A-C4A
27	BC	518	DGD	C1A-C2A-C3A-C4A
30	AE	102	LMG	O6-C5-C6-O5
27	BB	602	DGD	C8B-C9B-CAB-CBB
27	BC	516	DGD	C4A-C5A-C6A-C7A
30	AD	408	LMG	C36-C37-C38-C39
27	AC	516	DGD	C4A-C5A-C6A-C7A
27	BC	516	DGD	C2A-C3A-C4A-C5A
27	BC	517	DGD	C4A-C5A-C6A-C7A
30	BB	623	LMG	C36-C37-C38-C39
30	BB	623	LMG	C17-C18-C19-C20
29	BB	601	SQD	C8-C7-O47-C45
29	BL	101	SQD	C8-C7-O47-C45
30	AA	413	LMG	C11-C10-O7-C8
30	AE	102	LMG	C11-C10-O7-C8
30	BA	414	LMG	C11-C10-O7-C8
30	BE	102	LMG	C11-C10-O7-C8
30	BB	623	LMG	C18-C19-C20-C21
22	AA	404	CLA	C15-C16-C17-C18
22	AD	402	CLA	C5-C6-C7-C8
22	BC	506	CLA	C10-C11-C12-C13
22	BD	402	CLA	C5-C6-C7-C8
30	BD	408	LMG	C36-C37-C38-C39
27	BA	411	DGD	C7A-C8A-C9A-CAA
28	BC	521	LHG	C11-C10-C9-C8
30	AB	621	LMG	C18-C19-C20-C21
22	BC	512	CLA	C3-C5-C6-C7
32	AI	102	LMT	C5'-C4'-O1B-C1B
32	BI	102	LMT	C5'-C4'-O1B-C1B
27	AA	410	DGD	C5D-C6D-O5D-C1E
27	AC	517	DGD	C5D-C6D-O5D-C1E
27	BA	411	DGD	C5D-C6D-O5D-C1E
27	BC	517	DGD	C5D-C6D-O5D-C1E
30	AD	407	LMG	C36-C37-C38-C39
22	BB	609	CLA	C2A-CAA-CBA-CGA
27	AA	410	DGD	C7A-C8A-C9A-CAA
30	AA	416	LMG	C15-C16-C17-C18
30	AD	407	LMG	C34-C35-C36-C37
22	AB	610	CLA	C4-C3-C5-C6
27	AH	102	DGD	C7A-C8A-C9A-CAA
30	AA	416	LMG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
30	AB	621	LMG	C36-C37-C38-C39
30	AC	520	LMG	C29-C30-C31-C32
30	BC	520	LMG	C29-C30-C31-C32
30	BD	407	LMG	C36-C37-C38-C39
22	AC	504	CLA	C15-C16-C17-C18
32	AT	101	LMT	C2-C3-C4-C5
22	BC	509	CLA	C5-C6-C7-C8
23	AD	403	PHO	C10-C11-C12-C13
30	AB	623	LMG	C12-C13-C14-C15
30	AB	623	LMG	C15-C16-C17-C18
28	AC	521	LHG	C11-C10-C9-C8
30	AE	102	LMG	O9-C10-O7-C8
30	BE	102	LMG	O9-C10-O7-C8
22	BC	504	CLA	C15-C16-C17-C18
29	AA	412	SQD	O47-C45-C46-O48
29	AD	409	SQD	O6-C44-C45-O47
29	BA	413	SQD	O47-C45-C46-O48
29	BD	409	SQD	O6-C44-C45-O47
30	AA	413	LMG	O1-C7-C8-O7
30	BA	414	LMG	O1-C7-C8-O7
27	BH	101	DGD	C7A-C8A-C9A-CAA
30	AB	622	LMG	C34-C35-C36-C37
30	BD	408	LMG	C13-C14-C15-C16
30	BE	102	LMG	C18-C19-C20-C21
32	BT	101	LMT	C2-C3-C4-C5
22	BA	405	CLA	C15-C16-C17-C18
27	AC	518	DGD	C8B-C9B-CAB-CBB
27	BC	518	DGD	C8B-C9B-CAB-CBB
30	BB	624	LMG	C12-C13-C14-C15
30	BD	407	LMG	C34-C35-C36-C37
22	BB	613	CLA	C4-C3-C5-C6
29	BB	601	SQD	C9-C10-C11-C12
30	AA	413	LMG	C19-C20-C21-C22
30	BC	519	LMG	C12-C13-C14-C15
22	AB	606	CLA	C2A-CAA-CBA-CGA
22	BA	403	CLA	C2A-CAA-CBA-CGA
29	BL	101	SQD	C12-C13-C14-C15
30	AC	519	LMG	C12-C13-C14-C15
30	AD	408	LMG	C13-C14-C15-C16
30	AE	102	LMG	C18-C19-C20-C21
30	BB	624	LMG	C34-C35-C36-C37
22	AC	503	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
30	AA	416	LMG	O6-C5-C6-O5
22	BB	604	CLA	C4C-C3C-CAC-CBC
27	AC	518	DGD	CAB-CBB-CCB-CDB
27	BC	518	DGD	CEA-CFA-CGA-CHA
27	BC	518	DGD	CAB-CBB-CCB-CDB
22	AA	404	CLA	C3-C5-C6-C7
22	BB	605	CLA	C3-C5-C6-C7
32	AB	627	LMT	C5'-C4'-O1B-C1B
32	BB	603	LMT	C5'-C4'-O1B-C1B
22	AA	406	CLA	C1A-C2A-CAA-CBA
22	AC	501	CLA	C1A-C2A-CAA-CBA
22	AC	507	CLA	C1A-C2A-CAA-CBA
22	AC	512	CLA	C1A-C2A-CAA-CBA
22	BA	407	CLA	C1A-C2A-CAA-CBA
22	BC	501	CLA	C1A-C2A-CAA-CBA
22	BC	507	CLA	C1A-C2A-CAA-CBA
22	BC	512	CLA	C1A-C2A-CAA-CBA
22	AA	404	CLA	C5-C6-C7-C8
27	AC	517	DGD	C2B-C3B-C4B-C5B
30	BA	414	LMG	C19-C20-C21-C22
27	BC	517	DGD	CCB-CDB-CEB-CFB
29	BB	601	SQD	C12-C13-C14-C15
27	AC	517	DGD	CCB-CDB-CEB-CFB
22	AB	608	CLA	C5-C6-C7-C8
23	AD	403	PHO	C13-C15-C16-C17
29	BL	101	SQD	O49-C7-O47-C45
27	AC	518	DGD	CEA-CFA-CGA-CHA
30	AA	413	LMG	C16-C17-C18-C19
30	AB	622	LMG	C12-C13-C14-C15
22	AA	404	CLA	C6-C7-C8-C10
22	AB	602	CLA	C11-C10-C8-C7
22	AB	602	CLA	C12-C13-C15-C16
22	AB	609	CLA	C12-C13-C15-C16
22	AB	611	CLA	C6-C7-C8-C10
22	AB	615	CLA	C12-C13-C15-C16
22	AC	502	CLA	C12-C13-C15-C16
22	AC	505	CLA	C12-C13-C15-C16
22	AC	511	CLA	C11-C10-C8-C7
22	AC	512	CLA	C11-C12-C13-C15
22	BA	405	CLA	C6-C7-C8-C10
22	BB	605	CLA	C11-C10-C8-C7
22	BB	605	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
22	BB	612	CLA	C12-C13-C15-C16
22	BB	614	CLA	C6-C7-C8-C10
22	BB	618	CLA	C12-C13-C15-C16
22	BC	502	CLA	C12-C13-C15-C16
22	BC	505	CLA	C12-C13-C15-C16
22	BC	512	CLA	C11-C12-C13-C15
23	AD	403	PHO	C11-C10-C8-C7
23	AD	403	PHO	C12-C13-C15-C16
23	BD	403	PHO	C11-C10-C8-C7
23	BD	403	PHO	C12-C13-C15-C16
27	BB	602	DGD	C2A-C3A-C4A-C5A
29	BL	101	SQD	C9-C10-C11-C12
30	BA	414	LMG	C38-C39-C40-C41
22	AB	610	CLA	C8-C10-C11-C12
22	AC	509	CLA	C5-C6-C7-C8
22	BB	613	CLA	C8-C10-C11-C12
22	BC	503	CLA	C15-C16-C17-C18
22	BC	513	CLA	C13-C15-C16-C17
23	BD	403	PHO	C10-C11-C12-C13
29	AA	415	SQD	C17-C18-C19-C20
30	AD	407	LMG	C31-C32-C33-C34
30	AB	623	LMG	O6-C5-C6-O5
22	AB	605	CLA	C10-C11-C12-C13
22	AC	513	CLA	C13-C15-C16-C17
22	AA	402	CLA	C2A-CAA-CBA-CGA
22	AA	404	CLA	C6-C7-C8-C9
22	AB	602	CLA	C11-C10-C8-C9
22	AB	606	CLA	C14-C13-C15-C16
22	AB	609	CLA	C14-C13-C15-C16
22	AB	613	CLA	C11-C12-C13-C14
22	AC	502	CLA	C6-C7-C8-C9
22	AC	512	CLA	C11-C12-C13-C14
22	AC	513	CLA	C6-C7-C8-C9
22	AD	402	CLA	C14-C13-C15-C16
22	BB	612	CLA	C14-C13-C15-C16
22	BB	614	CLA	C6-C7-C8-C9
22	BB	616	CLA	C11-C12-C13-C14
22	BC	506	CLA	C14-C13-C15-C16
22	BC	512	CLA	C11-C12-C13-C14
22	BD	402	CLA	C14-C13-C15-C16
23	AD	403	PHO	C11-C10-C8-C9
23	BD	403	PHO	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
23	BD	403	PHO	C14-C13-C15-C16
29	BA	401	SQD	C17-C18-C19-C20
32	AB	627	LMT	C1-C2-C3-C4
32	BB	603	LMT	C1-C2-C3-C4
27	BH	101	DGD	C4B-C5B-C6B-C7B
30	BA	414	LMG	C16-C17-C18-C19
29	BB	601	SQD	O49-C7-O47-C45
30	AD	408	LMG	C2-C1-O1-C7
30	BD	408	LMG	C2-C1-O1-C7
30	BE	102	LMG	C2-C1-O1-C7
22	BA	405	CLA	C5-C6-C7-C8
22	BB	611	CLA	C5-C6-C7-C8
27	AH	102	DGD	O1G-C1G-C2G-C3G
27	BB	602	DGD	C1G-C2G-C3G-O3G
27	BC	517	DGD	C1G-C2G-C3G-O3G
27	BH	101	DGD	O1G-C1G-C2G-C3G
28	BA	412	LHG	C4-C5-C6-O8
29	AA	415	SQD	O6-C44-C45-C46
29	BA	401	SQD	O6-C44-C45-C46
29	BA	413	SQD	C44-C45-C46-O48
29	BB	601	SQD	C44-C45-C46-O48
29	BL	101	SQD	C44-C45-C46-O48
30	AC	519	LMG	C7-C8-C9-O8
30	AM	101	LMG	C7-C8-C9-O8
30	BA	414	LMG	O1-C7-C8-C9
30	BC	519	LMG	C7-C8-C9-O8
30	BM	102	LMG	C7-C8-C9-O8
27	AA	410	DGD	C5B-C6B-C7B-C8B
29	AA	412	SQD	C9-C10-C11-C12
30	BD	407	LMG	C31-C32-C33-C34
30	AA	413	LMG	C38-C39-C40-C41
27	AH	102	DGD	C4B-C5B-C6B-C7B
27	BB	602	DGD	C4B-C5B-C6B-C7B
27	BC	517	DGD	C2B-C3B-C4B-C5B
29	BA	413	SQD	C9-C10-C11-C12
29	BA	413	SQD	C15-C16-C17-C18
30	AA	413	LMG	C29-C30-C31-C32
30	AI	101	LMG	C18-C19-C20-C21
22	AB	602	CLA	C3-C5-C6-C7
30	BI	101	LMG	C18-C19-C20-C21
27	AC	518	DGD	CDB-CEB-CFB-CGB
27	BC	518	DGD	CDB-CEB-CFB-CGB

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Mol	Chain	Res	Type	Atoms
22	BB	608	CLA	C10-C11-C12-C13
22	BC	510	CLA	C13-C15-C16-C17
30	AA	413	LMG	O9-C10-O7-C8
30	BA	414	LMG	O9-C10-O7-C8
23	BD	403	PHO	C13-C15-C16-C17
27	BA	411	DGD	C5B-C6B-C7B-C8B
29	AA	412	SQD	C15-C16-C17-C18
22	AA	403	CLA	C3-C5-C6-C7
22	BA	404	CLA	C3-C5-C6-C7
27	AB	626	DGD	C2A-C3A-C4A-C5A
27	BA	411	DGD	C4B-C5B-C6B-C7B
30	BE	102	LMG	C31-C32-C33-C34
30	AD	407	LMG	C28-C29-C30-C31
22	AB	601	CLA	C4C-C3C-CAC-CBC
27	BB	602	DGD	C3A-C4A-C5A-C6A
30	AB	621	LMG	C32-C33-C34-C35
30	BA	414	LMG	C29-C30-C31-C32
30	BB	623	LMG	C32-C33-C34-C35
23	BA	406	PHO	C5-C6-C7-C8
27	AB	626	DGD	C4B-C5B-C6B-C7B
27	AA	410	DGD	C4B-C5B-C6B-C7B
27	BD	410	DGD	CBA-CCA-CDA-CEA
27	AC	517	DGD	C1A-C2A-C3A-C4A
28	BC	521	LHG	C23-C24-C25-C26
30	BD	407	LMG	C28-C29-C30-C31
30	BD	408	LMG	C14-C15-C16-C17
26	BZ	101	BCR	C6-C7-C8-C9
27	AC	517	DGD	C7A-C8A-C9A-CAA
30	AB	621	LMG	C19-C20-C21-C22
27	AC	518	DGD	C2A-C1A-O1G-C1G
27	AH	102	DGD	CAB-CBB-CCB-CDB
30	AA	413	LMG	C20-C21-C22-C23
30	BB	623	LMG	C19-C20-C21-C22
27	AD	410	DGD	CBA-CCA-CDA-CEA
27	BC	517	DGD	C7A-C8A-C9A-CAA
30	BA	414	LMG	C20-C21-C22-C23
30	AD	408	LMG	C14-C15-C16-C17
30	AM	101	LMG	C13-C14-C15-C16
30	BM	102	LMG	C13-C14-C15-C16
27	AB	626	DGD	C3A-C4A-C5A-C6A
30	AB	623	LMG	C13-C14-C15-C16
30	AD	407	LMG	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
30	AE	102	LMG	C31-C32-C33-C34
30	BC	519	LMG	C30-C31-C32-C33
30	BD	407	LMG	C14-C15-C16-C17
28	BC	521	LHG	C7-C8-C9-C10
27	AC	517	DGD	CBB-CCB-CDB-CEB
27	AC	517	DGD	O2G-C2G-C3G-O3G
27	BC	517	DGD	O2G-C2G-C3G-O3G
30	AD	408	LMG	O1-C7-C8-O7
30	BD	408	LMG	O1-C7-C8-O7
29	BA	401	SQD	C25-C26-C27-C28
27	BH	101	DGD	CAB-CBB-CCB-CDB
30	BE	102	LMG	C19-C20-C21-C22
29	AF	101	SQD	C12-C13-C14-C15
29	AA	415	SQD	C12-C13-C14-C15
29	BA	401	SQD	C12-C13-C14-C15
22	BA	405	CLA	C3-C5-C6-C7
27	AH	102	DGD	C2A-C3A-C4A-C5A
30	AC	519	LMG	C30-C31-C32-C33
22	BC	501	CLA	C10-C11-C12-C13
27	BA	411	DGD	C7B-C8B-C9B-CAB
22	AC	501	CLA	C10-C11-C12-C13
29	AA	415	SQD	C25-C26-C27-C28
29	AF	101	SQD	C15-C16-C17-C18
27	BH	101	DGD	C2A-C3A-C4A-C5A
30	AA	416	LMG	C13-C14-C15-C16
24	AD	405	PL9	C7-C8-C9-C10
32	BB	626	LMT	C2B-C1B-O1B-C4'
27	BD	410	DGD	CBB-CCB-CDB-CEB
28	BC	521	LHG	C11-C12-C13-C14
29	BF	101	SQD	C15-C16-C17-C18
30	AB	621	LMG	C30-C31-C32-C33
30	AE	102	LMG	C19-C20-C21-C22
28	AC	521	LHG	C7-C8-C9-C10
28	AC	521	LHG	C23-C24-C25-C26
29	AF	101	SQD	C29-C30-C31-C32
22	AB	610	CLA	C5-C6-C7-C8
22	AB	610	CLA	C13-C15-C16-C17
22	BB	613	CLA	C5-C6-C7-C8
29	BF	101	SQD	C29-C30-C31-C32
30	BD	407	LMG	C38-C39-C40-C41
30	AD	407	LMG	C38-C39-C40-C41
27	BC	517	DGD	CBB-CCB-CDB-CEB

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Mol	Chain	Res	Type	Atoms
28	AC	521	LHG	C11-C12-C13-C14
30	AC	520	LMG	C34-C35-C36-C37
22	AB	608	CLA	C11-C12-C13-C14
22	AB	611	CLA	C6-C7-C8-C9
22	AB	616	CLA	C11-C10-C8-C9
22	AC	506	CLA	C14-C13-C15-C16
22	AC	511	CLA	C11-C10-C8-C9
22	BA	405	CLA	C6-C7-C8-C9
22	BB	605	CLA	C11-C10-C8-C9
22	BB	609	CLA	C14-C13-C15-C16
22	BB	611	CLA	C11-C12-C13-C14
22	BC	502	CLA	C6-C7-C8-C9
22	BC	511	CLA	C11-C10-C8-C9
22	BC	513	CLA	C6-C7-C8-C9
23	AD	403	PHO	C14-C13-C15-C16
22	AC	510	CLA	C13-C15-C16-C17
22	AC	513	CLA	C5-C6-C7-C8
28	AA	411	LHG	C2-C3-O3-P
28	BA	412	LHG	C2-C3-O3-P
22	AB	610	CLA	C4B-C3B-CAB-CBB
22	AB	611	CLA	C4B-C3B-CAB-CBB
22	BB	613	CLA	C4B-C3B-CAB-CBB
22	BB	614	CLA	C4B-C3B-CAB-CBB
29	AF	101	SQD	C10-C11-C12-C13
32	AB	625	LMT	C2B-C1B-O1B-C4'
30	AC	519	LMG	C15-C16-C17-C18
29	BF	101	SQD	C12-C13-C14-C15
27	AC	518	DGD	C4B-C5B-C6B-C7B
29	AA	412	SQD	C17-C18-C19-C20
30	AB	622	LMG	C38-C39-C40-C41
30	BB	623	LMG	C13-C14-C15-C16
29	AD	409	SQD	C2-C1-O6-C44
29	BD	409	SQD	C2-C1-O6-C44
22	AC	505	CLA	C15-C16-C17-C18
27	AA	410	DGD	C7B-C8B-C9B-CAB
27	AC	518	DGD	CFA-CGA-CHA-CIA
27	BC	518	DGD	CFA-CGA-CHA-CIA
30	BC	519	LMG	C15-C16-C17-C18
22	AA	403	CLA	C6-C7-C8-C10
22	AA	403	CLA	C12-C13-C15-C16
22	AB	601	CLA	C11-C10-C8-C7
22	AB	606	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
22	AB	608	CLA	C6-C7-C8-C10
22	AB	608	CLA	C11-C12-C13-C15
22	AB	613	CLA	C11-C12-C13-C15
22	AB	615	CLA	C11-C10-C8-C7
22	AB	616	CLA	C11-C10-C8-C7
22	AC	506	CLA	C12-C13-C15-C16
22	AC	510	CLA	C6-C7-C8-C10
22	AC	512	CLA	C12-C13-C15-C16
22	AC	513	CLA	C6-C7-C8-C10
22	AD	402	CLA	C12-C13-C15-C16
22	AD	404	CLA	C11-C10-C8-C7
22	BA	404	CLA	C6-C7-C8-C10
22	BB	604	CLA	C11-C10-C8-C7
22	BB	609	CLA	C12-C13-C15-C16
22	BB	611	CLA	C6-C7-C8-C10
22	BB	611	CLA	C11-C12-C13-C15
22	BB	616	CLA	C11-C12-C13-C15
22	BB	618	CLA	C11-C10-C8-C7
22	BB	619	CLA	C11-C10-C8-C7
22	BC	508	CLA	C11-C10-C8-C7
22	BC	510	CLA	C6-C7-C8-C10
22	BC	512	CLA	C12-C13-C15-C16
22	BC	513	CLA	C6-C7-C8-C10
22	BD	402	CLA	C12-C13-C15-C16
22	BD	404	CLA	C11-C10-C8-C7
22	AC	506	CLA	C15-C16-C17-C18
22	BB	613	CLA	C13-C15-C16-C17
23	AA	405	PHO	C5-C6-C7-C8
30	BB	623	LMG	C30-C31-C32-C33
28	BA	412	LHG	C9-C10-C11-C12
32	AT	101	LMT	C6-C7-C8-C9
30	AA	416	LMG	C14-C15-C16-C17
30	BB	624	LMG	C38-C39-C40-C41
22	AC	513	CLA	C3A-C2A-CAA-CBA
22	BB	615	CLA	C4-C3-C5-C6
22	BC	513	CLA	C3A-C2A-CAA-CBA
30	AB	621	LMG	C13-C14-C15-C16
22	AC	511	CLA	C5-C6-C7-C8
27	BC	518	DGD	C2A-C1A-O1G-C1G
27	BC	517	DGD	C8B-C9B-CAB-CBB
30	AC	520	LMG	C36-C37-C38-C39
27	BC	518	DGD	CBA-CCA-CDA-CEA

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Mol	Chain	Res	Type	Atoms
28	AA	411	LHG	C9-C10-C11-C12
30	AB	623	LMG	C14-C15-C16-C17
27	AB	626	DGD	C1G-C2G-C3G-O3G
27	AD	410	DGD	C1G-C2G-C3G-O3G
27	BD	410	DGD	C1G-C2G-C3G-O3G
28	AA	411	LHG	C4-C5-C6-O8
29	AA	412	SQD	C44-C45-C46-O48
29	AD	409	SQD	O6-C44-C45-C46
29	BD	409	SQD	O6-C44-C45-C46
30	AA	413	LMG	O1-C7-C8-C9
30	AD	408	LMG	O1-C7-C8-C9
30	AE	102	LMG	O1-C7-C8-C9
30	BE	102	LMG	O1-C7-C8-C9
29	BB	601	SQD	C17-C18-C19-C20
30	AD	407	LMG	C19-C20-C21-C22
22	BC	506	CLA	C15-C16-C17-C18
22	BC	513	CLA	C5-C6-C7-C8
27	BC	517	DGD	C3A-C4A-C5A-C6A
27	BH	101	DGD	C5A-C6A-C7A-C8A
27	AC	517	DGD	CDB-CEB-CFB-CGB
27	AD	410	DGD	CBB-CCB-CDB-CEB
29	BA	413	SQD	C17-C18-C19-C20
22	AA	404	CLA	C1-C2-C3-C4
22	AB	604	CLA	C1-C2-C3-C4
22	AB	605	CLA	C1-C2-C3-C4
22	AC	506	CLA	C1-C2-C3-C4
22	AC	511	CLA	C1-C2-C3-C4
22	BA	405	CLA	C1-C2-C3-C4
22	BB	604	CLA	C1-C2-C3-C4
22	BB	607	CLA	C1-C2-C3-C4
22	BB	608	CLA	C1-C2-C3-C4
22	BC	506	CLA	C1-C2-C3-C4
22	BC	511	CLA	C1-C2-C3-C4
27	BH	101	DGD	CCA-CDA-CEA-CFA
27	AA	410	DGD	C3B-C4B-C5B-C6B
27	AC	517	DGD	C8B-C9B-CAB-CBB
22	AB	612	CLA	C4-C3-C5-C6
27	BC	518	DGD	C4B-C5B-C6B-C7B
27	AC	518	DGD	O1A-C1A-O1G-C1G
32	BT	101	LMT	C6-C7-C8-C9
27	BC	517	DGD	C1A-C2A-C3A-C4A
22	AC	503	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
27	AC	517	DGD	C3A-C4A-C5A-C6A
30	BD	407	LMG	C19-C20-C21-C22
22	AB	610	CLA	C2B-C3B-CAB-CBB
22	BB	613	CLA	C2B-C3B-CAB-CBB
22	BB	614	CLA	C2B-C3B-CAB-CBB
26	AB	618	BCR	C23-C24-C25-C26
26	AC	514	BCR	C23-C24-C25-C30
26	AT	102	BCR	C23-C24-C25-C26
26	BJ	102	BCR	C23-C24-C25-C26
30	BC	520	LMG	C34-C35-C36-C37
27	BC	517	DGD	CDB-CEB-CFB-CGB
22	AB	612	CLA	C10-C11-C12-C13
27	BA	411	DGD	C3B-C4B-C5B-C6B
30	BC	520	LMG	C36-C37-C38-C39
27	AC	516	DGD	C4E-C5E-C6E-O5E
27	AH	102	DGD	C5A-C6A-C7A-C8A
22	BC	512	CLA	C16-C17-C18-C19
22	BC	512	CLA	C16-C17-C18-C20
28	AA	411	LHG	O7-C5-C6-O8
28	BA	412	LHG	O7-C5-C6-O8
30	AB	621	LMG	O1-C7-C8-O7
30	BB	623	LMG	O1-C7-C8-O7
30	BE	102	LMG	O1-C7-C8-O7
30	AB	621	LMG	C16-C17-C18-C19
24	AA	407	PL9	C4-C3-C7-C8
24	BA	408	PL9	C4-C3-C7-C8
27	BH	101	DGD	C7B-C8B-C9B-CAB
27	AA	410	DGD	C1A-C2A-C3A-C4A
32	BB	626	LMT	O5B-C1B-O1B-C4'
27	BC	517	DGD	C6B-C7B-C8B-C9B
30	AB	623	LMG	C17-C18-C19-C20
30	AC	519	LMG	C32-C33-C34-C35
30	BI	101	LMG	C31-C32-C33-C34
22	BA	404	CLA	C5-C6-C7-C8
29	BL	101	SQD	C17-C18-C19-C20
30	BC	519	LMG	C32-C33-C34-C35
22	AA	406	CLA	C1-C2-C3-C5
22	AB	601	CLA	C1-C2-C3-C5
22	AB	604	CLA	C1-C2-C3-C5
22	AC	512	CLA	C1-C2-C3-C5
22	BA	407	CLA	C1-C2-C3-C5
22	BB	604	CLA	C1-C2-C3-C5

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Mol	Chain	Res	Type	Atoms
22	BB	607	CLA	C1-C2-C3-C5
22	BC	512	CLA	C1-C2-C3-C5
27	BA	411	DGD	C2A-C3A-C4A-C5A
30	AA	416	LMG	C17-C18-C19-C20
30	BB	623	LMG	C16-C17-C18-C19
22	BC	503	CLA	C8-C10-C11-C12
30	BC	519	LMG	C28-C29-C30-C31
22	AA	403	CLA	C14-C13-C15-C16
22	AB	601	CLA	C11-C10-C8-C9
22	AC	502	CLA	C14-C13-C15-C16
22	AD	404	CLA	C14-C13-C15-C16
22	BA	404	CLA	C14-C13-C15-C16
22	BB	604	CLA	C11-C10-C8-C9
22	BB	619	CLA	C11-C10-C8-C9
22	BC	506	CLA	C11-C12-C13-C14
22	BD	404	CLA	C14-C13-C15-C16
27	AB	626	DGD	C4A-C5A-C6A-C7A
32	AB	625	LMT	O5B-C1B-O1B-C4'
26	AZ	101	BCR	C6-C7-C8-C9
30	BA	414	LMG	C15-C16-C17-C18
27	AC	517	DGD	CBA-CCA-CDA-CEA
27	BB	602	DGD	C4A-C5A-C6A-C7A
30	AM	101	LMG	C2-C1-O1-C7
30	BI	101	LMG	C2-C1-O1-C7
30	BM	102	LMG	C2-C1-O1-C7
27	AH	102	DGD	CCA-CDA-CEA-CFA
24	BA	408	PL9	C24-C26-C27-C28
27	AC	517	DGD	C6B-C7B-C8B-C9B
27	BC	517	DGD	CBA-CCA-CDA-CEA
30	BM	102	LMG	C14-C15-C16-C17
30	BC	519	LMG	C20-C21-C22-C23
22	BC	501	CLA	C13-C15-C16-C17
27	AA	410	DGD	C2A-C3A-C4A-C5A
22	AB	612	CLA	C2-C3-C5-C6
22	BB	615	CLA	C2-C3-C5-C6
22	AC	512	CLA	C16-C17-C18-C19
22	AC	512	CLA	C16-C17-C18-C20
22	BC	505	CLA	C15-C16-C17-C18
22	BC	511	CLA	C5-C6-C7-C8
29	BF	101	SQD	C10-C11-C12-C13
30	AA	413	LMG	C15-C16-C17-C18
22	AC	501	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
30	AB	623	LMG	C29-C30-C31-C32
30	AI	101	LMG	C31-C32-C33-C34
22	BB	615	CLA	C10-C11-C12-C13
22	BC	501	CLA	C8-C10-C11-C12
27	AH	102	DGD	C7B-C8B-C9B-CAB
30	AC	519	LMG	C20-C21-C22-C23
22	AA	403	CLA	C5-C6-C7-C8
22	AC	501	CLA	C13-C15-C16-C17
22	AB	605	CLA	C6-C7-C8-C10
22	AB	605	CLA	C11-C10-C8-C7
22	AC	504	CLA	C6-C7-C8-C10
22	AC	506	CLA	C11-C12-C13-C15
22	AC	511	CLA	C6-C7-C8-C10
22	AC	513	CLA	C11-C10-C8-C7
22	AD	404	CLA	C12-C13-C15-C16
22	BA	404	CLA	C12-C13-C15-C16
22	BB	608	CLA	C6-C7-C8-C10
22	BB	608	CLA	C11-C10-C8-C7
22	BC	504	CLA	C6-C7-C8-C10
22	BC	506	CLA	C11-C12-C13-C15
22	BC	506	CLA	C12-C13-C15-C16
22	BC	511	CLA	C6-C7-C8-C10
22	BD	404	CLA	C12-C13-C15-C16
30	AC	519	LMG	C28-C29-C30-C31
30	AM	101	LMG	C14-C15-C16-C17
22	BB	616	CLA	C8-C10-C11-C12
30	AM	101	LMG	C34-C35-C36-C37
27	BC	517	DGD	CEB-CFB-CGB-CHB
27	BC	518	DGD	O1A-C1A-O1G-C1G
30	AD	408	LMG	C8-C7-O1-C1
30	BA	414	LMG	C8-C7-O1-C1
30	BD	408	LMG	C8-C7-O1-C1
30	AC	520	LMG	C13-C14-C15-C16
27	BA	411	DGD	C1A-C2A-C3A-C4A
22	BD	404	CLA	C2A-CAA-CBA-CGA
30	BM	102	LMG	C34-C35-C36-C37
27	BD	410	DGD	CAA-CBA-CCA-CDA
30	AC	519	LMG	C17-C18-C19-C20
30	BA	414	LMG	C36-C37-C38-C39
30	AA	416	LMG	C29-C30-C31-C32
30	AC	520	LMG	C9-C8-O7-C10
30	BD	408	LMG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
27	AC	518	DGD	CBA-CCA-CDA-CEA
30	AB	621	LMG	O1-C7-C8-C9
30	BB	623	LMG	O1-C7-C8-C9
30	BD	408	LMG	O1-C7-C8-C9
30	BB	624	LMG	C36-C37-C38-C39
27	BC	516	DGD	C4E-C5E-C6E-O5E
22	AD	404	CLA	C2A-CAA-CBA-CGA
29	AA	415	SQD	C19-C20-C21-C22
22	AB	613	CLA	C8-C10-C11-C12
27	AC	517	DGD	CEB-CFB-CGB-CHB
27	AH	102	DGD	O1G-C1G-C2G-O2G
27	BH	101	DGD	O1G-C1G-C2G-O2G
29	BB	601	SQD	O47-C45-C46-O48
29	BL	101	SQD	O47-C45-C46-O48
30	AE	102	LMG	O1-C7-C8-O7
22	AB	605	CLA	C6-C7-C8-C9
22	AC	506	CLA	C11-C12-C13-C14
22	AC	512	CLA	C14-C13-C15-C16
22	BB	608	CLA	C6-C7-C8-C9
22	BC	512	CLA	C14-C13-C15-C16
30	BC	520	LMG	C13-C14-C15-C16
27	AB	626	DGD	C5B-C6B-C7B-C8B
27	BB	602	DGD	C5B-C6B-C7B-C8B
30	AB	622	LMG	C36-C37-C38-C39
30	AI	101	LMG	C19-C20-C21-C22
30	BC	519	LMG	C17-C18-C19-C20
30	BI	101	LMG	C19-C20-C21-C22
28	AA	411	LHG	C35-C36-C37-C38
30	AD	407	LMG	C13-C14-C15-C16
29	BA	401	SQD	C10-C11-C12-C13
30	BB	624	LMG	C18-C19-C20-C21
22	AB	608	CLA	C13-C15-C16-C17
30	AA	413	LMG	C36-C37-C38-C39
30	AI	101	LMG	C2-C1-O1-C7
30	BM	102	LMG	C30-C31-C32-C33
22	AB	609	CLA	C4-C3-C5-C6
22	BB	612	CLA	C4-C3-C5-C6
30	AB	622	LMG	C18-C19-C20-C21
30	BD	407	LMG	C13-C14-C15-C16
30	AC	519	LMG	C38-C39-C40-C41
27	AH	102	DGD	C4D-C5D-C6D-O5D
32	AB	627	LMT	O1'-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
30	AD	408	LMG	C31-C32-C33-C34
22	BB	608	CLA	C3-C5-C6-C7
22	AC	505	CLA	C2C-C3C-CAC-CBC
29	AA	415	SQD	C10-C11-C12-C13
27	BC	516	DGD	C5A-C6A-C7A-C8A
32	BB	603	LMT	O1'-C1-C2-C3
28	BA	412	LHG	C35-C36-C37-C38
27	BH	101	DGD	C4D-C5D-C6D-O5D
22	AA	404	CLA	C1A-C2A-CAA-CBA
22	AB	616	CLA	C4B-C3B-CAB-CBB
22	BB	607	CLA	C1A-C2A-CAA-CBA
22	BB	612	CLA	C1A-C2A-CAA-CBA
22	BB	619	CLA	C4B-C3B-CAB-CBB
26	AC	515	BCR	C6-C7-C8-C9
26	BC	515	BCR	C6-C7-C8-C9
30	AM	101	LMG	C30-C31-C32-C33
29	BA	401	SQD	C19-C20-C21-C22
22	AC	501	CLA	C2A-CAA-CBA-CGA
29	AF	101	SQD	C11-C12-C13-C14
22	BC	505	CLA	C2C-C3C-CAC-CBC
24	BD	405	PL9	C7-C8-C9-C10
24	BD	405	PL9	C17-C18-C19-C20
30	BC	519	LMG	C16-C17-C18-C19
29	AA	412	SQD	C25-C26-C27-C28
29	BA	413	SQD	C25-C26-C27-C28
22	AA	406	CLA	C11-C10-C8-C7
22	AB	602	CLA	C6-C7-C8-C10
22	AB	603	CLA	C11-C10-C8-C7
22	AB	607	CLA	C11-C10-C8-C7
22	AB	611	CLA	C11-C10-C8-C7
22	AC	502	CLA	C11-C10-C8-C7
22	AC	504	CLA	C11-C10-C8-C7
22	AC	506	CLA	C6-C7-C8-C10
22	AC	507	CLA	C11-C12-C13-C15
22	AC	507	CLA	C12-C13-C15-C16
22	AC	508	CLA	C11-C10-C8-C7
22	BA	407	CLA	C11-C10-C8-C7
22	BB	605	CLA	C6-C7-C8-C10
22	BB	606	CLA	C11-C10-C8-C7
22	BB	614	CLA	C11-C10-C8-C7
22	BC	502	CLA	C11-C10-C8-C7
22	BC	504	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
22	BC	506	CLA	C6-C7-C8-C10
22	BC	507	CLA	C12-C13-C15-C16
30	BC	519	LMG	C38-C39-C40-C41
30	BA	414	LMG	C12-C13-C14-C15
29	AA	412	SQD	C24-C25-C26-C27
29	AF	101	SQD	C9-C10-C11-C12
27	AC	516	DGD	C5A-C6A-C7A-C8A
27	AD	410	DGD	CAA-CBA-CCA-CDA
27	BB	602	DGD	CAB-CBB-CCB-CDB
22	BC	501	CLA	C2A-CAA-CBA-CGA
22	AB	605	CLA	C11-C10-C8-C9
22	AB	615	CLA	C11-C10-C8-C9
22	AC	504	CLA	C6-C7-C8-C9
22	AC	513	CLA	C11-C10-C8-C9
22	BB	608	CLA	C11-C10-C8-C9
22	BB	618	CLA	C11-C10-C8-C9
22	BB	618	CLA	C14-C13-C15-C16
22	BC	502	CLA	C14-C13-C15-C16
22	BC	504	CLA	C6-C7-C8-C9
22	BC	507	CLA	C14-C13-C15-C16
22	BC	510	CLA	C6-C7-C8-C9
27	AB	626	DGD	CAB-CBB-CCB-CDB
30	BD	408	LMG	C34-C35-C36-C37
29	AA	415	SQD	O5-C5-C6-S
29	BA	401	SQD	O5-C5-C6-S
30	AA	413	LMG	C12-C13-C14-C15
30	BD	408	LMG	C20-C21-C22-C23
22	AB	605	CLA	C3-C5-C6-C7
30	AD	408	LMG	C22-C23-C24-C25
29	AA	415	SQD	C11-C10-C9-C8
29	BA	413	SQD	C24-C25-C26-C27
22	BB	611	CLA	C13-C15-C16-C17
30	AD	408	LMG	C34-C35-C36-C37
22	BB	614	CLA	C8-C10-C11-C12
22	AB	609	CLA	C2-C3-C5-C6
22	AB	614	CLA	CAD-CBD-CGD-O2D
22	BB	617	CLA	CAD-CBD-CGD-O2D
22	AB	613	CLA	C10-C11-C12-C13
30	BD	408	LMG	C22-C23-C24-C25
30	AB	621	LMG	C28-C29-C30-C31
22	AB	614	CLA	CAD-CBD-CGD-O1D
22	AC	509	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	BB	617	CLA	CAD-CBD-CGD-O1D
22	BC	509	CLA	CHA-CBD-CGD-O1D
22	BC	509	CLA	CHA-CBD-CGD-O2D
28	AC	521	LHG	C3-O3-P-O6
28	BC	521	LHG	C3-O3-P-O4
30	AD	407	LMG	C29-C30-C31-C32
30	BD	407	LMG	C29-C30-C31-C32
22	AB	602	CLA	C2B-C3B-CAB-CBB
22	AB	613	CLA	C2B-C3B-CAB-CBB
22	AB	616	CLA	C2B-C3B-CAB-CBB
22	BB	605	CLA	C2B-C3B-CAB-CBB
22	BB	616	CLA	C2B-C3B-CAB-CBB
22	BB	619	CLA	C2B-C3B-CAB-CBB
26	AJ	102	BCR	C23-C24-C25-C30
26	BJ	102	BCR	C5-C6-C7-C8
30	AE	102	LMG	O7-C10-C11-C12
22	BB	612	CLA	C2-C3-C5-C6
29	BF	101	SQD	C9-C10-C11-C12
27	BA	411	DGD	C3A-C4A-C5A-C6A
30	AD	408	LMG	C20-C21-C22-C23
30	AM	101	LMG	C18-C19-C20-C21
30	BC	519	LMG	C29-C30-C31-C32
29	BA	401	SQD	C11-C10-C9-C8
30	AC	519	LMG	C16-C17-C18-C19
27	AC	518	DGD	C3G-C2G-O2G-C1B
27	BC	518	DGD	C3G-C2G-O2G-C1B
28	AA	411	LHG	C4-C5-O7-C7
30	BC	520	LMG	C9-C8-O7-C10
30	BE	102	LMG	O7-C10-C11-C12
24	AA	407	PL9	C24-C26-C27-C28
22	BB	617	CLA	C13-C15-C16-C17
30	BB	623	LMG	C28-C29-C30-C31
30	BM	102	LMG	C18-C19-C20-C21
27	AD	410	DGD	C9B-CAB-CBB-CCB
22	AB	607	CLA	C15-C16-C17-C18
22	AB	615	CLA	C14-C13-C15-C16
22	AC	503	CLA	C11-C10-C8-C9
22	AC	505	CLA	C14-C13-C15-C16
22	AC	507	CLA	C14-C13-C15-C16
22	AC	508	CLA	C6-C7-C8-C9
22	AC	510	CLA	C6-C7-C8-C9
22	AD	404	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
22	BC	503	CLA	C11-C10-C8-C9
22	BC	508	CLA	C6-C7-C8-C9
22	BC	513	CLA	C11-C10-C8-C9
22	BD	404	CLA	C11-C10-C8-C9
22	AB	601	CLA	C12-C13-C15-C16
22	BB	604	CLA	C12-C13-C15-C16
22	BC	507	CLA	C11-C12-C13-C15
22	BC	513	CLA	C11-C10-C8-C7
27	BD	410	DGD	C9B-CAB-CBB-CCB
26	BC	515	BCR	C22-C23-C24-C25
22	BB	608	CLA	C2A-CAA-CBA-CGA
22	BC	513	CLA	C2A-CAA-CBA-CGA
22	AB	616	CLA	C8-C10-C11-C12
27	AA	410	DGD	C3A-C4A-C5A-C6A
29	BA	413	SQD	C10-C11-C12-C13
29	AA	412	SQD	C10-C11-C12-C13
27	AD	410	DGD	O2G-C2G-C3G-O3G
27	BD	410	DGD	O2G-C2G-C3G-O3G
30	AC	519	LMG	O7-C8-C9-O8
30	BC	519	LMG	O7-C8-C9-O8
30	BM	102	LMG	O7-C8-C9-O8
22	AB	611	CLA	C8-C10-C11-C12
22	BB	606	CLA	C13-C15-C16-C17
32	AB	624	LMT	O1'-C1-C2-C3
22	AC	505	CLA	C4-C3-C5-C6
22	BC	505	CLA	C4-C3-C5-C6
22	AB	605	CLA	C15-C16-C17-C18
30	AC	519	LMG	C29-C30-C31-C32
32	BB	625	LMT	O1'-C1-C2-C3
30	AA	413	LMG	C8-C7-O1-C1
30	AB	621	LMG	C8-C7-O1-C1
30	BB	623	LMG	C8-C7-O1-C1
29	BF	101	SQD	C25-C26-C27-C28
30	BA	414	LMG	C40-C41-C42-C43
22	AB	614	CLA	C13-C15-C16-C17
22	BB	616	CLA	C10-C11-C12-C13
32	BI	102	LMT	C7-C8-C9-C10
22	AB	605	CLA	C2A-CAA-CBA-CGA
22	AC	513	CLA	C2A-CAA-CBA-CGA
32	AI	102	LMT	C7-C8-C9-C10
22	BC	508	CLA	C13-C15-C16-C17
22	AC	505	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	BC	505	CLA	C2-C3-C5-C6
30	BI	101	LMG	C17-C18-C19-C20
30	BA	414	LMG	C11-C12-C13-C14
27	AC	518	DGD	CCB-CDB-CEB-CFB
22	AA	406	CLA	C11-C10-C8-C9
22	AB	601	CLA	C6-C7-C8-C9
22	AB	601	CLA	C14-C13-C15-C16
22	AC	506	CLA	C6-C7-C8-C9
22	AC	508	CLA	C11-C10-C8-C9
22	BA	407	CLA	C11-C10-C8-C9
22	BB	604	CLA	C6-C7-C8-C9
22	BC	505	CLA	C14-C13-C15-C16
22	BC	506	CLA	C6-C7-C8-C9
22	BC	508	CLA	C11-C10-C8-C9
22	AA	403	CLA	C10-C11-C12-C13
22	AD	402	CLA	C4B-C3B-CAB-CBB
22	BC	509	CLA	C4B-C3B-CAB-CBB
22	BD	402	CLA	C4B-C3B-CAB-CBB
30	AD	407	LMG	C32-C33-C34-C35
30	AA	413	LMG	C11-C12-C13-C14
22	AB	611	CLA	C4-C3-C5-C6
22	BB	614	CLA	C4-C3-C5-C6
29	BF	101	SQD	C11-C12-C13-C14
22	AC	509	CLA	C10-C11-C12-C13
32	AB	624	LMT	C4-C5-C6-C7
30	AA	413	LMG	C40-C41-C42-C43
29	BB	601	SQD	C27-C28-C29-C30
29	BL	101	SQD	C27-C28-C29-C30
22	AB	612	CLA	C12-C13-C15-C16
22	AC	503	CLA	C11-C10-C8-C7
22	AC	513	CLA	C12-C13-C15-C16
22	BB	615	CLA	C12-C13-C15-C16
22	BB	616	CLA	C11-C10-C8-C7
22	BC	505	CLA	C6-C7-C8-C10
22	BC	513	CLA	C12-C13-C15-C16
32	BB	625	LMT	C4-C5-C6-C7
22	AC	512	CLA	CAA-CBA-CGA-O2A
22	BC	512	CLA	CAA-CBA-CGA-O2A
27	AC	517	DGD	C7B-C8B-C9B-CAB
22	AC	512	CLA	C10-C11-C12-C13
22	AB	601	CLA	C3A-C2A-CAA-CBA
22	AB	616	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	BB	604	CLA	C3A-C2A-CAA-CBA
22	BB	604	CLA	C4-C3-C5-C6
22	BB	619	CLA	C3A-C2A-CAA-CBA
22	BC	512	CLA	C4-C3-C5-C6
27	BD	410	DGD	C5B-C6B-C7B-C8B
22	AC	503	CLA	C2A-CAA-CBA-CGA
26	AB	617	BCR	C6-C7-C8-C9
26	BB	620	BCR	C6-C7-C8-C9
22	BB	614	CLA	C5-C6-C7-C8
22	BC	512	CLA	C10-C11-C12-C13
29	AA	415	SQD	C9-C10-C11-C12
29	AA	415	SQD	C30-C31-C32-C33
22	AB	614	CLA	C2-C1-O2A-CGA
22	BC	502	CLA	C2-C1-O2A-CGA
22	BB	619	CLA	C8-C10-C11-C12
30	BD	408	LMG	C16-C17-C18-C19
27	BB	602	DGD	C1B-C2B-C3B-C4B
22	BB	607	CLA	C15-C16-C17-C18
22	AB	601	CLA	C4-C3-C5-C6
22	AC	512	CLA	C4-C3-C5-C6
27	BA	411	DGD	O6E-C5E-C6E-O5E
29	AD	409	SQD	C44-C45-C46-O48
29	BD	409	SQD	C44-C45-C46-O48
30	BC	520	LMG	C15-C16-C17-C18
22	AB	613	CLA	C11-C10-C8-C9
22	AC	503	CLA	C6-C7-C8-C9
22	AC	505	CLA	C6-C7-C8-C9
22	AC	507	CLA	C11-C12-C13-C14
22	AC	509	CLA	C14-C13-C15-C16
22	BB	604	CLA	C14-C13-C15-C16
22	BB	613	CLA	C14-C13-C15-C16
22	BC	503	CLA	C6-C7-C8-C9
22	BC	505	CLA	C6-C7-C8-C9
22	BC	507	CLA	C11-C12-C13-C14
23	AD	403	PHO	C6-C7-C8-C9
23	BD	403	PHO	C6-C7-C8-C9
29	AA	412	SQD	C19-C20-C21-C22
27	BC	517	DGD	C7B-C8B-C9B-CAB
29	AF	101	SQD	C25-C26-C27-C28
22	AB	603	CLA	C13-C15-C16-C17
22	AB	604	CLA	C15-C16-C17-C18
30	BD	407	LMG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
28	BA	412	LHG	C4-C5-O7-C7
22	AA	406	CLA	C1-C2-C3-C4
22	AB	612	CLA	C1-C2-C3-C4
22	AC	502	CLA	C1-C2-C3-C4
22	AC	510	CLA	C1-C2-C3-C4
22	AC	512	CLA	C1-C2-C3-C4
22	BA	407	CLA	C1-C2-C3-C4
22	BB	615	CLA	C1-C2-C3-C4
22	BC	502	CLA	C1-C2-C3-C4
22	BC	510	CLA	C1-C2-C3-C4
22	BC	512	CLA	C1-C2-C3-C4
27	BH	101	DGD	C8B-C9B-CAB-CBB
22	AB	611	CLA	C2-C3-C5-C6
22	BB	614	CLA	C2-C3-C5-C6
22	BC	503	CLA	C2A-CAA-CBA-CGA
22	AB	601	CLA	C1A-C2A-CAA-CBA
22	AB	604	CLA	C1A-C2A-CAA-CBA
22	AC	513	CLA	C1A-C2A-CAA-CBA
22	BA	405	CLA	C1A-C2A-CAA-CBA
22	BB	604	CLA	C1A-C2A-CAA-CBA
22	BC	513	CLA	C1A-C2A-CAA-CBA
29	BB	601	SQD	C10-C11-C12-C13
22	BA	404	CLA	C10-C11-C12-C13
30	AC	520	LMG	C15-C16-C17-C18
22	BC	509	CLA	C2B-C3B-CAB-CBB
26	AB	618	BCR	C23-C24-C25-C30
26	AC	514	BCR	C23-C24-C25-C26
26	AT	102	BCR	C23-C24-C25-C30
26	BC	514	BCR	C23-C24-C25-C26
30	AI	101	LMG	C17-C18-C19-C20
22	BC	512	CLA	C2-C3-C5-C6
22	AB	601	CLA	C6-C7-C8-C10
22	AB	613	CLA	C11-C10-C8-C7
22	AB	614	CLA	C11-C10-C8-C7
22	AC	503	CLA	C6-C7-C8-C10
22	AC	505	CLA	C6-C7-C8-C10
22	AC	510	CLA	C11-C12-C13-C15
22	AD	402	CLA	C11-C10-C8-C7
22	BB	604	CLA	C6-C7-C8-C10
22	BB	610	CLA	C11-C10-C8-C7
22	BB	617	CLA	C11-C10-C8-C7
22	BC	503	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
22	BC	503	CLA	C11-C10-C8-C7
22	BC	510	CLA	C11-C12-C13-C15
22	BD	402	CLA	C11-C10-C8-C7
23	AD	403	PHO	C6-C7-C8-C10
23	BD	403	PHO	C6-C7-C8-C10
22	AB	614	CLA	C2A-CAA-CBA-CGA
22	BB	617	CLA	C2A-CAA-CBA-CGA
30	AM	101	LMG	O7-C8-C9-O8
30	AD	408	LMG	C16-C17-C18-C19
27	AC	518	DGD	C7A-C8A-C9A-CAA
29	BA	413	SQD	C19-C20-C21-C22
22	AB	601	CLA	C2-C3-C5-C6
22	AC	512	CLA	C2-C3-C5-C6
22	BB	604	CLA	C2-C3-C5-C6
27	BC	518	DGD	CCB-CDB-CEB-CFB
22	AB	608	CLA	C1-C2-C3-C5
22	AB	611	CLA	C1-C2-C3-C5
22	AC	505	CLA	C1-C2-C3-C5
22	BB	611	CLA	C1-C2-C3-C5
22	BB	614	CLA	C1-C2-C3-C5
22	BC	505	CLA	C1-C2-C3-C5
22	BB	609	CLA	C15-C16-C17-C18
22	BC	509	CLA	C10-C11-C12-C13
30	AA	413	LMG	C33-C34-C35-C36
29	BA	401	SQD	C9-C10-C11-C12
22	AC	507	CLA	C11-C10-C8-C9
22	BB	616	CLA	C11-C10-C8-C9
22	BC	507	CLA	C11-C10-C8-C9
22	BB	610	CLA	C15-C16-C17-C18
27	AH	102	DGD	C8B-C9B-CAB-CBB
29	BL	101	SQD	C10-C11-C12-C13
26	AC	515	BCR	C22-C23-C24-C25
22	BC	510	CLA	C4-C3-C5-C6
22	BB	608	CLA	C15-C16-C17-C18
22	AB	611	CLA	C5-C6-C7-C8
34	BV	201	HEM	CAD-CBD-CGD-O2D
29	BL	101	SQD	C15-C16-C17-C18
29	BA	401	SQD	C30-C31-C32-C33
29	AA	415	SQD	C15-C16-C17-C18
29	BA	401	SQD	O49-C7-O47-C45
22	AB	606	CLA	C15-C16-C17-C18
22	AC	508	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
22	BB	613	CLA	C10-C11-C12-C13
27	AD	410	DGD	C5B-C6B-C7B-C8B
22	AC	509	CLA	C4B-C3B-CAB-CBB
30	BA	414	LMG	C33-C34-C35-C36
27	AB	626	DGD	C1B-C2B-C3B-C4B
22	AC	510	CLA	C4-C3-C5-C6
30	AB	622	LMG	O7-C8-C9-O8
23	BA	406	PHO	C8-C10-C11-C12
34	AV	201	HEM	CAD-CBD-CGD-O2D
22	BB	615	CLA	C8-C10-C11-C12
22	AC	503	CLA	C11-C12-C13-C15
27	AA	410	DGD	C4A-C5A-C6A-C7A
22	AB	602	CLA	C11-C12-C13-C14
22	AC	502	CLA	C11-C10-C8-C9
22	AC	503	CLA	C11-C12-C13-C14
22	AC	510	CLA	C11-C12-C13-C14
22	AC	511	CLA	C14-C13-C15-C16
22	AC	513	CLA	C14-C13-C15-C16
22	BB	605	CLA	C11-C12-C13-C14
22	BB	606	CLA	C11-C10-C8-C9
22	BB	614	CLA	C11-C10-C8-C9
22	BC	503	CLA	C11-C12-C13-C14
22	BC	509	CLA	C14-C13-C15-C16
22	BC	511	CLA	C14-C13-C15-C16
22	BC	513	CLA	C14-C13-C15-C16
27	BD	410	DGD	O6D-C5D-C6D-O5D
29	BA	401	SQD	C45-C44-O6-C1
29	BL	101	SQD	C45-C44-O6-C1
29	BB	601	SQD	C15-C16-C17-C18
22	AB	606	CLA	C2-C1-O2A-CGA
22	AC	502	CLA	C2-C1-O2A-CGA
22	BB	617	CLA	C2-C1-O2A-CGA
22	BA	403	CLA	C3A-C2A-CAA-CBA
32	BM	101	LMT	C1-C2-C3-C4
27	BA	411	DGD	C4A-C5A-C6A-C7A
30	BI	101	LMG	C15-C16-C17-C18
34	BV	201	HEM	CAD-CBD-CGD-O1D
30	BD	408	LMG	C11-C12-C13-C14
22	AB	610	CLA	C10-C11-C12-C13
34	AV	201	HEM	CAD-CBD-CGD-O1D
32	AM	102	LMT	C1-C2-C3-C4
22	BA	407	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
34	AE	101	HEM	CAA-CBA-CGA-O1A
34	BE	101	HEM	CAA-CBA-CGA-O1A
30	BB	624	LMG	C39-C40-C41-C42
27	AD	410	DGD	O6D-C5D-C6D-O5D
22	AC	509	CLA	C13-C15-C16-C17
22	BB	605	CLA	CAA-CBA-CGA-O2A
22	BC	509	CLA	C13-C15-C16-C17
27	AA	410	DGD	O6E-C5E-C6E-O5E
29	BL	101	SQD	C24-C25-C26-C27
27	BC	517	DGD	CFB-CGB-CHB-CIB
22	AC	505	CLA	C8-C10-C11-C12
29	AD	409	SQD	C11-C12-C13-C14
30	AI	101	LMG	C15-C16-C17-C18
22	AB	603	CLA	C11-C10-C8-C9
22	AB	610	CLA	C14-C13-C15-C16
22	AB	611	CLA	C11-C10-C8-C9
22	AC	504	CLA	C11-C10-C8-C9
22	BC	502	CLA	C11-C10-C8-C9
22	BC	504	CLA	C11-C10-C8-C9
22	BC	510	CLA	C11-C12-C13-C14
30	AD	408	LMG	C11-C12-C13-C14
29	BA	401	SQD	O47-C7-C8-C9
34	BE	101	HEM	CAA-CBA-CGA-O2A
22	AB	602	CLA	C11-C12-C13-C15
22	AB	604	CLA	C11-C10-C8-C7
22	AB	606	CLA	C11-C10-C8-C7
22	AC	501	CLA	C6-C7-C8-C10
22	AC	507	CLA	C11-C10-C8-C7
22	AC	511	CLA	C12-C13-C15-C16
22	BB	605	CLA	C11-C12-C13-C15
22	BB	609	CLA	C11-C10-C8-C7
22	BB	611	CLA	C11-C10-C8-C7
22	BC	503	CLA	C11-C12-C13-C15
22	BC	507	CLA	C11-C10-C8-C7
22	BC	511	CLA	C12-C13-C15-C16
23	AA	405	PHO	C6-C7-C8-C10
23	BA	406	PHO	C6-C7-C8-C10
22	AD	402	CLA	C2B-C3B-CAB-CBB
22	BD	402	CLA	C2B-C3B-CAB-CBB
26	BJ	102	BCR	C1-C6-C7-C8
26	BJ	102	BCR	C23-C24-C25-C30
29	BA	401	SQD	C8-C7-O47-C45

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Mol	Chain	Res	Type	Atoms
22	AB	610	CLA	C2-C1-O2A-CGA
22	BB	604	CLA	C2-C1-O2A-CGA
27	AC	516	DGD	C2B-C3B-C4B-C5B
30	AE	102	LMG	C14-C15-C16-C17
29	AA	415	SQD	O47-C7-C8-C9
22	BC	512	CLA	C8-C10-C11-C12
28	BC	521	LHG	O7-C7-C8-C9
34	AE	101	HEM	CAA-CBA-CGA-O2A
29	AA	415	SQD	O49-C7-O47-C45
22	AB	603	CLA	C2A-CAA-CBA-CGA
22	BB	606	CLA	C2A-CAA-CBA-CGA
29	AA	415	SQD	C8-C7-O47-C45
22	AB	602	CLA	CAA-CBA-CGA-O2A
22	AB	610	CLA	CAA-CBA-CGA-O2A
29	BB	601	SQD	C24-C25-C26-C27
22	AC	512	CLA	C8-C10-C11-C12
23	AA	405	PHO	C8-C10-C11-C12
22	BB	613	CLA	CAA-CBA-CGA-O2A
22	BB	617	CLA	CAA-CBA-CGA-O2A
28	AC	521	LHG	O7-C7-C8-C9
29	AA	415	SQD	C32-C33-C34-C35
30	AM	101	LMG	C32-C33-C34-C35
32	AB	624	LMT	C3-C4-C5-C6
22	AB	614	CLA	CAA-CBA-CGA-O2A
30	AA	413	LMG	O7-C10-C11-C12
22	AB	613	CLA	C6-C7-C8-C9
22	AD	402	CLA	C11-C10-C8-C9
22	BB	610	CLA	C11-C10-C8-C9
22	BD	402	CLA	C11-C10-C8-C9
22	AB	612	CLA	C8-C10-C11-C12
22	AC	506	CLA	C8-C10-C11-C12
22	AA	402	CLA	C1A-C2A-CAA-CBA
22	AB	609	CLA	C1A-C2A-CAA-CBA
22	BA	403	CLA	C1A-C2A-CAA-CBA
22	BB	604	CLA	C4B-C3B-CAB-CBB
30	AA	413	LMG	C35-C36-C37-C38
26	AA	409	BCR	C6-C7-C8-C9
26	BA	410	BCR	C6-C7-C8-C9
22	BC	505	CLA	CAA-CBA-CGA-O2A
27	BC	518	DGD	O1G-C1A-C2A-C3A
29	BA	413	SQD	O6-C44-C45-O47
27	BC	516	DGD	C2B-C3B-C4B-C5B

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Mol	Chain	Res	Type	Atoms
30	BE	102	LMG	C14-C15-C16-C17
30	AA	413	LMG	C8-C9-O8-C28
32	BB	625	LMT	C3-C4-C5-C6
22	AC	505	CLA	CAA-CBA-CGA-O2A
27	BB	602	DGD	O2G-C1B-C2B-C3B
30	BA	414	LMG	O7-C10-C11-C12
29	BA	401	SQD	C15-C16-C17-C18
22	AD	404	CLA	C8-C10-C11-C12
27	AD	410	DGD	C8B-C9B-CAB-CBB
27	AB	626	DGD	O2G-C1B-C2B-C3B
30	AC	519	LMG	O8-C28-C29-C30
29	AA	412	SQD	C5-C6-S-O9
29	BA	413	SQD	C5-C6-S-O9
30	BM	102	LMG	C16-C17-C18-C19
22	AB	611	CLA	C2-C1-O2A-CGA
22	AB	616	CLA	C2-C1-O2A-CGA
22	BB	609	CLA	C2-C1-O2A-CGA
22	BB	612	CLA	C2-C1-O2A-CGA
22	BB	613	CLA	C2-C1-O2A-CGA
22	BB	614	CLA	C2-C1-O2A-CGA
22	BB	615	CLA	C2-C1-O2A-CGA
27	AC	518	DGD	O1G-C1A-C2A-C3A
22	AB	608	CLA	C11-C10-C8-C7
22	AC	508	CLA	C12-C13-C15-C16
22	BB	607	CLA	C11-C10-C8-C7
22	BB	608	CLA	C11-C12-C13-C15
22	BB	610	CLA	C6-C7-C8-C10
22	BC	501	CLA	C6-C7-C8-C10
22	BC	508	CLA	C12-C13-C15-C16
30	BA	414	LMG	C35-C36-C37-C38
23	AD	403	PHO	O2A-C1-C2-C3
23	BD	403	PHO	O2A-C1-C2-C3
27	AC	517	DGD	C8A-C9A-CAA-CBA
30	AM	101	LMG	C16-C17-C18-C19
30	BC	519	LMG	O8-C28-C29-C30
22	AB	614	CLA	C10-C11-C12-C13
30	BI	101	LMG	C34-C35-C36-C37
30	AB	622	LMG	C32-C33-C34-C35
22	AA	406	CLA	C15-C16-C17-C18
22	BC	506	CLA	C8-C10-C11-C12
22	AA	402	CLA	C4-C3-C5-C6
22	AD	404	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
24	AD	405	PL9	C15-C14-C16-C17
22	AC	512	CLA	C15-C16-C17-C18
27	BC	517	DGD	C8A-C9A-CAA-CBA
27	BC	518	DGD	C7A-C8A-C9A-CAA
29	BD	409	SQD	C11-C12-C13-C14
29	BA	401	SQD	C32-C33-C34-C35
22	BB	613	CLA	CAA-CBA-CGA-O1A
30	AC	519	LMG	O10-C28-C29-C30
27	BD	410	DGD	CCA-CDA-CEA-CFA
22	BC	505	CLA	C8-C10-C11-C12
22	AB	605	CLA	C11-C12-C13-C14
22	AB	606	CLA	C11-C10-C8-C9
22	AB	607	CLA	C11-C10-C8-C9
22	AC	508	CLA	C14-C13-C15-C16
22	BB	608	CLA	C11-C12-C13-C14
22	BB	609	CLA	C11-C10-C8-C9
22	BC	508	CLA	C14-C13-C15-C16
23	AA	405	PHO	C14-C13-C15-C16
23	BA	406	PHO	C14-C13-C15-C16
22	AB	614	CLA	CAA-CBA-CGA-O1A
28	BC	521	LHG	O9-C7-C8-C9
22	AB	602	CLA	CAA-CBA-CGA-O1A
22	AB	610	CLA	CAA-CBA-CGA-O1A
22	BB	617	CLA	CAA-CBA-CGA-O1A
30	BM	102	LMG	C32-C33-C34-C35
27	AD	410	DGD	CCA-CDA-CEA-CFA
29	BA	401	SQD	O49-C7-C8-C9
30	BI	101	LMG	O7-C10-C11-C12
34	AV	201	HEM	CAA-CBA-CGA-O2A
22	BB	605	CLA	CAA-CBA-CGA-O1A
29	AA	415	SQD	O49-C7-C8-C9
22	AC	502	CLA	C13-C15-C16-C17
22	BC	512	CLA	C15-C16-C17-C18
27	AB	626	DGD	C2G-C3G-O3G-C1D
27	BB	602	DGD	C2G-C3G-O3G-C1D
27	BD	410	DGD	C2G-C3G-O3G-C1D
29	AA	415	SQD	C45-C44-O6-C1
29	BB	601	SQD	C45-C44-O6-C1
34	BV	201	HEM	CAA-CBA-CGA-O2A
30	AD	407	LMG	C2-C1-O1-C7
22	BC	505	CLA	CAA-CBA-CGA-O1A
27	BB	602	DGD	O1B-C1B-C2B-C3B

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Mol	Chain	Res	Type	Atoms
30	AI	101	LMG	O7-C10-C11-C12
22	BB	608	CLA	C13-C15-C16-C17
22	BC	502	CLA	C13-C15-C16-C17
30	BE	102	LMG	C12-C13-C14-C15
30	AB	622	LMG	C7-C8-C9-O8
28	AC	521	LHG	O9-C7-C8-C9
30	BA	414	LMG	O9-C10-C11-C12
30	BC	519	LMG	O10-C28-C29-C30
22	BD	402	CLA	CAD-CBD-CGD-O2D
29	BD	409	SQD	O47-C7-C8-C9
34	BV	201	HEM	CAA-CBA-CGA-O1A
30	BB	624	LMG	C32-C33-C34-C35
27	AB	626	DGD	O1B-C1B-C2B-C3B
30	AA	413	LMG	C10-C11-C12-C13
22	AB	601	CLA	C2-C1-O2A-CGA
29	AA	415	SQD	C11-C12-C13-C14
29	AD	409	SQD	O47-C7-C8-C9
30	AA	416	LMG	O8-C28-C29-C30
30	AB	623	LMG	O8-C28-C29-C30
22	AB	613	CLA	C1-C2-C3-C4
22	BB	616	CLA	C1-C2-C3-C4
22	BD	402	CLA	CAA-CBA-CGA-O2A
27	AC	516	DGD	O2G-C1B-C2B-C3B
27	AC	517	DGD	O2G-C1B-C2B-C3B
27	BC	516	DGD	O2G-C1B-C2B-C3B
30	AB	622	LMG	C40-C41-C42-C43
22	AB	605	CLA	C13-C15-C16-C17
27	AC	518	DGD	O1A-C1A-C2A-C3A
22	AA	406	CLA	CAA-CBA-CGA-O2A
22	AD	402	CLA	CAA-CBA-CGA-O2A
27	BC	517	DGD	O2G-C1B-C2B-C3B
30	AE	102	LMG	C12-C13-C14-C15
22	AC	505	CLA	CAA-CBA-CGA-O1A
30	AA	413	LMG	O9-C10-C11-C12

There are no ring outliers.

165 monomers are involved in 591 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	AB	622	LMG	1	0
22	BA	407	CLA	3	0
26	AD	406	BCR	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	AB	614	CLA	1	0
22	AC	511	CLA	7	0
32	AT	101	LMT	3	0
22	BB	619	CLA	5	0
22	BC	510	CLA	1	0
27	AB	626	DGD	3	0
24	BD	405	PL9	8	0
26	AH	101	BCR	2	0
22	BA	404	CLA	7	0
22	BD	404	CLA	3	0
26	AB	617	BCR	3	0
29	BB	601	SQD	2	0
26	AC	515	BCR	5	0
30	BB	624	LMG	1	0
22	BC	511	CLA	9	0
22	AB	616	CLA	4	0
22	BC	502	CLA	2	0
22	AC	506	CLA	2	0
24	AA	407	PL9	5	0
22	BC	501	CLA	2	0
34	BV	201	HEM	3	0
27	AC	516	DGD	3	0
26	BX	101	BCR	4	0
29	BL	101	SQD	2	0
30	AB	621	LMG	1	0
22	BC	508	CLA	7	0
22	AC	507	CLA	3	0
22	BB	608	CLA	3	0
22	BB	615	CLA	4	0
29	AD	409	SQD	2	0
23	AA	405	PHO	5	0
22	BB	612	CLA	5	0
33	BD	401	BCT	1	0
26	BB	620	BCR	3	0
30	AI	101	LMG	3	0
22	BD	402	CLA	8	0
22	AC	512	CLA	8	0
32	AD	411	LMT	1	0
28	BC	521	LHG	4	0
27	AC	518	DGD	8	0
27	AC	517	DGD	8	0
28	AA	411	LHG	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	BB	626	LMT	2	0
34	AE	101	HEM	5	0
22	AC	508	CLA	8	0
22	AA	402	CLA	8	0
22	AC	501	CLA	2	0
22	BB	614	CLA	8	0
22	BC	503	CLA	2	0
23	BA	406	PHO	5	0
34	AV	201	HEM	3	0
22	BB	605	CLA	6	0
30	AB	623	LMG	2	0
30	BC	520	LMG	5	0
22	BC	512	CLA	6	0
30	AA	413	LMG	1	0
22	AB	607	CLA	13	0
26	AK	102	BCR	13	0
30	BC	519	LMG	3	0
22	AD	404	CLA	3	0
32	AM	102	LMT	1	0
22	AB	601	CLA	3	0
30	AM	101	LMG	4	0
32	AB	625	LMT	2	0
26	BZ	101	BCR	4	0
26	BK	102	BCR	13	0
29	AF	101	SQD	2	0
30	BM	102	LMG	4	0
23	AD	403	PHO	3	0
22	AB	603	CLA	7	0
22	BA	403	CLA	8	0
22	AB	608	CLA	10	0
22	AA	404	CLA	2	0
34	BE	101	HEM	6	0
26	BJ	102	BCR	5	0
29	AA	412	SQD	5	0
22	AB	610	CLA	4	0
26	AB	620	BCR	2	0
30	AE	102	LMG	4	0
23	BD	403	PHO	6	0
22	AC	513	CLA	2	0
22	BB	617	CLA	1	0
33	AD	401	BCT	1	0
28	BA	412	LHG	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	AC	520	LMG	4	0
22	AC	505	CLA	9	0
27	BC	517	DGD	10	0
24	BA	408	PL9	6	0
26	AJ	102	BCR	5	0
22	AC	504	CLA	5	0
32	BT	101	LMT	3	0
26	AA	409	BCR	6	0
22	AB	615	CLA	5	0
22	BC	506	CLA	2	0
26	BB	622	BCR	2	0
32	BB	625	LMT	1	0
24	AD	405	PL9	9	0
29	BA	401	SQD	2	0
22	AB	613	CLA	1	0
22	BC	513	CLA	3	0
22	AA	406	CLA	3	0
26	AC	514	BCR	8	0
22	AB	602	CLA	5	0
22	AB	609	CLA	4	0
22	AB	612	CLA	4	0
30	BA	414	LMG	2	0
22	BB	616	CLA	1	0
22	BB	618	CLA	4	0
28	AC	521	LHG	5	0
30	AD	408	LMG	7	0
32	AI	102	LMT	4	0
26	AB	618	BCR	4	0
30	AA	416	LMG	4	0
22	BC	507	CLA	4	0
22	AD	402	CLA	7	0
27	BH	101	DGD	1	0
22	BB	613	CLA	4	0
30	BB	623	LMG	1	0
22	AB	606	CLA	4	0
26	AZ	101	BCR	4	0
22	BB	609	CLA	5	0
26	BD	406	BCR	3	0
22	BC	505	CLA	10	0
32	BM	101	LMT	1	0
22	AC	509	CLA	2	0
26	AT	102	BCR	7	0

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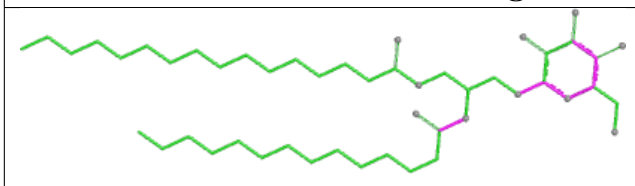
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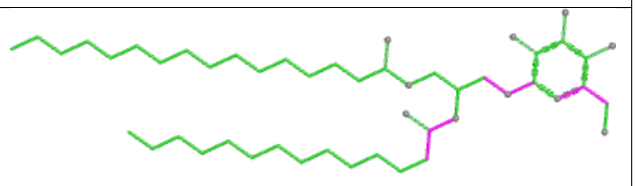
Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	AB	627	LMT	3	0
29	BD	409	SQD	2	0
22	BB	611	CLA	10	0
32	AB	624	LMT	2	0
32	BI	102	LMT	3	0
27	BC	516	DGD	4	0
29	BF	101	SQD	1	0
22	AC	510	CLA	1	0
22	BC	504	CLA	5	0
22	AC	502	CLA	3	0
29	AA	415	SQD	5	0
30	BD	408	LMG	8	0
22	AA	403	CLA	7	0
22	AC	503	CLA	2	0
27	AH	102	DGD	1	0
27	BB	602	DGD	3	0
30	BI	101	LMG	3	0
22	AB	604	CLA	5	0
26	BA	410	BCR	3	0
26	BC	514	BCR	10	0
22	BA	405	CLA	3	0
29	BA	413	SQD	4	0
30	AC	519	LMG	2	0
22	AB	611	CLA	5	0
30	BD	407	LMG	2	0
30	AD	407	LMG	2	0
27	BC	518	DGD	8	0
30	BE	102	LMG	4	0
22	AB	605	CLA	3	0
22	BB	610	CLA	12	0
22	BB	604	CLA	3	0
26	BC	515	BCR	6	0
22	BC	509	CLA	2	0
22	BB	607	CLA	5	0
22	BB	606	CLA	7	0
32	BB	603	LMT	3	0

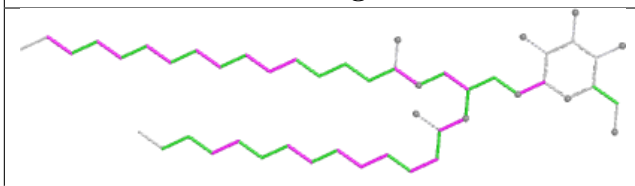
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

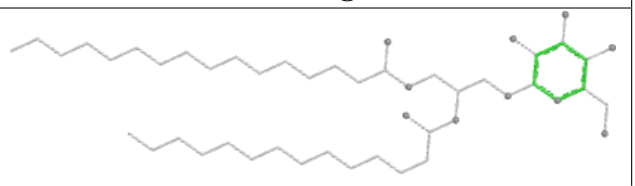
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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 LMG AB 622

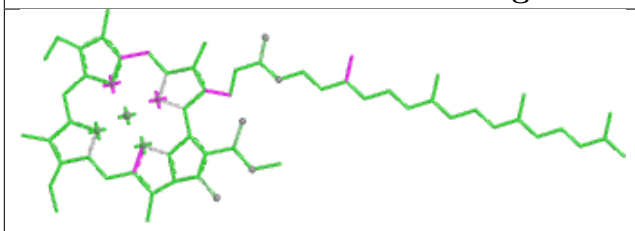

Bond lengths

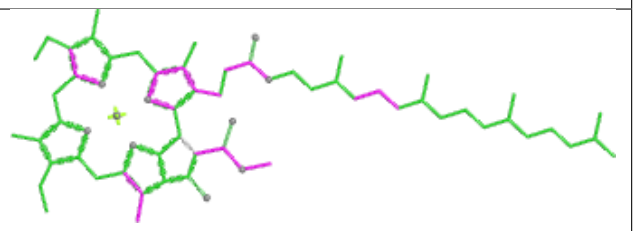

Bond angles

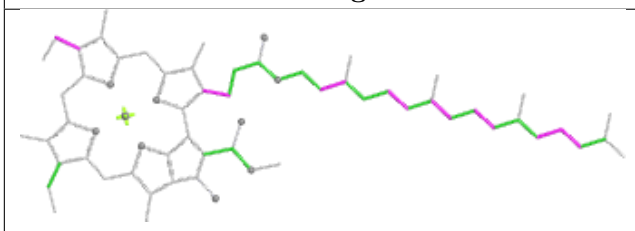

Torsions

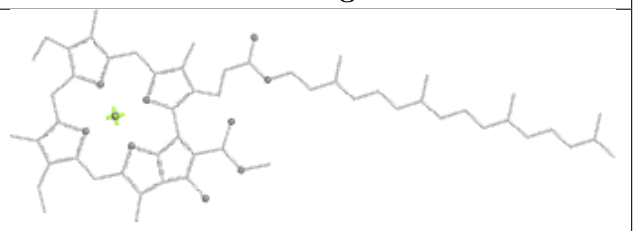

Rings

Ligand CLA BA 407

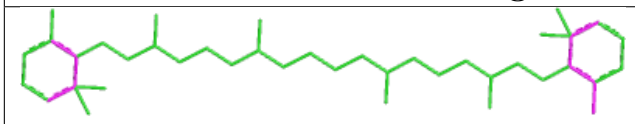

Bond lengths

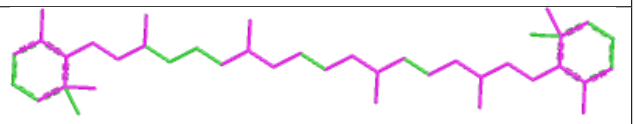

Bond angles

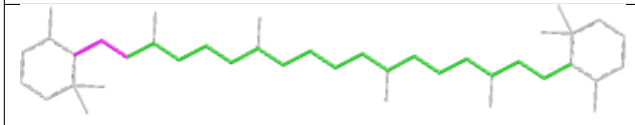

Torsions

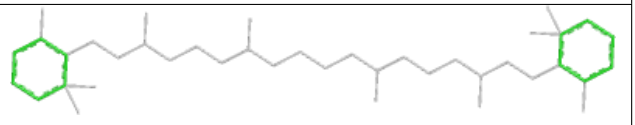

Rings

Ligand BCR AD 406

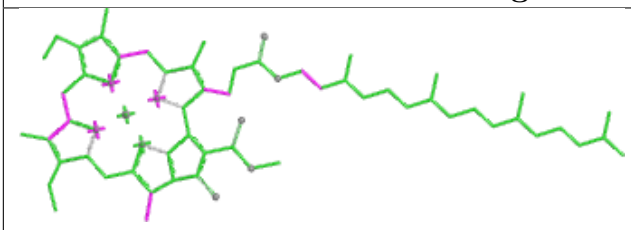

Bond lengths


Bond angles

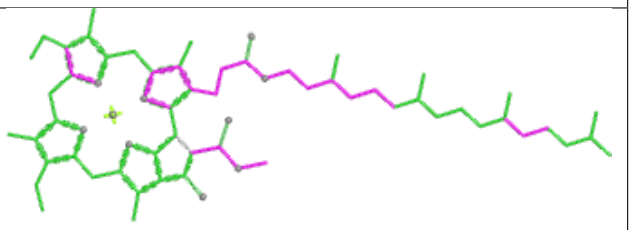

Torsions


Rings

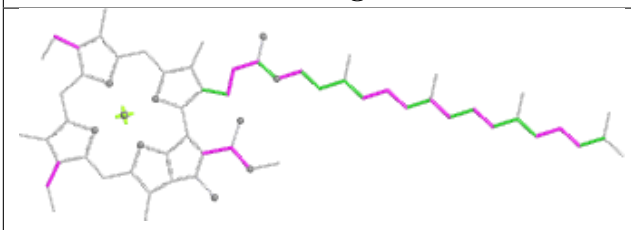
Ligand CLA AB 614



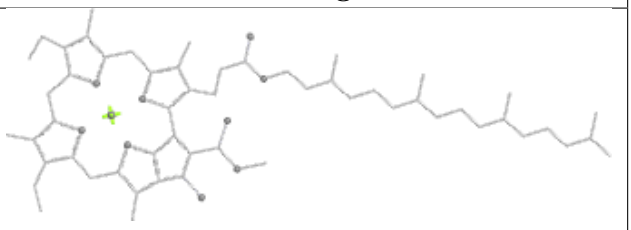
Bond lengths



Bond angles

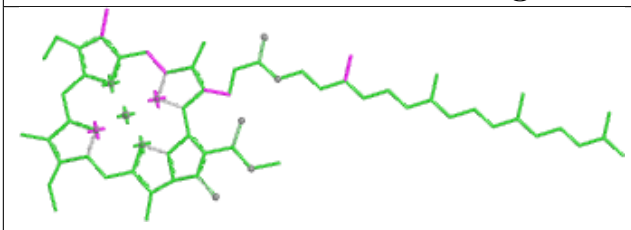


Torsions

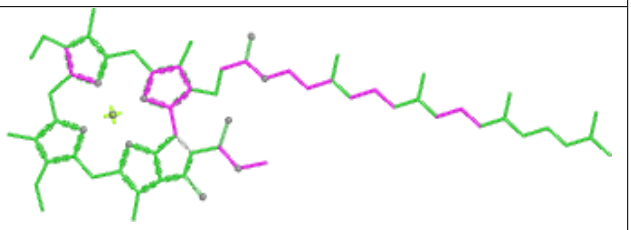


Rings

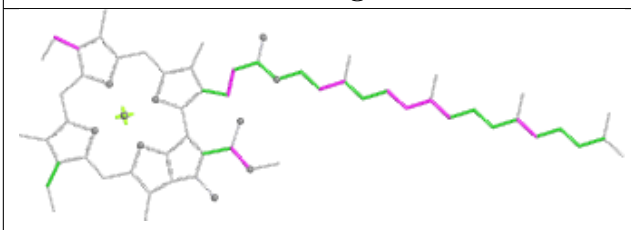
Ligand CLA AC 511



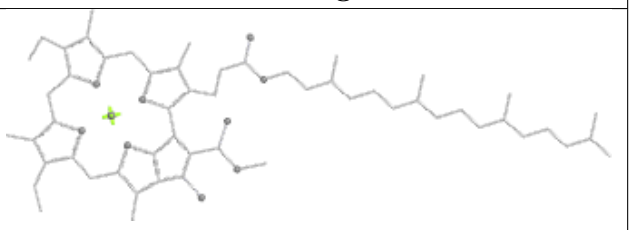
Bond lengths



Bond angles

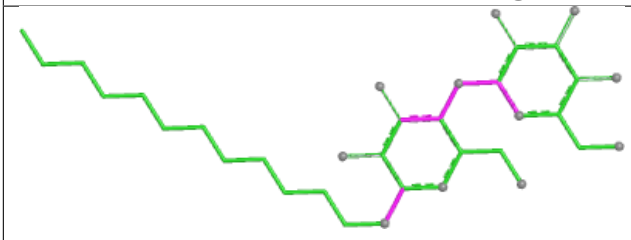


Torsions

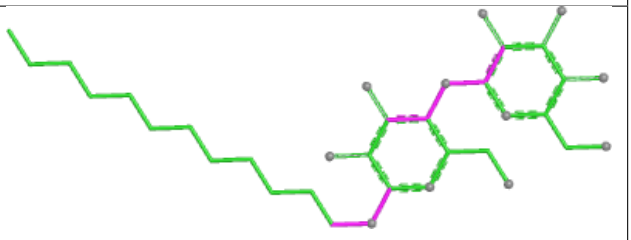


Rings

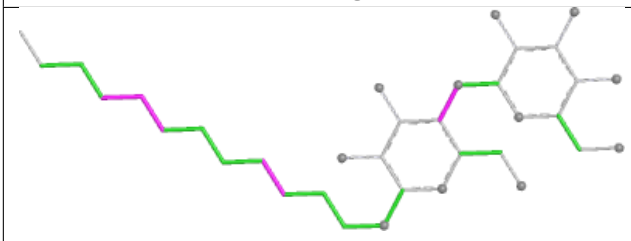
Ligand LMT AT 101



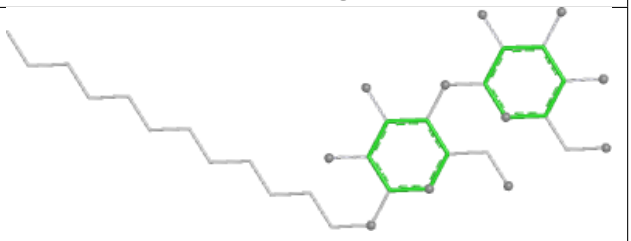
Bond lengths



Bond angles

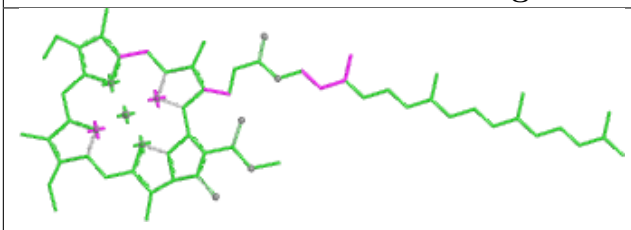


Torsions

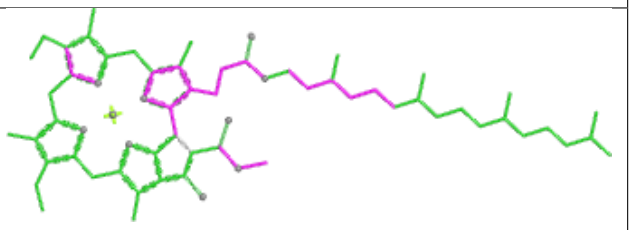


Rings

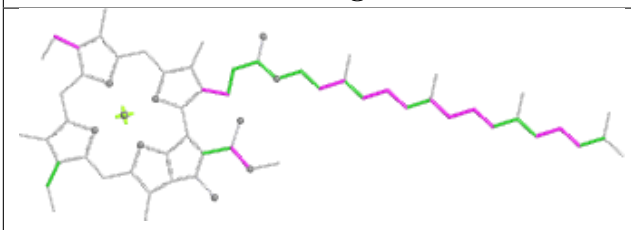
Ligand CLA BB 619



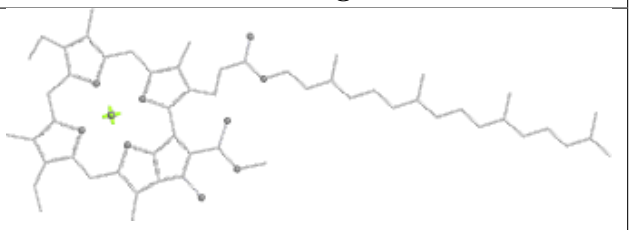
Bond lengths



Bond angles

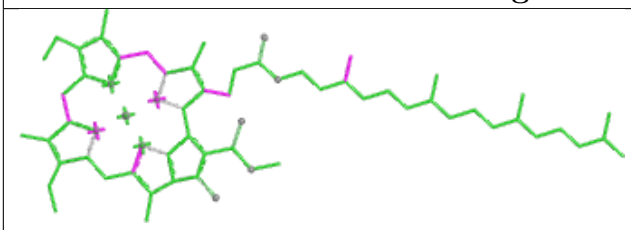


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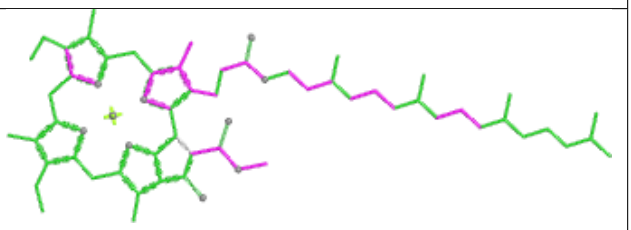


Rings

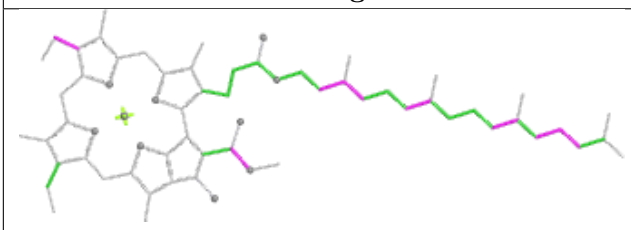
Ligand CLA BC 510



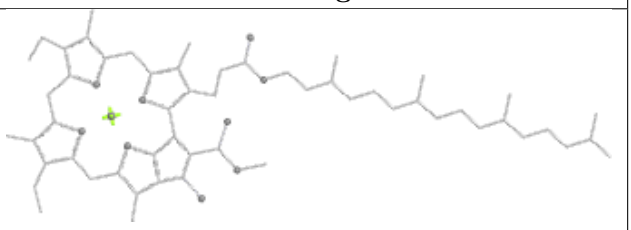
Bond lengths



Bond angles

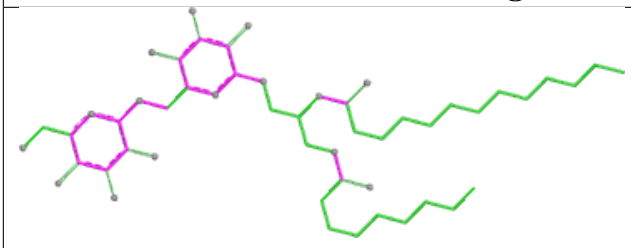


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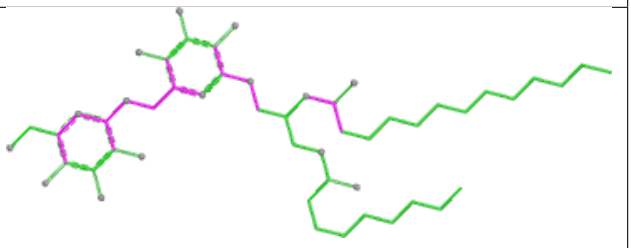


Rings

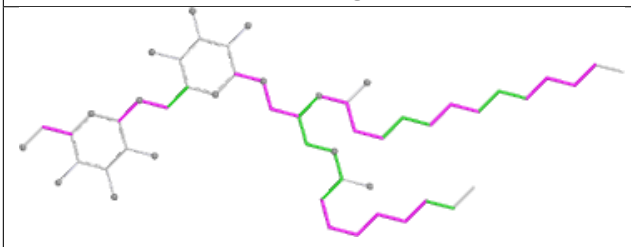
Ligand DGD AB 626



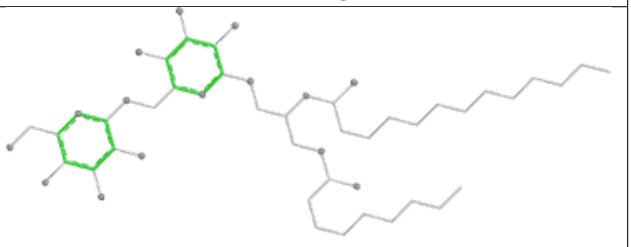
Bond lengths



Bond angles

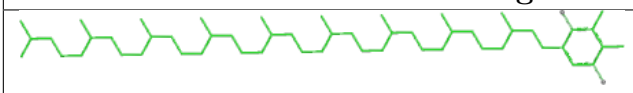


Torsions

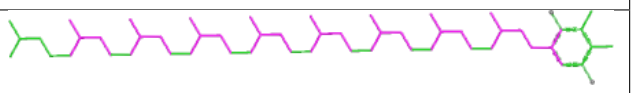


Rings

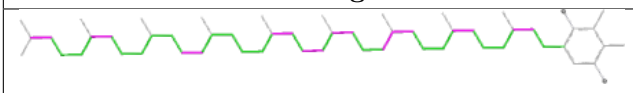
Ligand PL9 BD 405



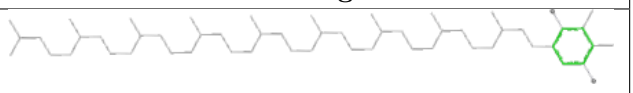
Bond lengths



Bond angles

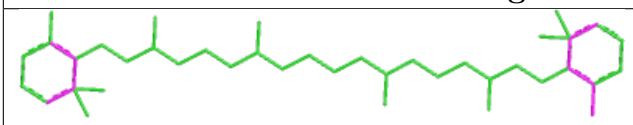


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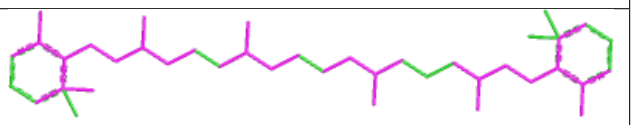


Rings

Ligand BCR AH 101



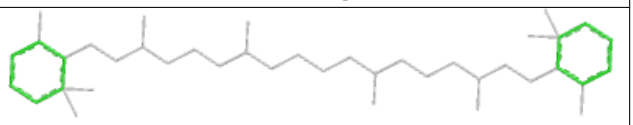
Bond lengths



Bond angles

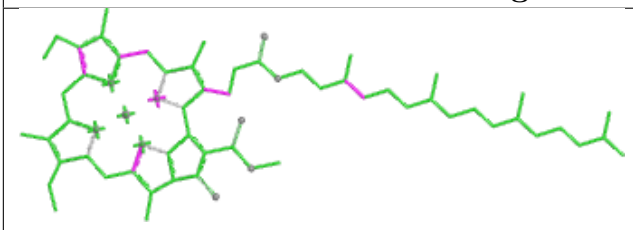


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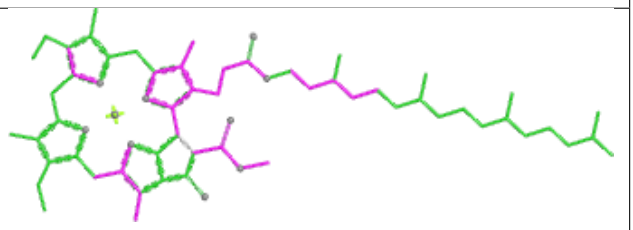


Rings

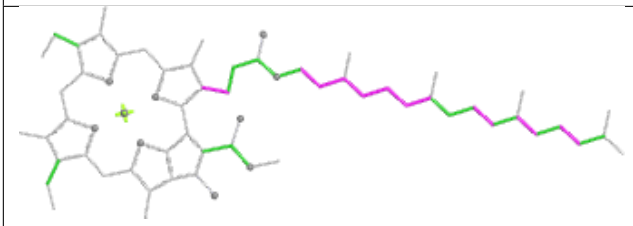
Ligand CLA BA 404



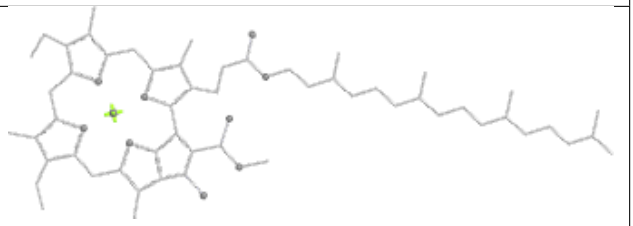
Bond lengths



Bond angles

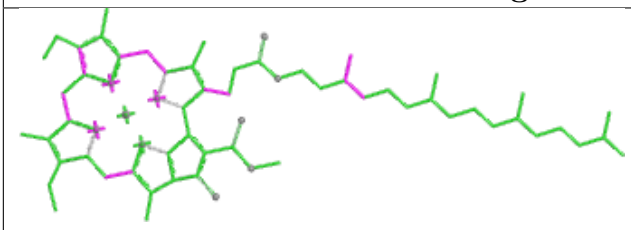


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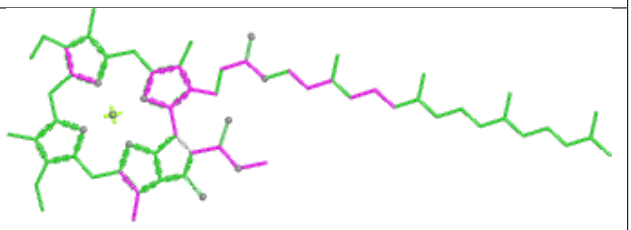


Rings

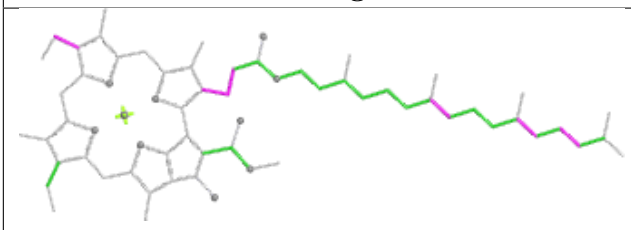
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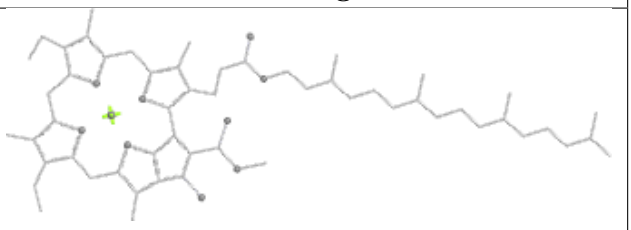
Bond lengths



Bond angles

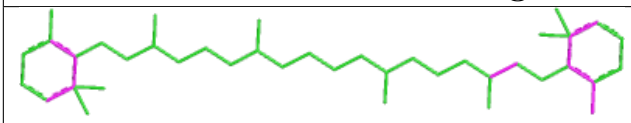


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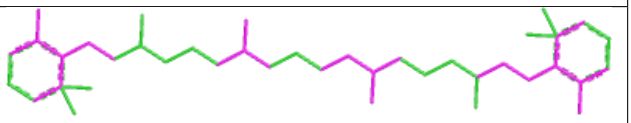


Rings

Ligand BCR AB 617



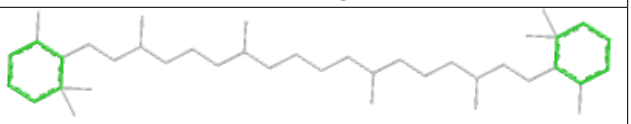
Bond lengths



Bond angles

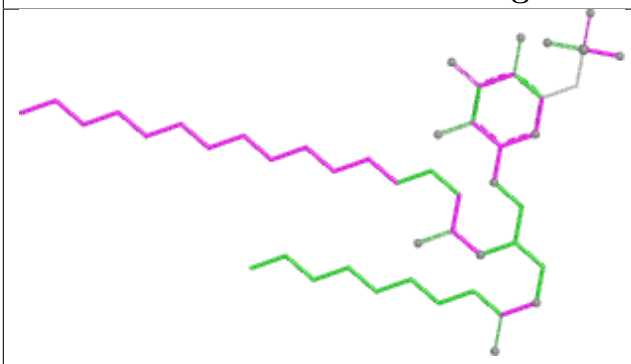


Torsions

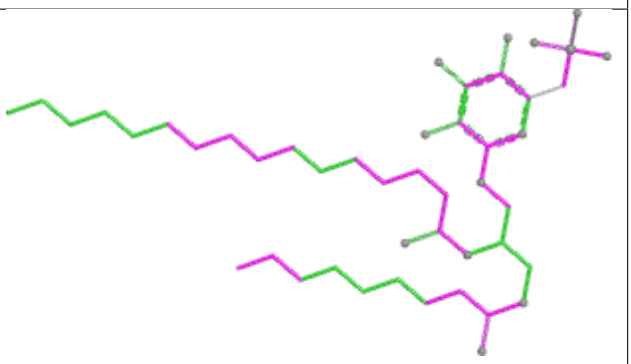


Rings

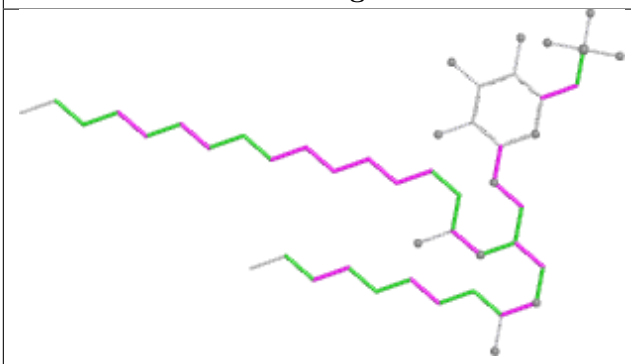
Ligand SQD BB 601



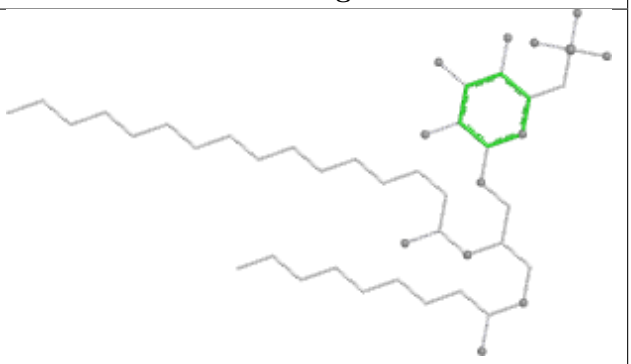
Bond lengths



Bond angles

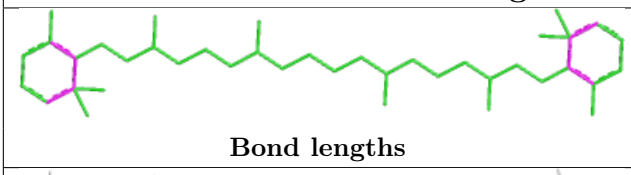


Torsions

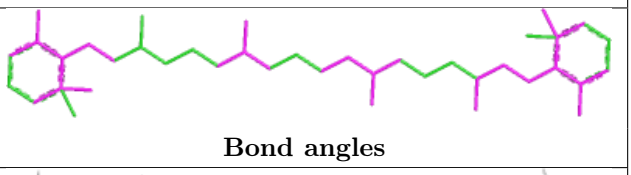


Rings

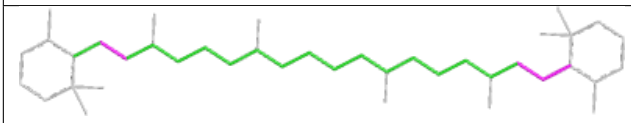
Ligand BCR AC 515



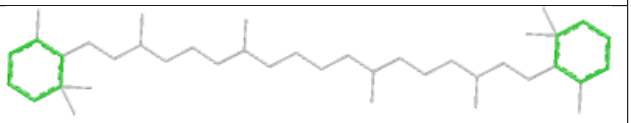
Bond lengths



Bond angles

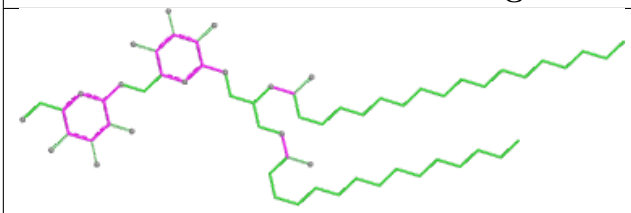


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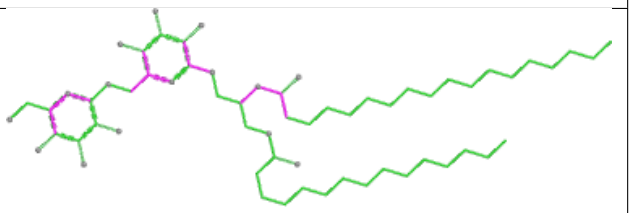


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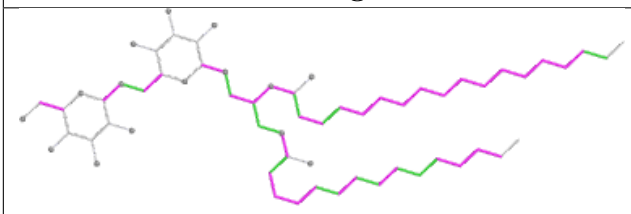
Ligand DGD AD 410



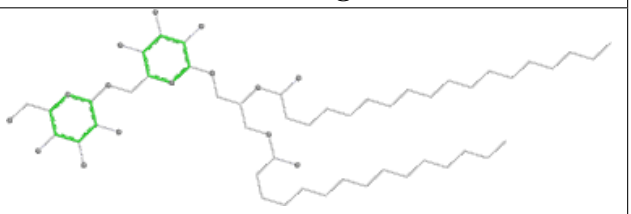
Bond lengths



Bond angles

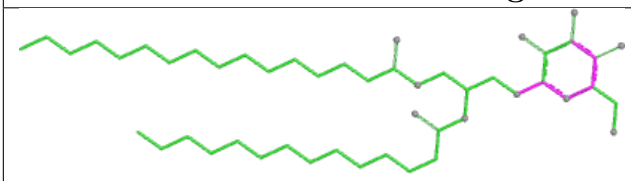


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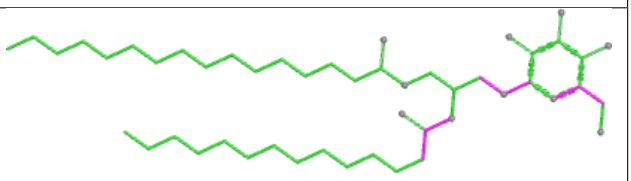


Rings

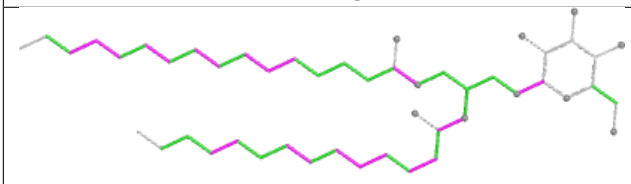
Ligand LMG BB 624



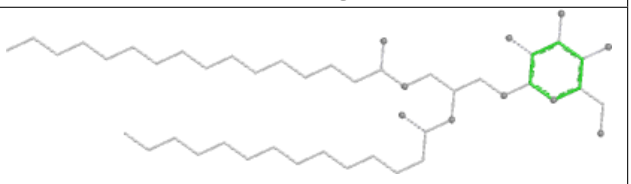
Bond lengths



Bond angles

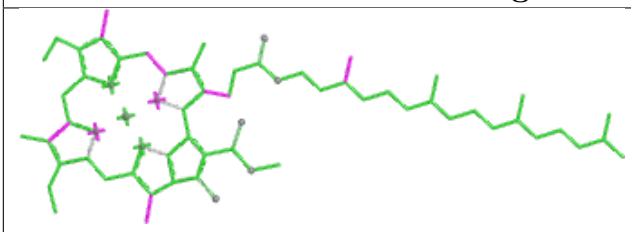


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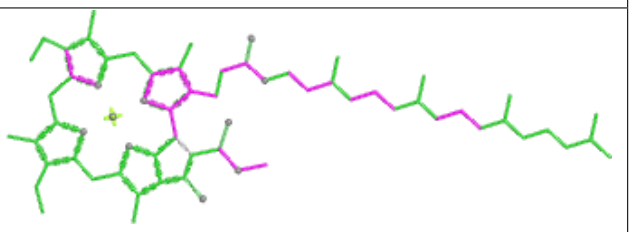


Rings

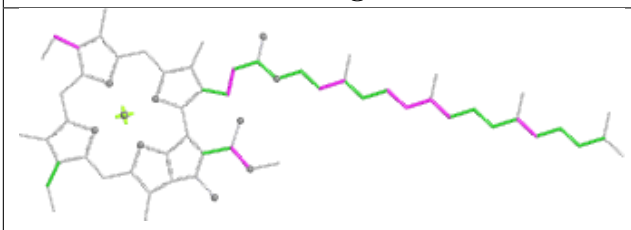
Ligand CLA BC 511



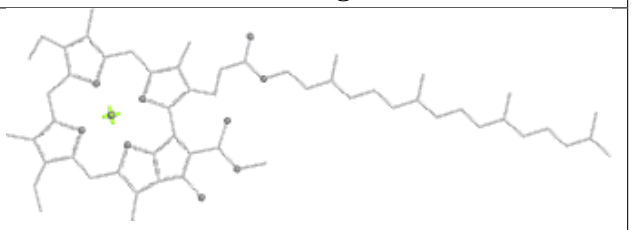
Bond lengths



Bond angles

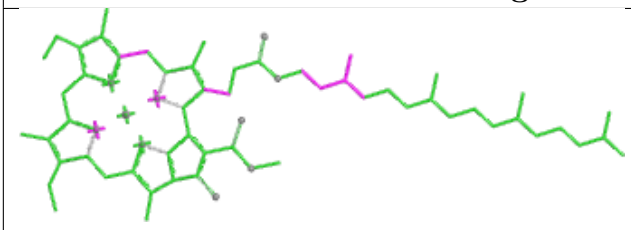


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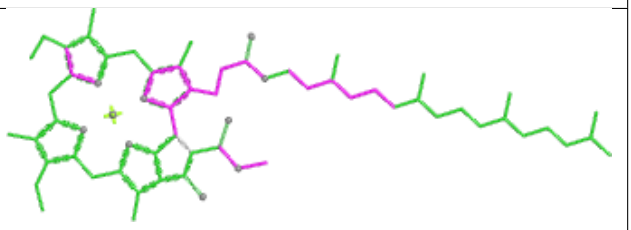


Rings

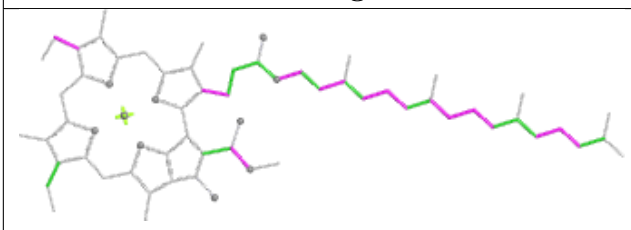
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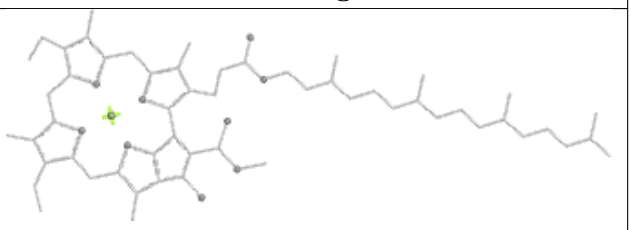
Bond lengths



Bond angles

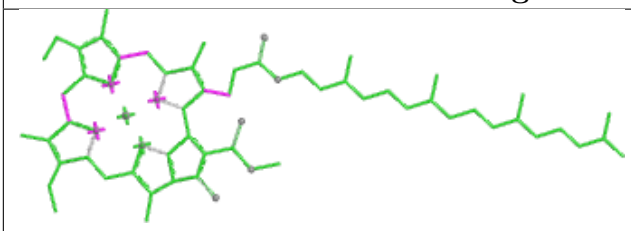


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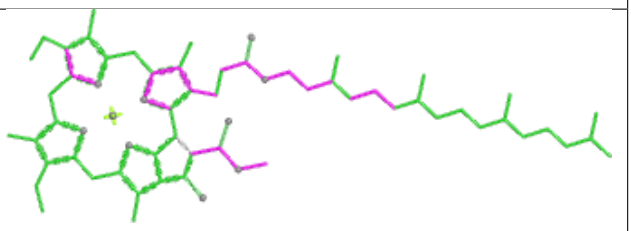


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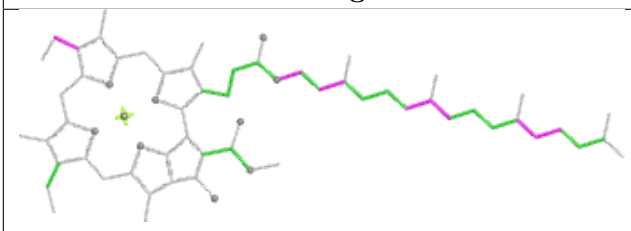
Ligand CLA BC 502



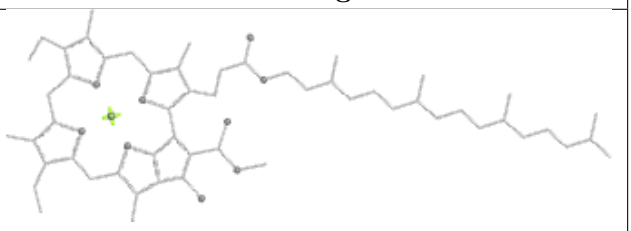
Bond lengths



Bond angles

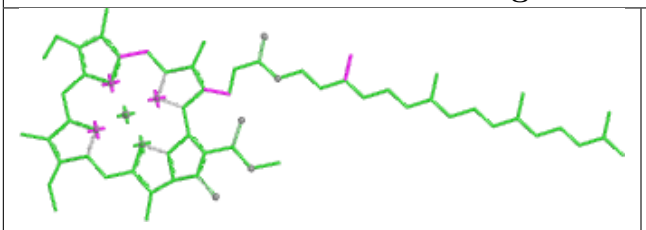


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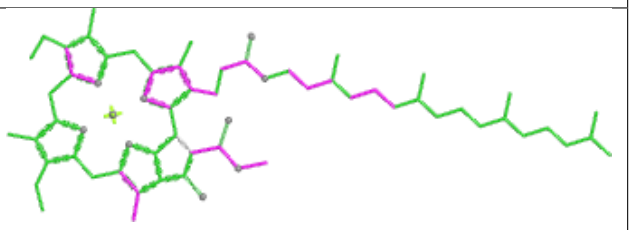


Rings

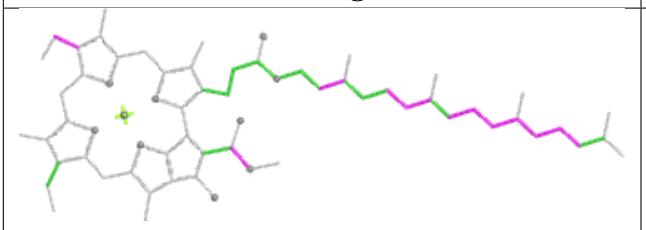
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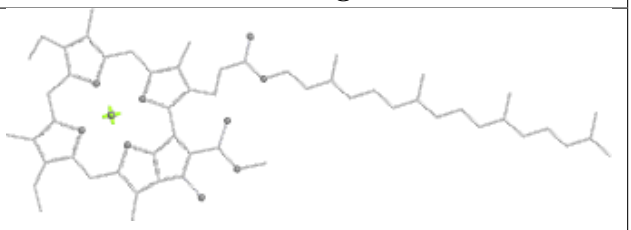
Bond lengths



Bond angles

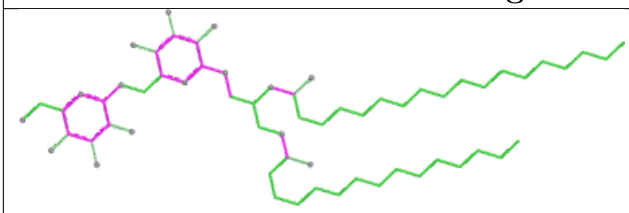


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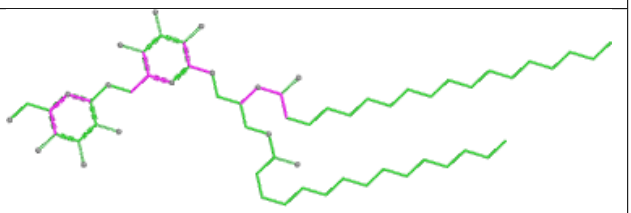


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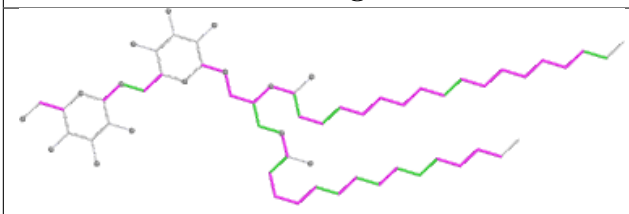
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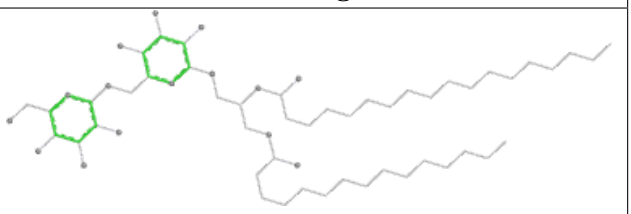
Bond lengths



Bond angles

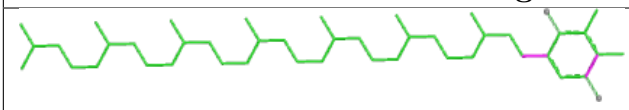


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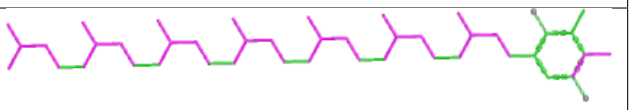


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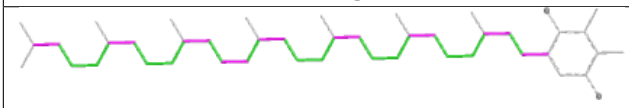
Ligand PL9 AA 407



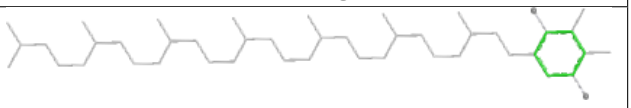
Bond lengths



Bond angles

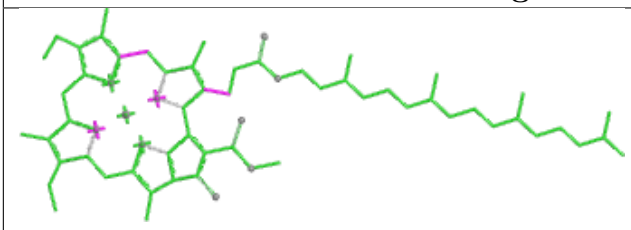


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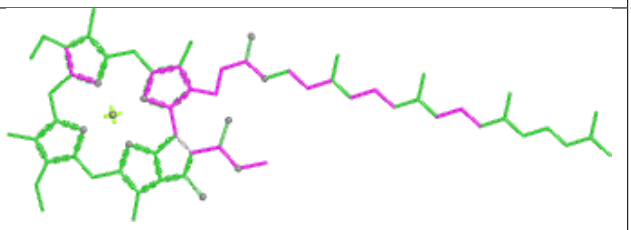


Rings

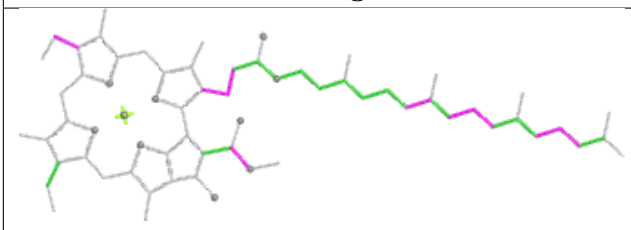
Ligand CLA BC 501



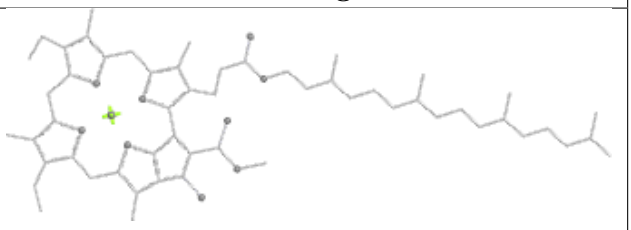
Bond lengths



Bond angles

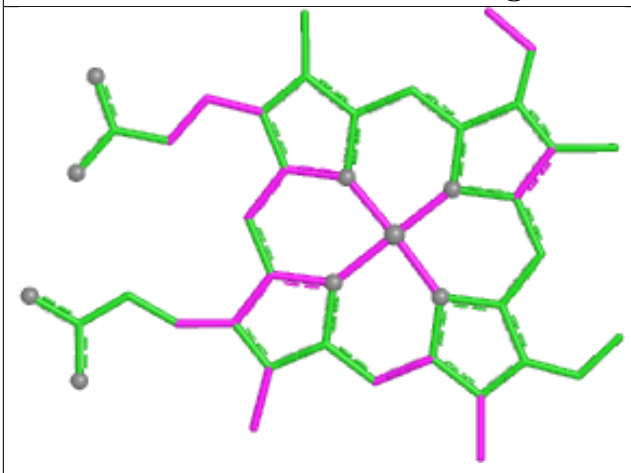


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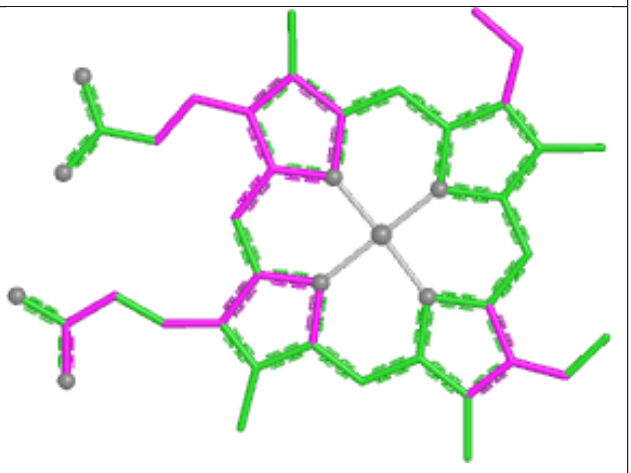


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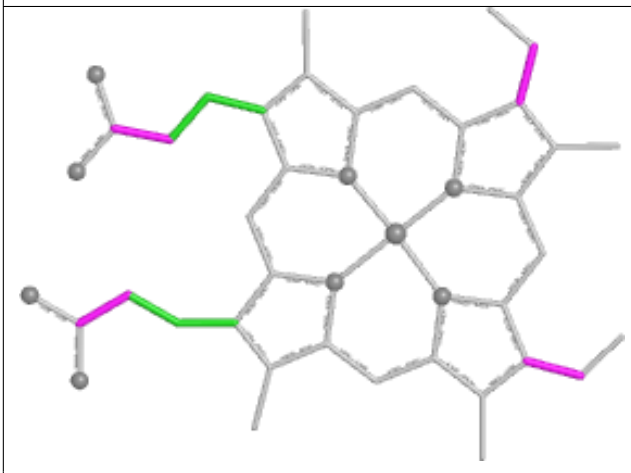
Ligand HEM BV 201



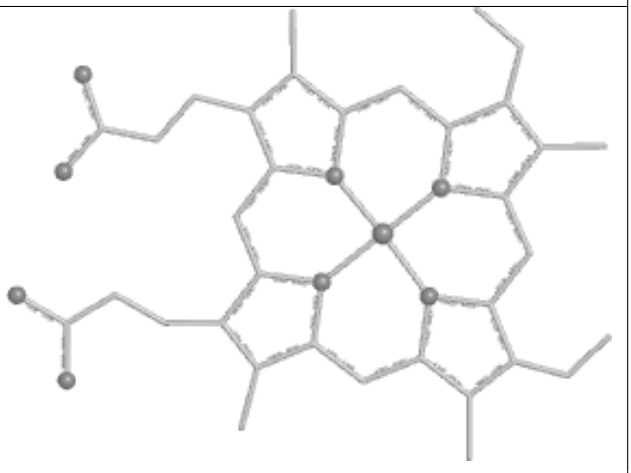
Bond lengths



Bond angles

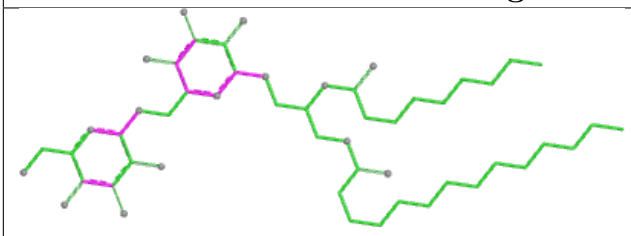


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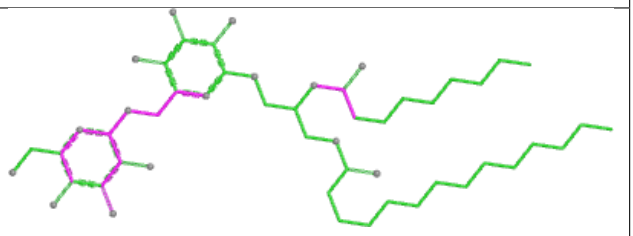


Rings

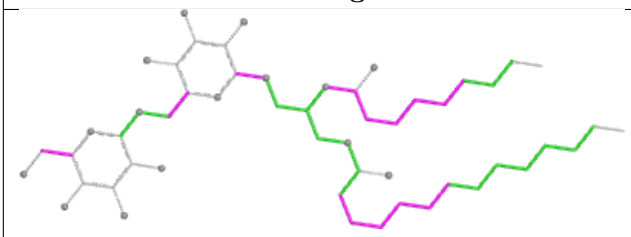
Ligand DGD AC 516



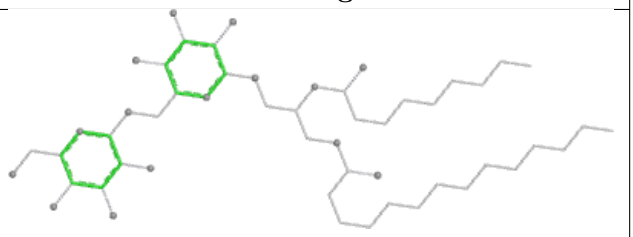
Bond lengths



Bond angles

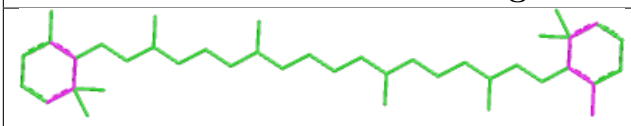


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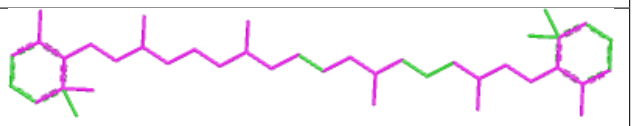


Rings

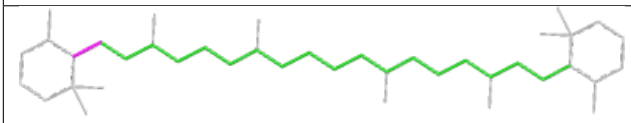
Ligand BCR BX 101



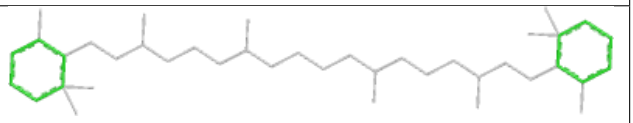
Bond lengths



Bond angles

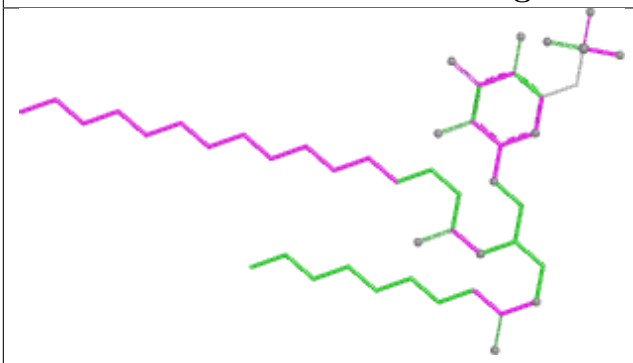


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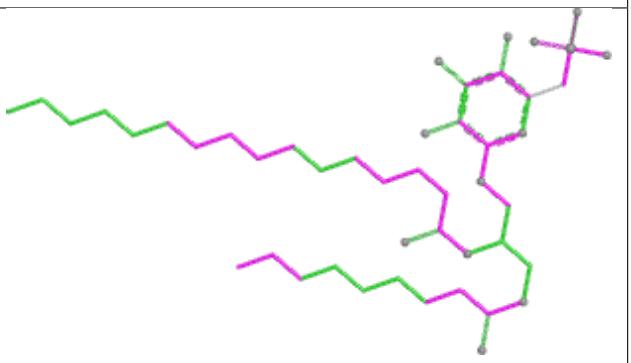


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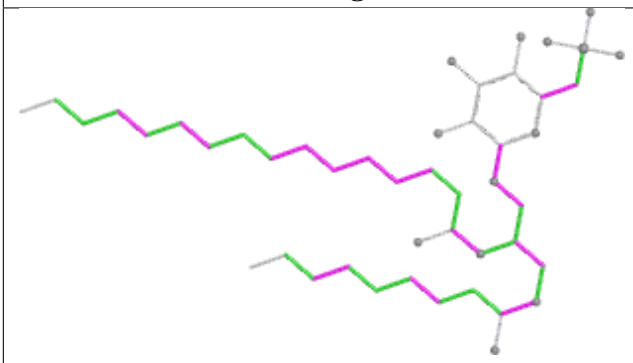
Ligand SQD BL 101



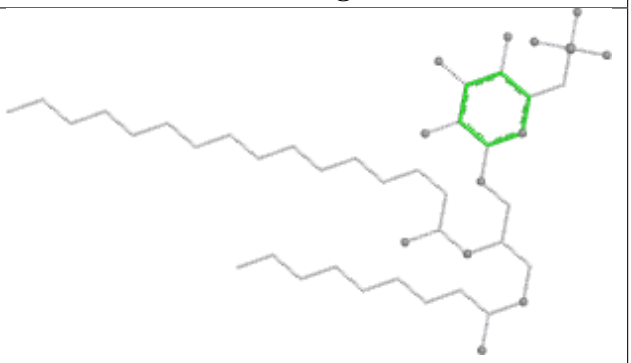
Bond lengths



Bond angles

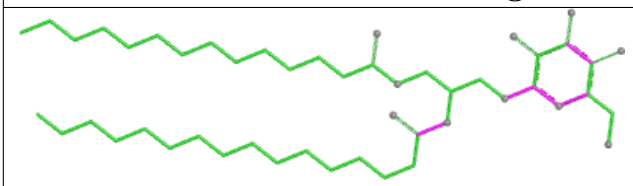


Torsions

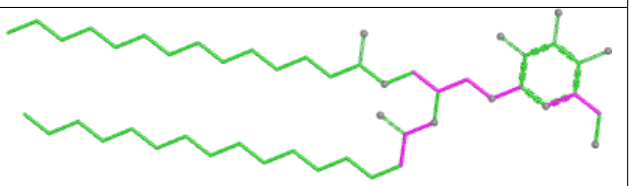


Rings

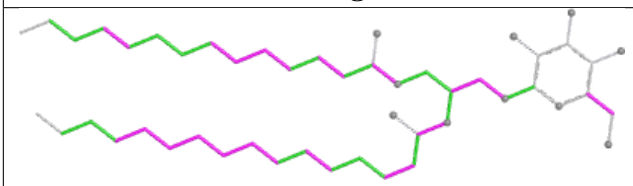
Ligand LMG AB 621



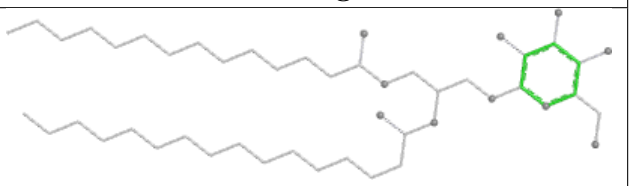
Bond lengths



Bond angles

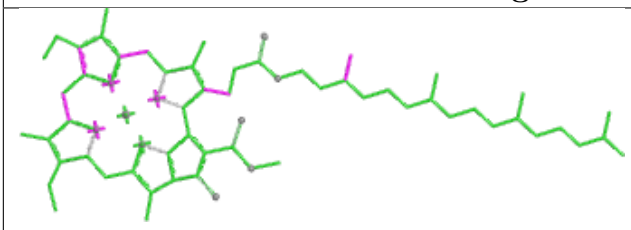


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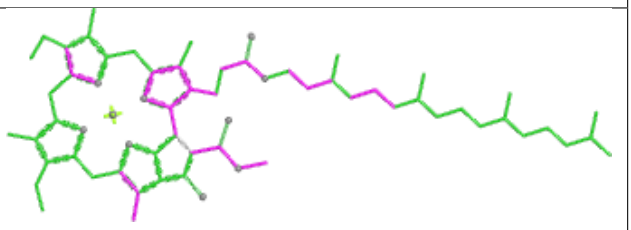


Rings

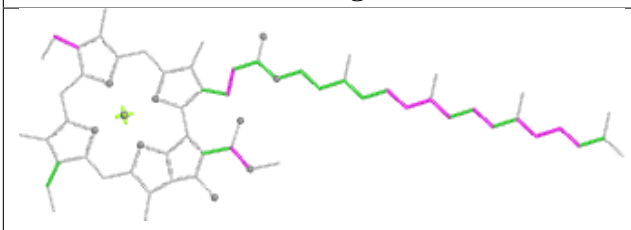
Ligand CLA BC 508



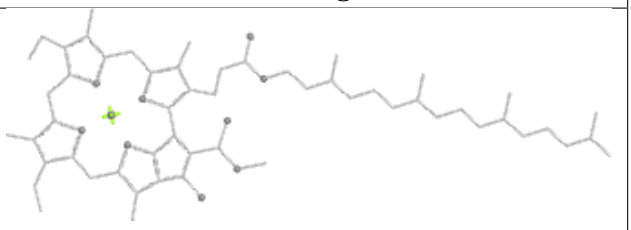
Bond lengths



Bond angles

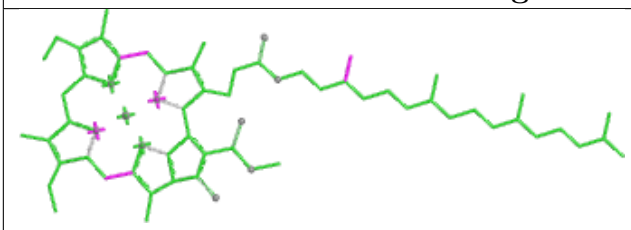


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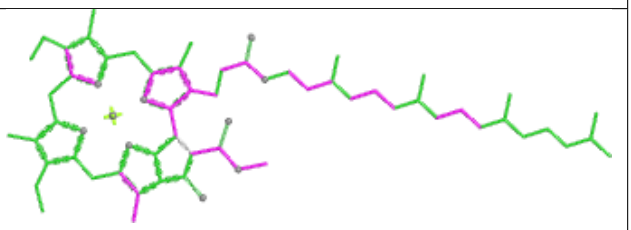


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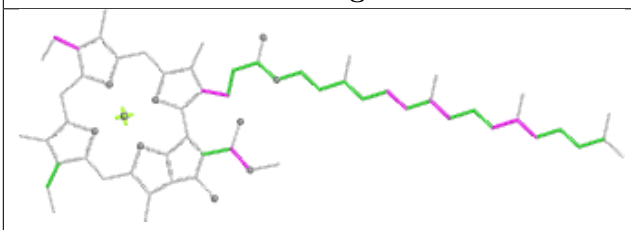
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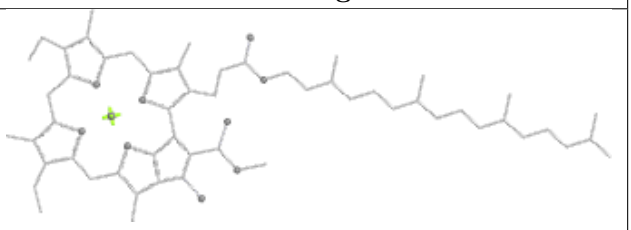
Bond lengths



Bond angles

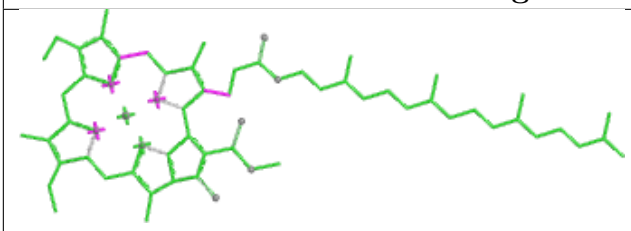


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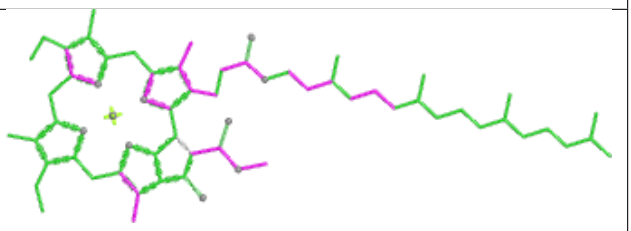


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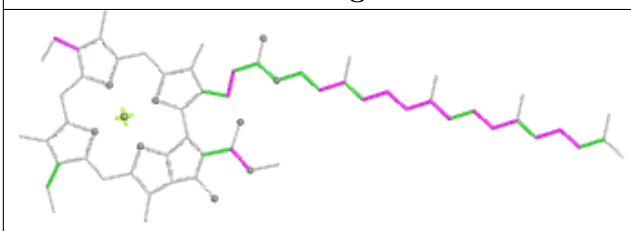
Ligand CLA BB 608



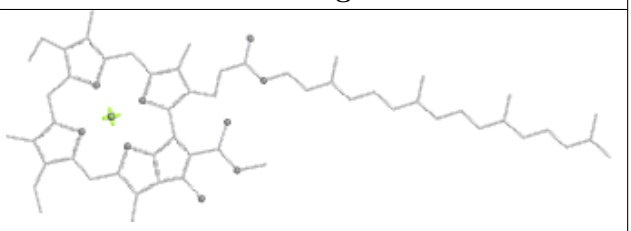
Bond lengths



Bond angles

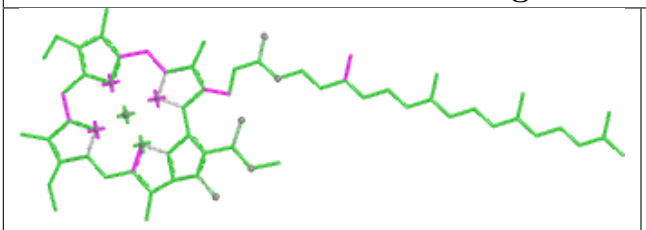


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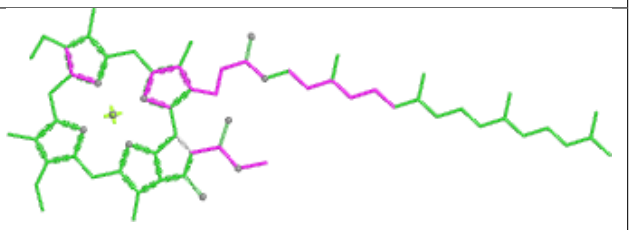


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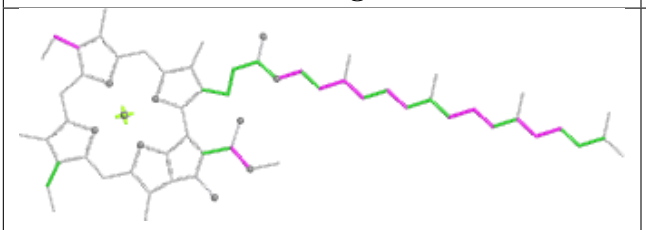
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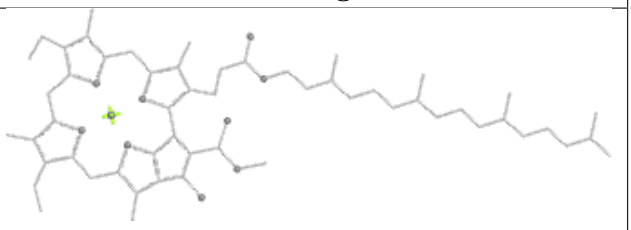
Bond lengths



Bond angles

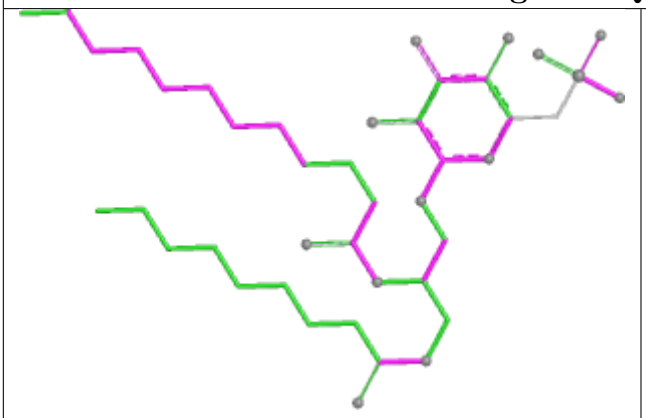


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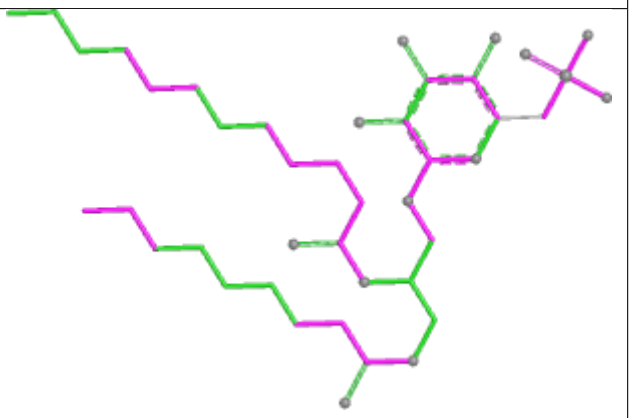


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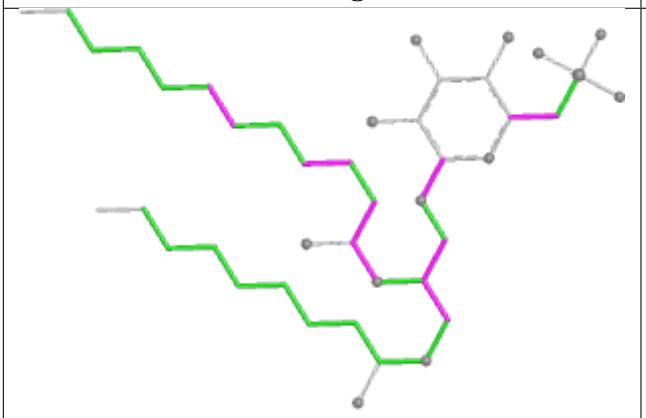
Ligand SQD AD 409



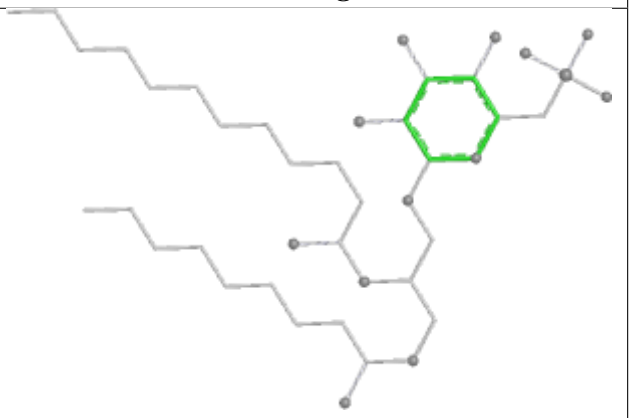
Bond lengths



Bond angles

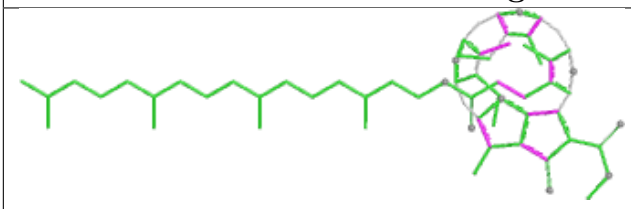


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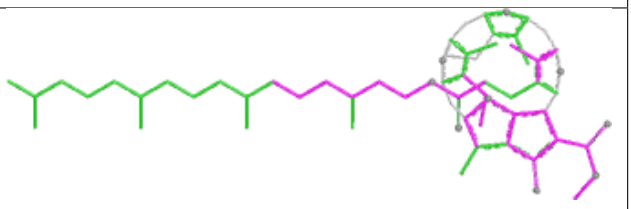


Rings

Ligand PHO AA 405



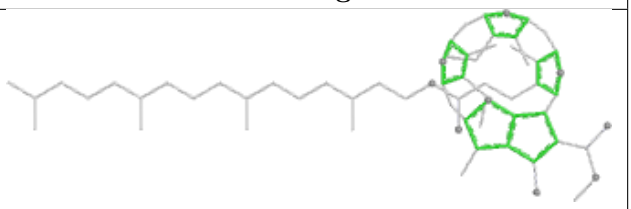
Bond lengths



Bond angles

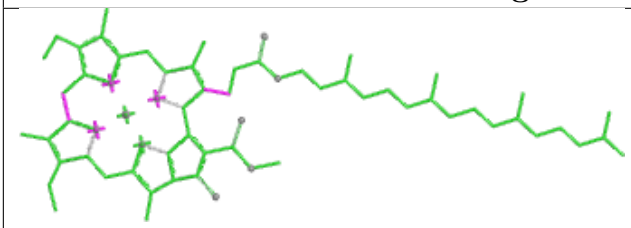


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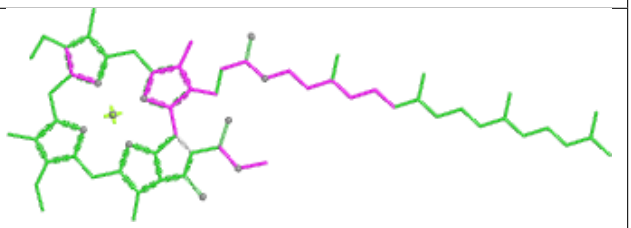


Rings

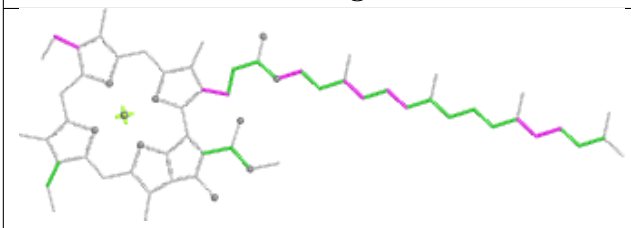
Ligand CLA BB 612



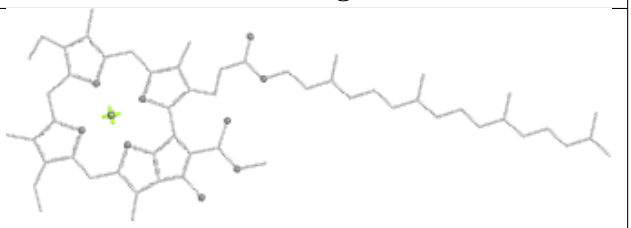
Bond lengths



Bond angles

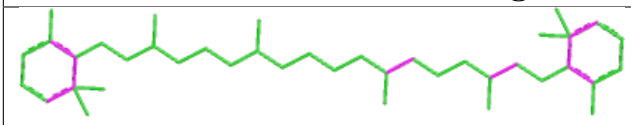


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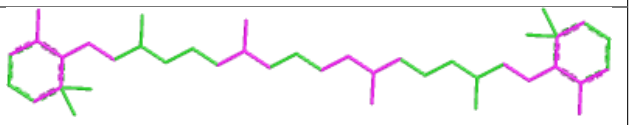


Rings

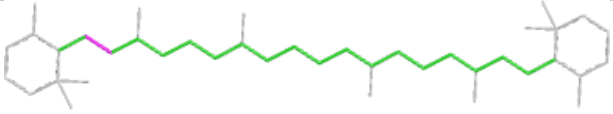
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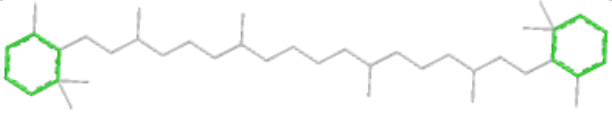
Bond lengths



Bond angles

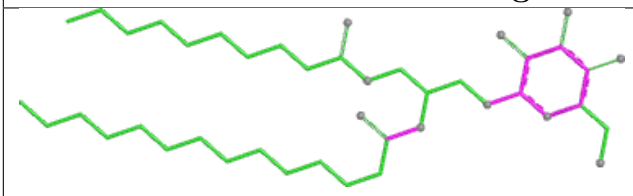


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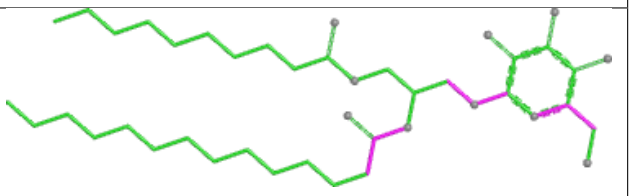


Rings

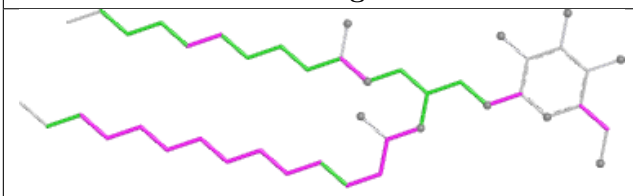
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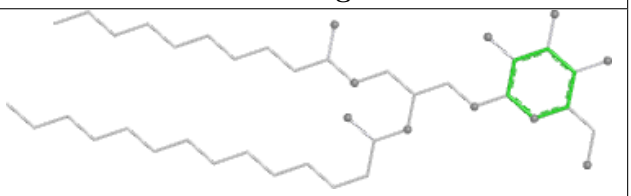
Bond lengths



Bond angles

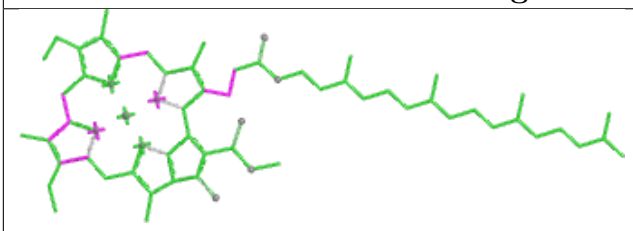


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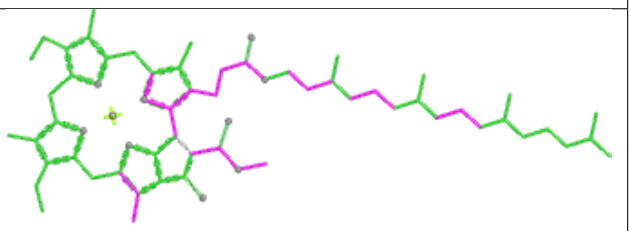


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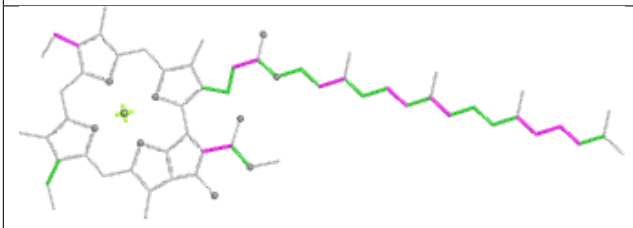
Ligand CLA BD 402



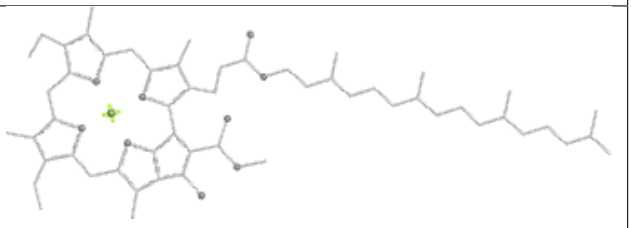
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Bond angles

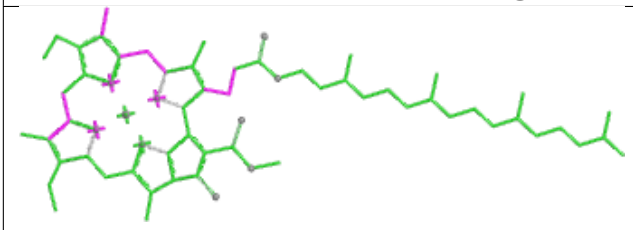


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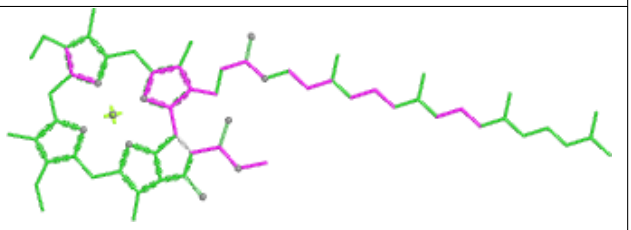


Rings

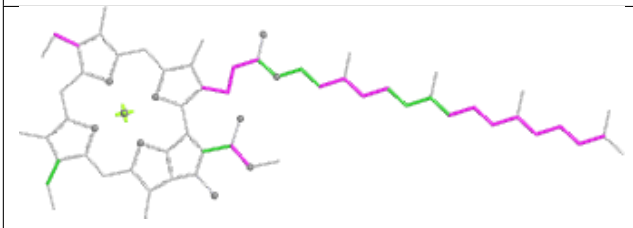
Ligand CLA AC 512



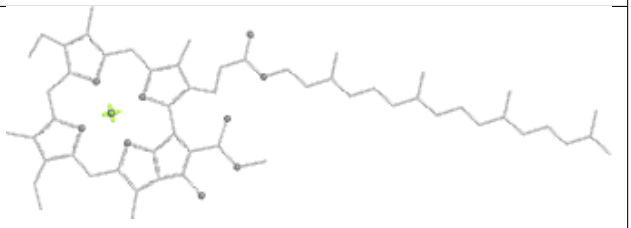
Bond lengths



Bond angles

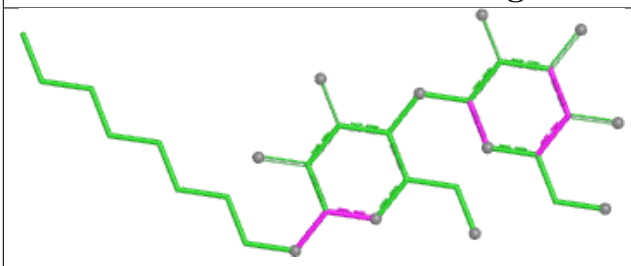


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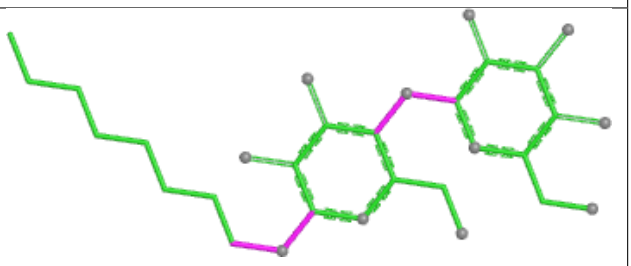


Rings

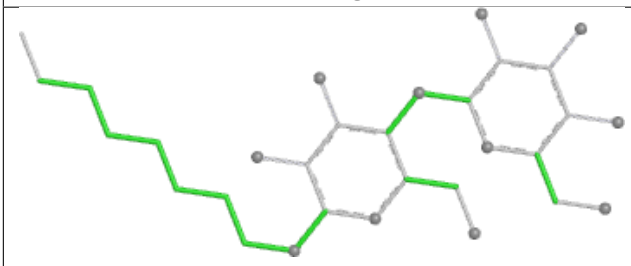
Ligand LMT AD 411



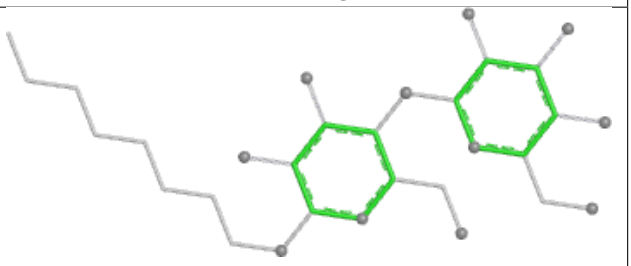
Bond lengths



Bond angles

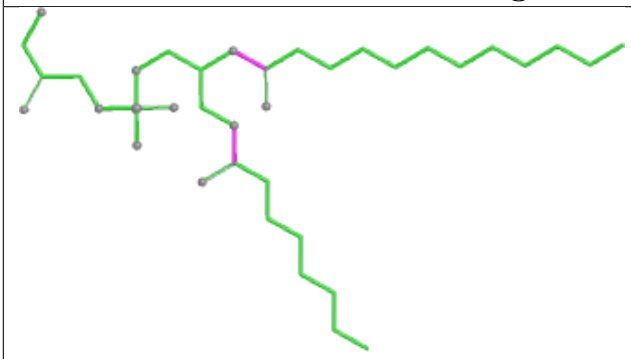


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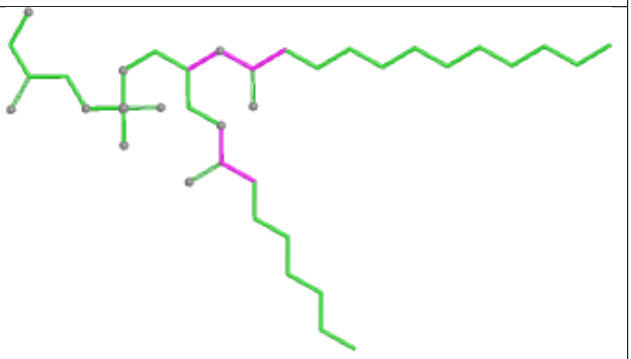


Rings

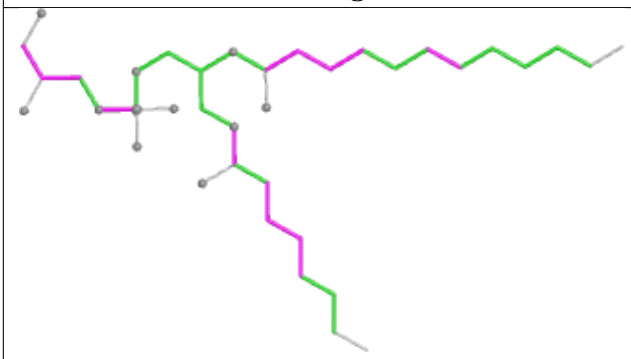
Ligand LHG BC 521



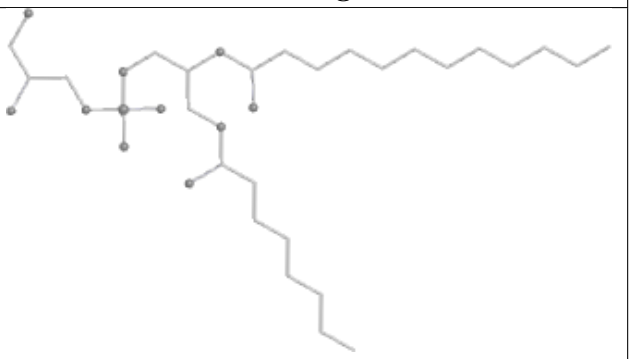
Bond lengths



Bond angles

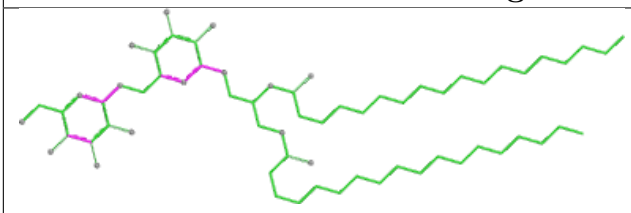


Torsions

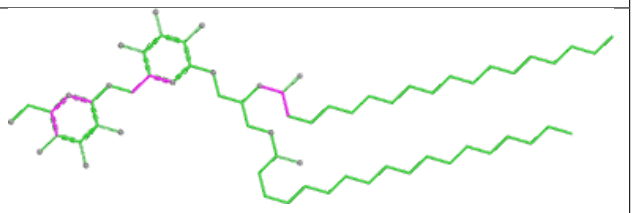


Rings

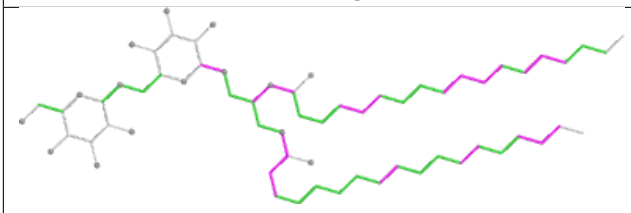
Ligand DGD AC 518



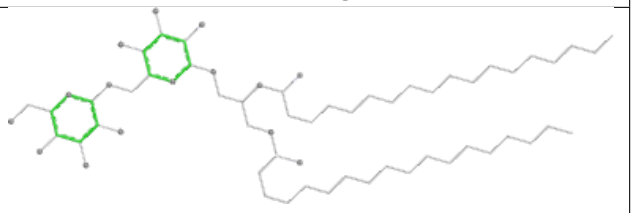
Bond lengths



Bond angles

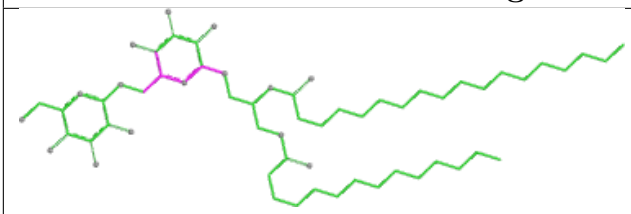


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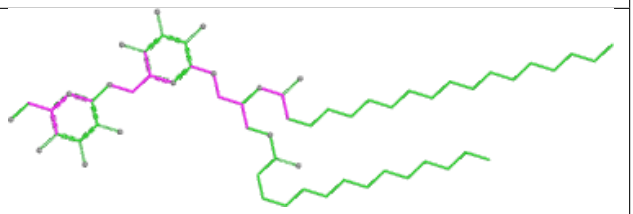


Rings

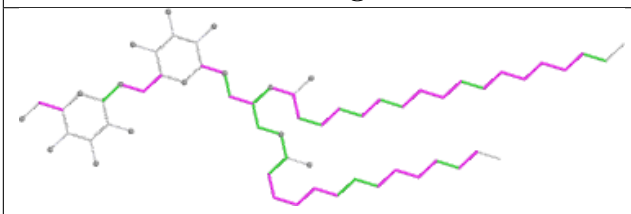
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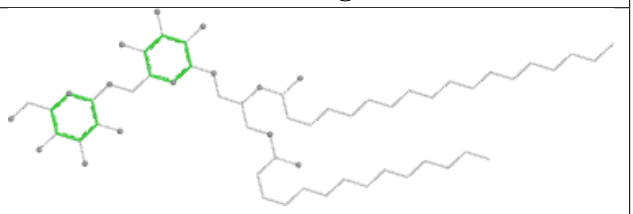
Bond lengths



Bond angles

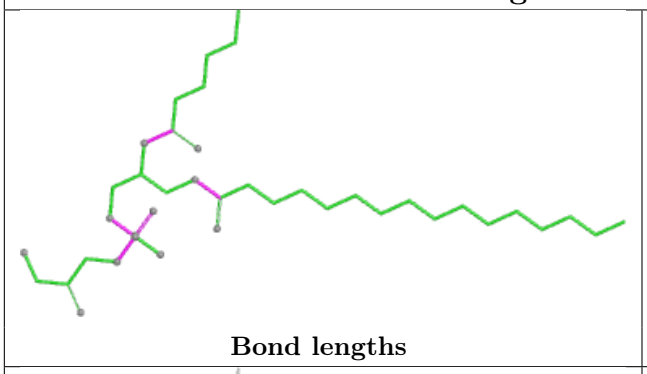


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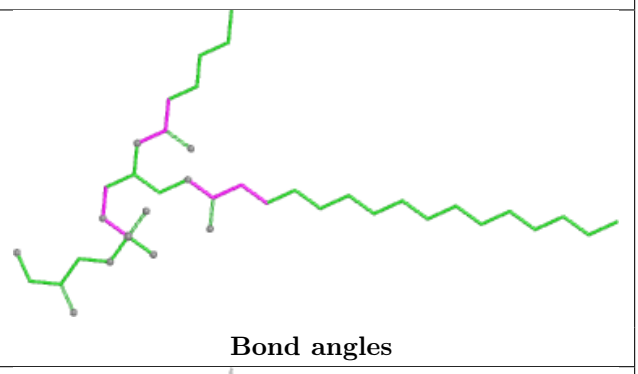


Rings

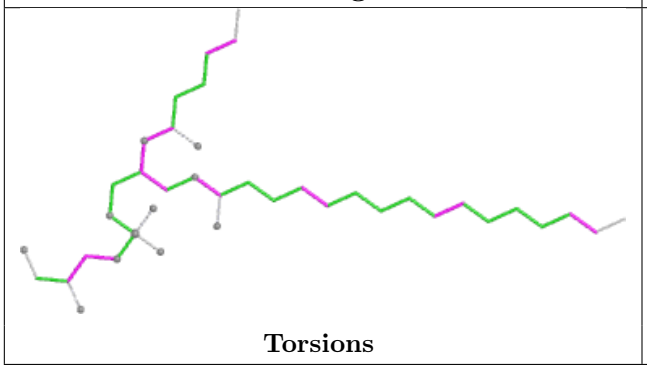
Ligand LHG AA 411



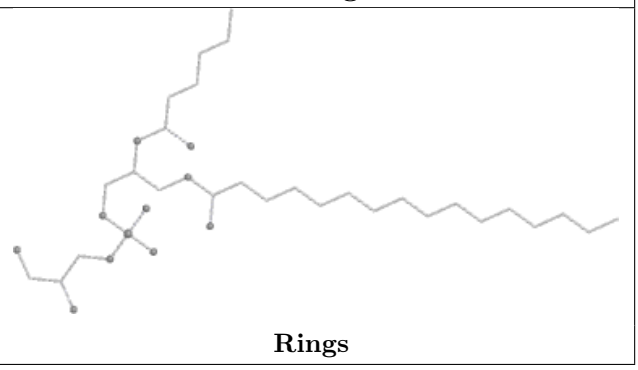
Bond lengths



Bond angles

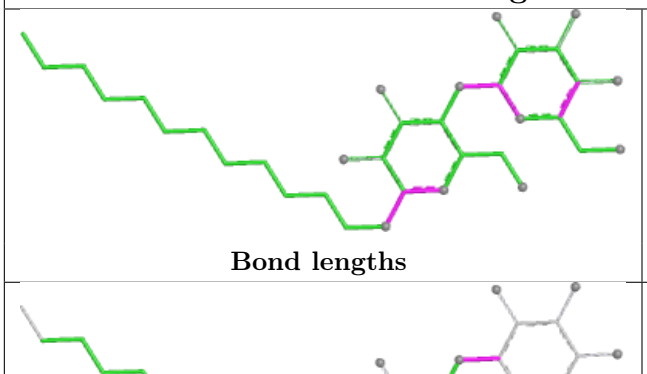


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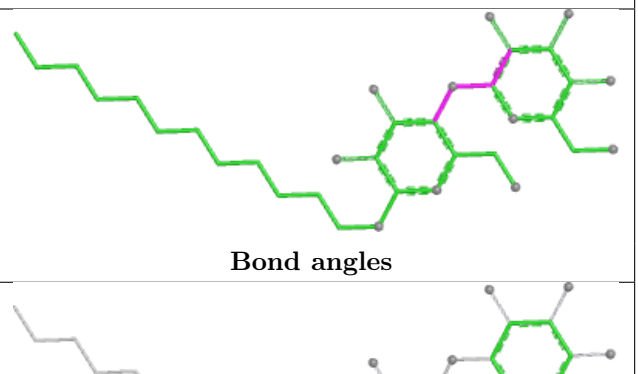


Rings

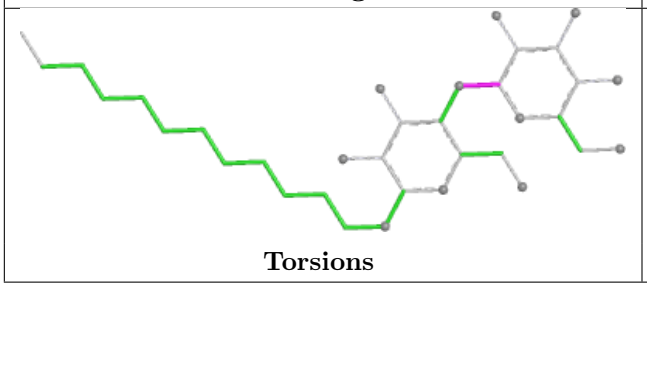
Ligand LMT BB 626



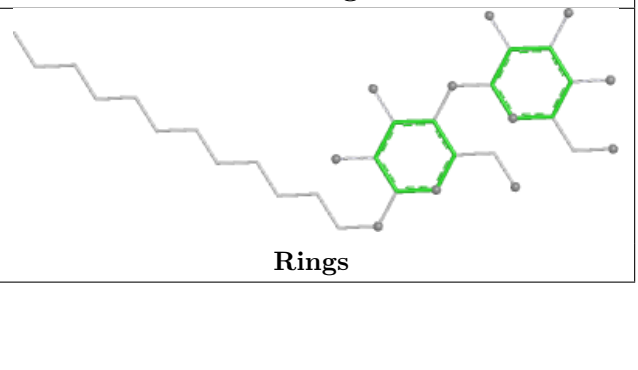
Bond lengths



Bond angles

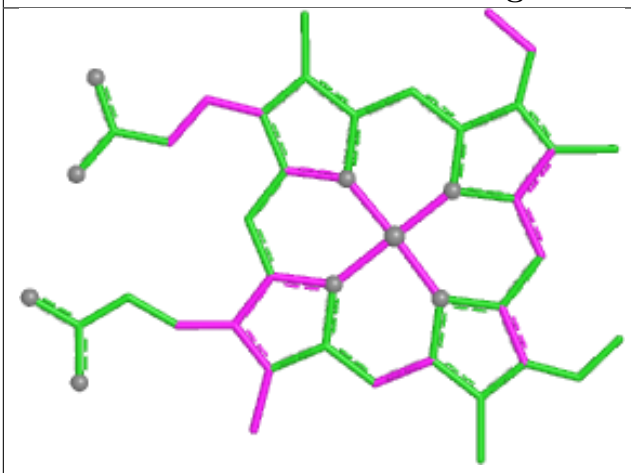


Torsions

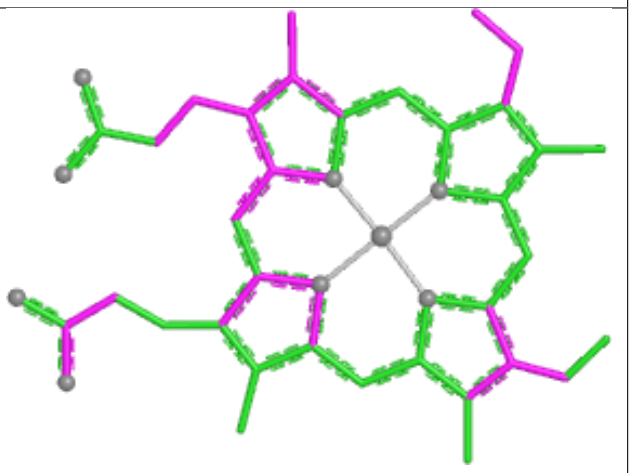


Rings

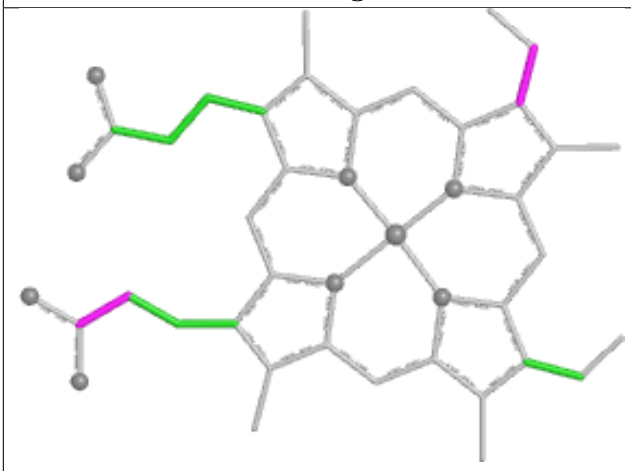
Ligand HEM AE 101



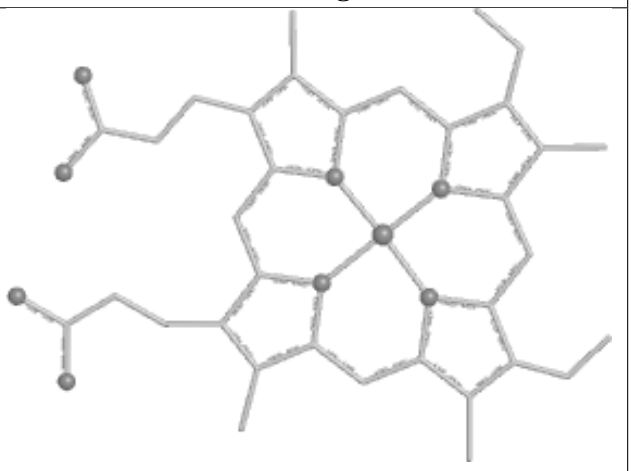
Bond lengths



Bond angles

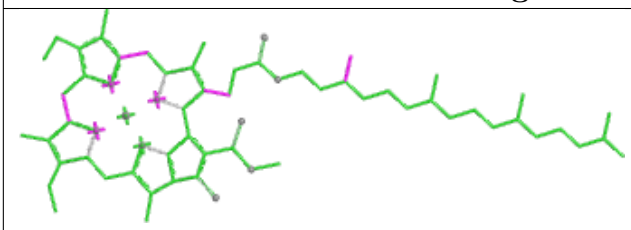


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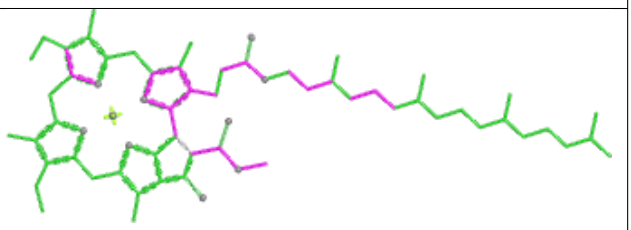


Rings

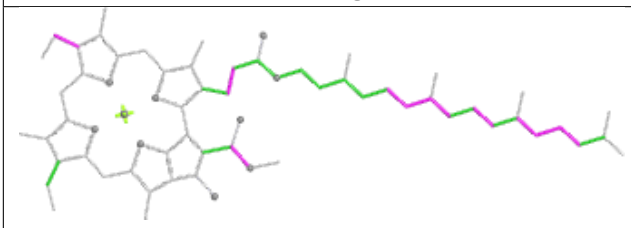
Ligand CLA AC 508



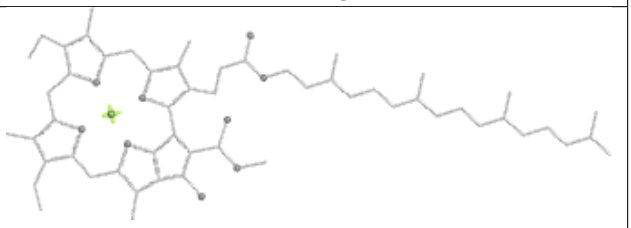
Bond lengths



Bond angles

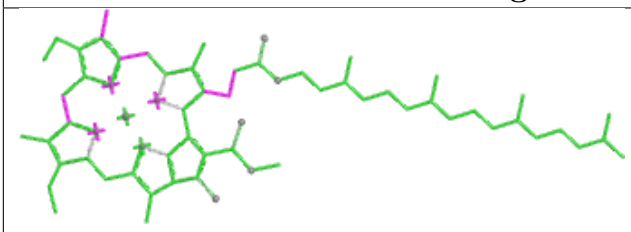


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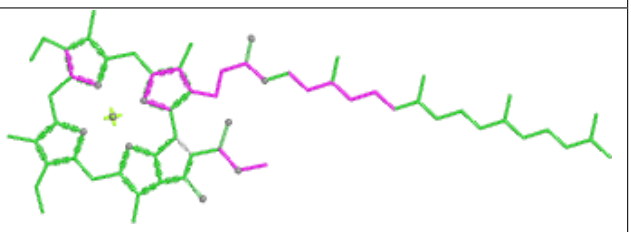


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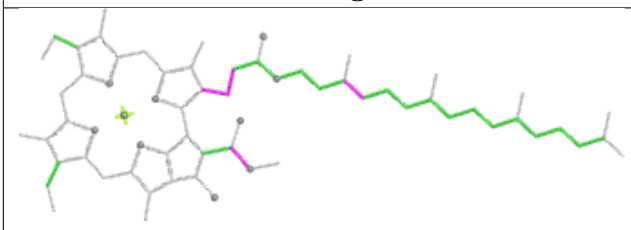
Ligand CLA AA 402



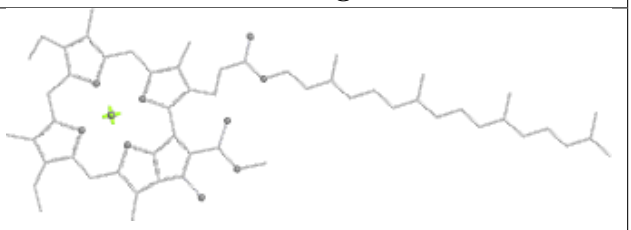
Bond lengths



Bond angles



Torsions

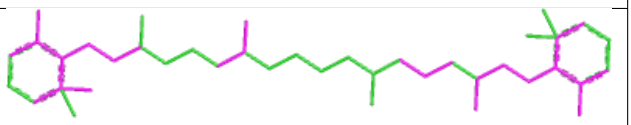


Rings

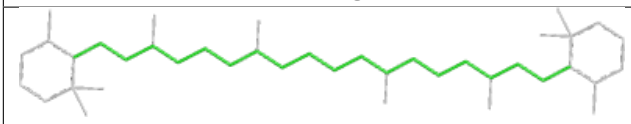
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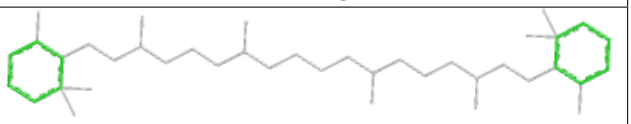
Bond lengths



Bond angles

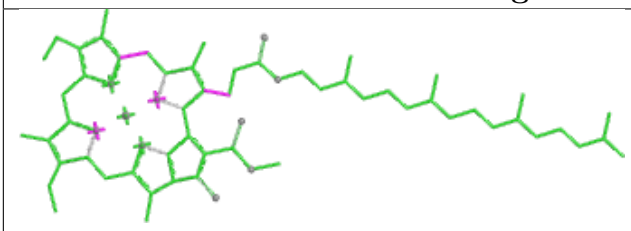


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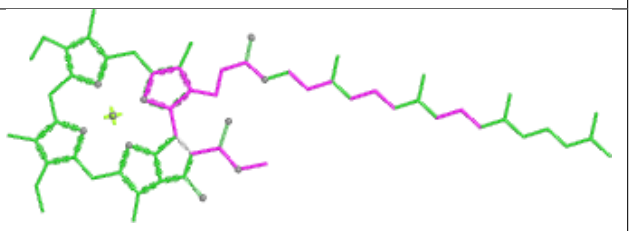


Rings

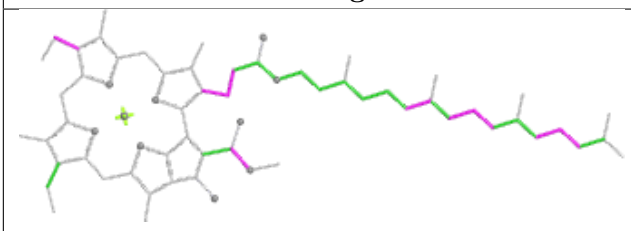
Ligand CLA AC 501



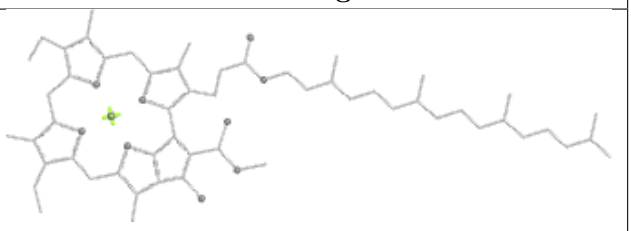
Bond lengths



Bond angles

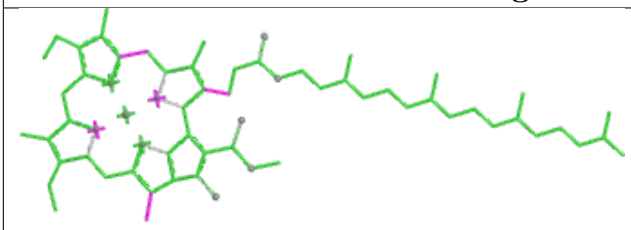


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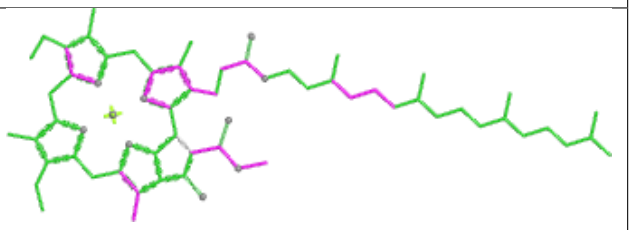


Rings

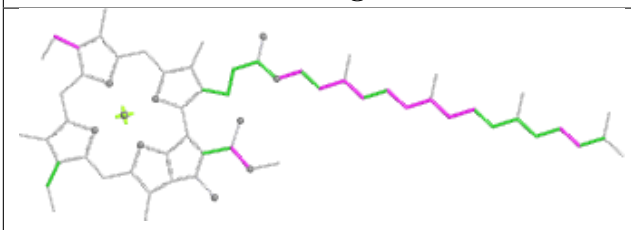
Ligand CLA BB 614



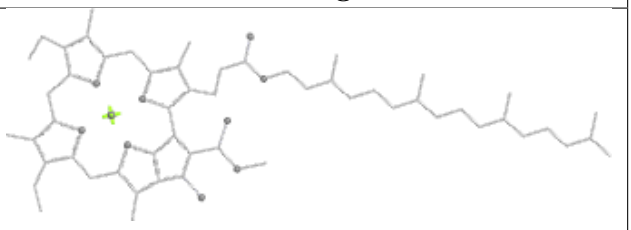
Bond lengths



Bond angles

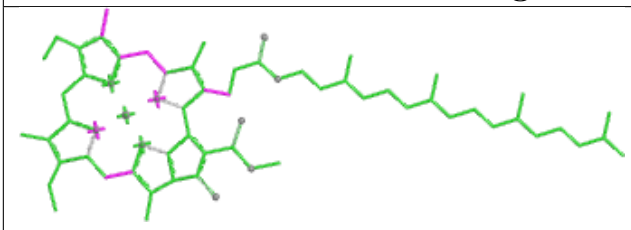


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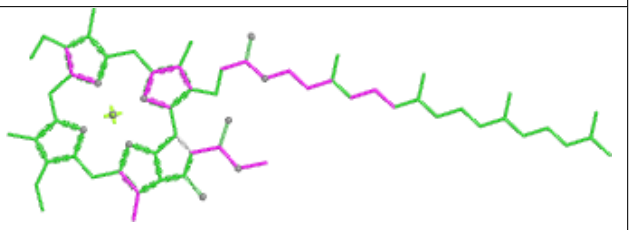


Rings

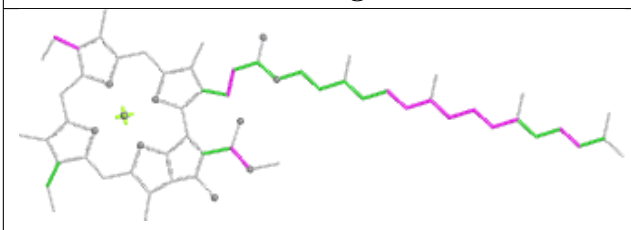
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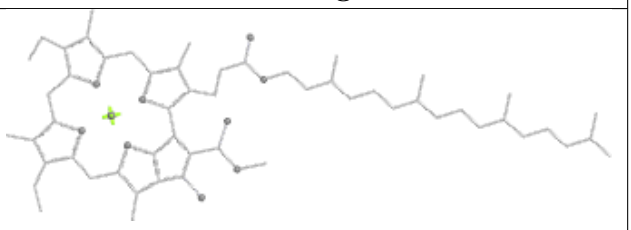
Bond lengths



Bond angles

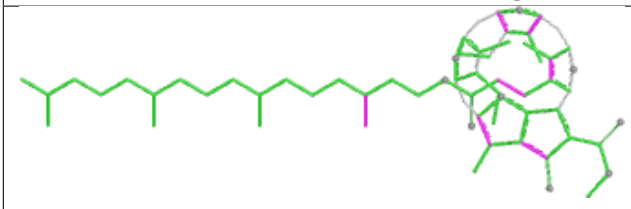


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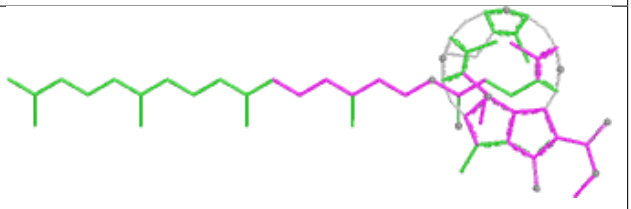


Rings

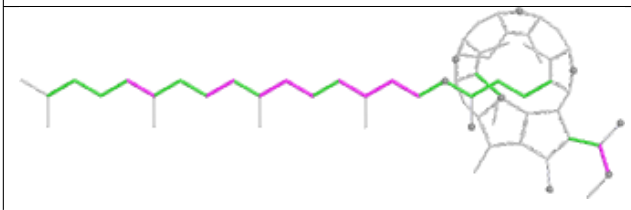
Ligand PHO BA 406



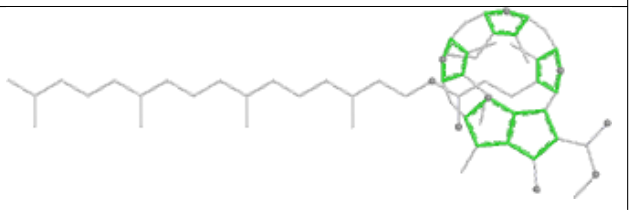
Bond lengths



Bond angles

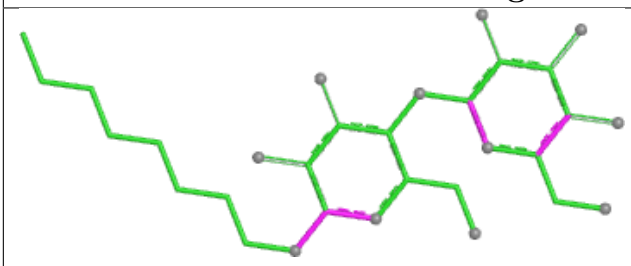


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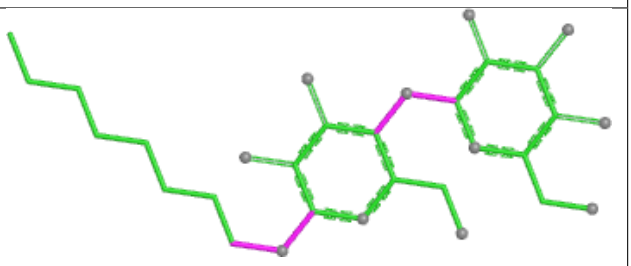


Rings

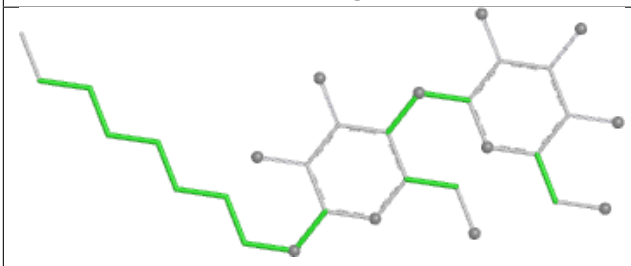
Ligand LMT BD 411



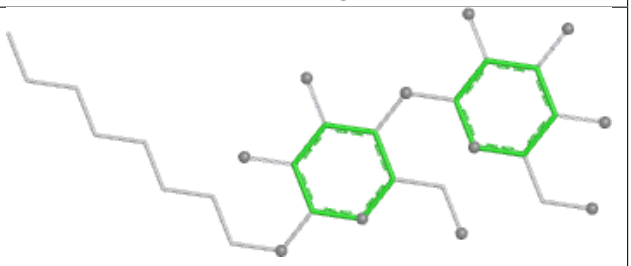
Bond lengths



Bond angles

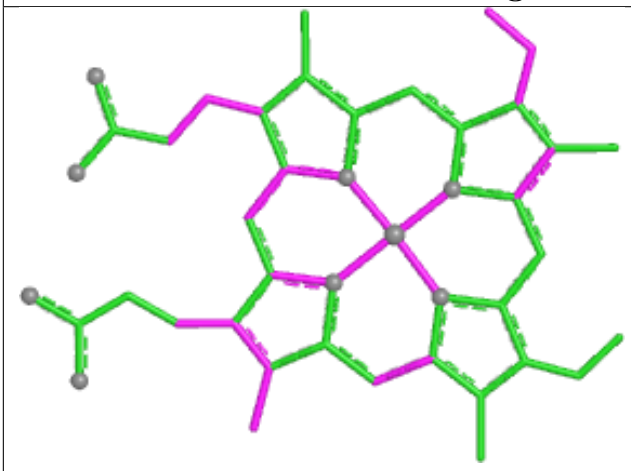


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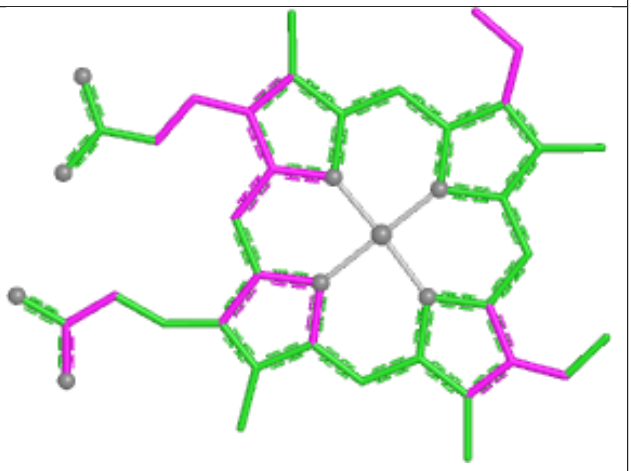


Rings

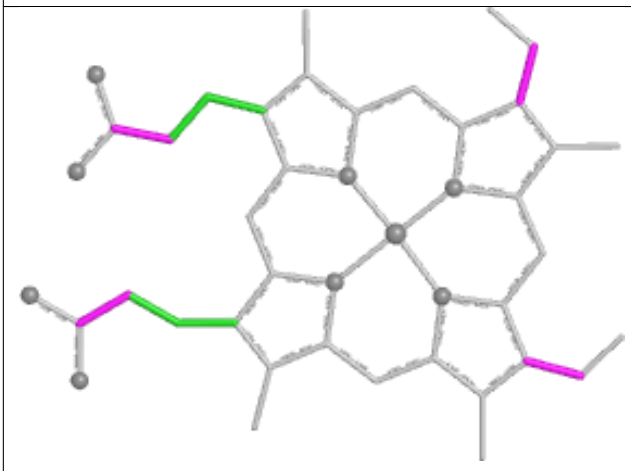
Ligand HEM AV 201



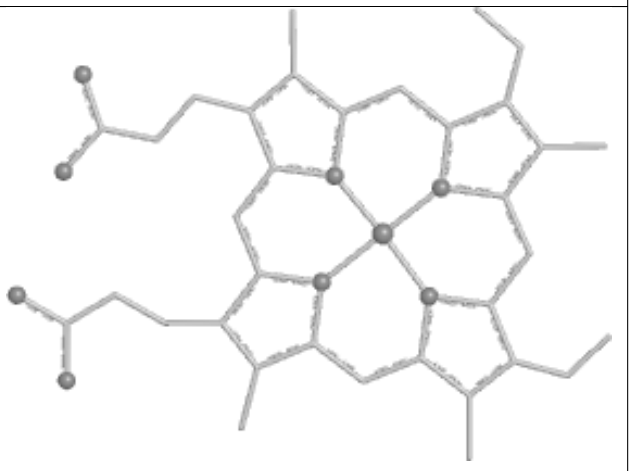
Bond lengths



Bond angles

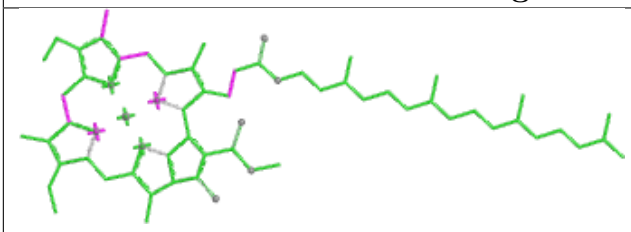


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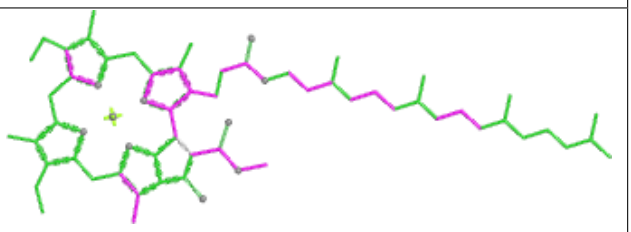


Rings

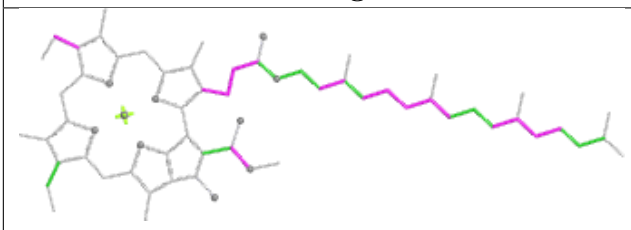
Ligand CLA BB 605



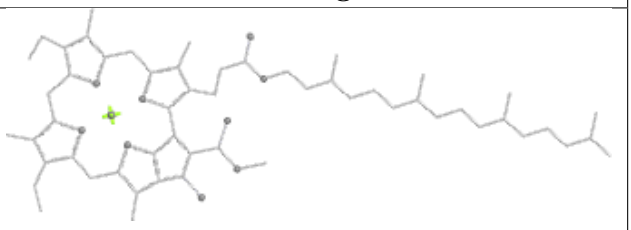
Bond lengths



Bond angles

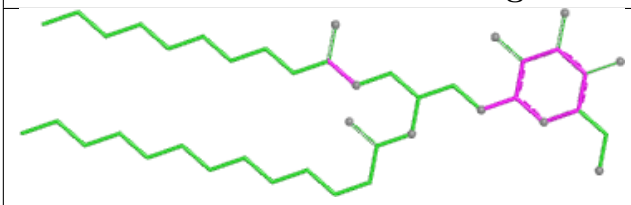


Torsions

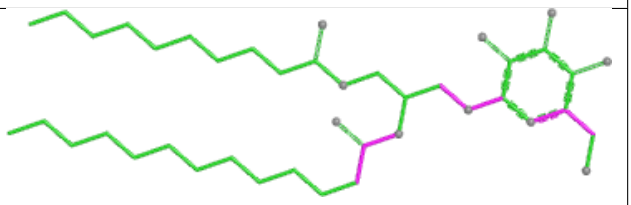


Rings

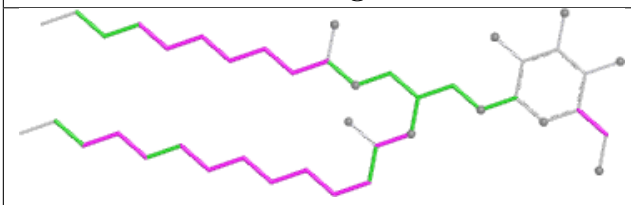
Ligand LMG AB 623



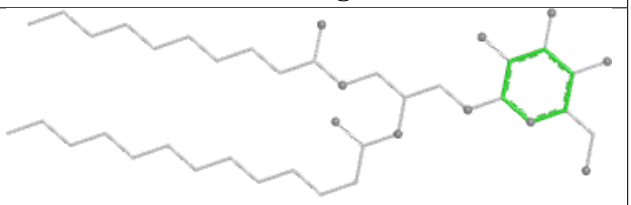
Bond lengths



Bond angles

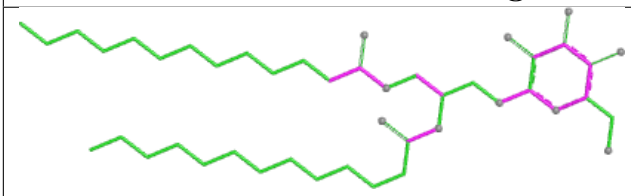


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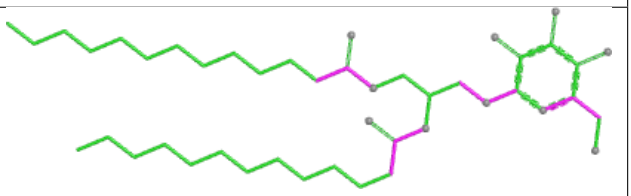


Rings

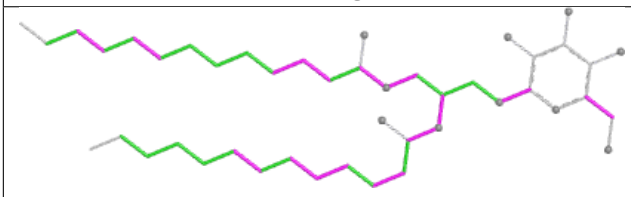
Ligand LMG BC 520



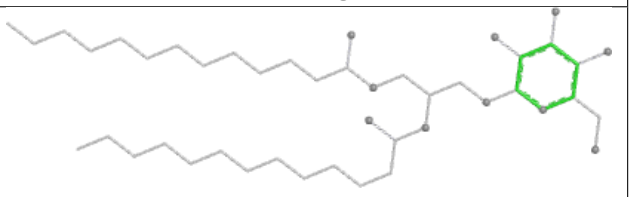
Bond lengths



Bond angles

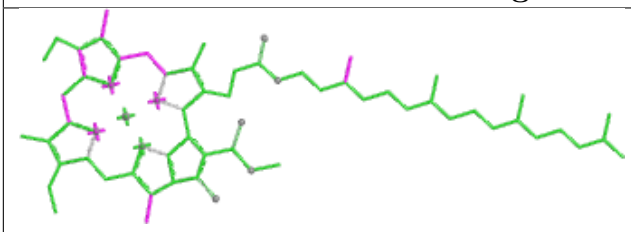


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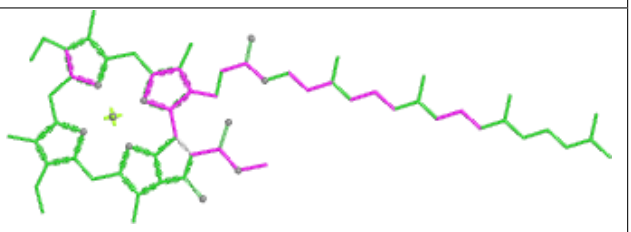


Rings

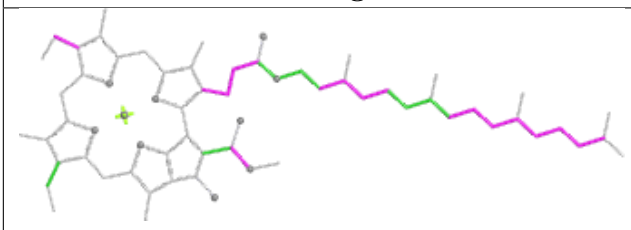
Ligand CLA BC 512



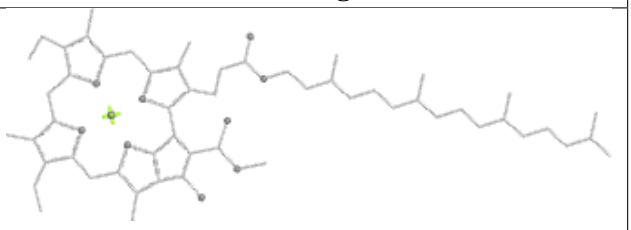
Bond lengths



Bond angles

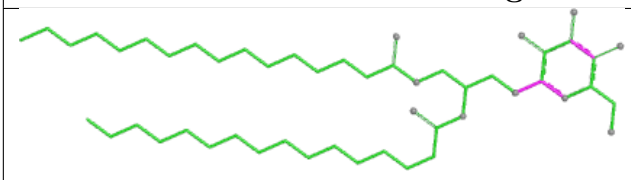


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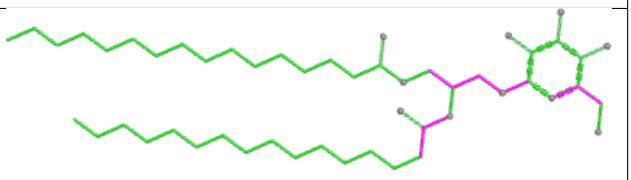


Rings

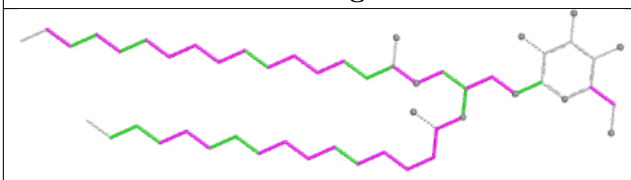
Ligand LMG AA 413



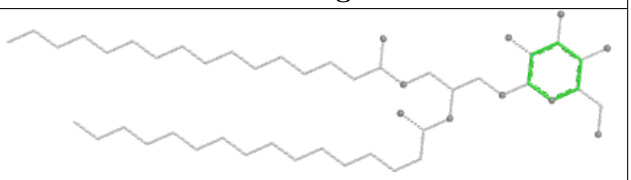
Bond lengths



Bond angles

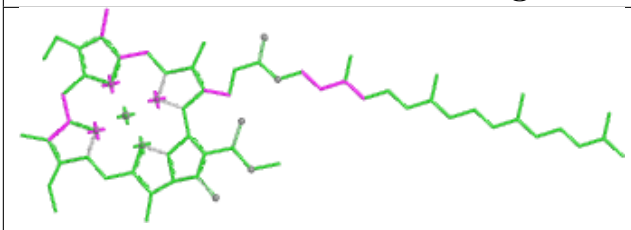


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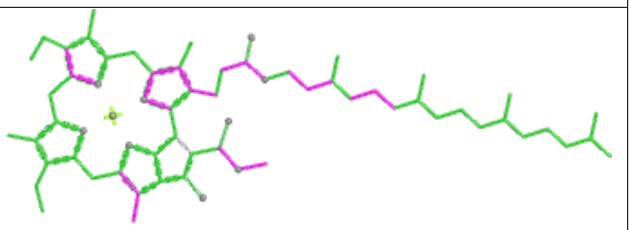


Rings

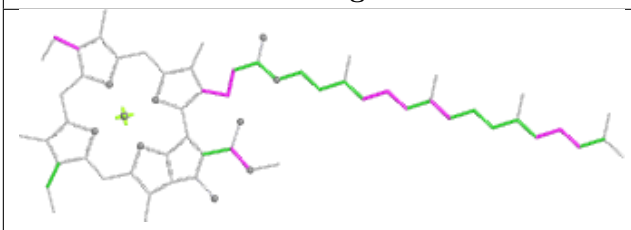
Ligand CLA AB 607



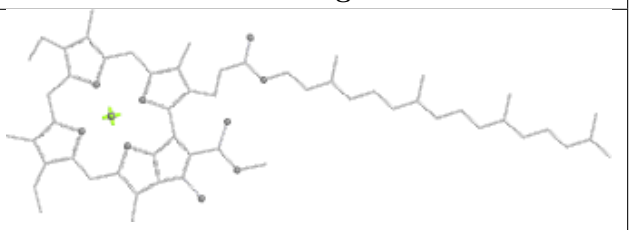
Bond lengths



Bond angles

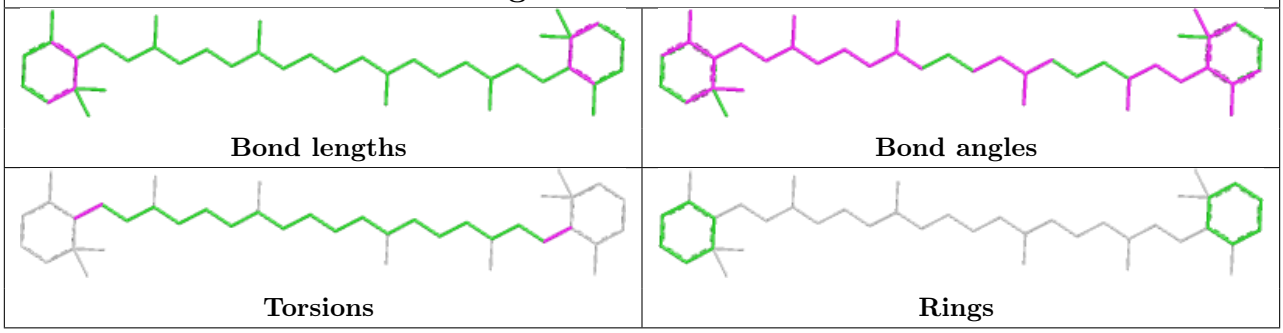


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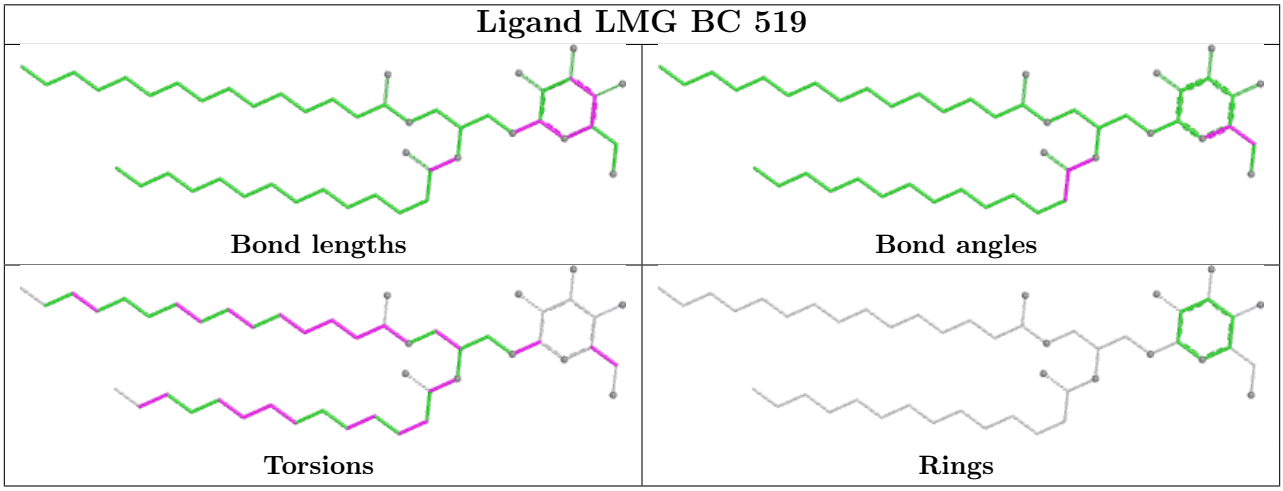


Rings

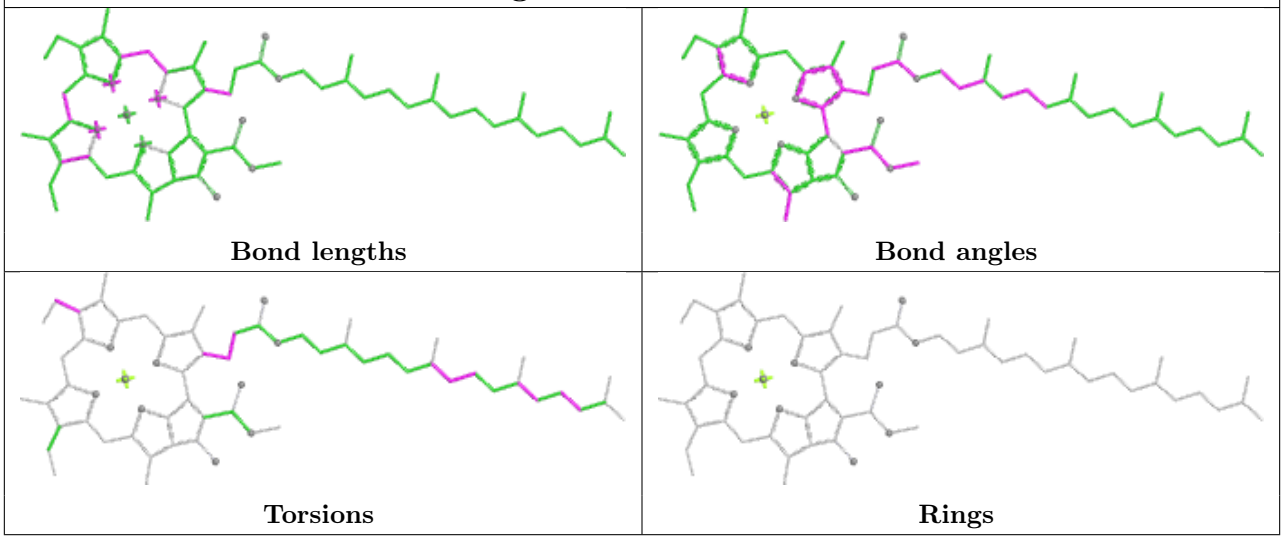
Ligand BCR AK 102



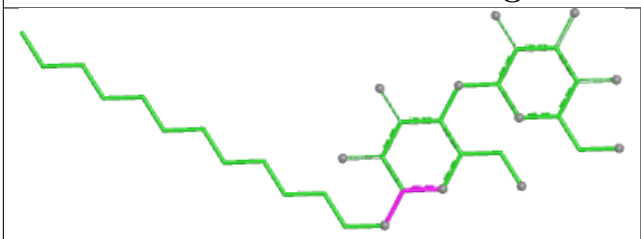
Ligand LMG BC 519



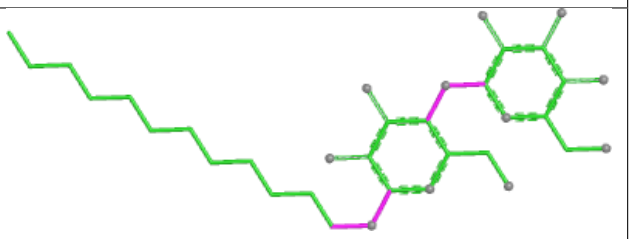
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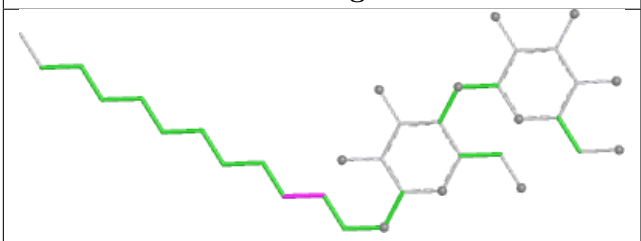
Ligand LMT AM 102



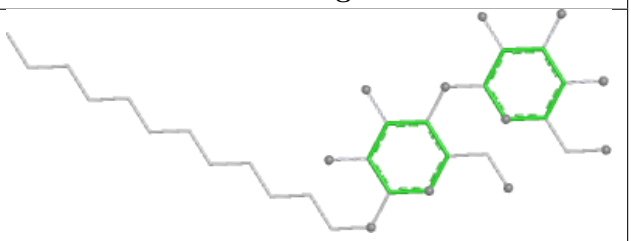
Bond lengths



Bond angles

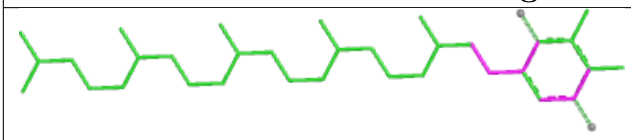


Torsions

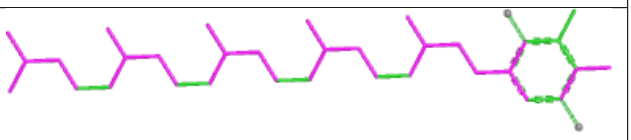


Rings

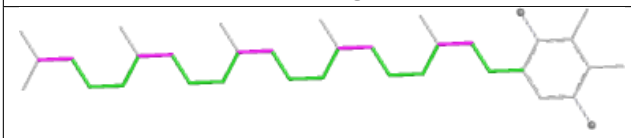
Ligand PL9 BJ 101



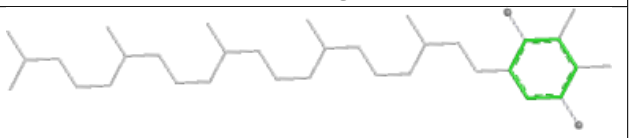
Bond lengths



Bond angles

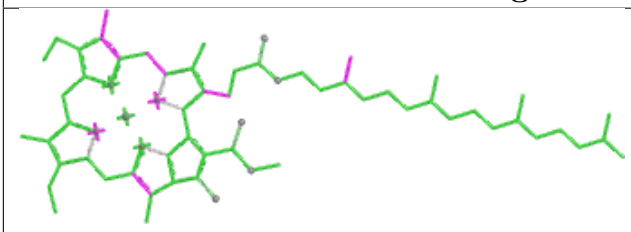


Torsions

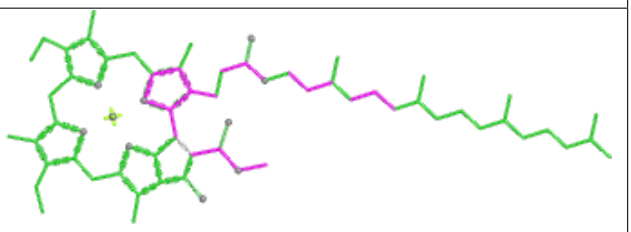


Rings

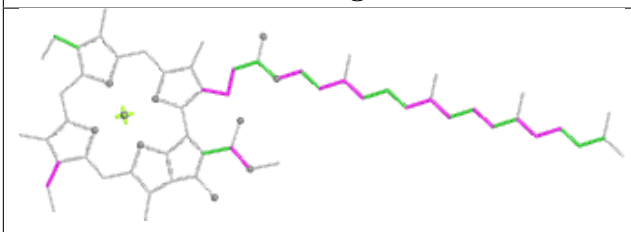
Ligand CLA AB 601



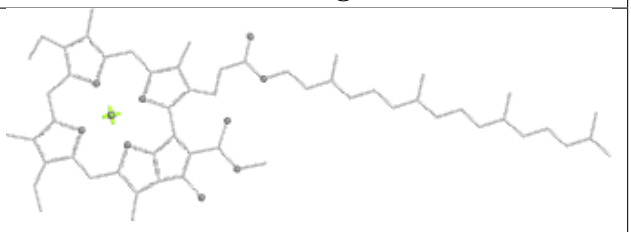
Bond lengths



Bond angles

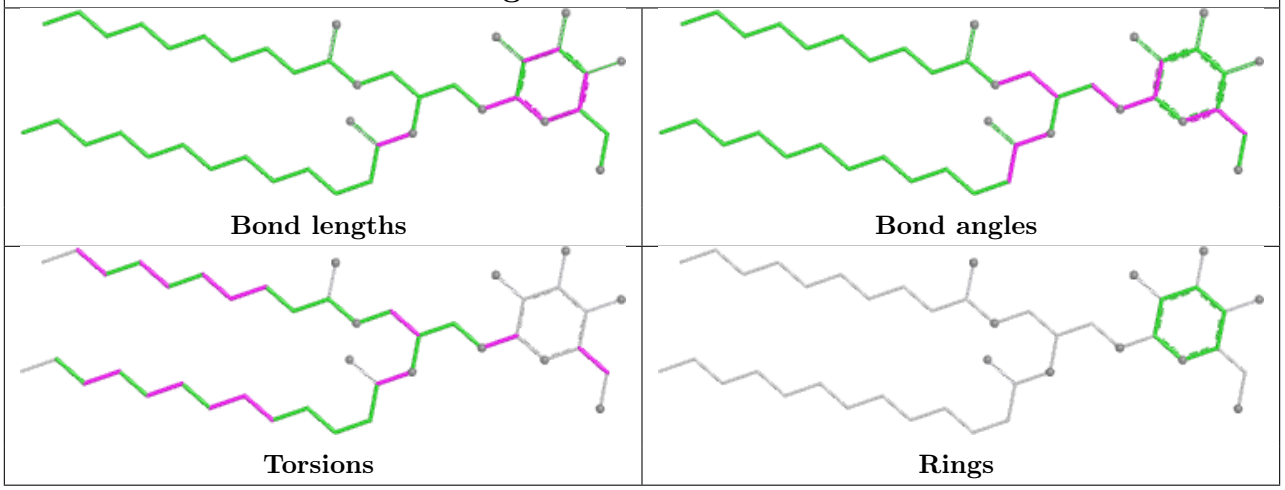


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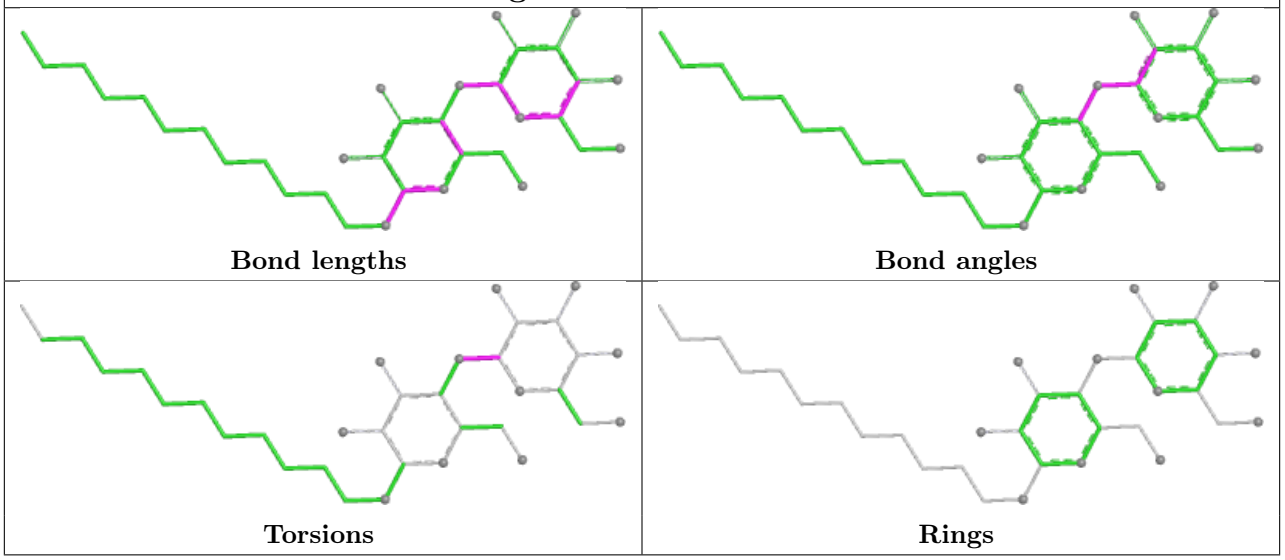


Rings

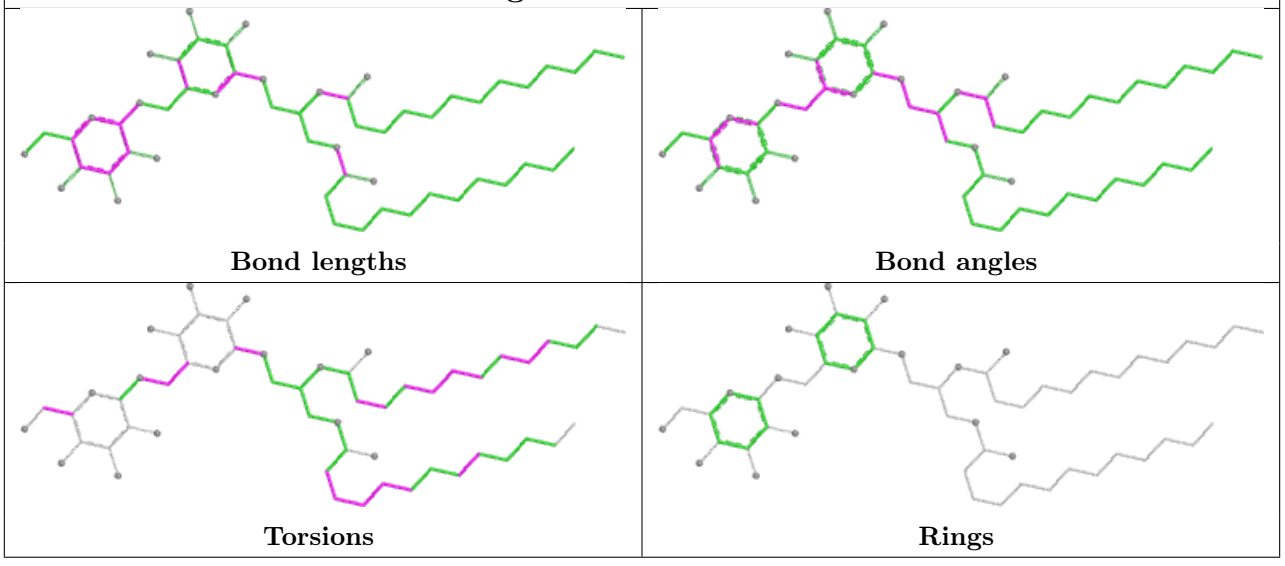
Ligand LMG AM 101



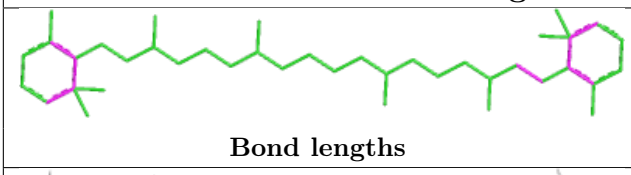
Ligand LMT AB 625

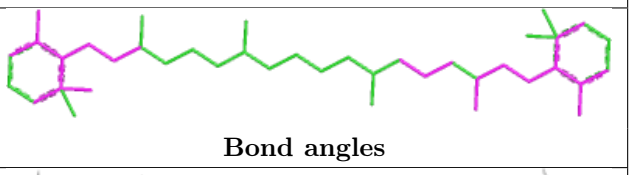


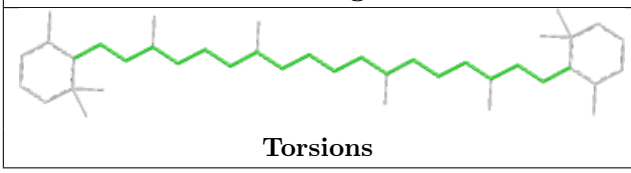
Ligand DGD AA 410

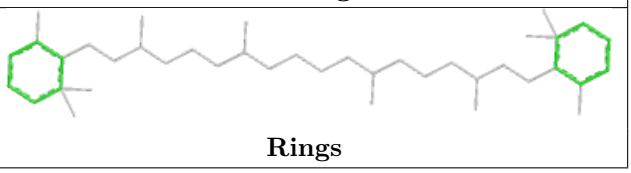


Ligand BCR AB 619

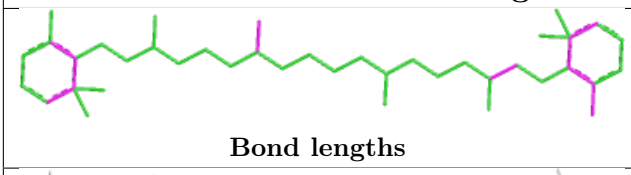

Bond lengths

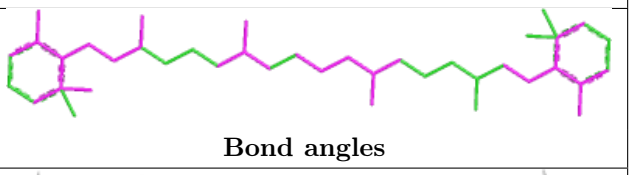

Bond angles

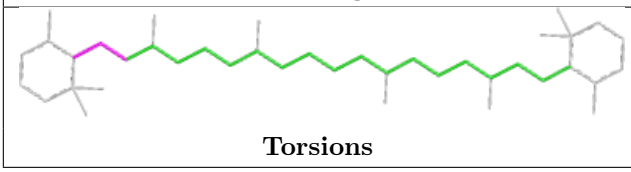

Torsions

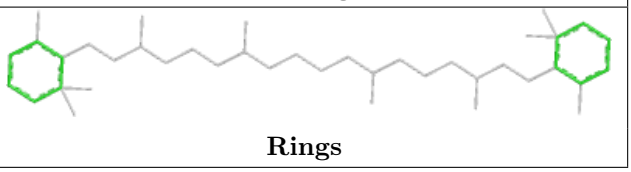

Rings

Ligand BCR BZ 101

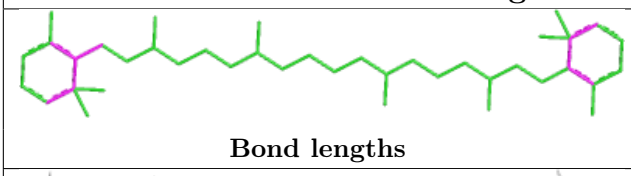

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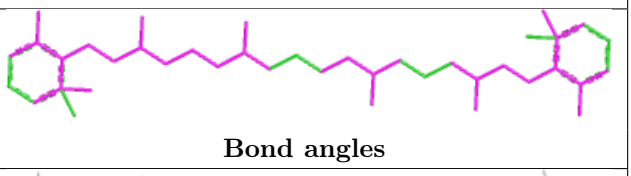

Bond angles

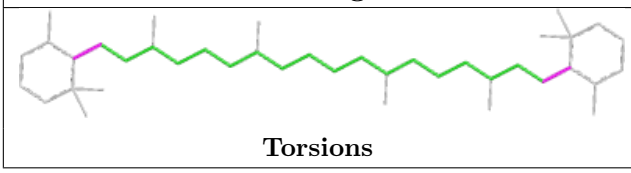

Torsions

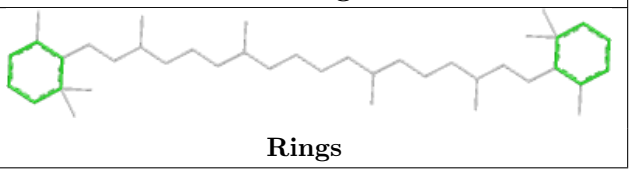

Rings

Ligand BCR BK 102

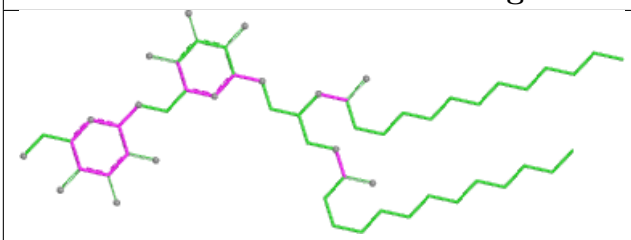

Bond lengths

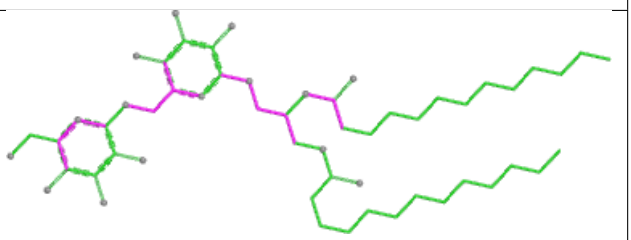

Bond angles

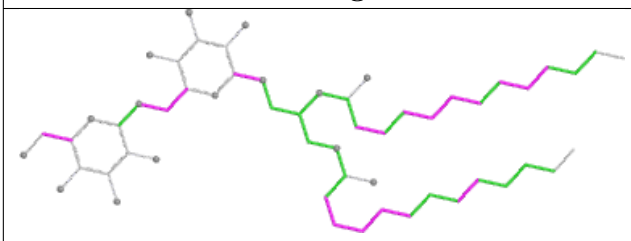

Torsions

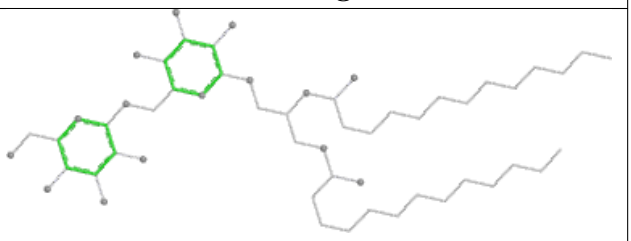

Rings

Ligand DGD BA 411

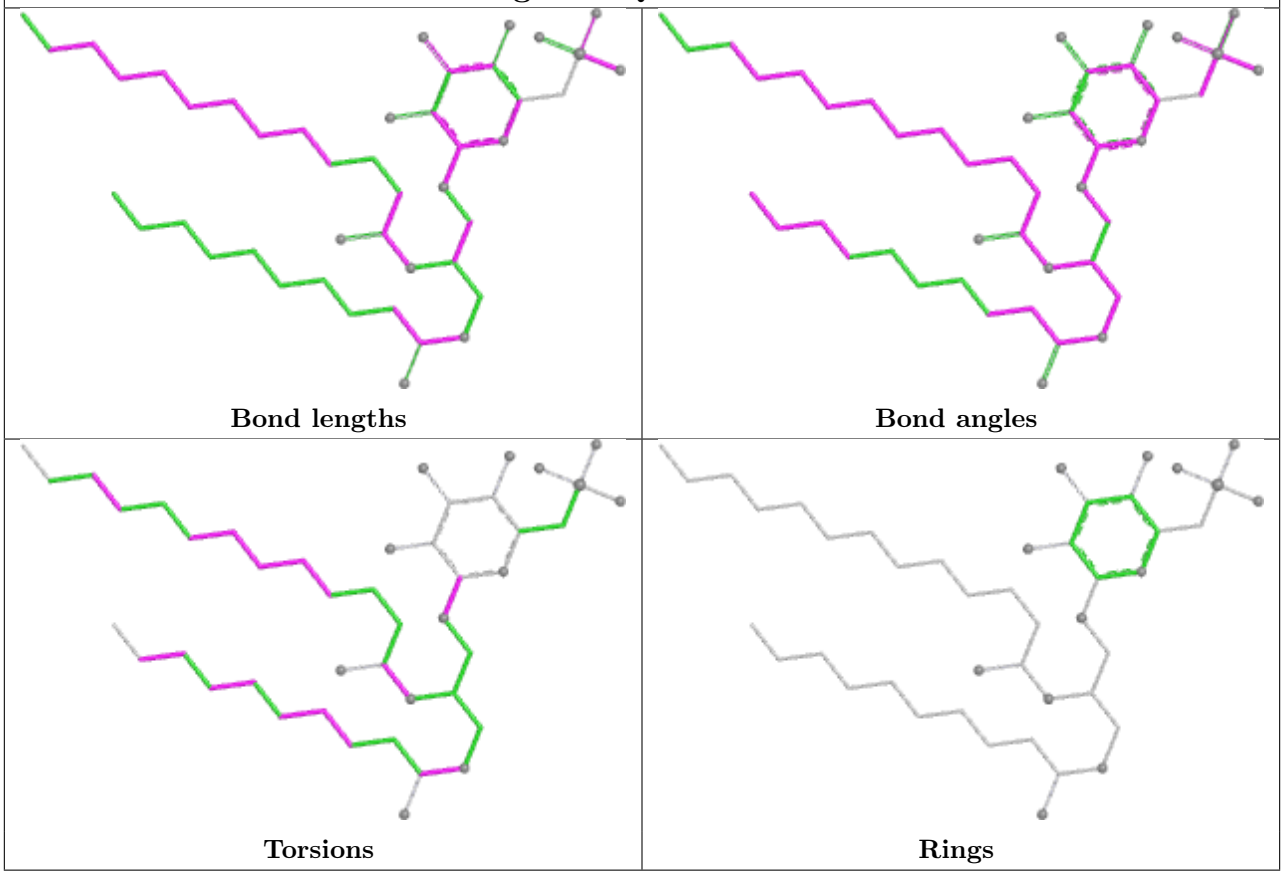

Bond lengths


Bond angles

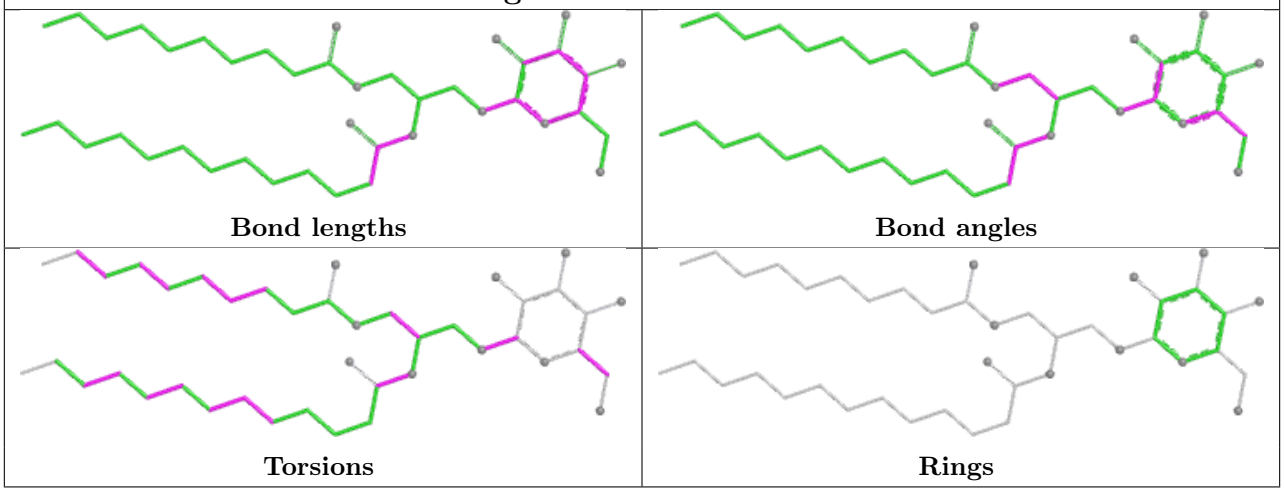

Torsions


Rings

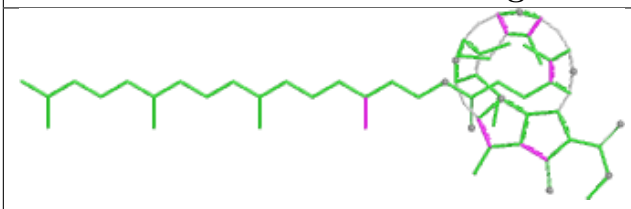
Ligand SQD AF 101



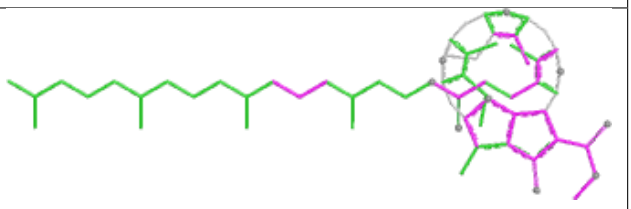
Ligand LMG BM 102



Ligand PHO AD 403



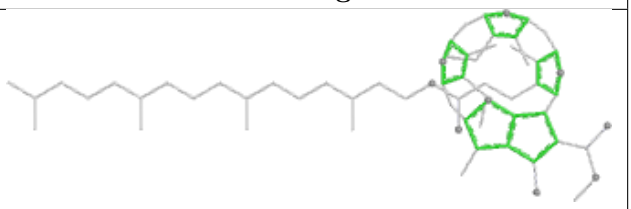
Bond lengths



Bond angles

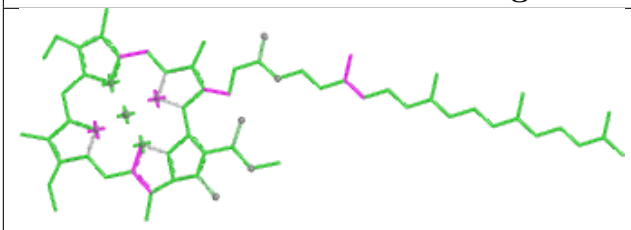


Torsions

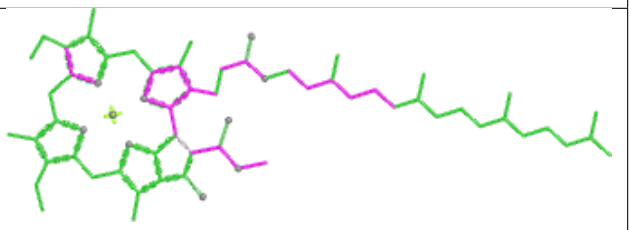


Rings

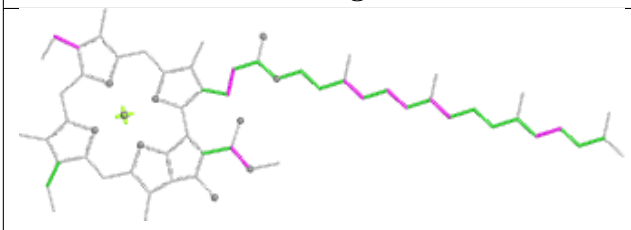
Ligand CLA AB 603



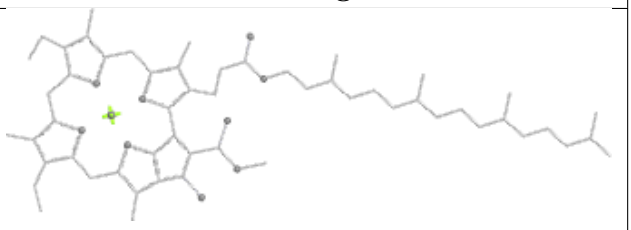
Bond lengths



Bond angles

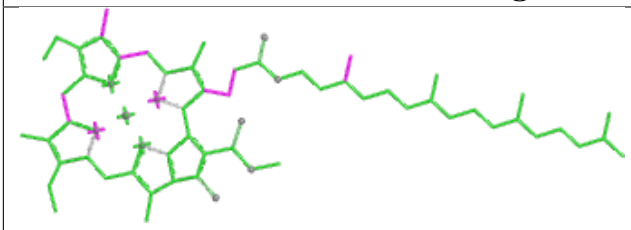


Torsions

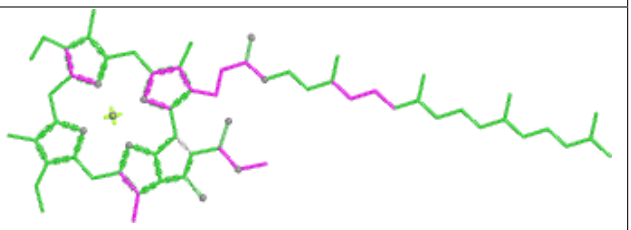


Rings

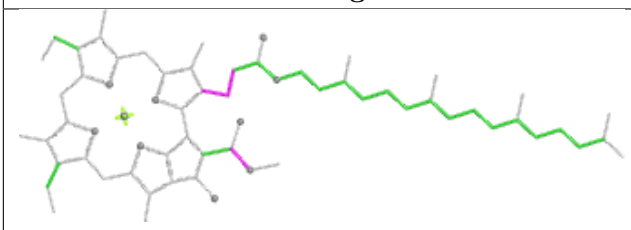
Ligand CLA BA 403



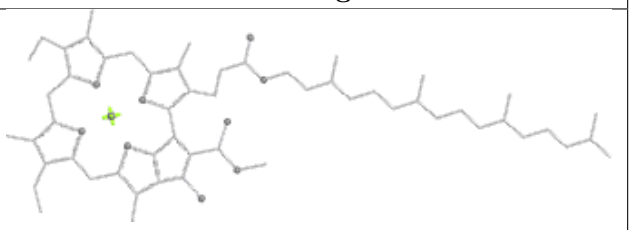
Bond lengths



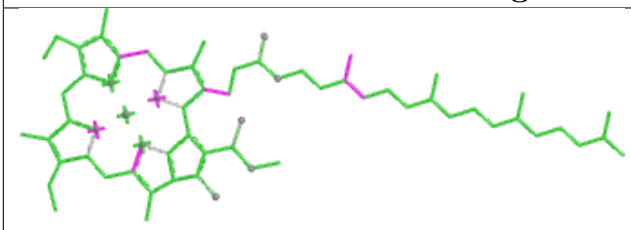
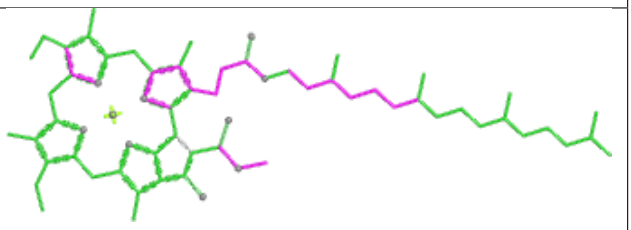
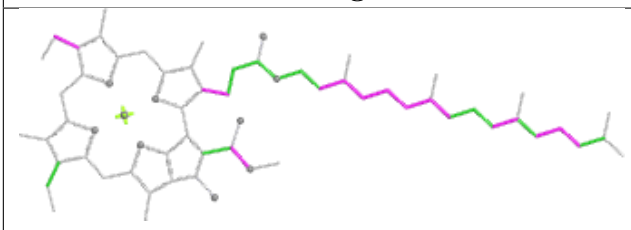
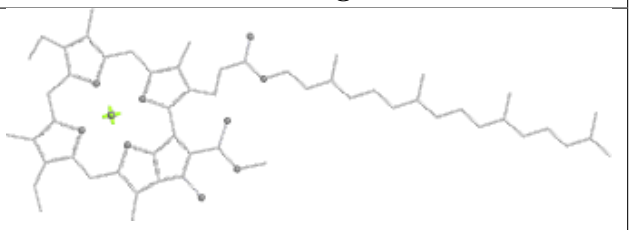
Bond angles

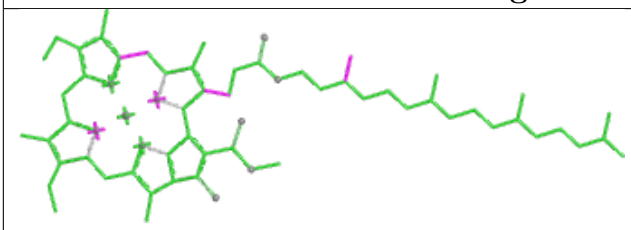
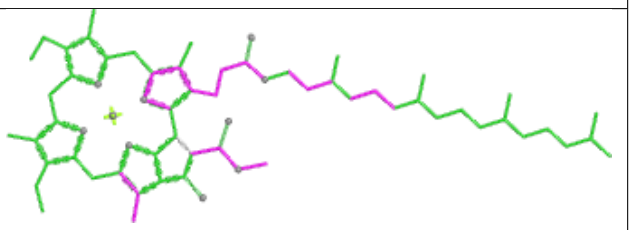
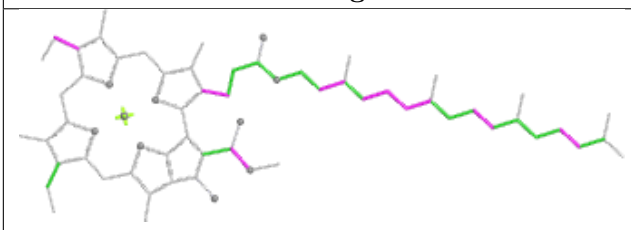
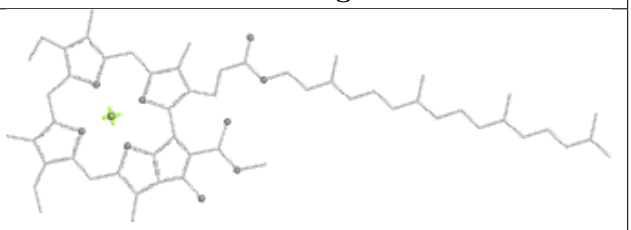


Torsions

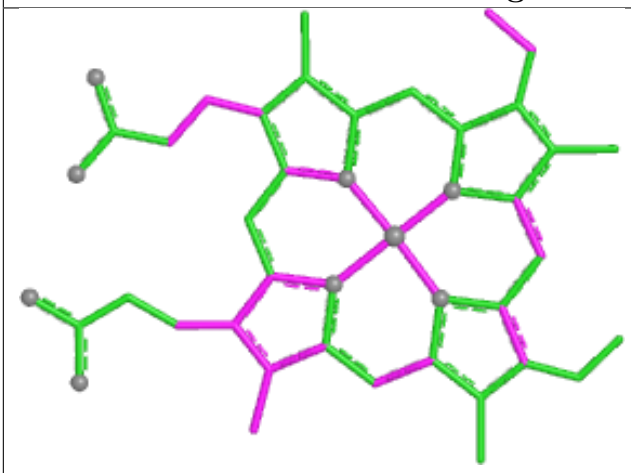


Rings

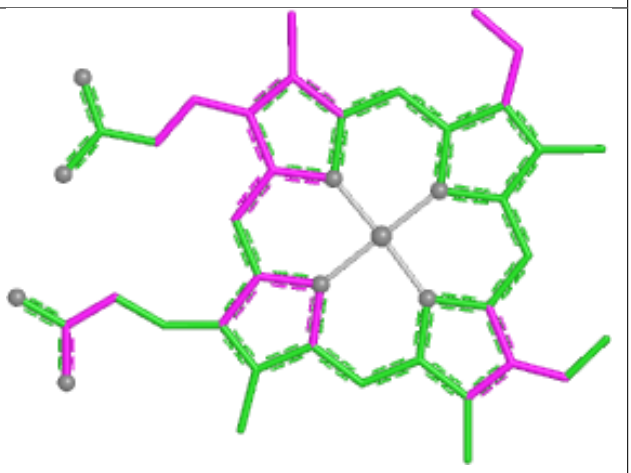
Ligand CLA AB 608	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA AA 404	
 Bond lengths	 Bond angles
 Torsions	 Rings

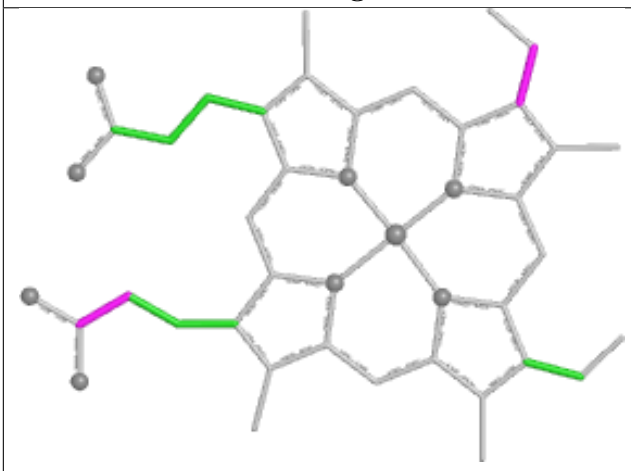
Ligand HEM BE 101



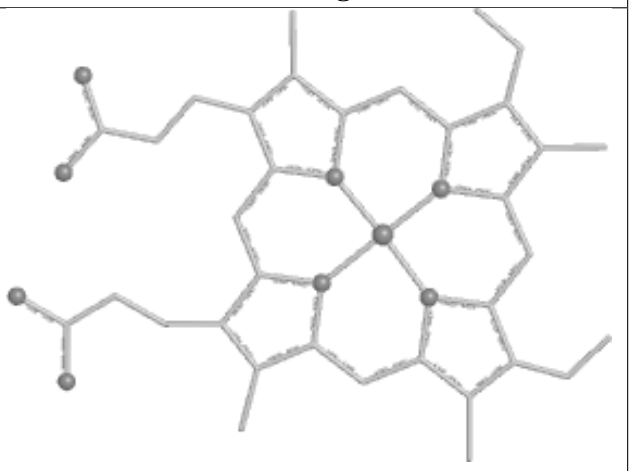
Bond lengths



Bond angles

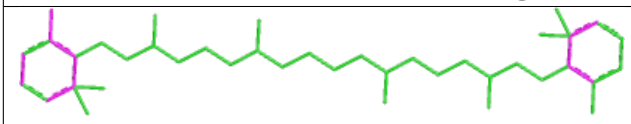


Torsions

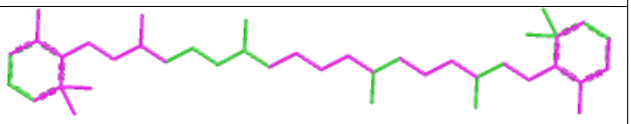


Rings

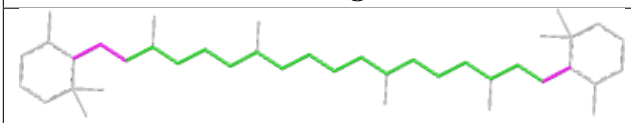
Ligand BCR BJ 102



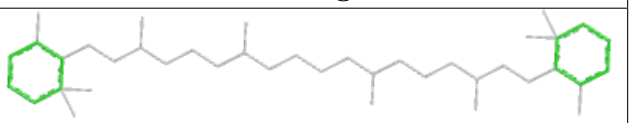
Bond lengths



Bond angles

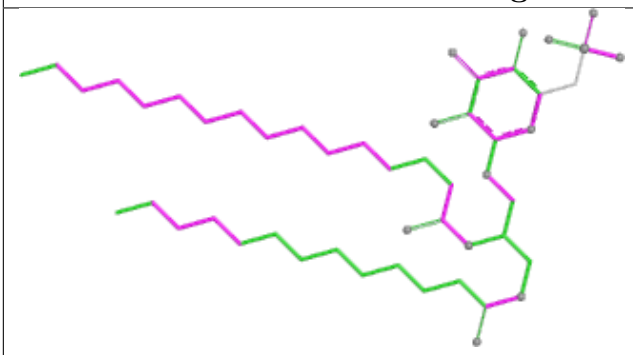


Torsions

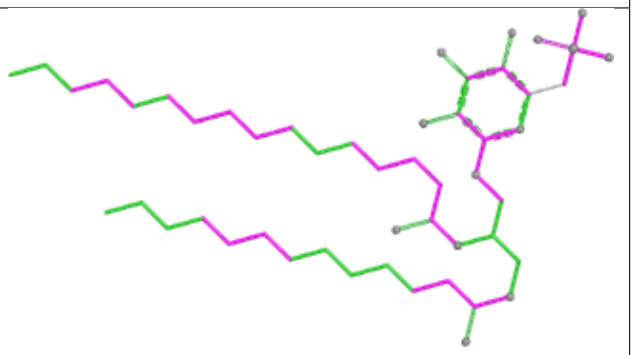


Rings

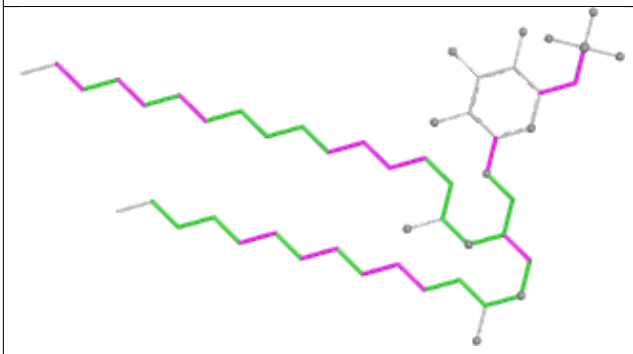
Ligand SQD AA 412



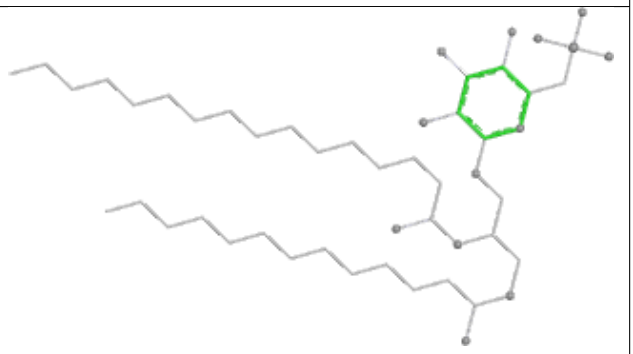
Bond lengths



Bond angles

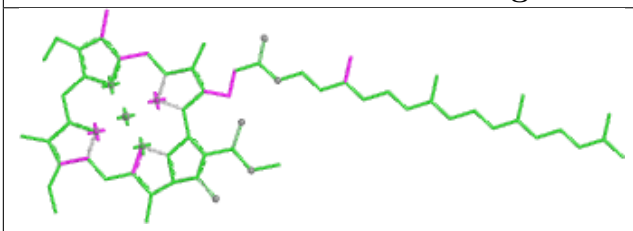


Torsions

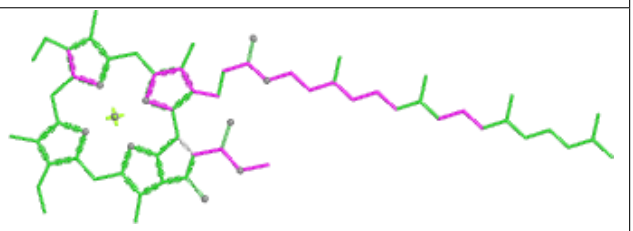


Rings

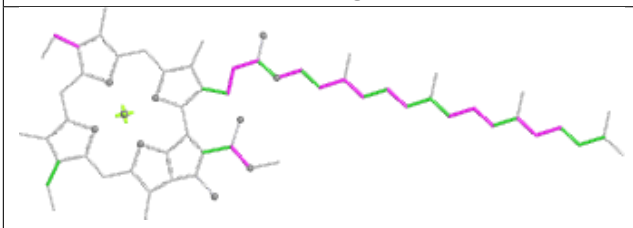
Ligand CLA AB 610



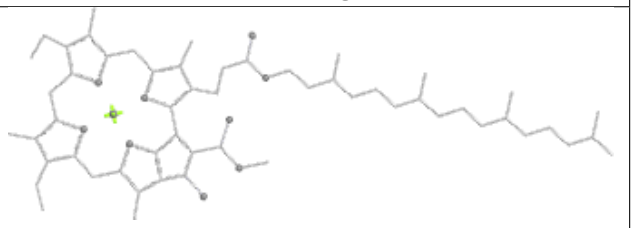
Bond lengths



Bond angles



Torsions

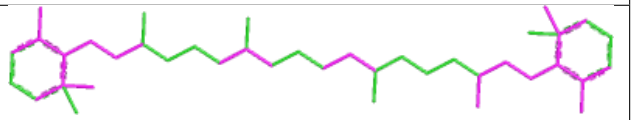


Rings

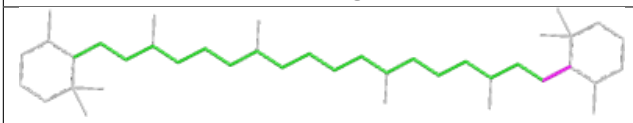
Ligand BCR AB 620



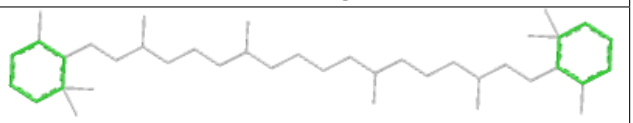
Bond lengths



Bond angles

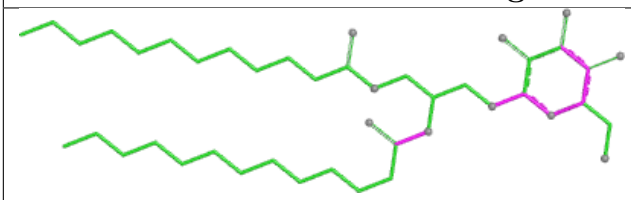


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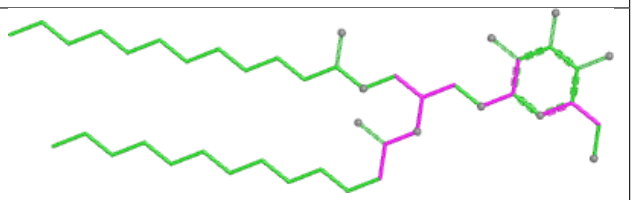


Rings

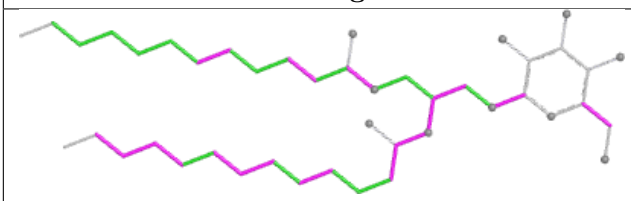
Ligand LMG AE 102



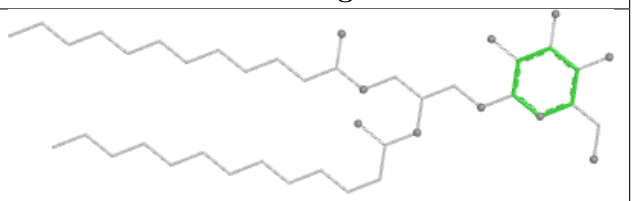
Bond lengths



Bond angles

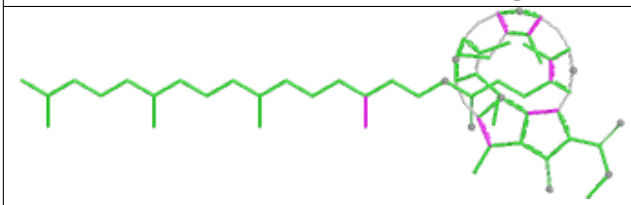


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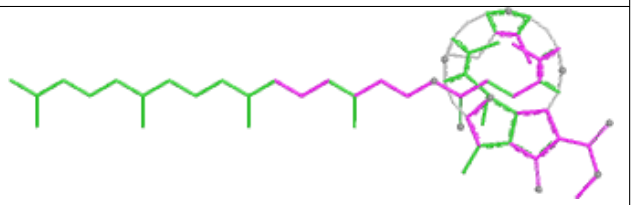


Rings

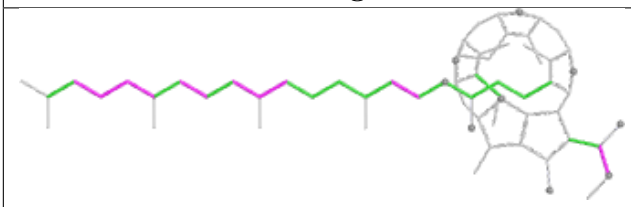
Ligand PHO BD 403



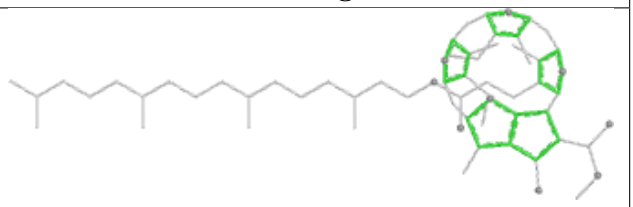
Bond lengths



Bond angles

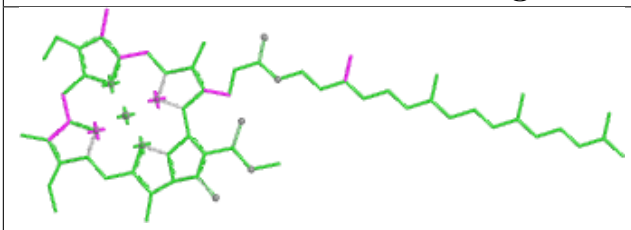


Torsions

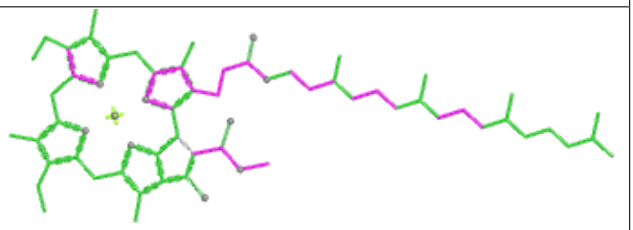


Rings

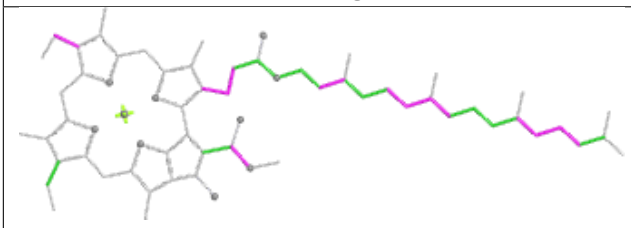
Ligand CLA AC 513



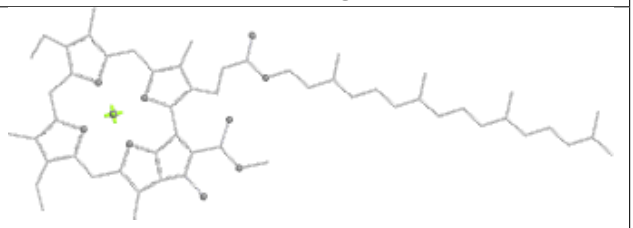
Bond lengths



Bond angles

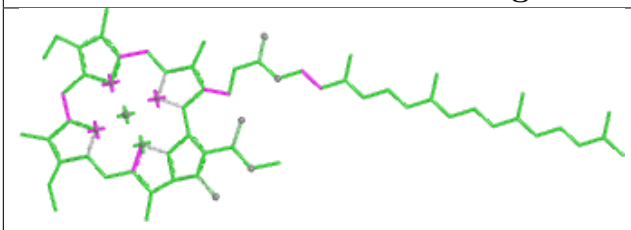


Torsions

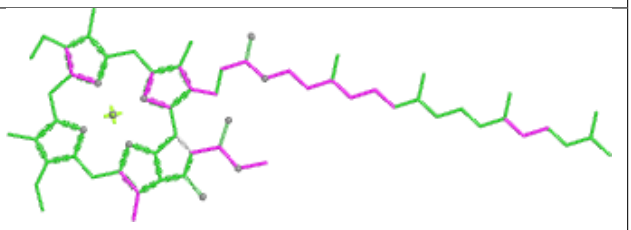


Rings

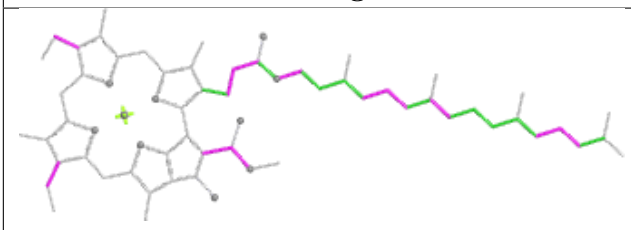
Ligand CLA BB 617



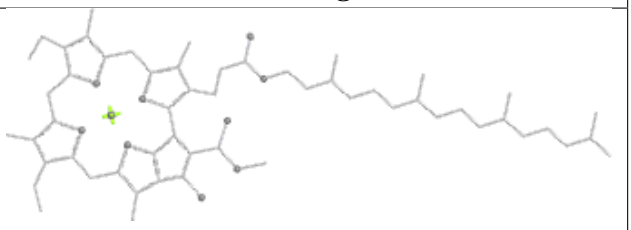
Bond lengths



Bond angles

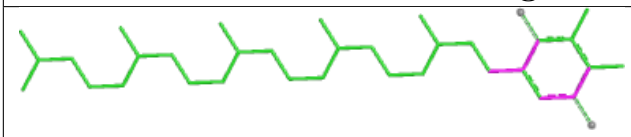


Torsions

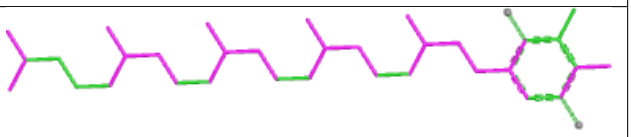


Rings

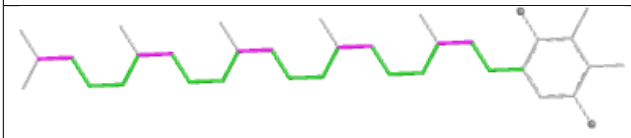
Ligand PL9 AJ 101



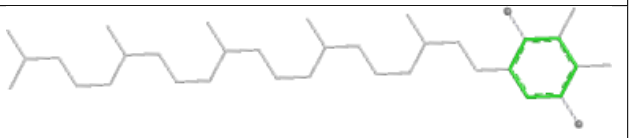
Bond lengths



Bond angles

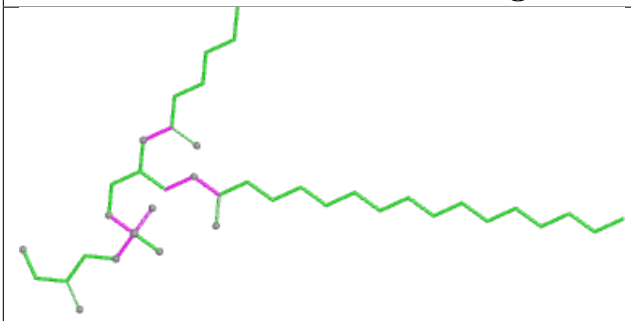


Torsions

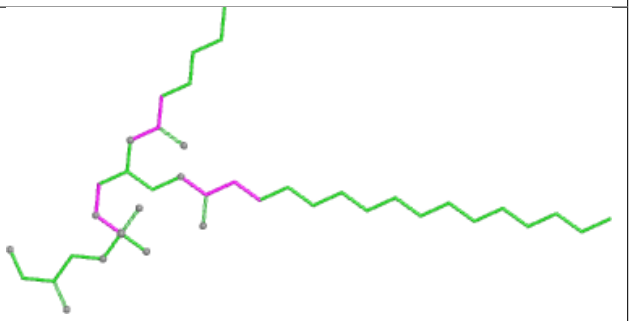


Rings

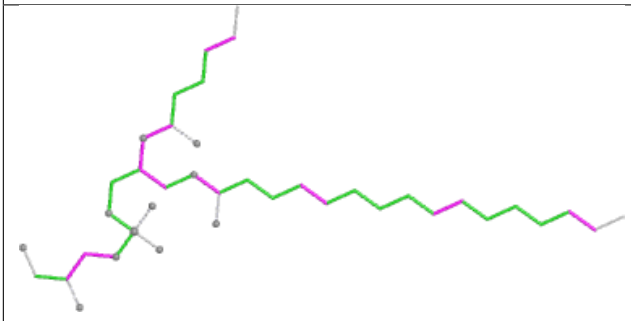
Ligand LHG BA 412



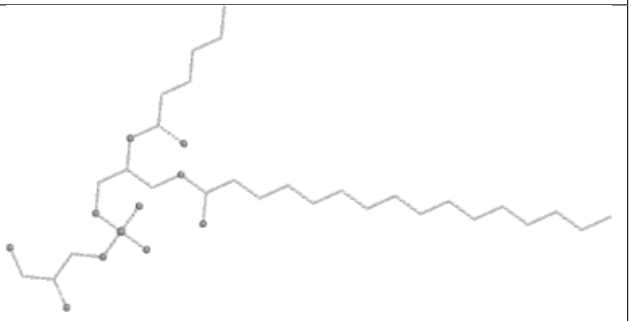
Bond lengths



Bond angles

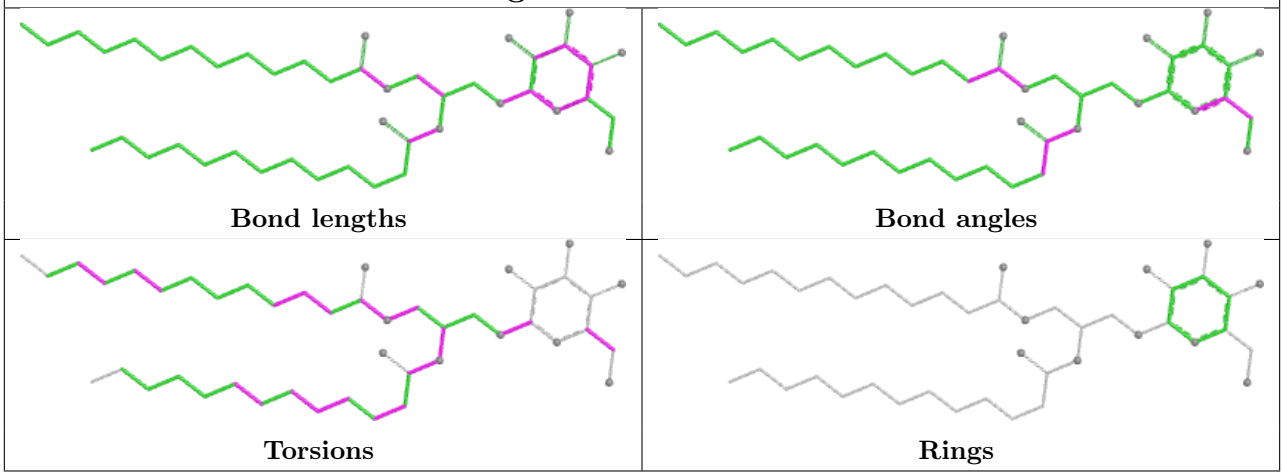


Torsions

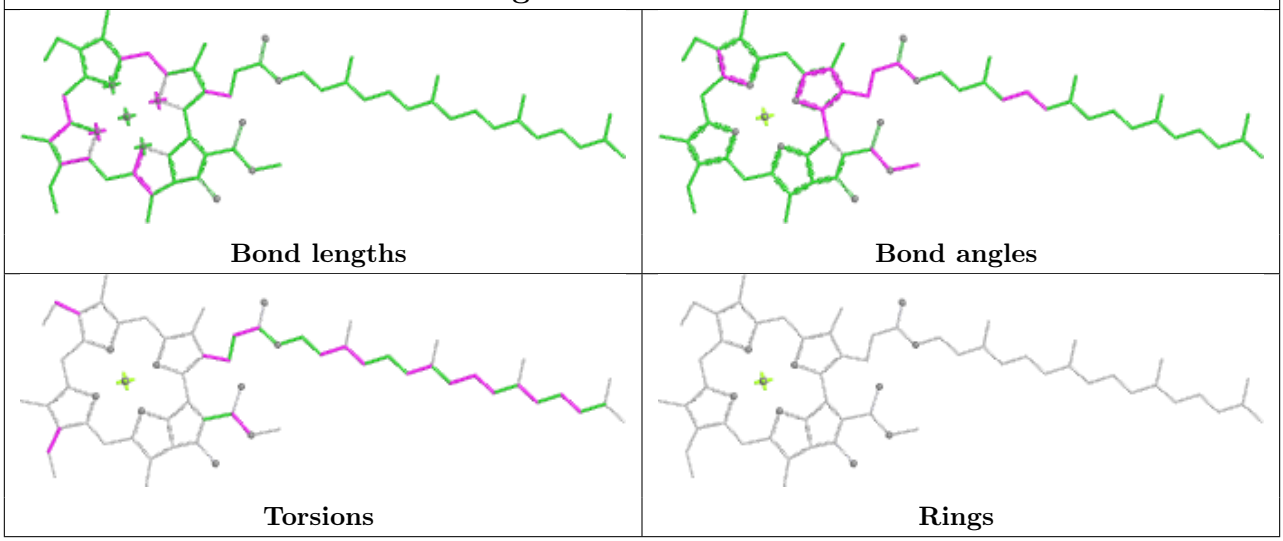


Rings

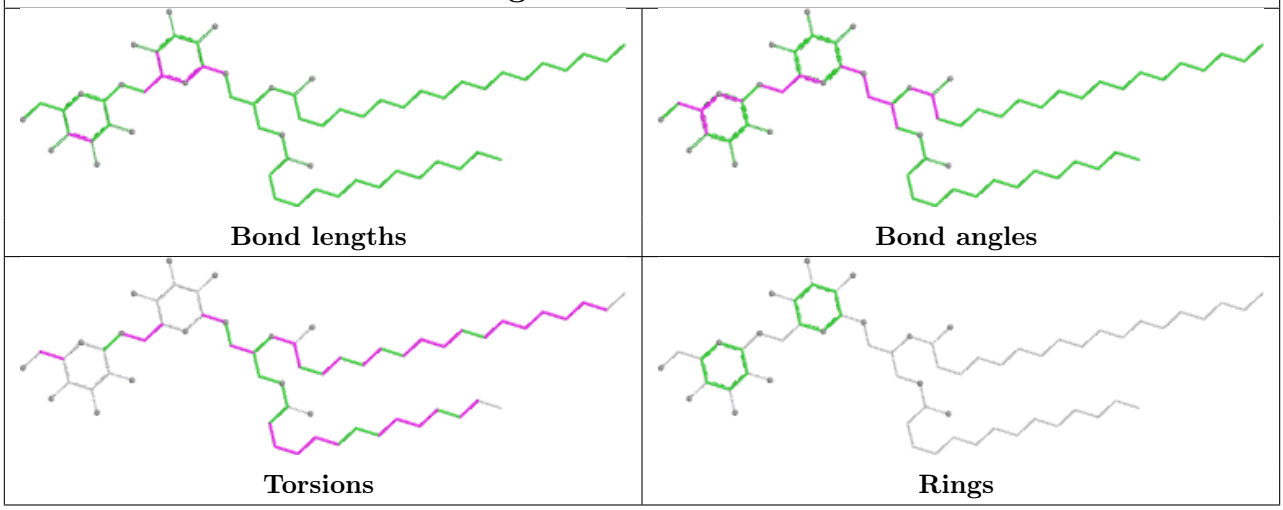
Ligand LMG AC 520



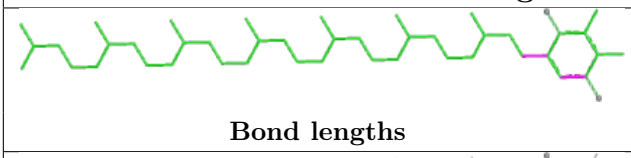
Ligand CLA AC 505



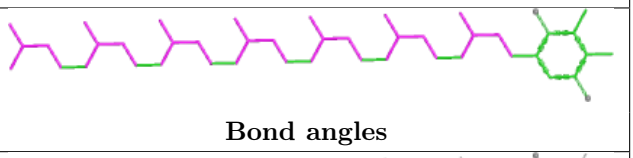
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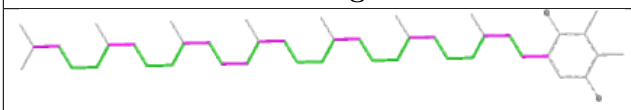
Ligand PL9 BA 408



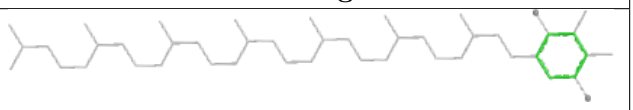
Bond lengths



Bond angles

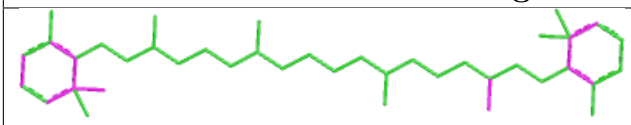


Torsions

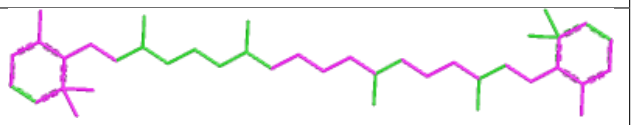


Rings

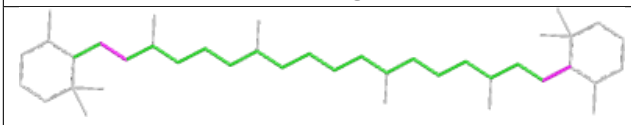
Ligand BCR AJ 102



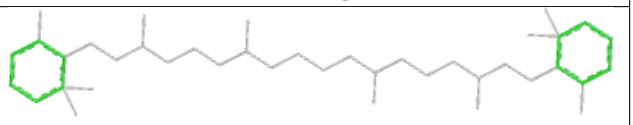
Bond lengths



Bond angles

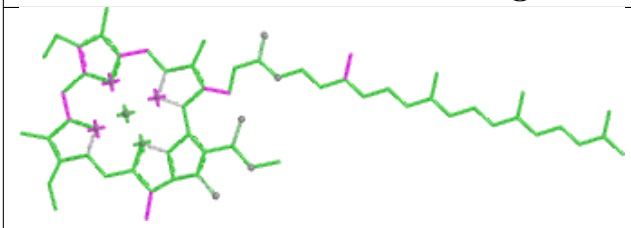


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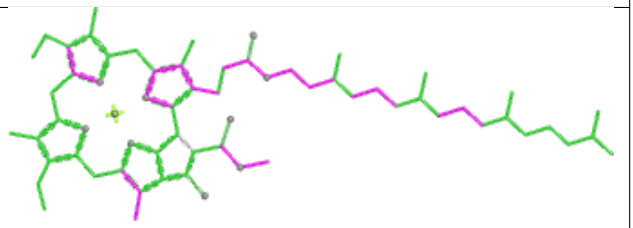


Rings

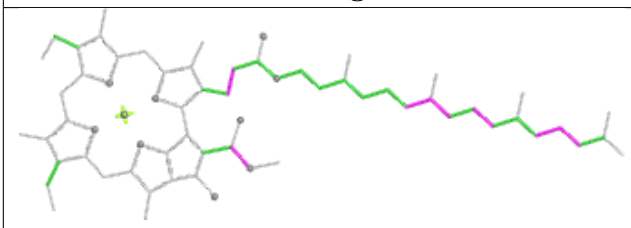
Ligand CLA AC 504



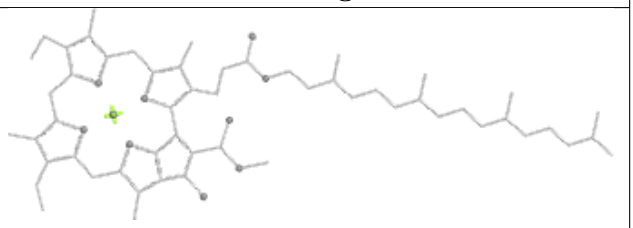
Bond lengths



Bond angles

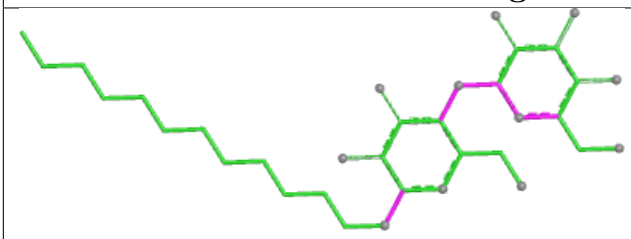


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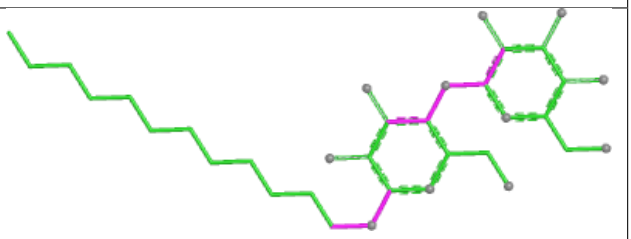


Rings

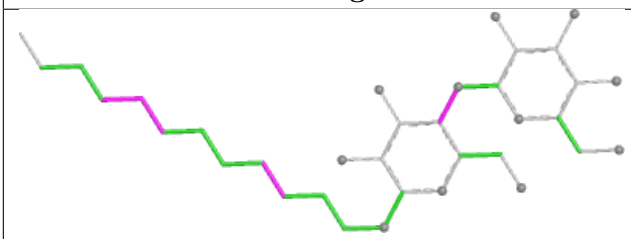
Ligand LMT BT 101



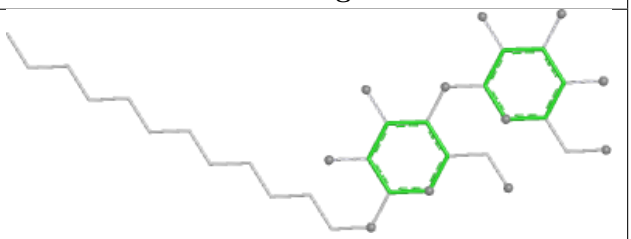
Bond lengths



Bond angles

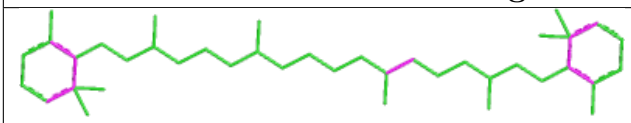


Torsions

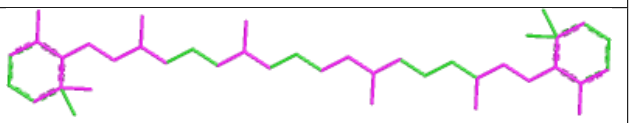


Rings

Ligand BCR AA 409



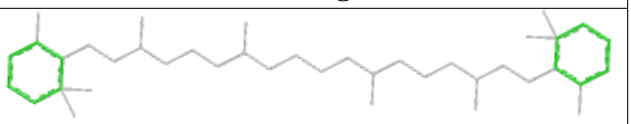
Bond lengths



Bond angles

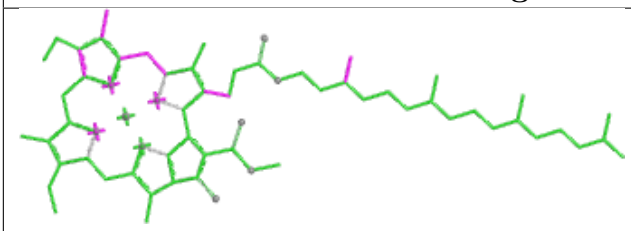


Torsions

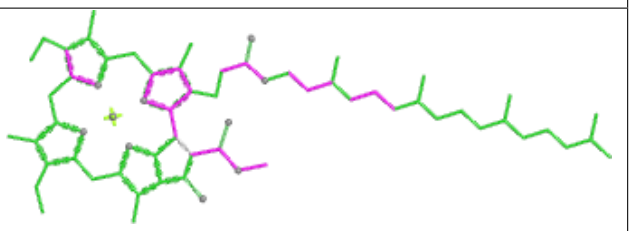


Rings

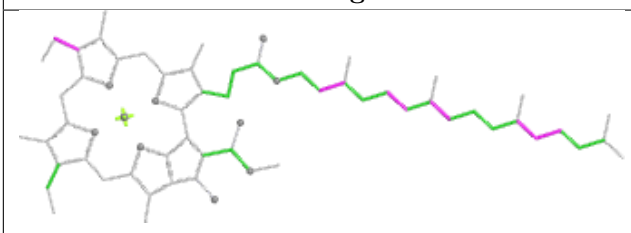
Ligand CLA AB 615



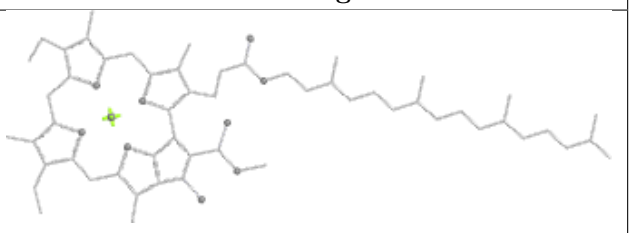
Bond lengths



Bond angles

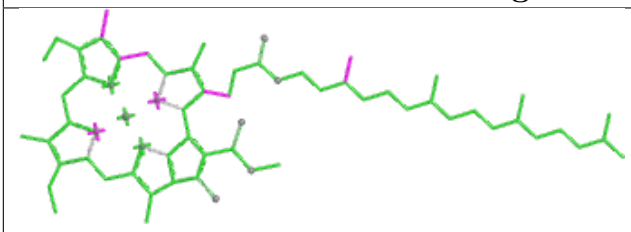


Torsions

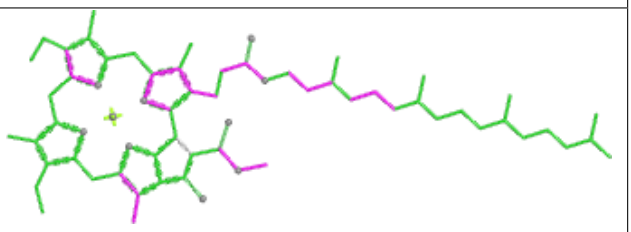


Rings

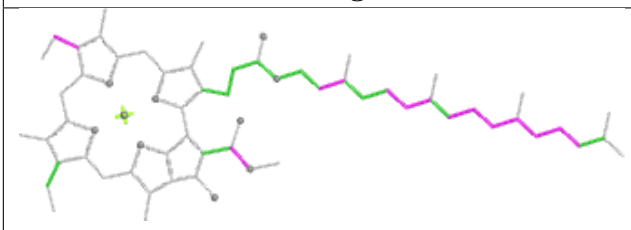
Ligand CLA BC 506



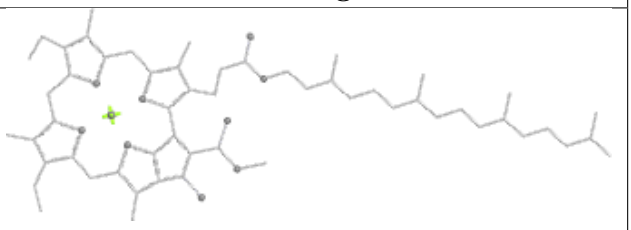
Bond lengths



Bond angles



Torsions

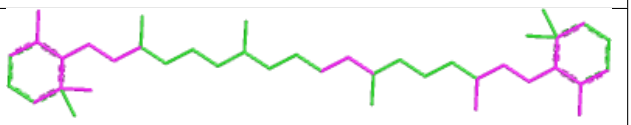


Rings

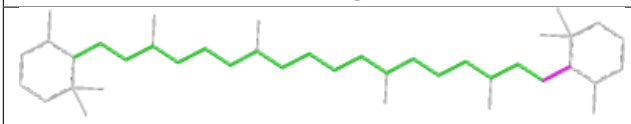
Ligand BCR BB 622



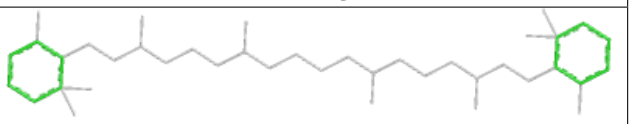
Bond lengths



Bond angles

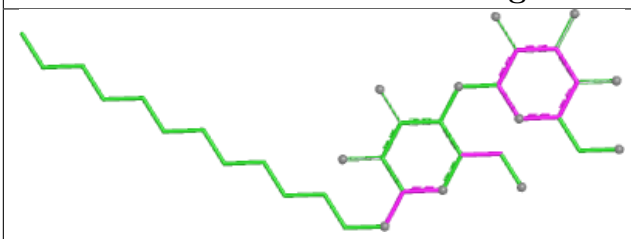


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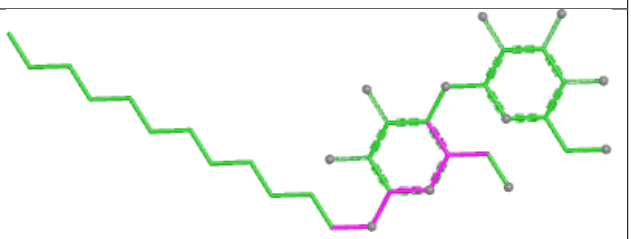


Rings

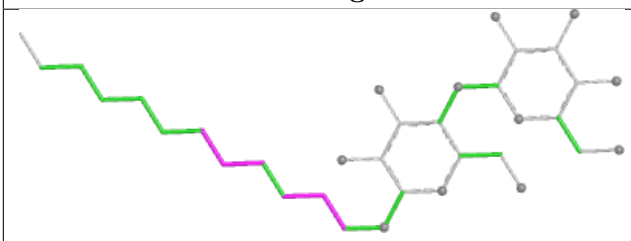
Ligand LMT BB 625



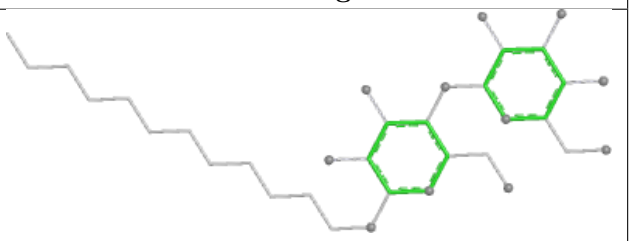
Bond lengths



Bond angles

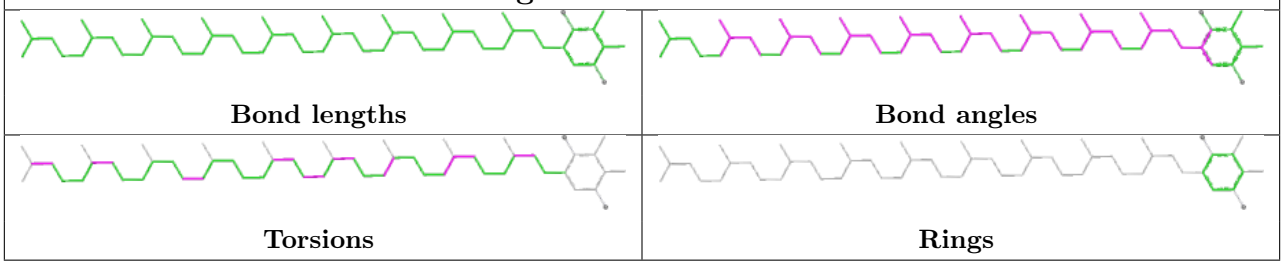


Torsions

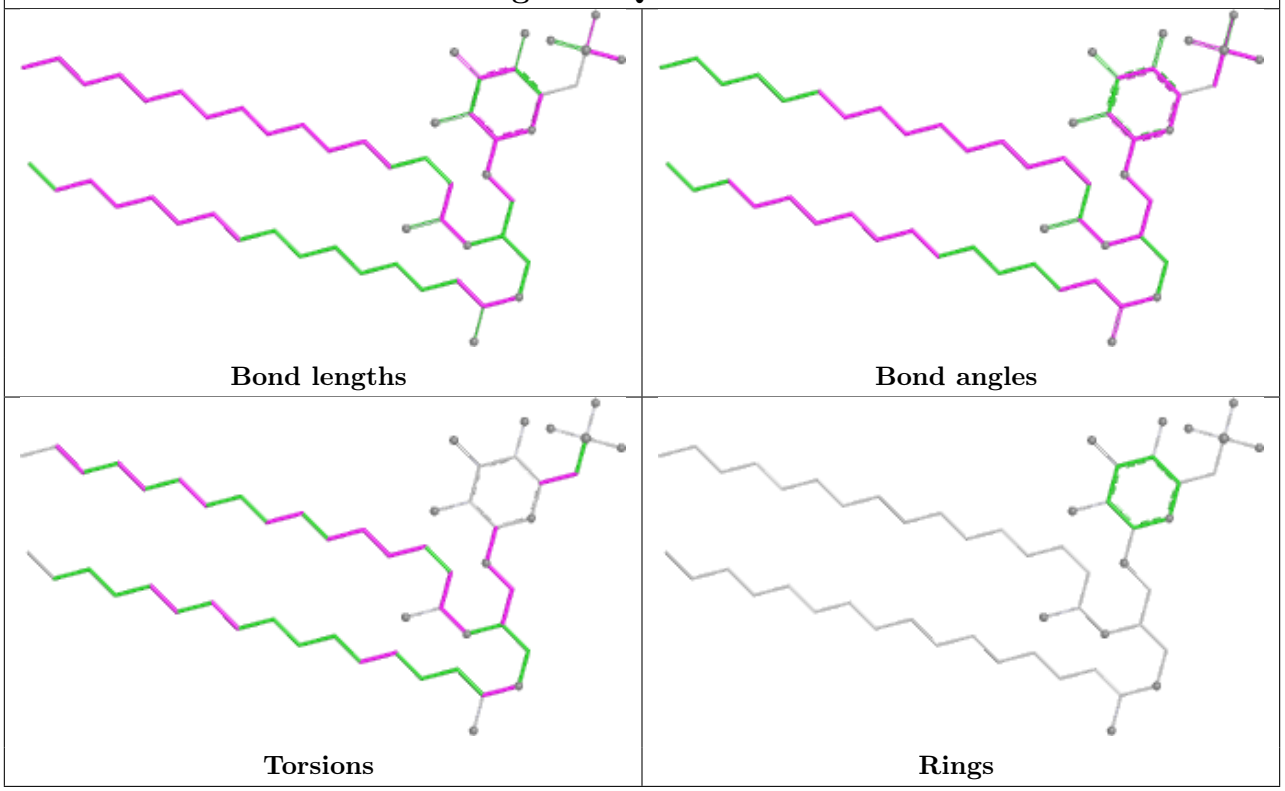


Rings

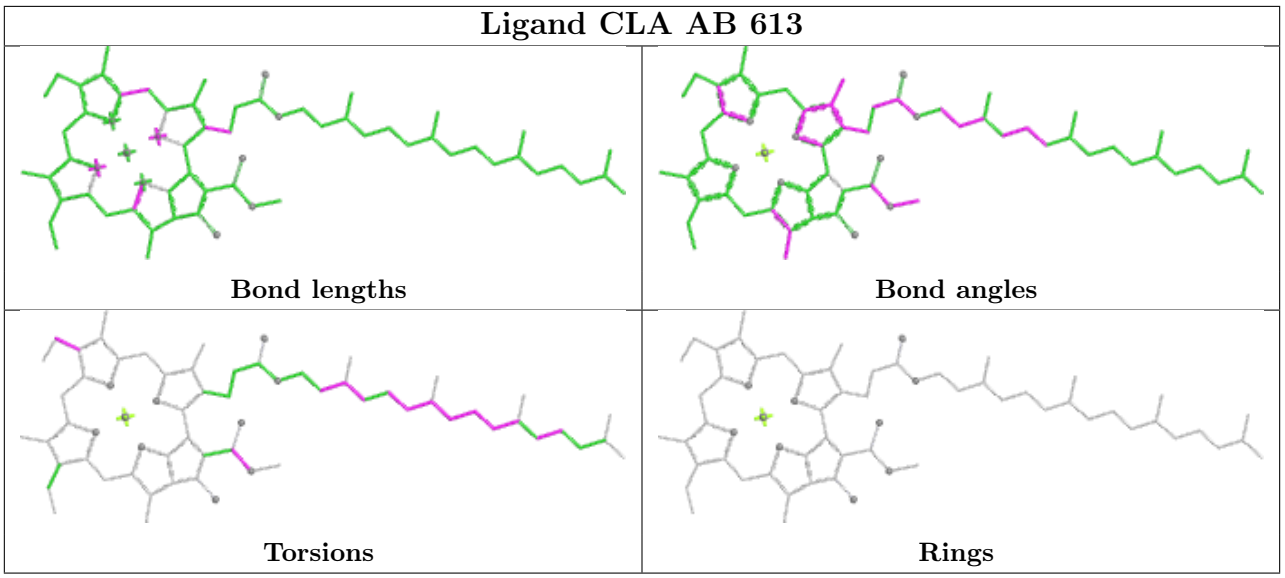
Ligand PL9 AD 405



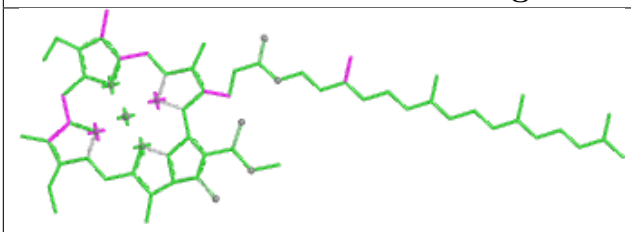
Ligand SQD BA 401



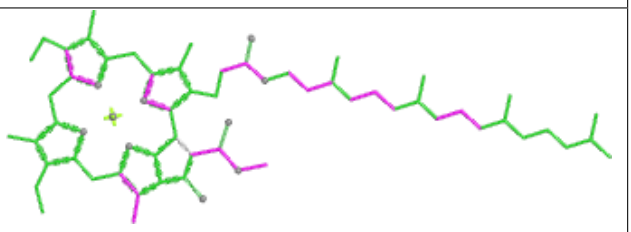
Ligand CLA AB 613



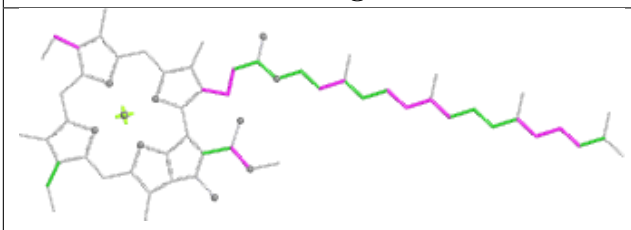
Ligand CLA BC 513



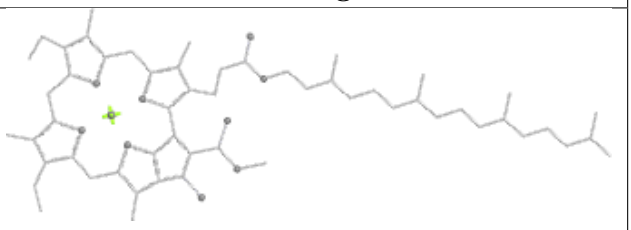
Bond lengths



Bond angles

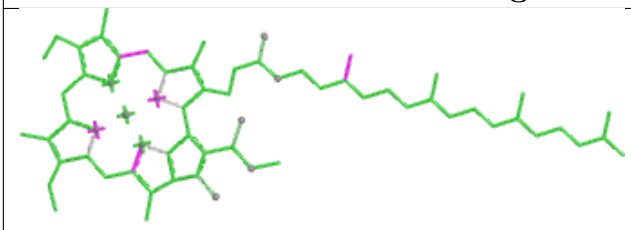


Torsions

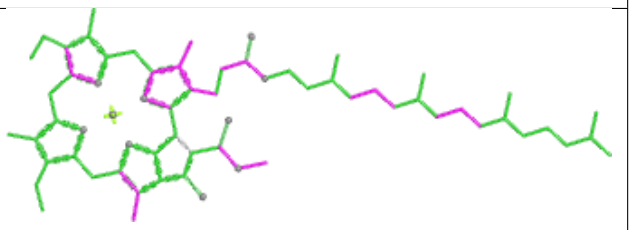


Rings

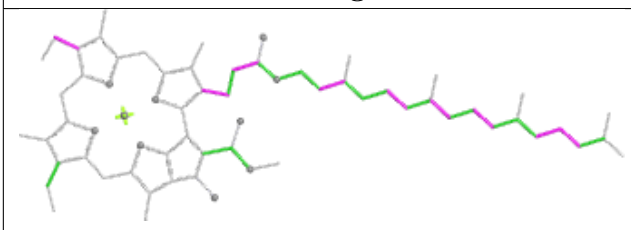
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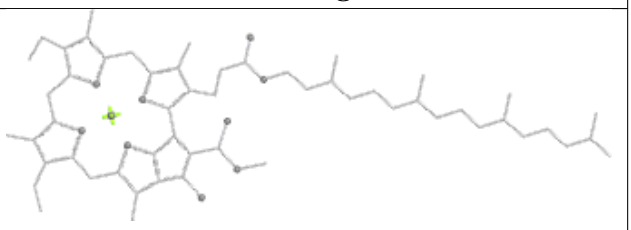
Bond lengths



Bond angles

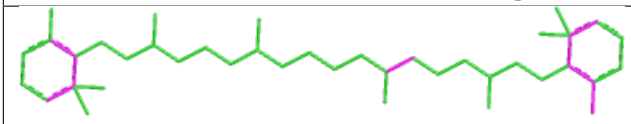


Torsions

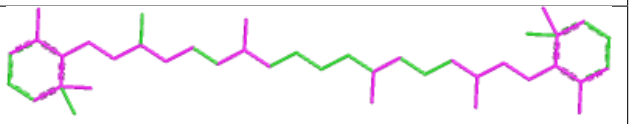


Rings

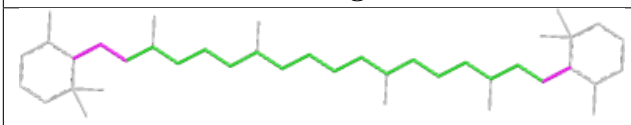
Ligand BCR AC 514



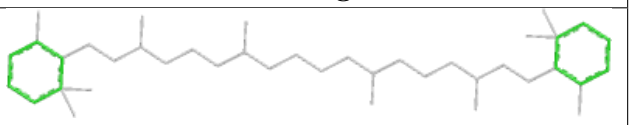
Bond lengths



Bond angles

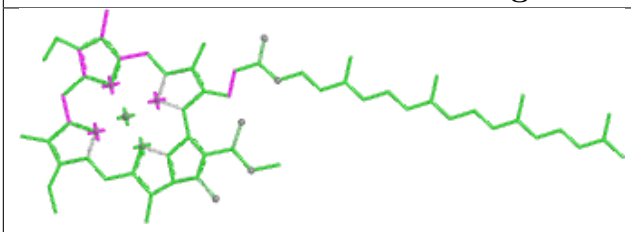


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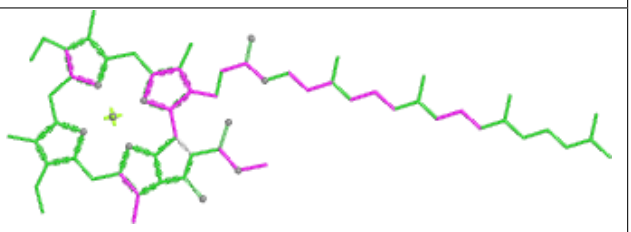


Rings

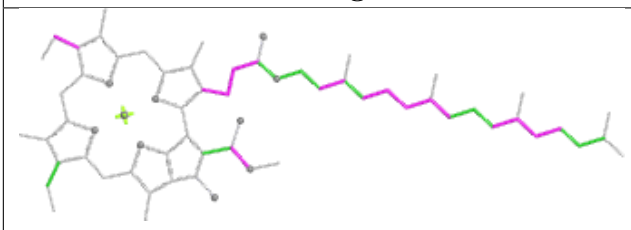
Ligand CLA AB 602



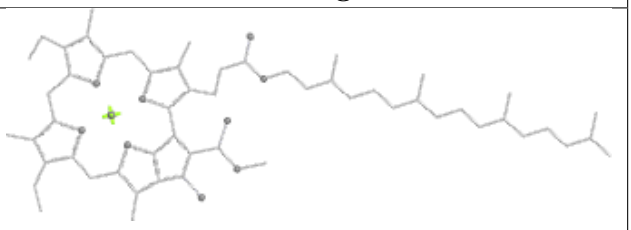
Bond lengths



Bond angles

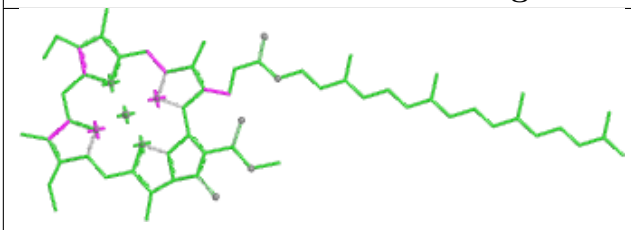


Torsions

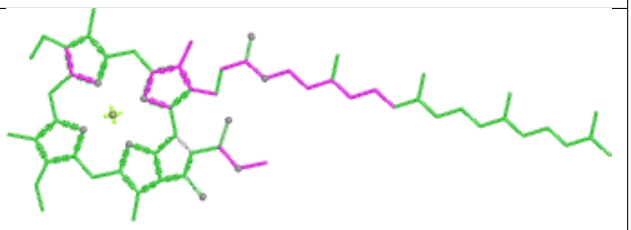


Rings

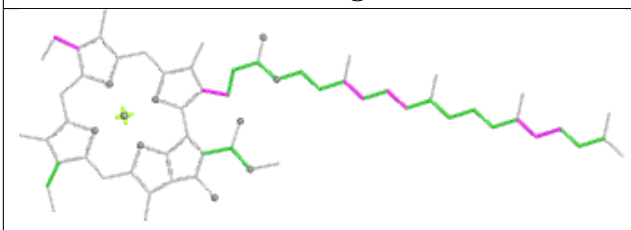
Ligand CLA AB 609



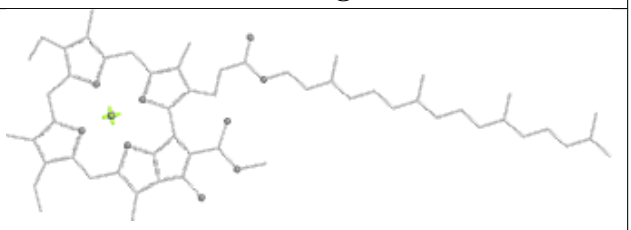
Bond lengths



Bond angles

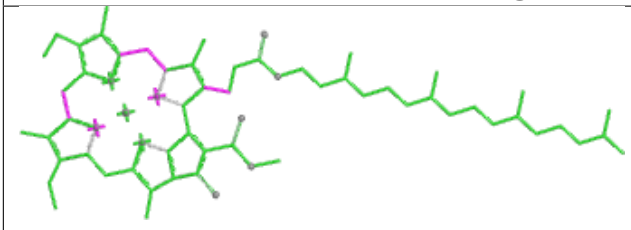


Torsions

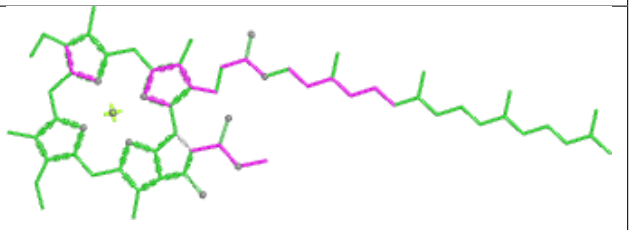


Rings

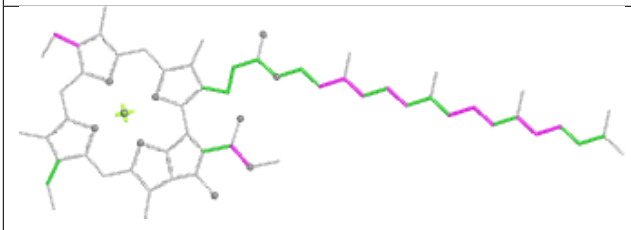
Ligand CLA AB 612



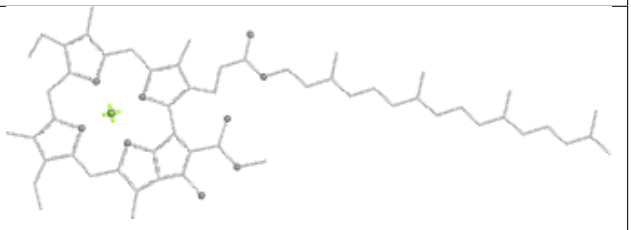
Bond lengths



Bond angles

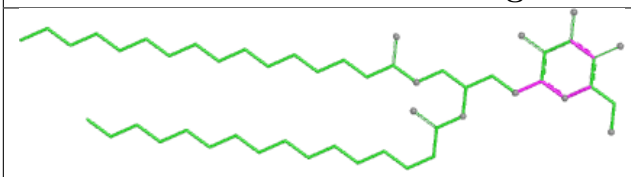


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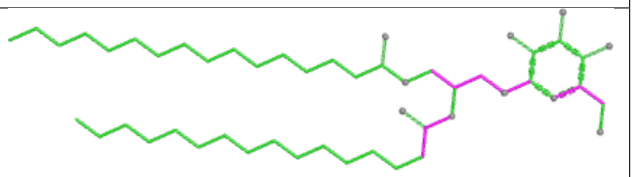


Rings

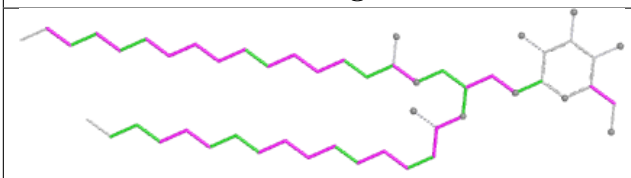
Ligand LMG BA 414



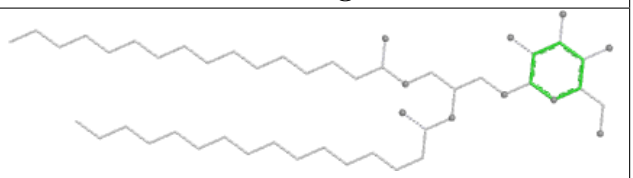
Bond lengths



Bond angles

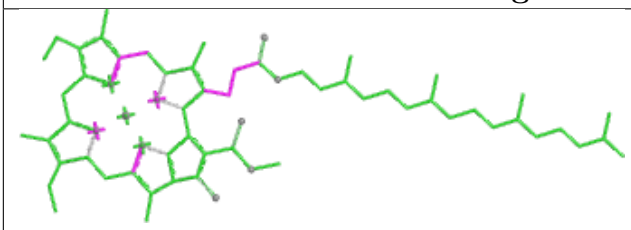


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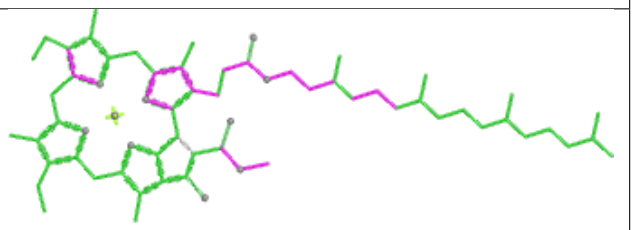


Rings

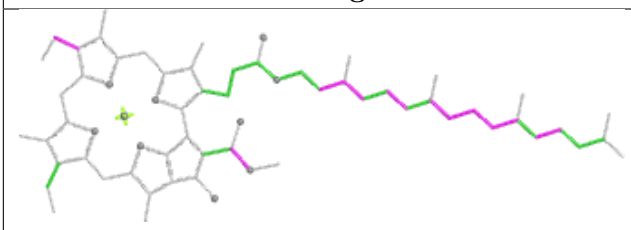
Ligand CLA BB 616



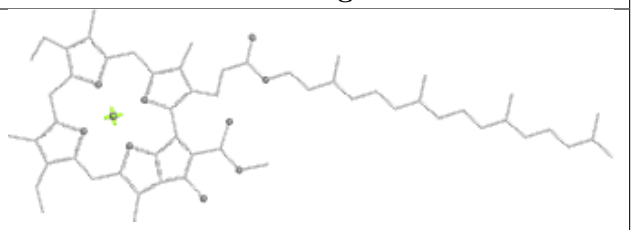
Bond lengths



Bond angles

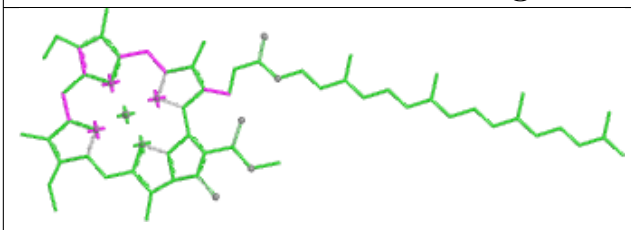


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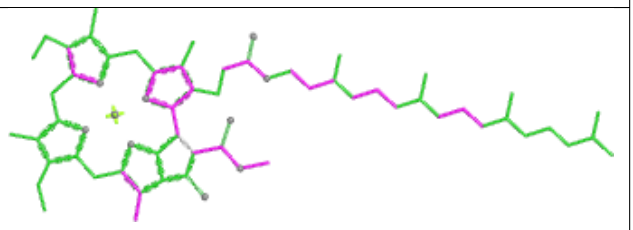


Rings

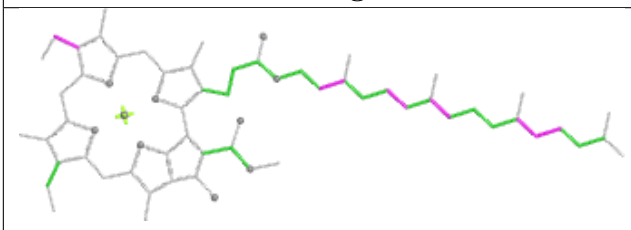
Ligand CLA BB 618



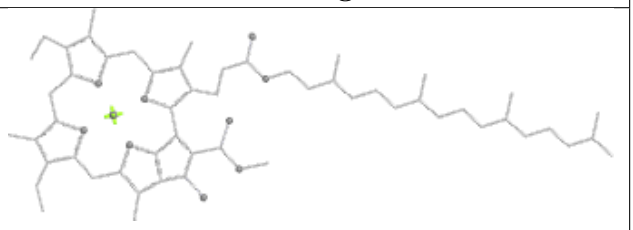
Bond lengths



Bond angles

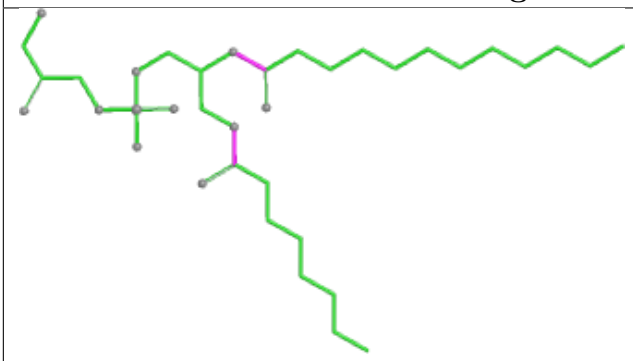


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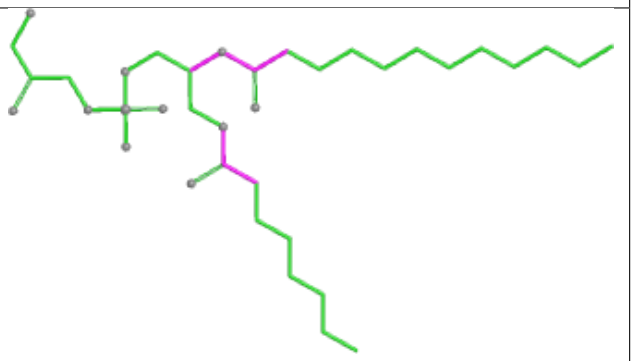


Rings

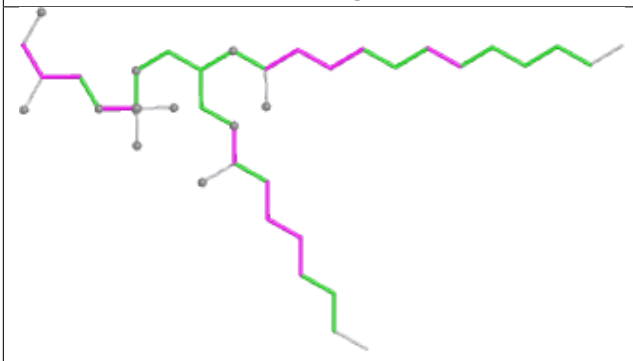
Ligand LHG AC 521



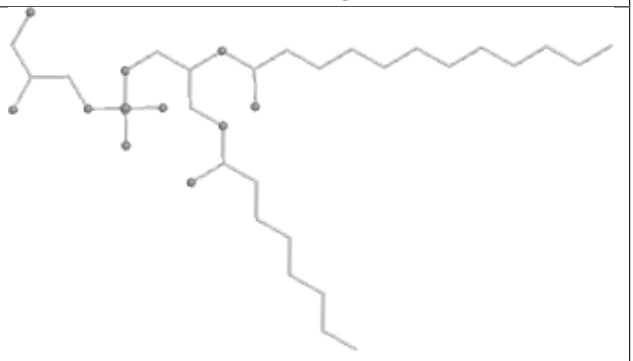
Bond lengths



Bond angles

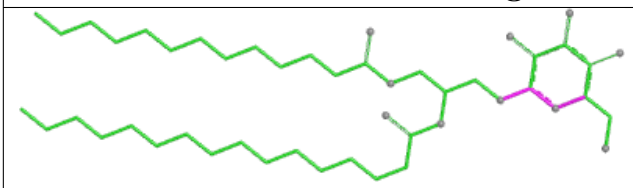


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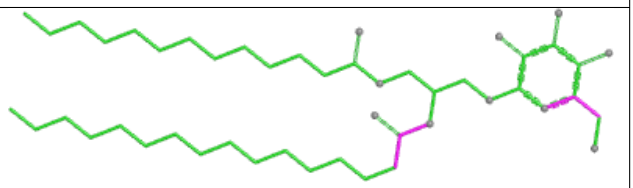


Rings

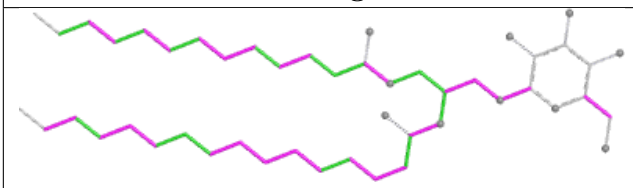
Ligand LMG AD 408



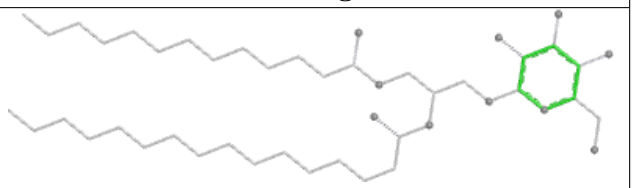
Bond lengths



Bond angles

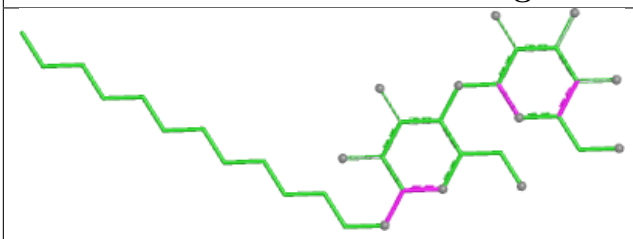


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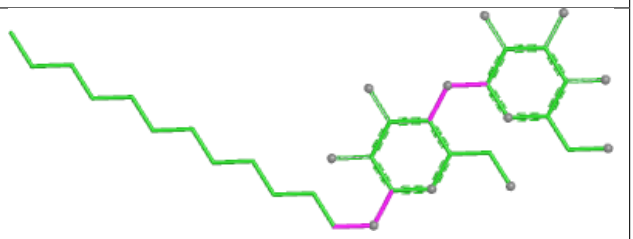


Rings

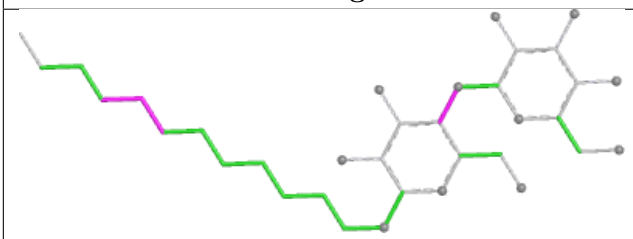
Ligand LMT AI 102



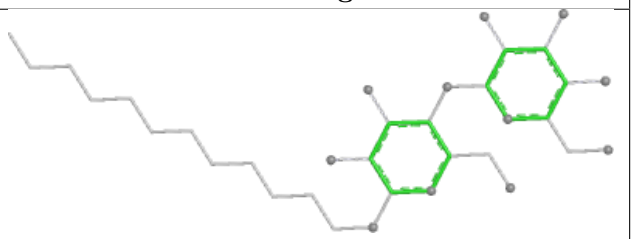
Bond lengths



Bond angles

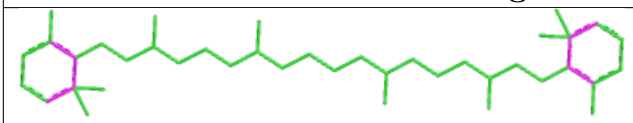


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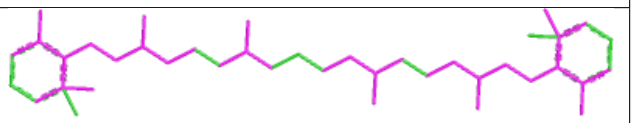


Rings

Ligand BCR AB 618



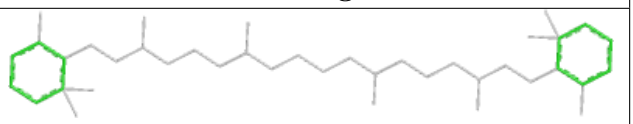
Bond lengths



Bond angles

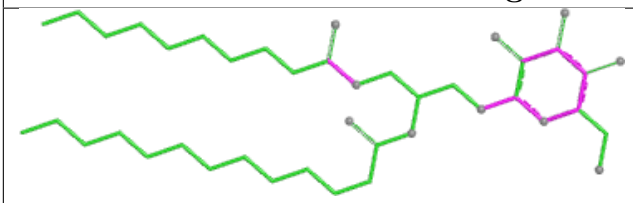


Torsions

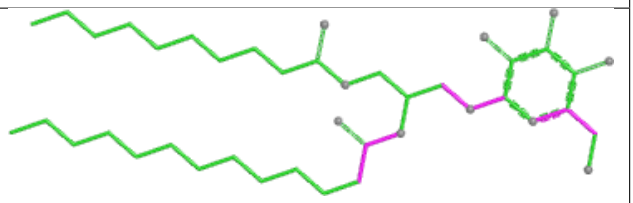


Rings

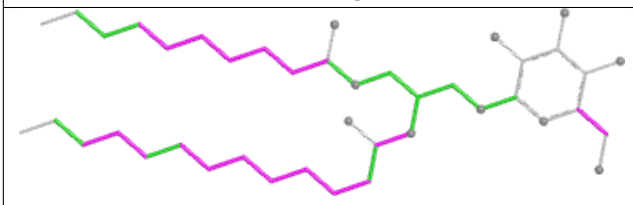
Ligand LMG AA 416



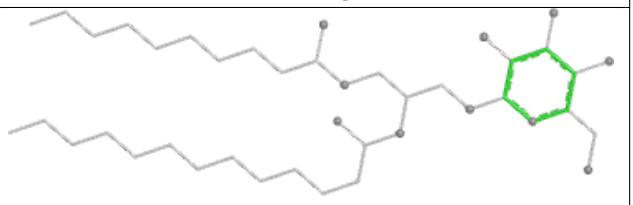
Bond lengths



Bond angles

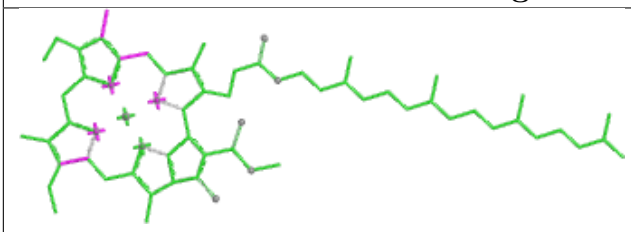


Torsions

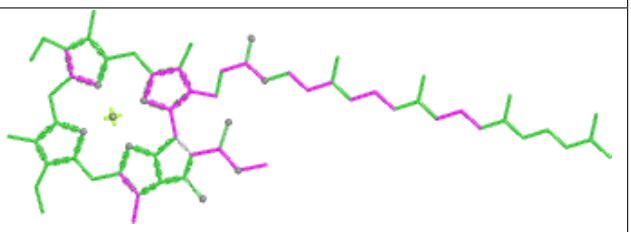


Rings

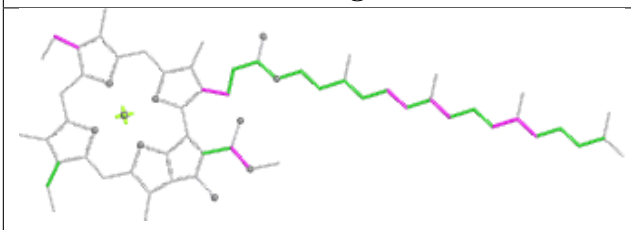
Ligand CLA BC 507



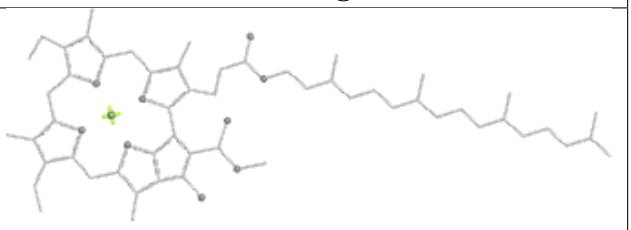
Bond lengths



Bond angles

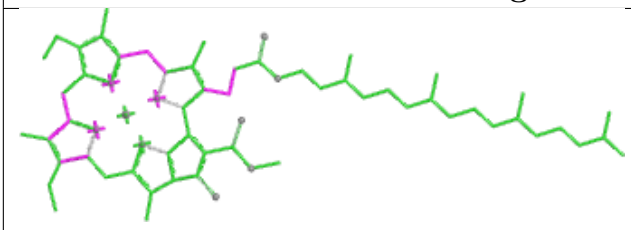


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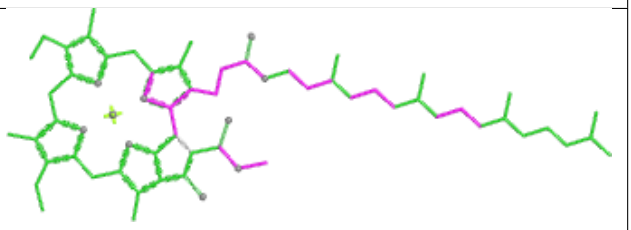


Rings

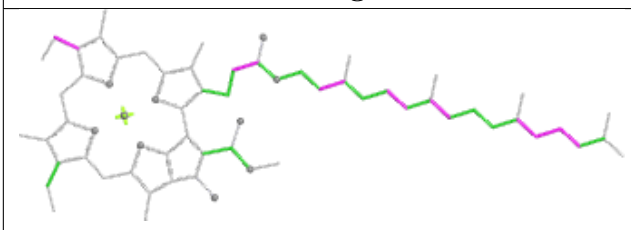
Ligand CLA AD 402



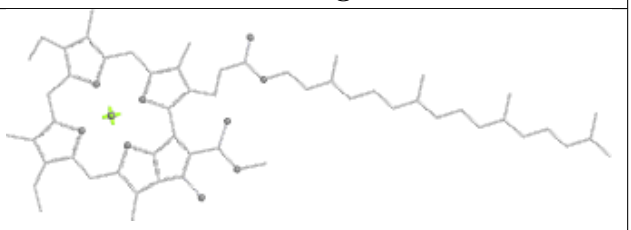
Bond lengths



Bond angles

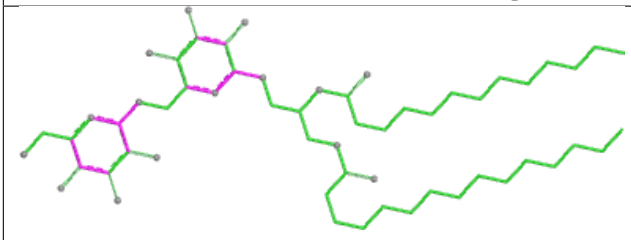


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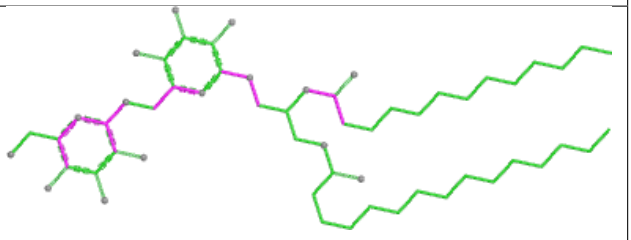


Rings

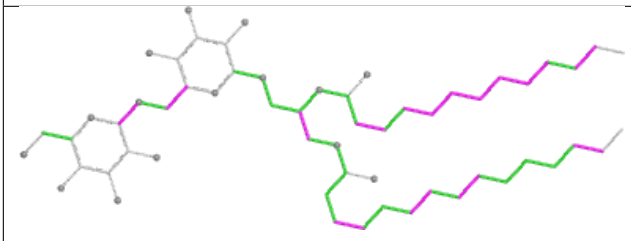
Ligand DGD BH 101



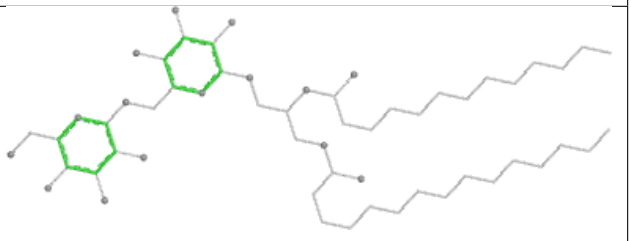
Bond lengths



Bond angles

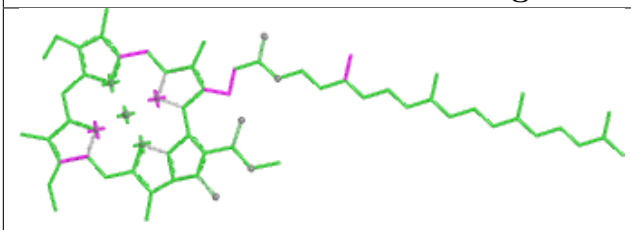


Torsions

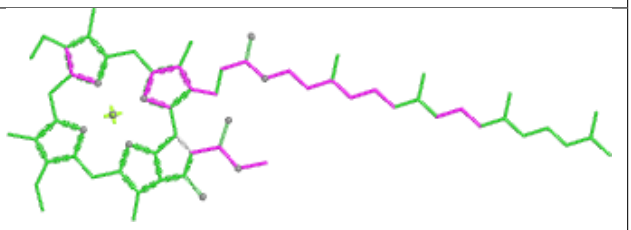


Rings

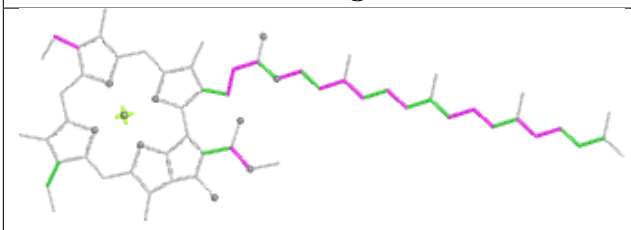
Ligand CLA BB 613



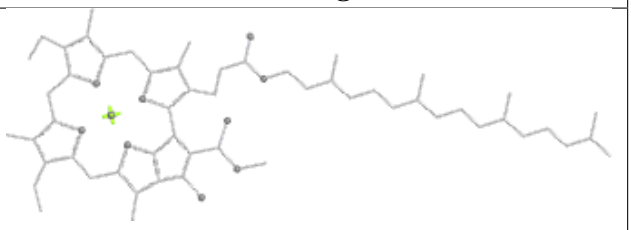
Bond lengths



Bond angles

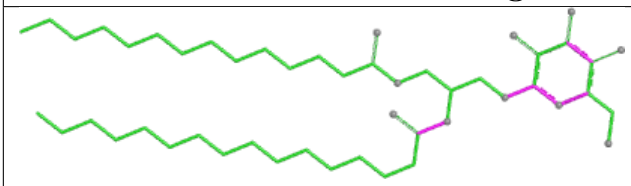


Torsions

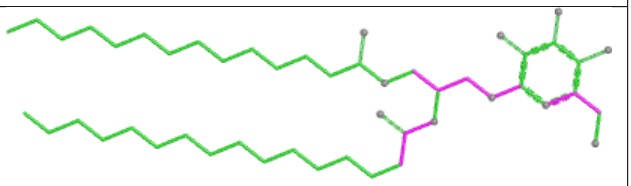


Rings

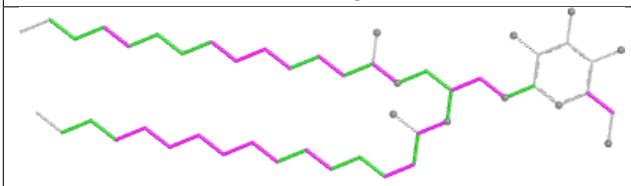
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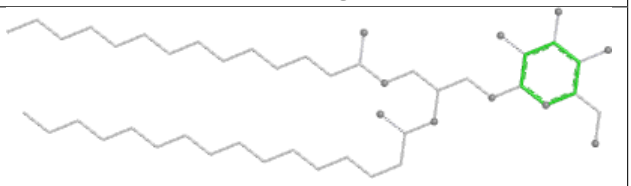
Bond lengths



Bond angles

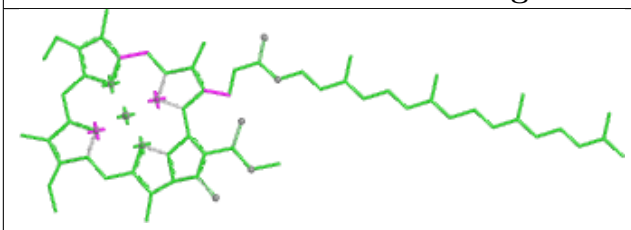


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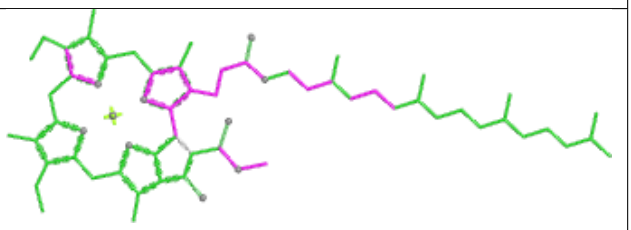


Rings

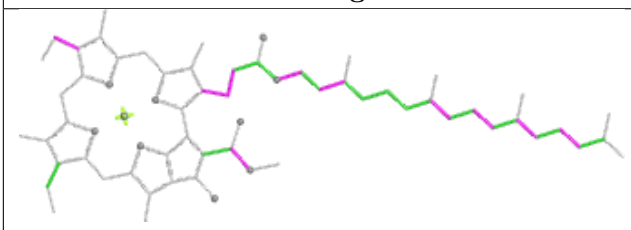
Ligand CLA AB 606



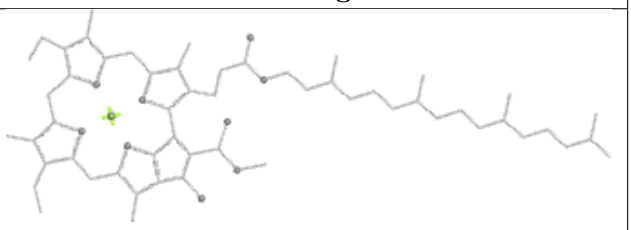
Bond lengths



Bond angles

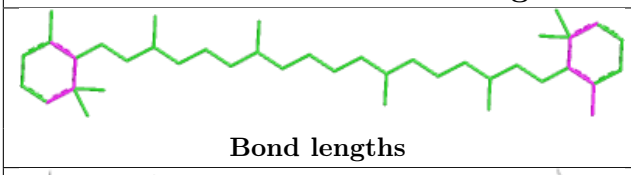


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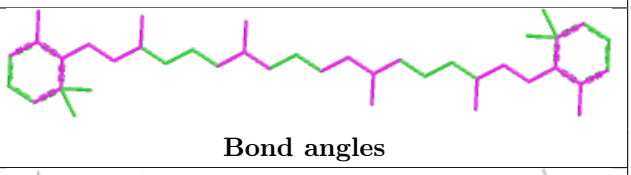


Rings

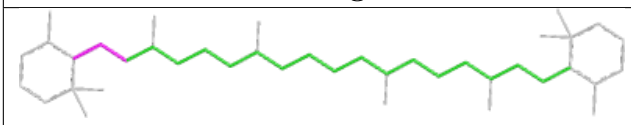
Ligand BCR AZ 101



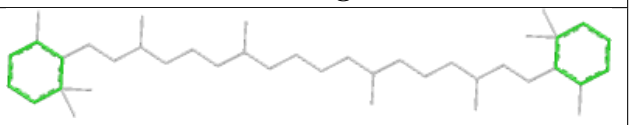
Bond lengths



Bond angles

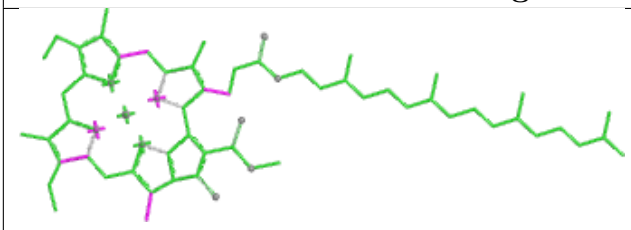


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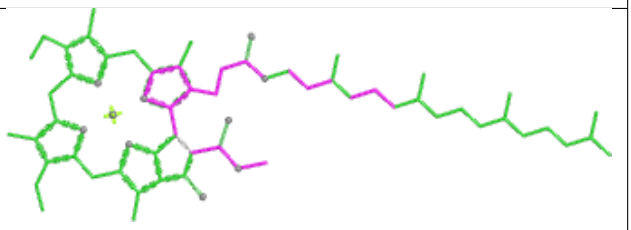


Rings

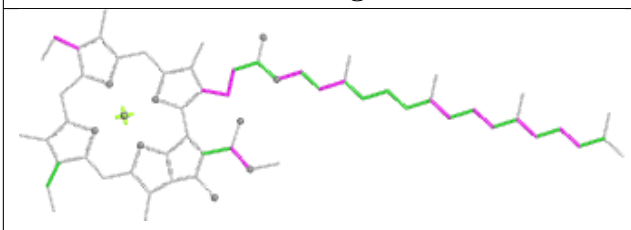
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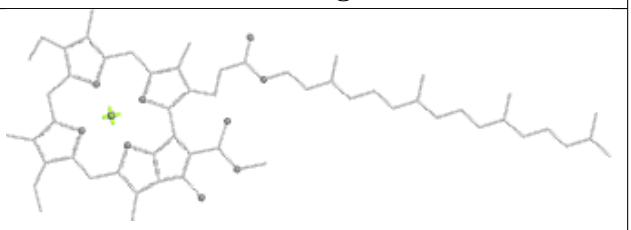
Bond lengths



Bond angles

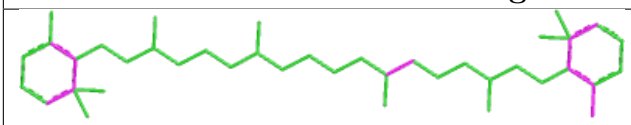


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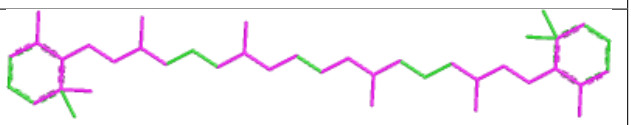


Rings

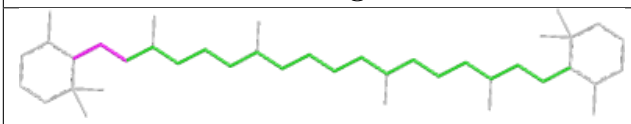
Ligand BCR BD 406



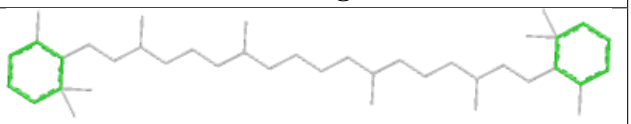
Bond lengths



Bond angles

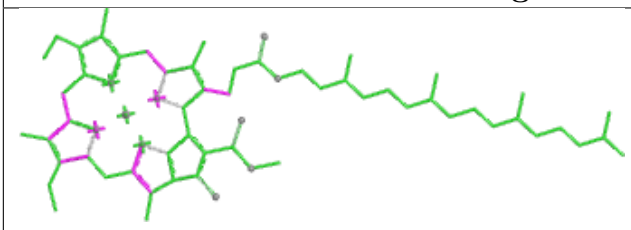


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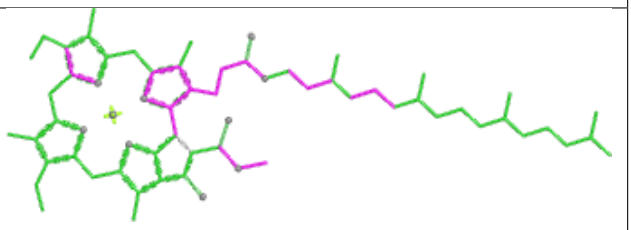


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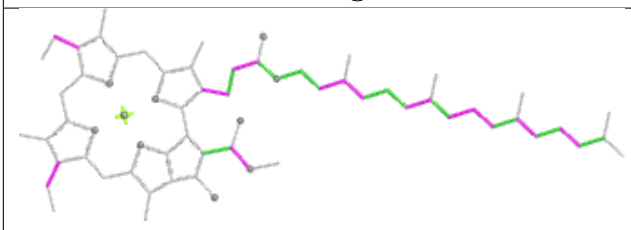
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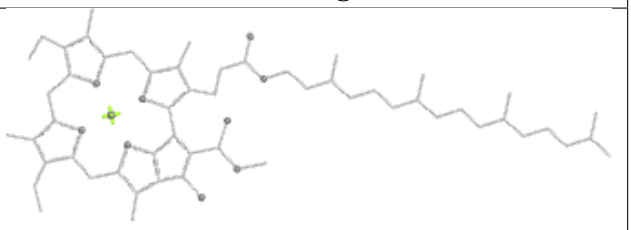
Bond lengths



Bond angles

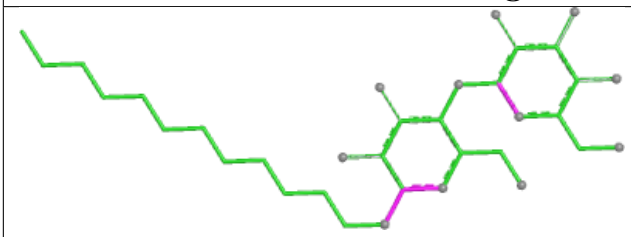


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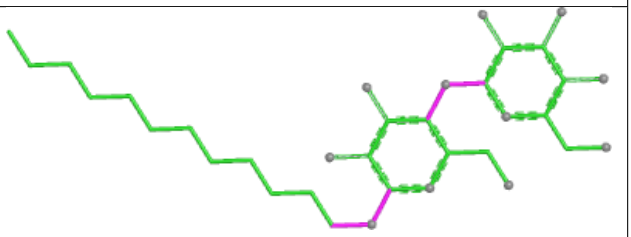


Rings

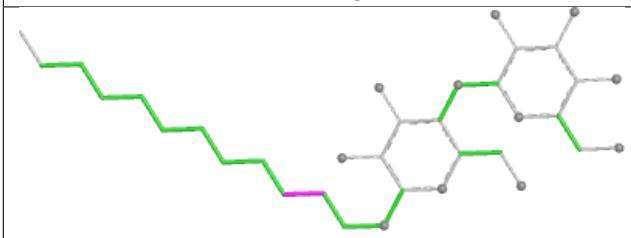
Ligand LMT BM 101



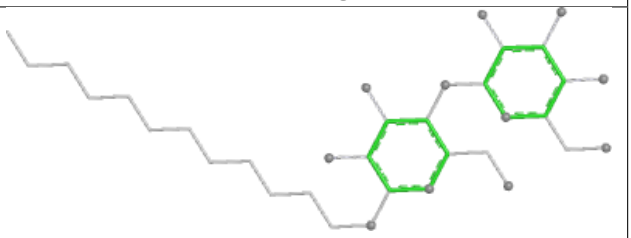
Bond lengths



Bond angles

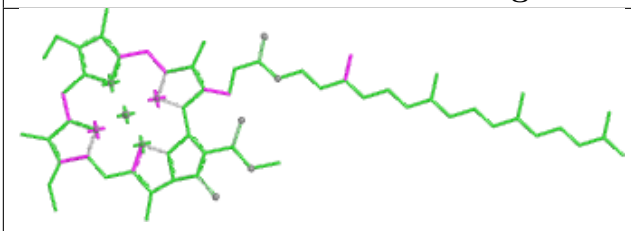


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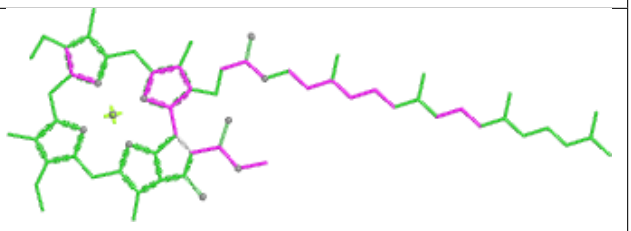


Rings

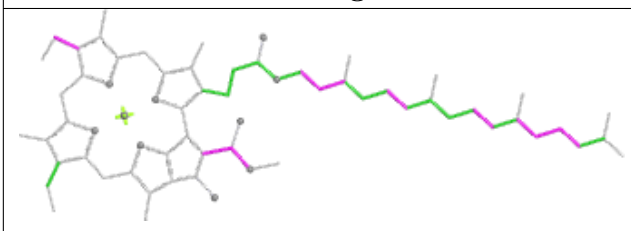
Ligand CLA AC 509



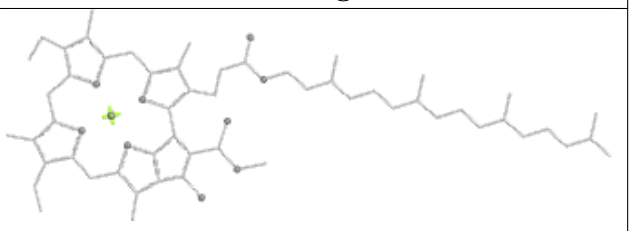
Bond lengths



Bond angles

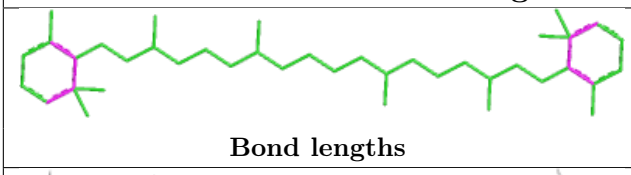


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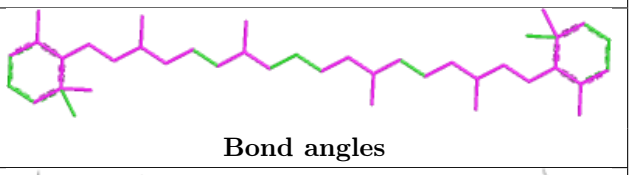


Rings

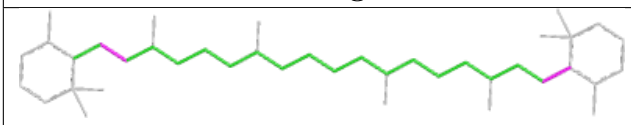
Ligand BCR AT 102



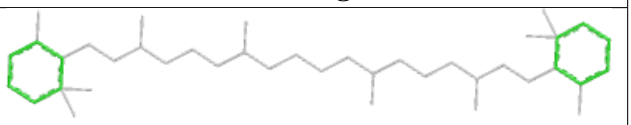
Bond lengths



Bond angles

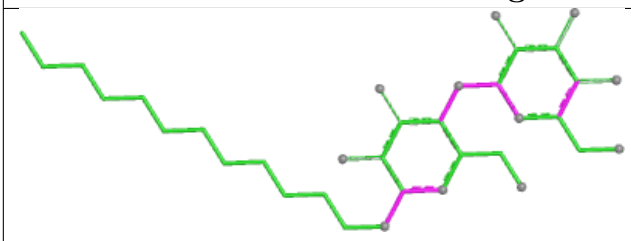


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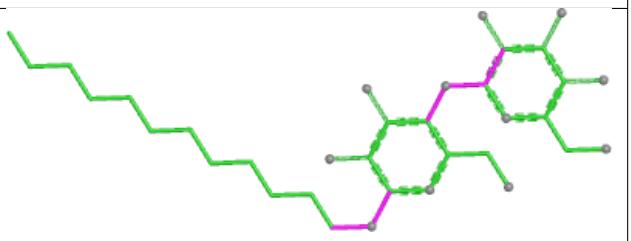


Rings

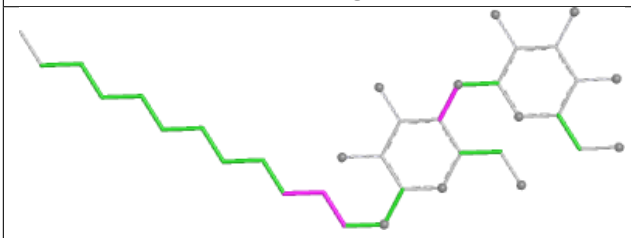
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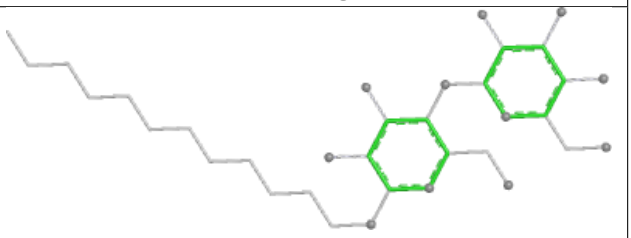
Bond lengths



Bond angles

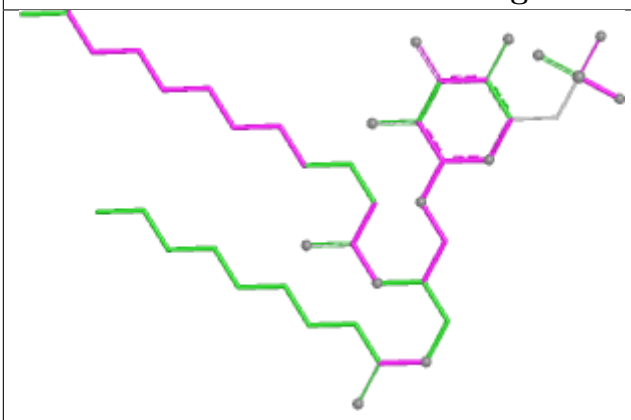


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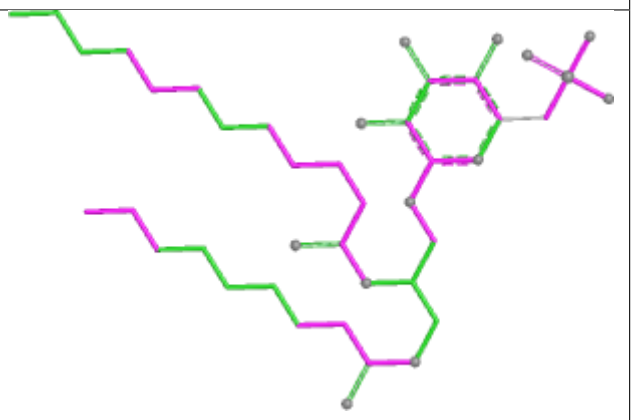


Rings

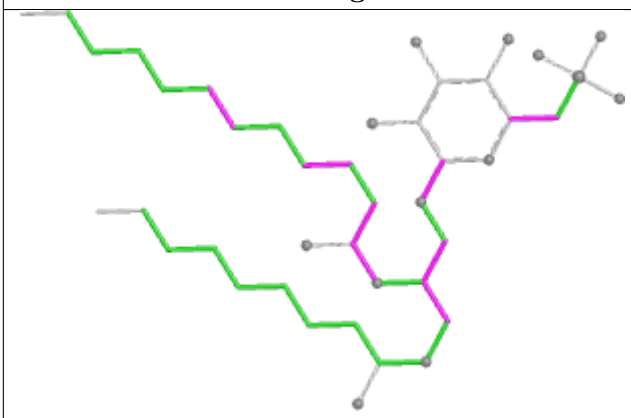
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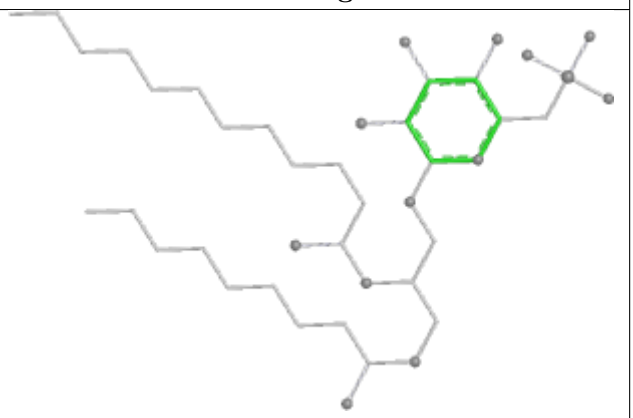
Bond lengths



Bond angles

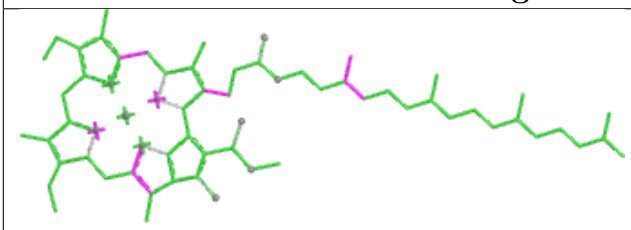


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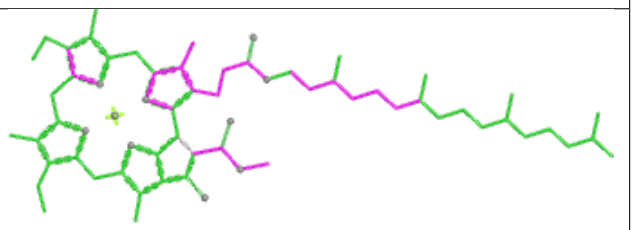


Rings

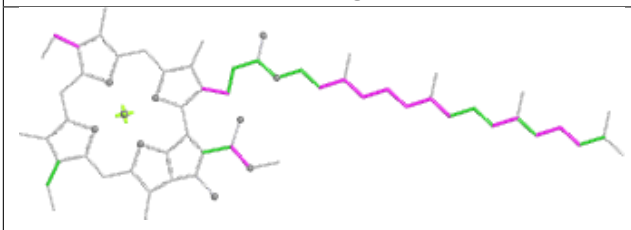
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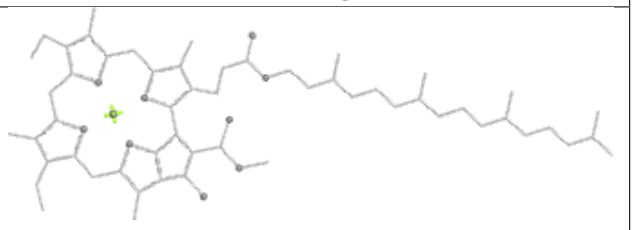
Bond lengths



Bond angles

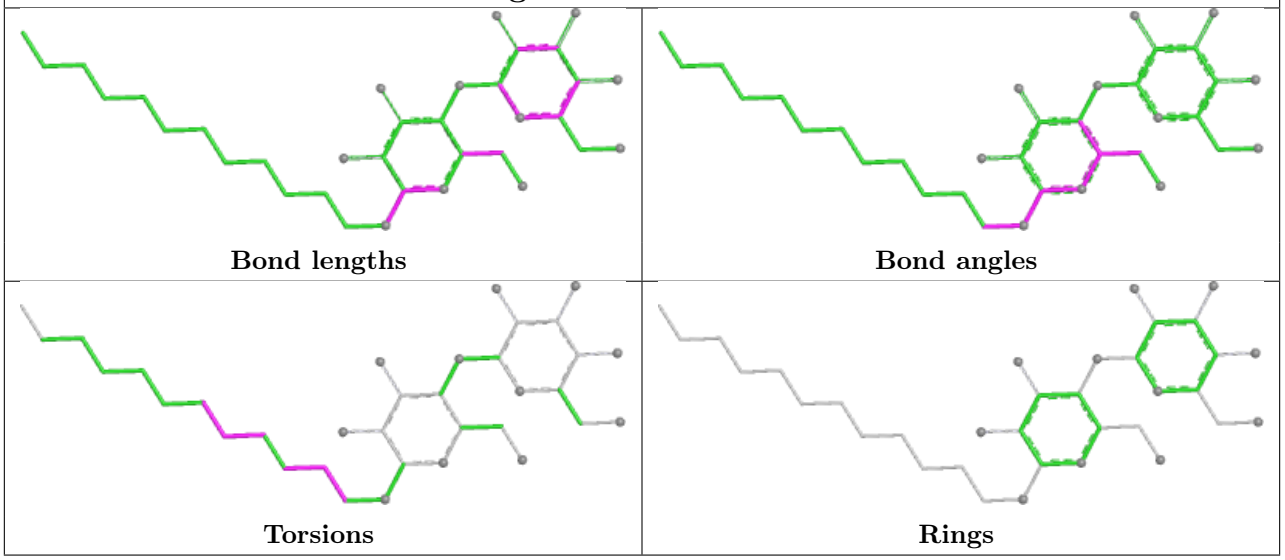


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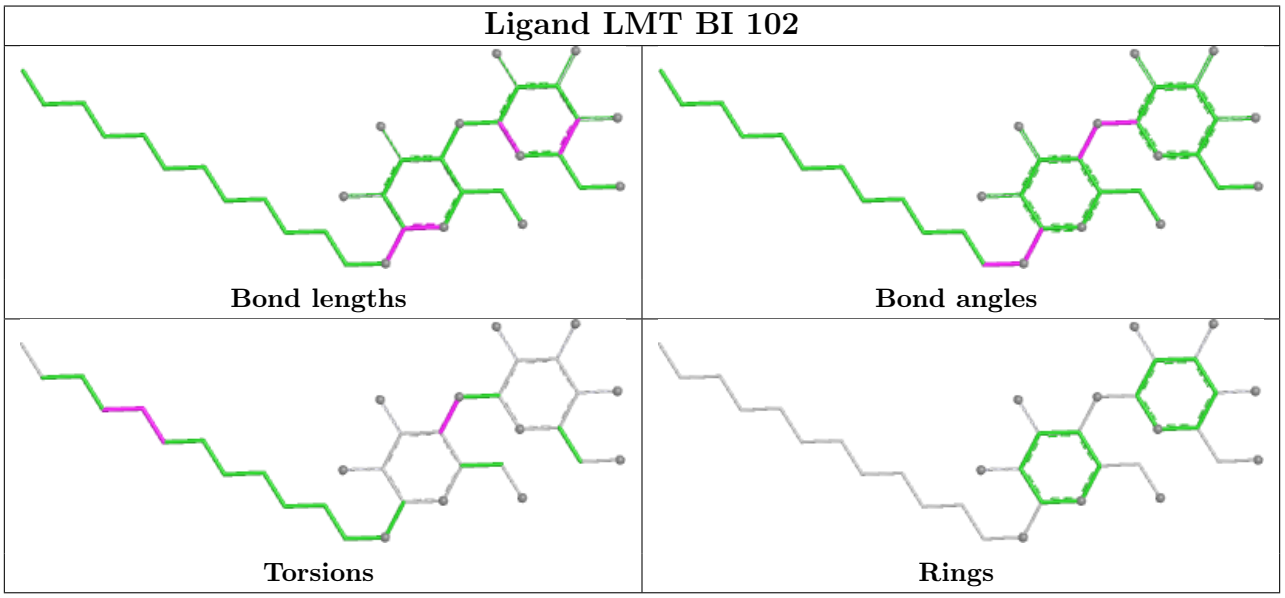


Rings

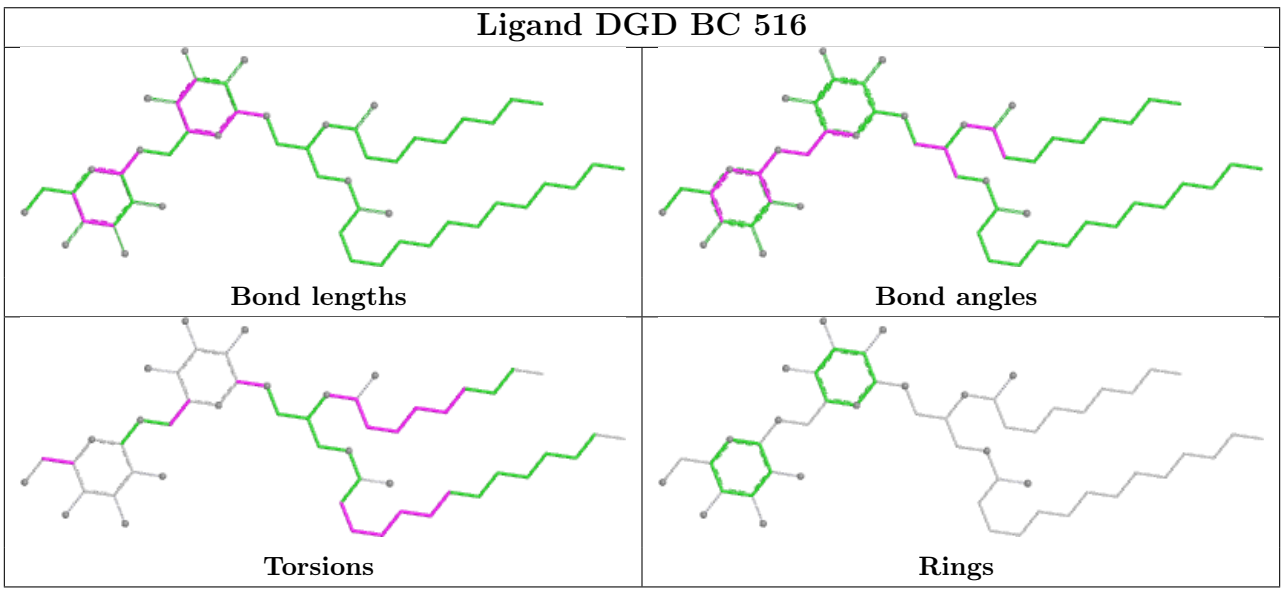
Ligand LMT AB 624



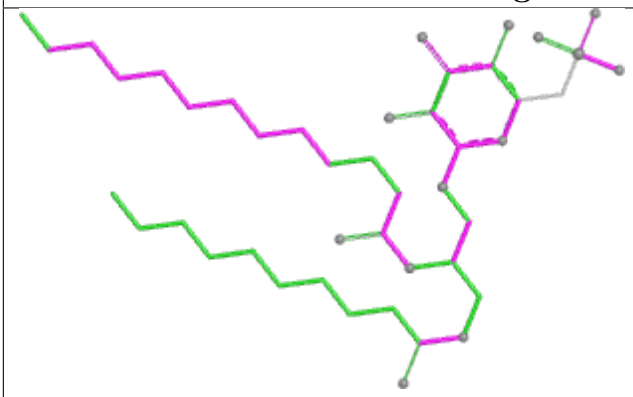
Ligand LMT BI 102



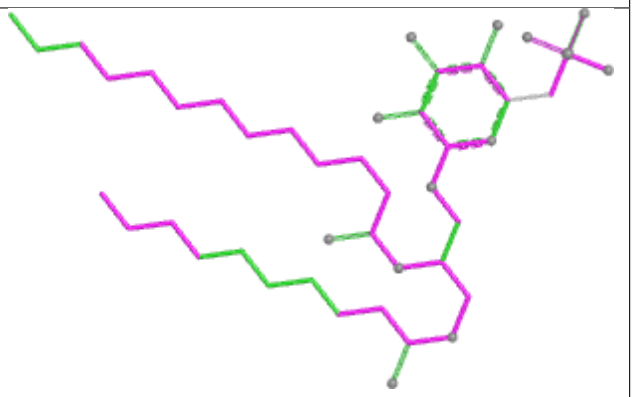
Ligand DGD BC 516



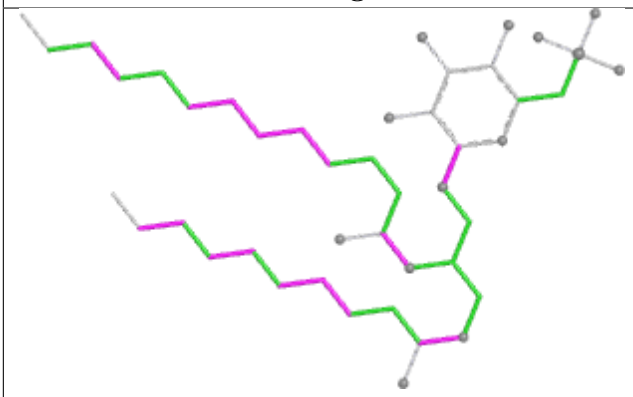
Ligand SQD BF 101



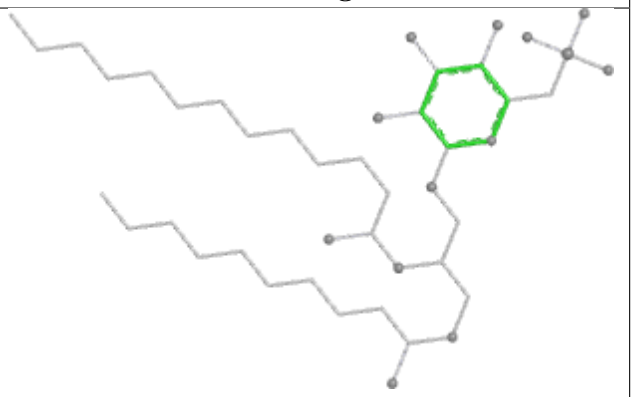
Bond lengths



Bond angles

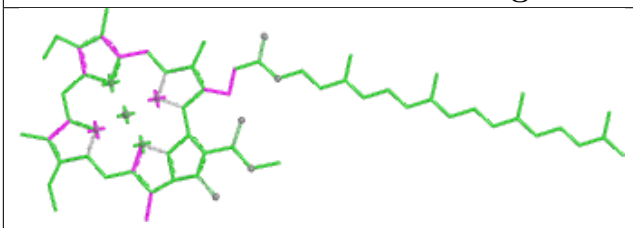


Torsions

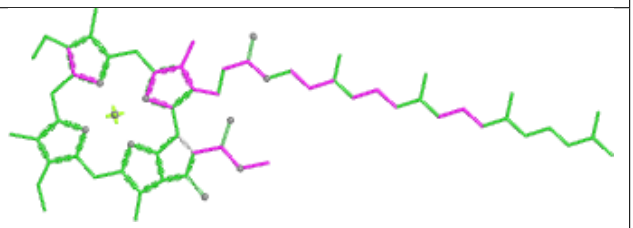


Rings

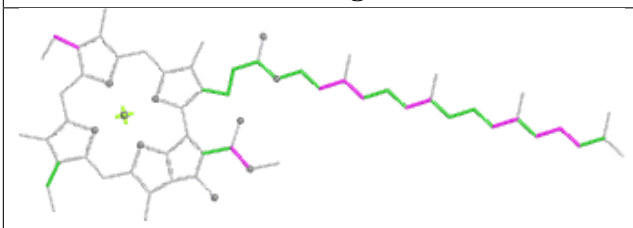
Ligand CLA AC 510



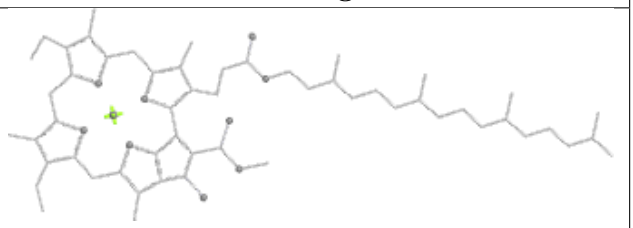
Bond lengths



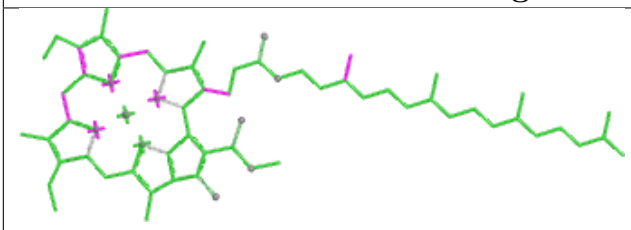
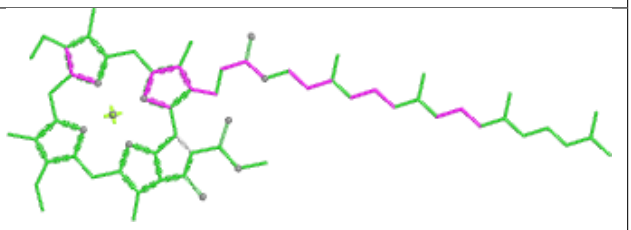
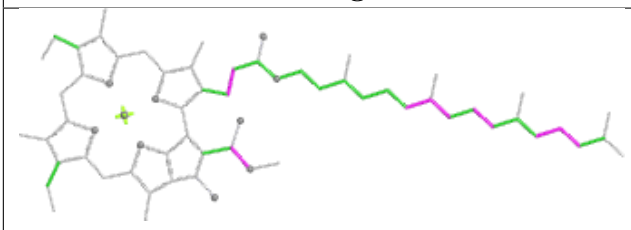
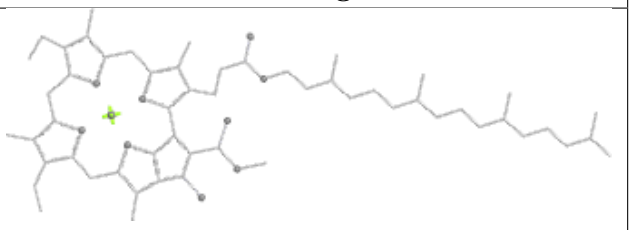
Bond angles

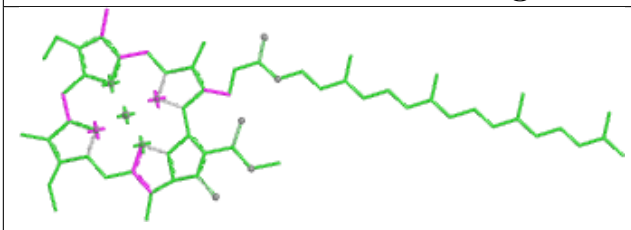
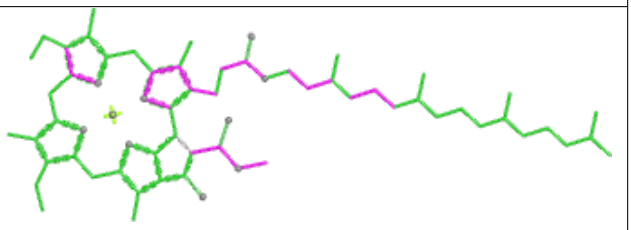
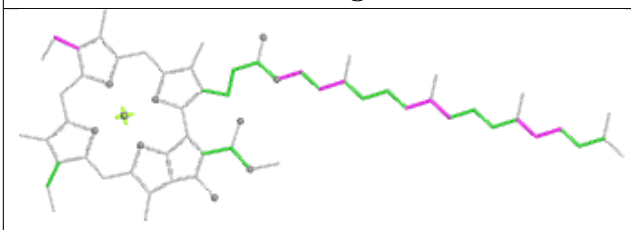
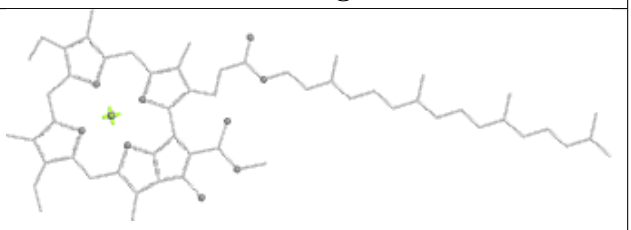


Torsions

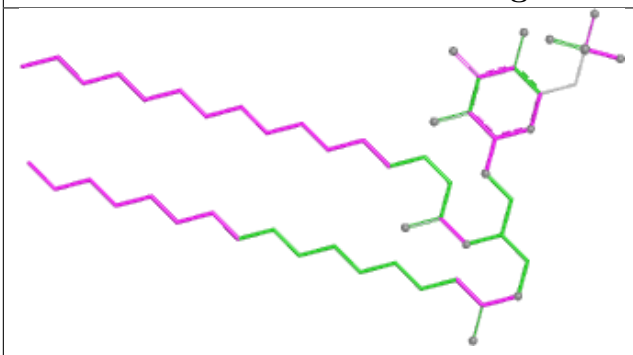


Rings

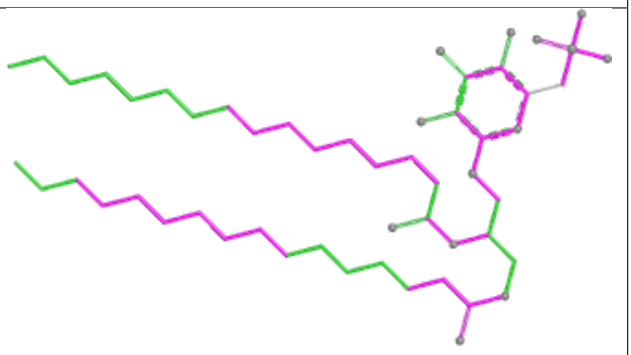
Ligand CLA BC 504	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA AC 502	
 Bond lengths	 Bond angles
 Torsions	 Rings

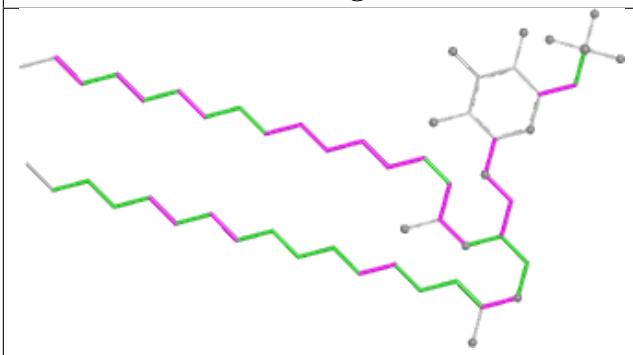
Ligand SQD AA 415



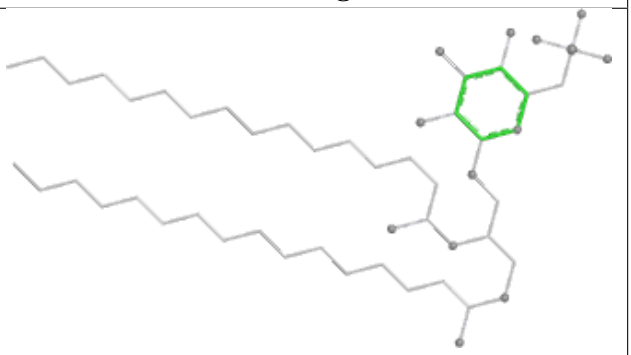
Bond lengths



Bond angles

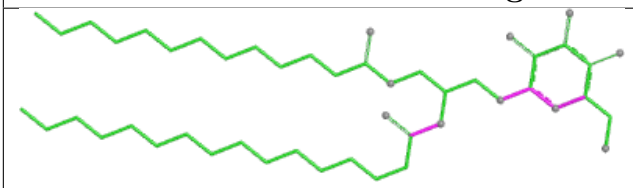


Torsions

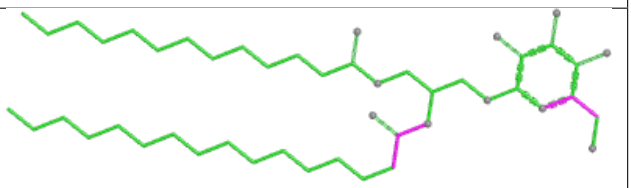


Rings

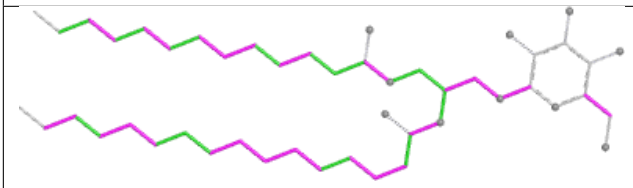
Ligand LMG BD 408



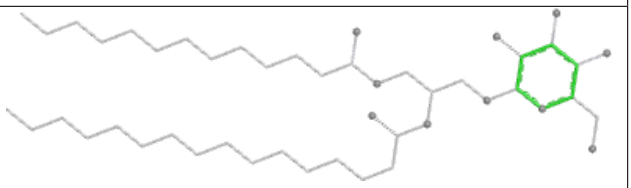
Bond lengths



Bond angles

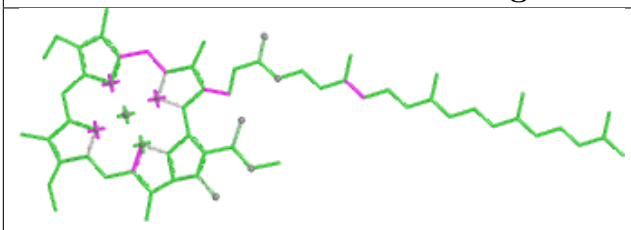


Torsions

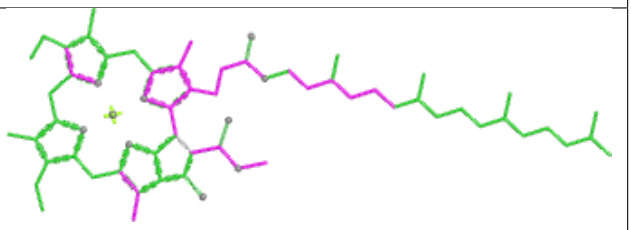


Rings

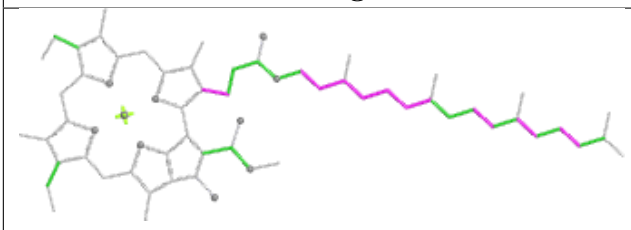
Ligand CLA AA 403



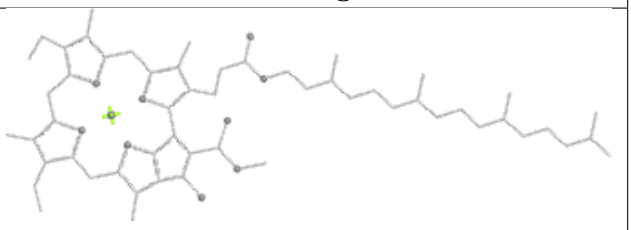
Bond lengths



Bond angles

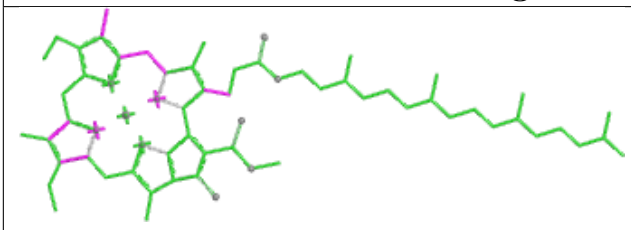


Torsions

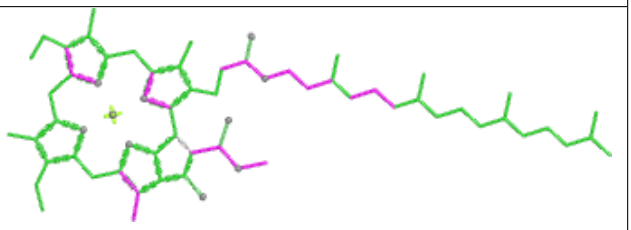


Rings

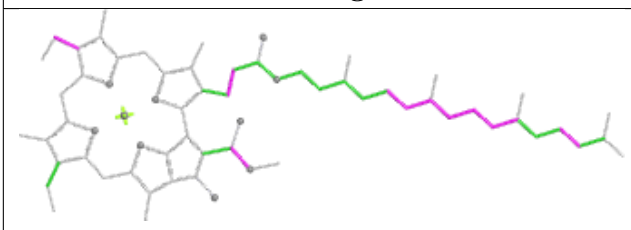
Ligand CLA AC 503



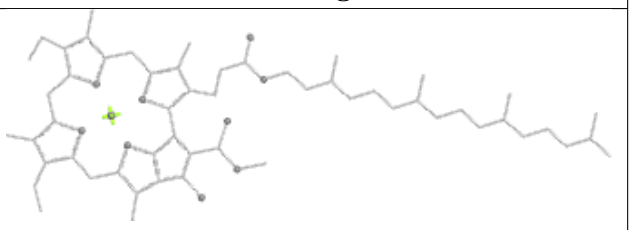
Bond lengths



Bond angles

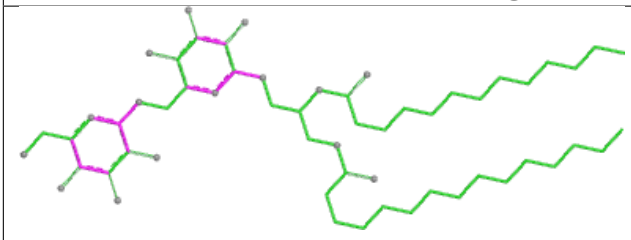


Torsions

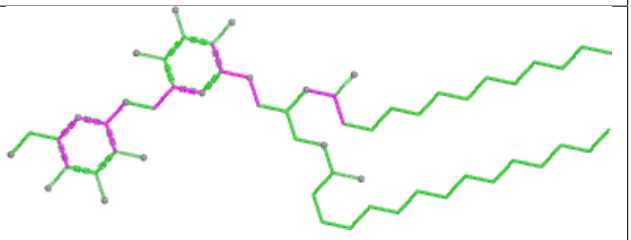


Rings

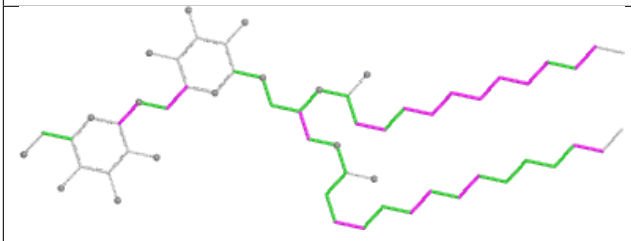
Ligand DGD AH 102



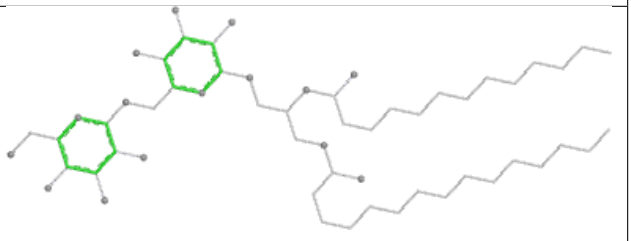
Bond lengths



Bond angles

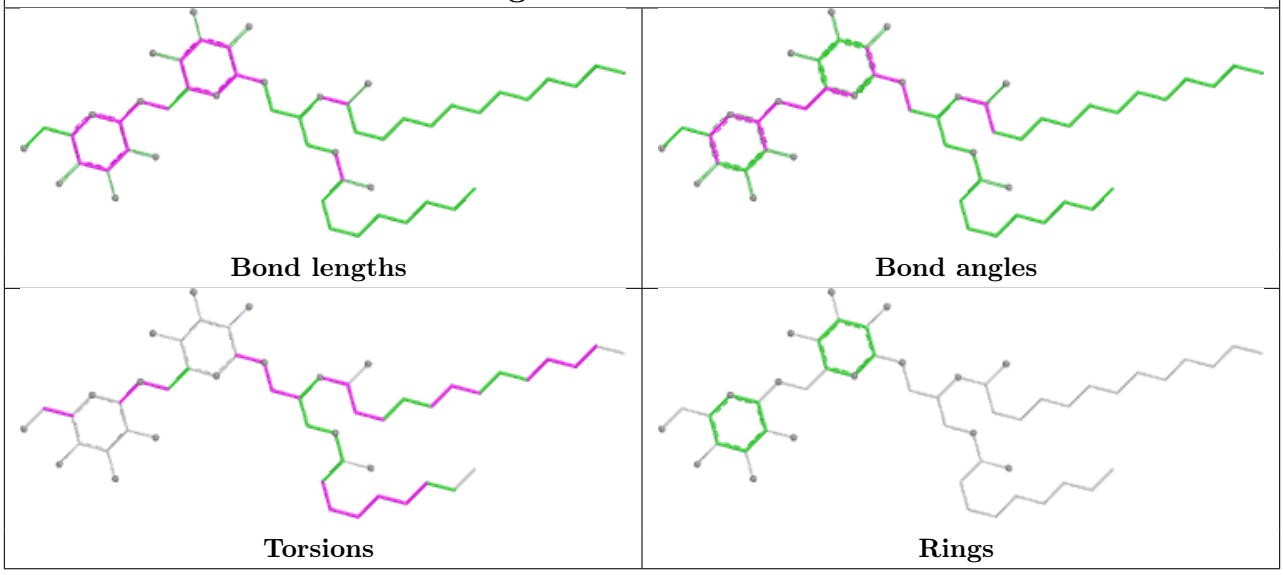


Torsions

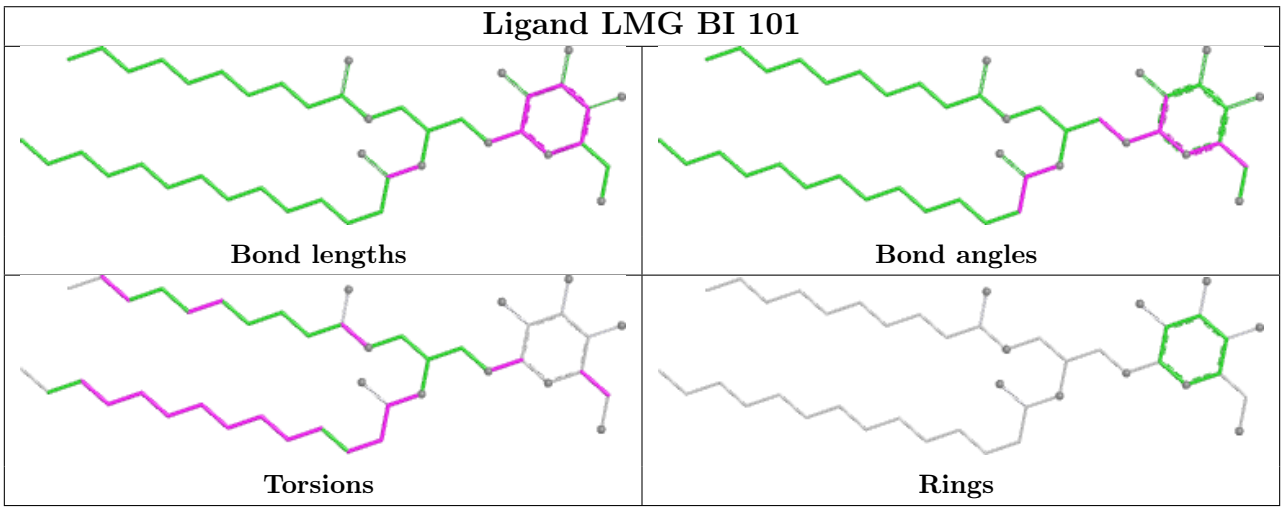


Rings

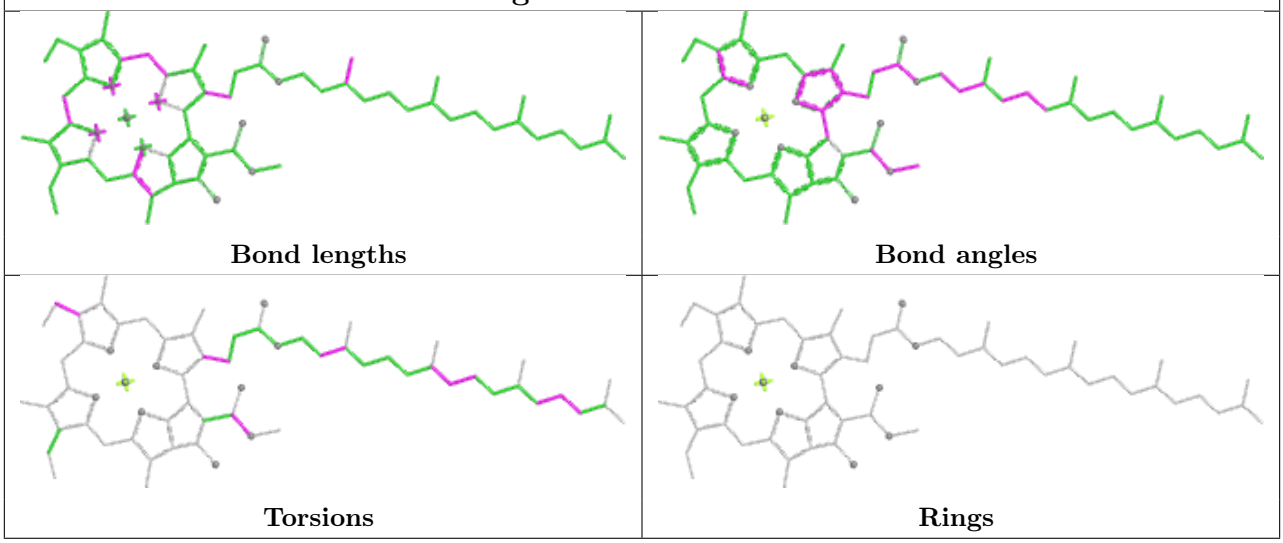
Ligand DGD BB 602



Ligand LMG BI 101



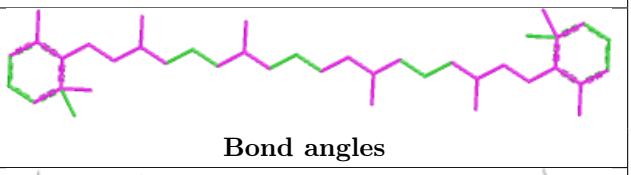
Ligand CLA AB 604



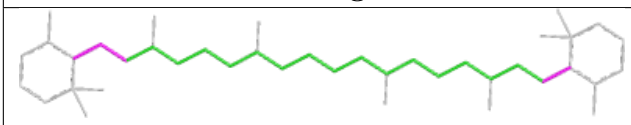
Ligand BCR BA 410



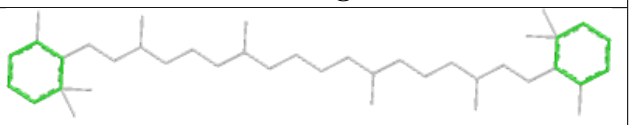
Bond lengths



Bond angles



Torsions

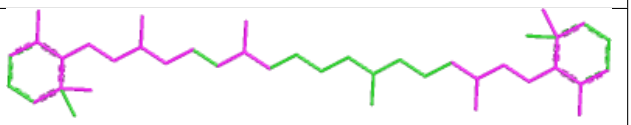


Rings

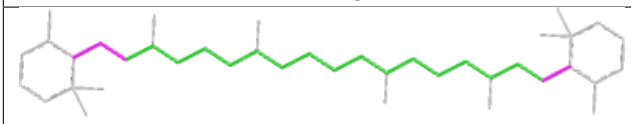
Ligand BCR BC 514



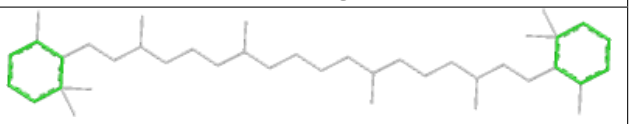
Bond lengths



Bond angles

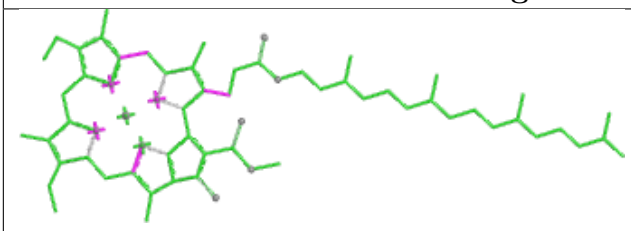


Torsions

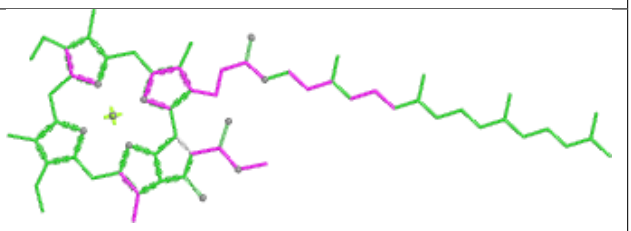


Rings

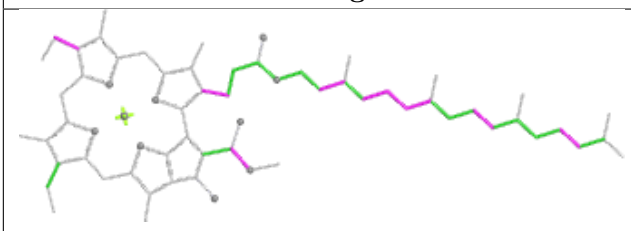
Ligand CLA BA 405



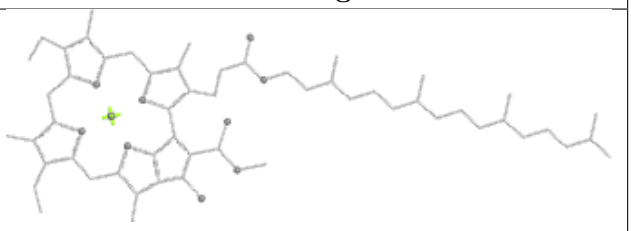
Bond lengths



Bond angles

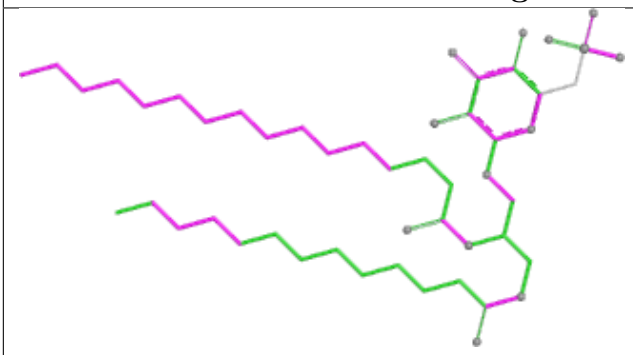


Torsions

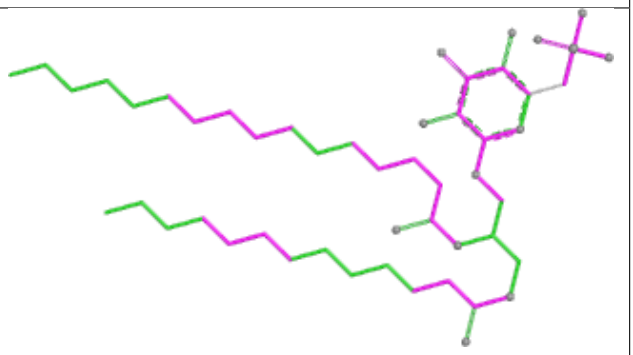


Rings

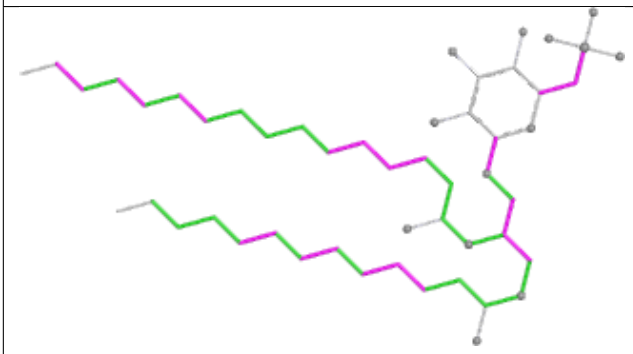
Ligand SQD BA 413



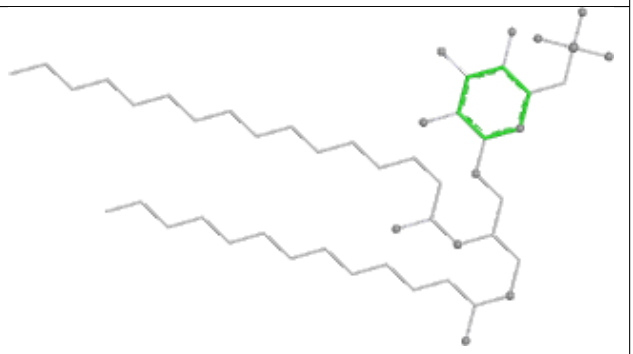
Bond lengths



Bond angles

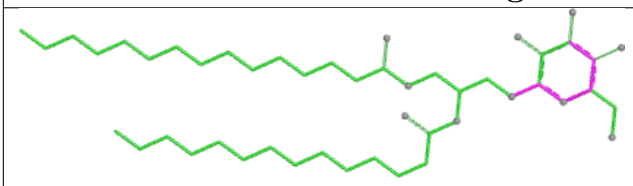


Torsions

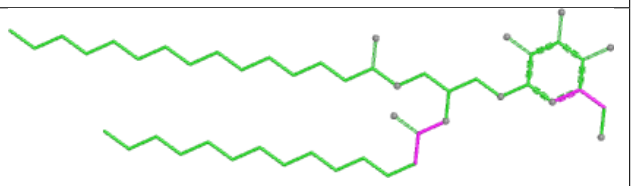


Rings

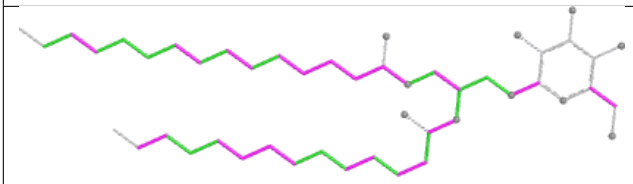
Ligand LMG AC 519



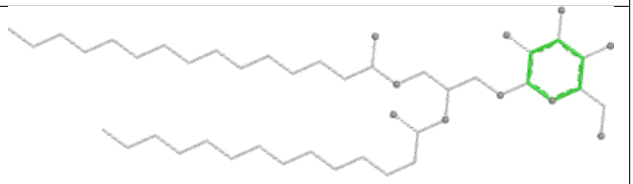
Bond lengths



Bond angles

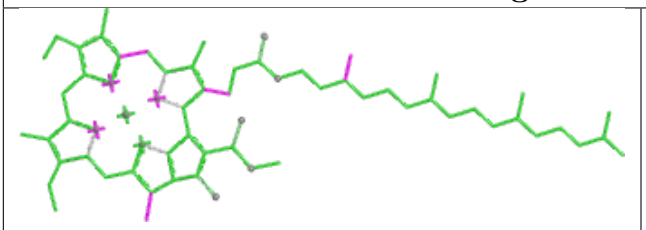


Torsions

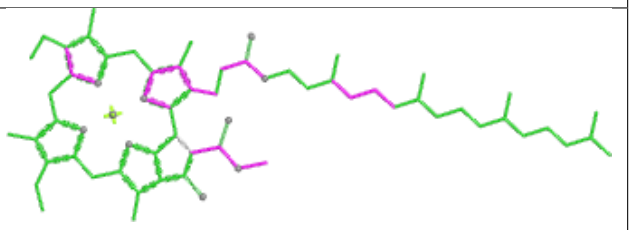


Rings

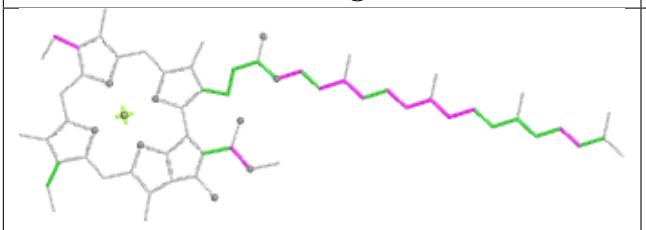
Ligand CLA AB 611



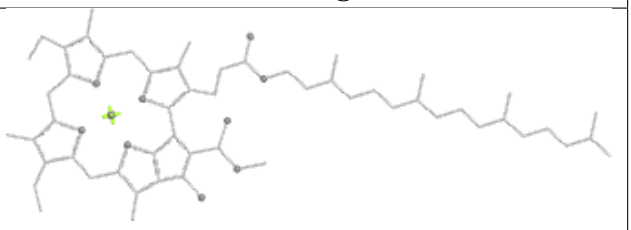
Bond lengths



Bond angles

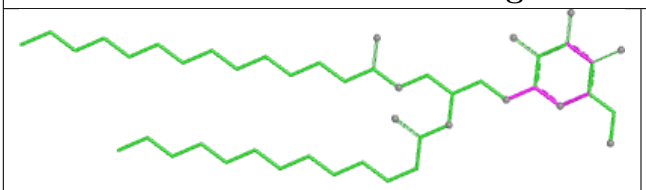


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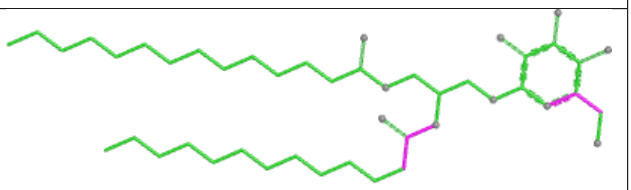


Rings

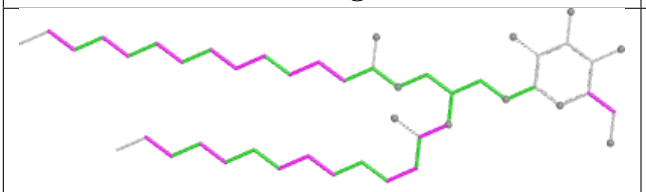
Ligand LMG BD 407



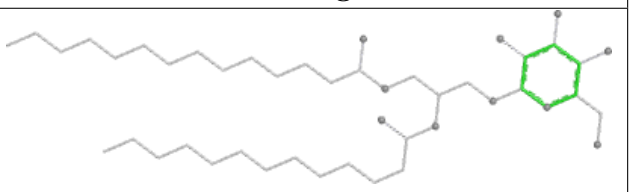
Bond lengths



Bond angles

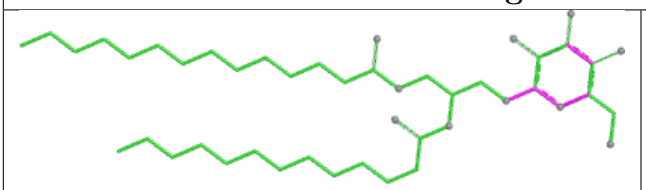


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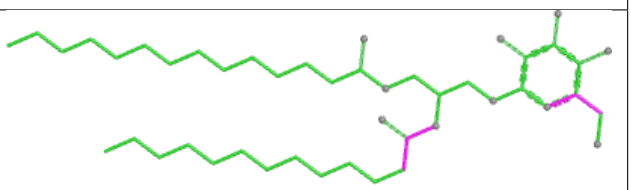


Rings

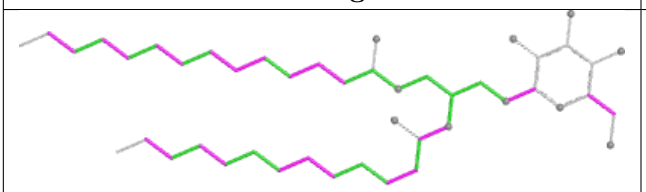
Ligand LMG AD 407



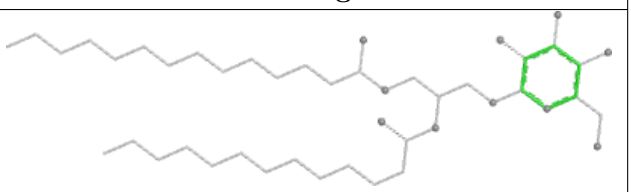
Bond lengths



Bond angles

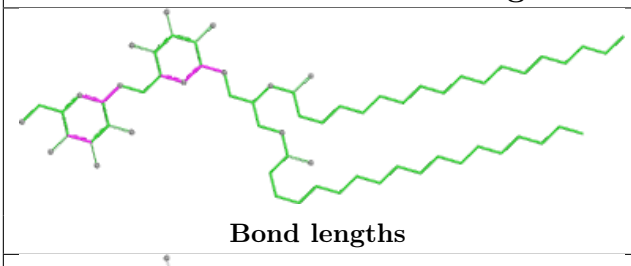


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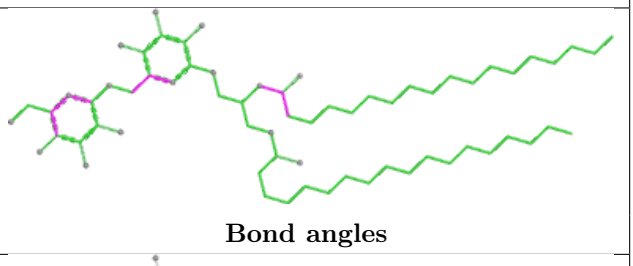


Rings

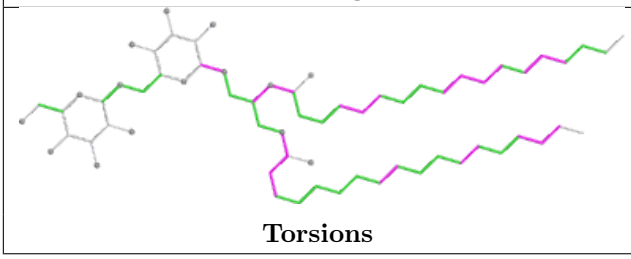
Ligand DGD BC 518



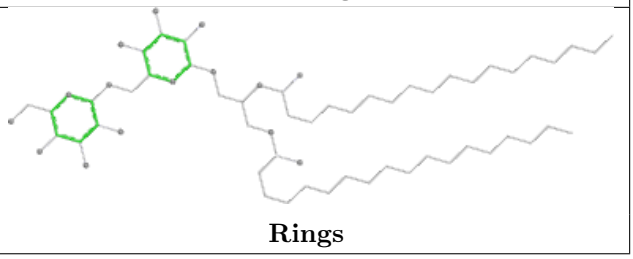
Bond lengths



Bond angles

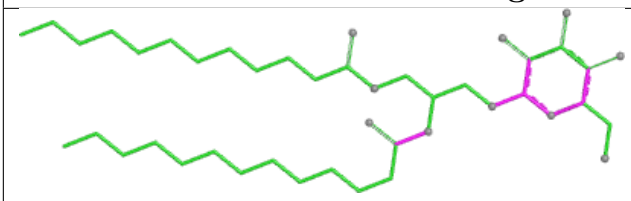


Torsions

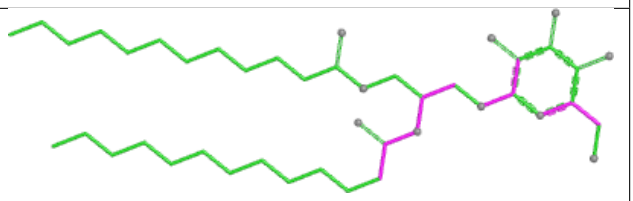


Rings

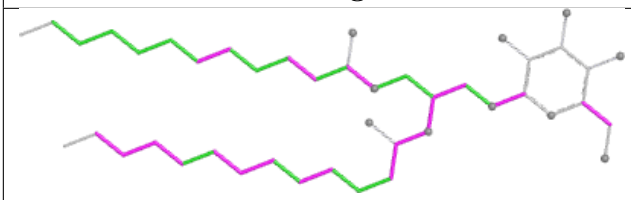
Ligand LMG BE 102



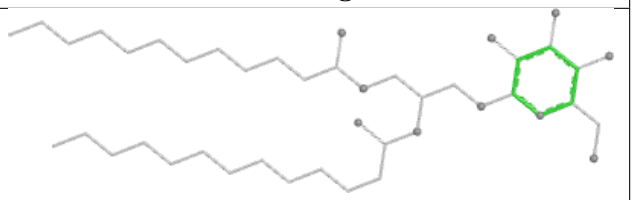
Bond lengths



Bond angles

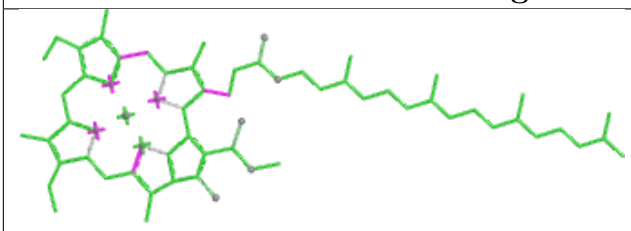


Torsions

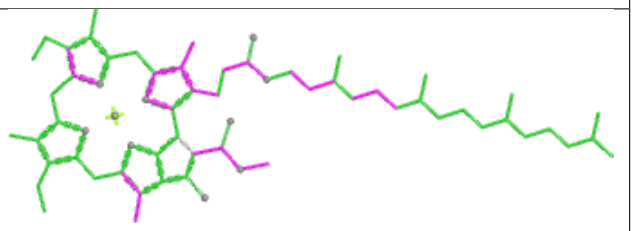


Rings

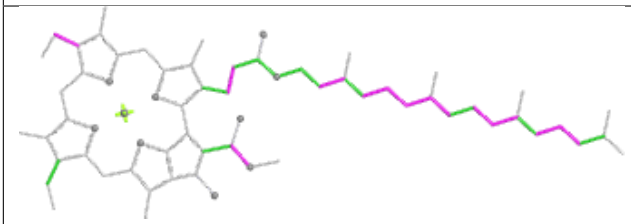
Ligand CLA AB 605



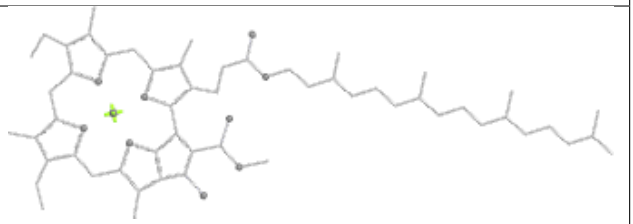
Bond lengths



Bond angles

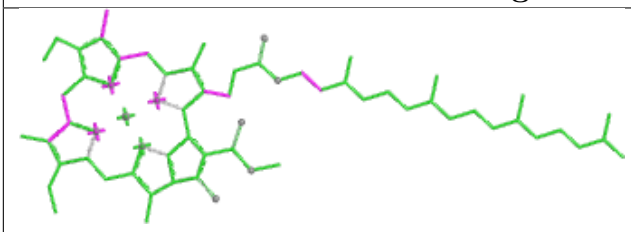


Torsions

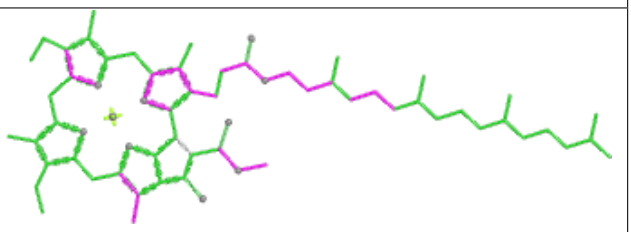


Rings

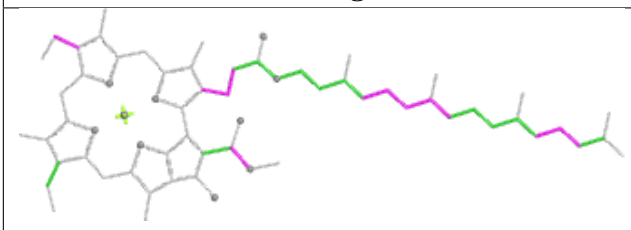
Ligand CLA BB 610



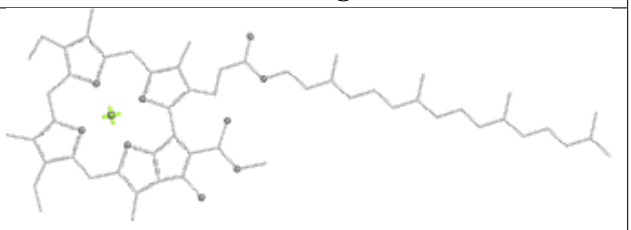
Bond lengths



Bond angles

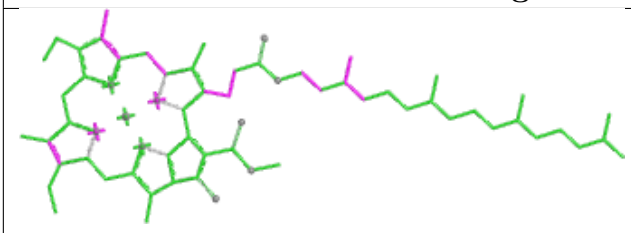


Torsions

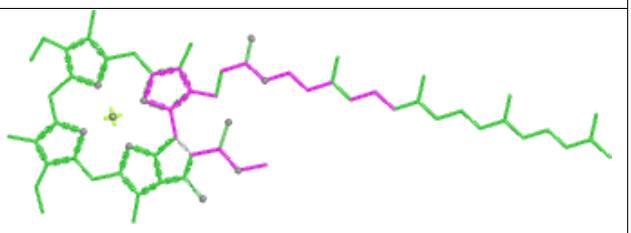


Rings

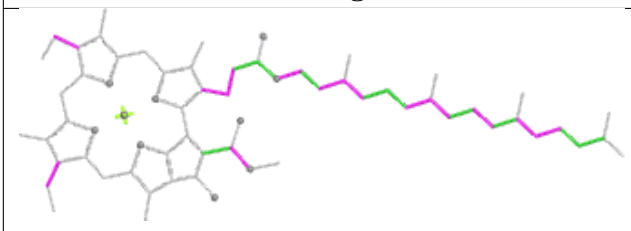
Ligand CLA BB 604



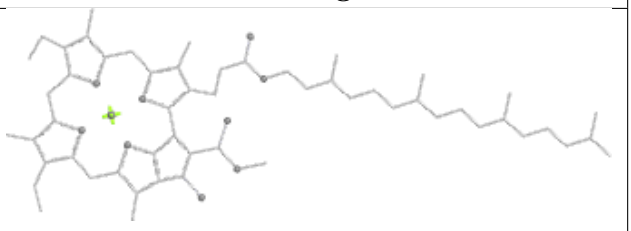
Bond lengths



Bond angles

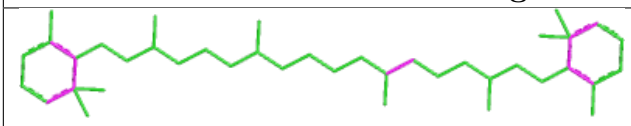


Torsions

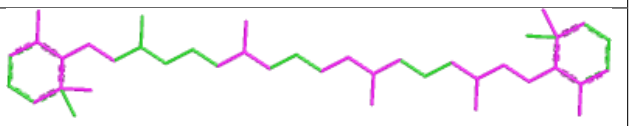


Rings

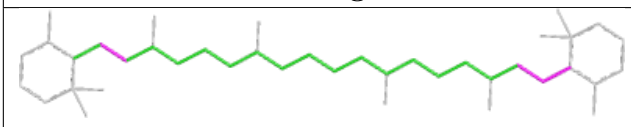
Ligand BCR BC 515



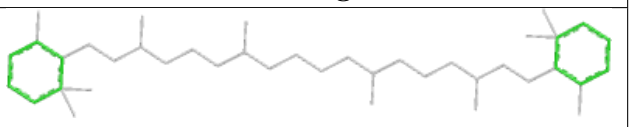
Bond lengths



Bond angles

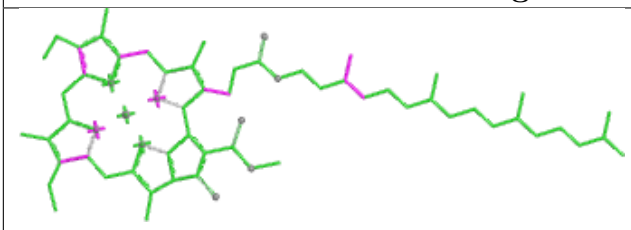


Torsions

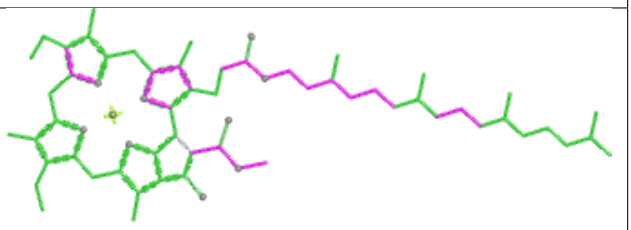


Rings

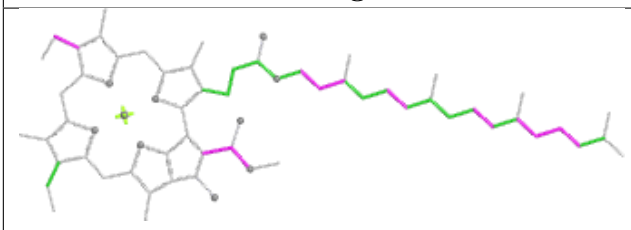
Ligand CLA BC 509



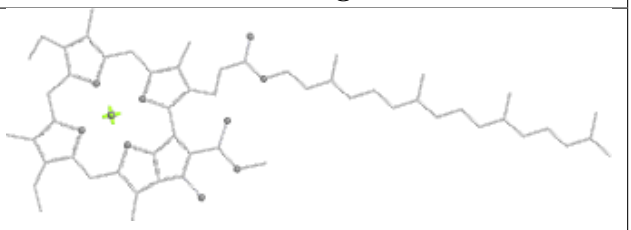
Bond lengths



Bond angles

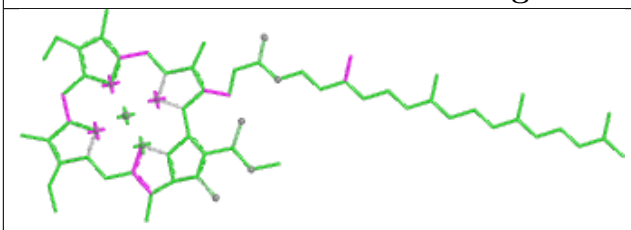


Torsions

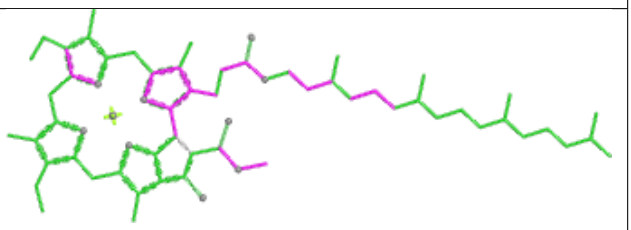


Rings

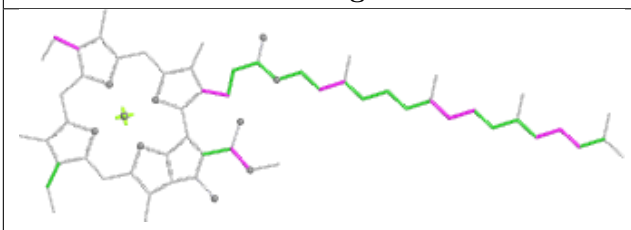
Ligand CLA BB 607



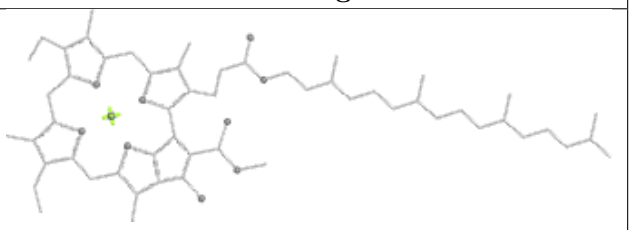
Bond lengths



Bond angles

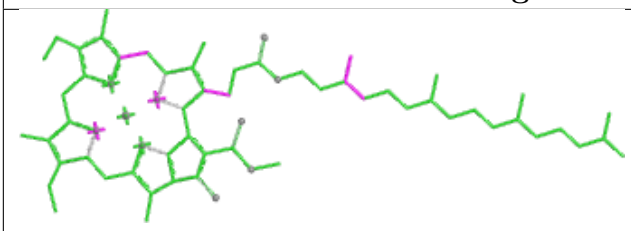


Torsions

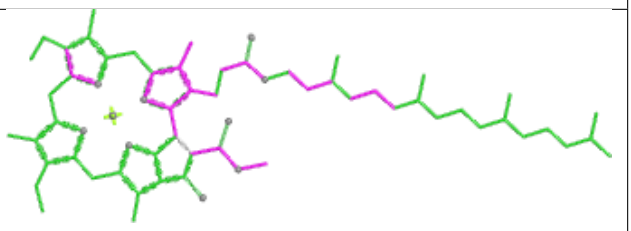


Rings

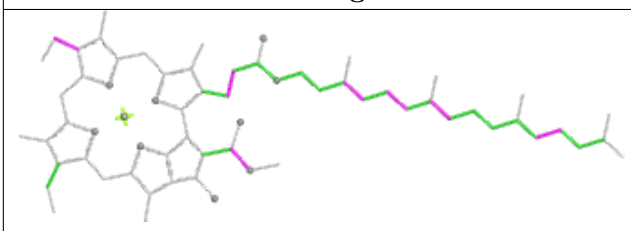
Ligand CLA BB 606



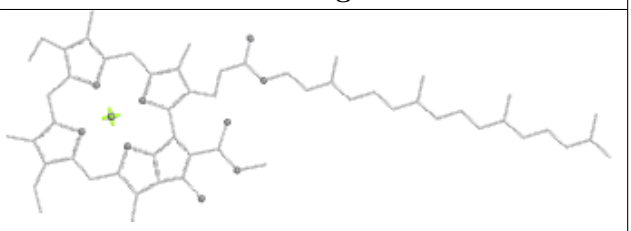
Bond lengths



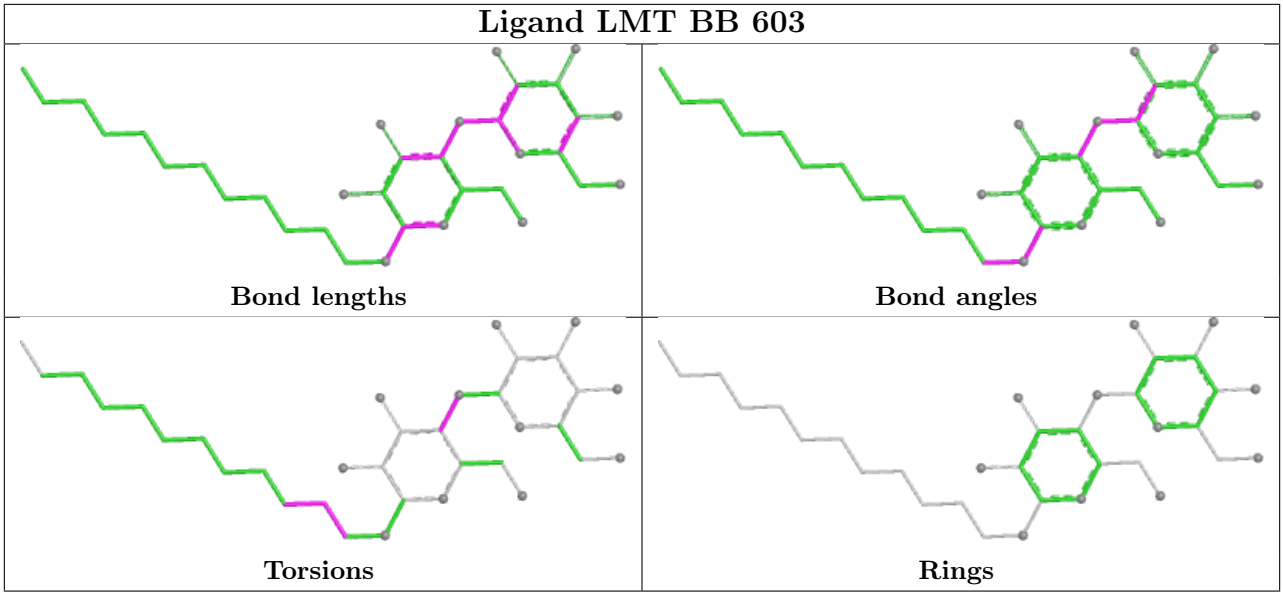
Bond angles



Torsions



Rings



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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, 95^{th} 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	AA	335/344 (97%)	-0.56	0 100 100	23, 59, 88, 103	0
1	BA	335/344 (97%)	-0.42	1 (0%) 90 87	47, 70, 89, 103	0
2	AB	490/510 (96%)	-0.48	1 (0%) 91 89	37, 63, 86, 99	0
2	BB	490/510 (96%)	-0.51	0 100 100	41, 64, 87, 103	0
3	AC	447/473 (94%)	-0.42	2 (0%) 88 85	43, 72, 87, 102	0
3	BC	447/473 (94%)	-0.24	4 (0%) 81 75	54, 83, 95, 101	0
4	AD	340/352 (96%)	-0.61	1 (0%) 90 87	29, 59, 84, 95	0
4	BD	340/352 (96%)	-0.49	0 100 100	40, 69, 91, 101	0
5	AE	82/84 (97%)	-0.10	1 (1%) 76 69	54, 75, 93, 99	0
5	BE	82/84 (97%)	-0.15	1 (1%) 76 69	71, 85, 98, 104	0
6	AF	35/45 (77%)	-0.48	0 100 100	56, 73, 94, 97	0
6	BF	35/45 (77%)	-0.13	1 (2%) 53 45	75, 82, 97, 99	0
7	AH	65/66 (98%)	-0.21	0 100 100	57, 76, 92, 97	0
7	BH	65/66 (98%)	-0.23	1 (1%) 72 64	62, 80, 91, 103	0
8	AI	35/38 (92%)	-0.31	0 100 100	57, 70, 87, 94	0
8	BI	35/38 (92%)	-0.22	0 100 100	69, 80, 92, 95	0
9	AJ	34/40 (85%)	-0.09	1 (2%) 53 45	65, 74, 83, 89	0
9	BJ	34/40 (85%)	-0.23	0 100 100	73, 81, 93, 98	0
10	AK	37/37 (100%)	-0.51	0 100 100	67, 75, 86, 93	0
10	BK	37/37 (100%)	-0.24	0 100 100	84, 90, 96, 101	0
11	AL	37/37 (100%)	-0.43	0 100 100	45, 60, 98, 107	0
11	BL	37/37 (100%)	-0.41	0 100 100	46, 62, 94, 102	0
12	AM	34/36 (94%)	-0.42	0 100 100	51, 65, 94, 100	0
12	BM	34/36 (94%)	-0.55	0 100 100	55, 61, 76, 91	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	AO	243/247 (98%)	-0.35	1 (0%) 88 85	39, 70, 93, 107	0
13	BO	243/247 (98%)	-0.23	3 (1%) 76 69	48, 76, 97, 107	0
14	AT	32/32 (100%)	-0.23	1 (3%) 51 42	53, 63, 102, 104	0
14	BT	32/32 (100%)	-0.25	0 100 100	57, 67, 93, 103	0
15	AU	97/104 (93%)	-0.47	0 100 100	43, 63, 78, 86	0
15	BU	97/104 (93%)	-0.48	0 100 100	55, 67, 77, 87	0
16	AV	137/137 (100%)	-0.53	1 (0%) 84 79	49, 66, 76, 79	0
16	BV	137/137 (100%)	-0.32	1 (0%) 84 79	64, 79, 95, 102	0
17	Ay	28/46 (60%)	0.08	1 (3%) 46 38	79, 91, 97, 99	0
17	By	28/46 (60%)	0.14	0 100 100	89, 98, 102, 106	0
18	AX	37/50 (74%)	-0.10	0 100 100	70, 79, 93, 95	0
18	BX	37/50 (74%)	-0.25	0 100 100	75, 82, 91, 94	0
19	AY	0/28	-	-	-	-
19	BY	0/28	-	-	-	-
20	AZ	62/62 (100%)	-0.17	0 100 100	76, 85, 103, 110	0
20	BZ	62/62 (100%)	0.25	0 100 100	86, 96, 105, 110	0
All	All	5214/5536 (94%)	-0.39	22 (0%) 88 85	23, 71, 94, 110	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
14	AT	30	THR	3.2
6	BF	17	THR	3.0
3	AC	32	GLY	2.7
1	BA	11	ALA	2.7
3	AC	31	SER	2.5
5	BE	84	LYS	2.4
5	AE	84	LYS	2.4
3	BC	31	SER	2.3
4	AD	133	ALA	2.3
3	BC	194	GLY	2.3
3	BC	38	GLY	2.2
13	BO	165	SER	2.2
13	BO	84	ASN	2.1
9	AJ	31	GLY	2.1
16	AV	158	GLY	2.1
13	AO	165	SER	2.1

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Mol	Chain	Res	Type	RSRZ
17	Ay	35	ILE	2.1
13	BO	232	GLY	2.1
16	BV	39	ASN	2.0
2	AB	232	GLY	2.0
7	BH	65	LEU	2.0
3	BC	32	GLY	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 oligosaccharides 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, 95^{th} 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
24	PL9	AJ	101	35/55	0.39	0.15	93,101,107,109	0
24	PL9	BJ	101	35/55	0.44	0.14	78,99,111,112	0
26	BCR	BJ	102	40/40	0.46	0.14	93,98,101,102	0
28	LHG	AC	521	37/49	0.50	0.13	78,99,109,109	0
28	LHG	BC	521	37/49	0.50	0.14	90,100,113,114	0
27	DGD	BD	410	63/66	0.53	0.11	84,100,105,105	0
25	OEC	BA	409	5/9	0.54	0.10	30,74,79,92	0
27	DGD	AD	410	63/66	0.55	0.12	91,97,107,108	0
22	CLA	BB	604	65/65	0.55	0.15	86,98,107,109	0
30	LMG	AI	101	43/55	0.56	0.13	83,92,97,98	0
32	LMT	BI	102	35/35	0.56	0.11	90,104,106,106	0
30	LMG	BI	101	43/55	0.59	0.11	84,90,99,100	0
30	LMG	AC	520	45/55	0.62	0.10	75,92,97,98	0
32	LMT	AB	627	35/35	0.64	0.12	73,103,106,107	0
32	LMT	AI	102	35/35	0.64	0.10	74,92,95,95	0
26	BCR	AJ	102	40/40	0.64	0.12	85,91,101,102	0
27	DGD	BB	602	52/66	0.65	0.12	71,85,104,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	LMT	AB	624	35/35	0.66	0.12	71,100,106,107	0
27	DGD	AB	626	52/66	0.68	0.11	79,94,105,107	0
29	SQD	AD	409	43/54	0.69	0.11	68,92,108,111	0
32	LMT	BB	625	35/35	0.69	0.12	66,103,111,111	0
22	CLA	AB	601	65/65	0.69	0.12	88,97,102,105	0
32	LMT	BB	603	35/35	0.70	0.10	68,86,95,96	0
30	LMG	BC	520	45/55	0.71	0.09	86,93,101,102	0
32	LMT	BD	411	31/35	0.71	0.12	67,91,99,100	0
32	LMT	AD	411	31/35	0.71	0.13	52,96,104,104	0
29	SQD	BD	409	43/54	0.72	0.10	73,88,110,111	0
29	SQD	BF	101	45/54	0.73	0.10	95,98,103,104	0
32	LMT	AT	101	35/35	0.73	0.12	72,91,97,98	0
29	SQD	AF	101	45/54	0.73	0.10	82,97,102,103	0
30	LMG	AM	101	42/55	0.74	0.10	68,86,93,95	0
27	DGD	AA	410	56/66	0.74	0.12	78,86,91,92	0
30	LMG	AA	416	42/55	0.74	0.11	67,92,96,99	0
27	DGD	BA	411	56/66	0.75	0.10	76,85,103,104	0
30	LMG	BE	102	44/55	0.77	0.11	75,92,98,99	0
29	SQD	BA	401	54/54	0.77	0.09	82,91,107,108	0
30	LMG	BM	102	42/55	0.77	0.09	72,90,95,98	0
30	LMG	AC	519	48/55	0.77	0.09	75,84,89,90	0
30	LMG	BC	519	48/55	0.78	0.08	83,90,94,95	0
26	BCR	BZ	101	40/40	0.78	0.10	81,90,93,94	0
32	LMT	AB	625	35/35	0.79	0.09	82,98,100,101	0
30	LMG	AB	623	42/55	0.79	0.10	70,89,92,93	0
30	LMG	AE	102	44/55	0.79	0.10	81,91,96,96	0
32	LMT	BT	101	35/35	0.79	0.11	77,91,94,95	0
27	DGD	BC	517	62/66	0.80	0.12	78,82,100,101	0
30	LMG	BB	623	49/55	0.80	0.10	70,78,88,91	0
29	SQD	BA	413	51/54	0.80	0.09	73,90,103,104	0
29	SQD	BL	101	47/54	0.81	0.09	75,91,115,116	0
29	SQD	AA	415	54/54	0.81	0.09	71,87,105,105	0
32	LMT	BM	101	35/35	0.81	0.09	70,88,97,101	0
32	LMT	BB	626	35/35	0.81	0.09	76,93,101,102	0
29	SQD	AA	412	51/54	0.82	0.10	73,83,98,99	0
31	CL	AA	414	1/1	0.82	0.07	73,73,73,73	0
30	LMG	BD	407	46/55	0.82	0.10	70,80,92,94	0
26	BCR	BC	515	40/40	0.82	0.08	74,80,91,92	0
24	PL9	AA	407	45/55	0.82	0.09	83,87,94,95	0
26	BCR	AK	102	40/40	0.83	0.10	73,77,81,81	0
22	CLA	AC	513	65/65	0.83	0.10	92,98,104,106	0
22	CLA	BB	617	65/65	0.83	0.12	75,79,99,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
30	LMG	BD	408	48/55	0.83	0.09	68,75,85,87	0
22	CLA	BC	505	65/65	0.83	0.09	88,93,94,95	0
22	CLA	BC	508	65/65	0.83	0.09	92,97,101,106	0
22	CLA	BC	513	65/65	0.83	0.10	96,99,106,107	0
26	BCR	BX	101	40/40	0.84	0.10	76,79,89,90	0
22	CLA	BC	512	65/65	0.84	0.10	95,99,109,110	0
22	CLA	AC	512	65/65	0.84	0.10	91,95,106,106	0
30	LMG	AA	413	51/55	0.84	0.09	70,74,77,79	0
22	CLA	BD	404	65/65	0.84	0.10	89,92,101,102	0
27	DGD	AC	516	53/66	0.84	0.10	57,72,91,92	0
22	CLA	AB	614	65/65	0.84	0.11	78,85,98,99	0
22	CLA	AC	506	65/65	0.84	0.09	83,87,101,102	0
24	PL9	BA	408	45/55	0.84	0.07	82,88,90,92	0
26	BCR	BK	102	40/40	0.84	0.08	76,81,85,85	0
29	SQD	BB	601	47/54	0.84	0.08	74,87,109,111	0
26	BCR	AZ	101	40/40	0.85	0.08	75,82,90,91	0
27	DGD	BC	518	66/66	0.85	0.09	71,78,89,90	0
30	LMG	AD	408	48/55	0.85	0.09	63,68,74,80	0
26	BCR	AH	101	40/40	0.85	0.10	76,88,95,95	0
22	CLA	BB	619	65/65	0.85	0.09	75,81,93,95	0
22	CLA	BC	511	65/65	0.85	0.09	91,99,104,105	0
27	DGD	BC	516	53/66	0.85	0.10	69,77,96,97	0
28	LHG	AA	411	39/49	0.86	0.09	63,68,76,78	0
30	LMG	BA	414	51/55	0.86	0.08	62,71,78,80	0
22	CLA	BC	506	65/65	0.86	0.09	81,85,97,99	0
27	DGD	AC	517	62/66	0.86	0.11	70,78,91,92	0
30	LMG	AB	621	49/55	0.86	0.08	62,75,80,83	0
26	BCR	BD	406	40/40	0.86	0.08	66,78,92,92	0
25	OEC	AA	408	5/9	0.87	0.07	56,62,67,75	0
22	CLA	AB	616	65/65	0.87	0.09	73,85,105,106	0
30	LMG	AD	407	46/55	0.87	0.08	63,71,90,92	0
27	DGD	BH	101	58/66	0.87	0.09	66,73,80,81	0
22	CLA	AC	511	65/65	0.87	0.09	77,85,89,90	0
22	CLA	BB	618	65/65	0.88	0.10	69,84,87,88	0
22	CLA	AC	507	65/65	0.88	0.09	83,90,95,97	0
22	CLA	AB	609	65/65	0.88	0.08	76,87,91,92	0
22	CLA	AB	615	65/65	0.88	0.09	83,93,97,99	0
22	CLA	BC	507	65/65	0.88	0.09	84,92,96,97	0
32	LMT	AM	102	35/35	0.88	0.07	67,89,93,96	0
27	DGD	AC	518	66/66	0.88	0.09	62,68,84,86	0
35	CA	BO	301	1/1	0.88	0.07	100,100,100,100	0
28	LHG	BA	412	39/49	0.89	0.07	72,77,80,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
26	BCR	AB	620	40/40	0.89	0.08	75,77,83,84	0
26	BCR	AD	406	40/40	0.89	0.07	64,72,85,85	0
22	CLA	AB	604	65/65	0.89	0.09	67,73,91,91	0
22	CLA	AC	504	65/65	0.89	0.10	78,86,107,107	0
22	CLA	BC	503	65/65	0.89	0.10	82,97,100,101	0
27	DGD	AH	102	58/66	0.89	0.09	57,72,85,86	0
22	CLA	AB	606	65/65	0.89	0.09	73,87,96,96	0
26	BCR	BB	620	40/40	0.89	0.08	66,69,72,73	0
22	CLA	AB	608	65/65	0.89	0.08	72,79,87,91	0
22	CLA	BB	609	65/65	0.89	0.10	72,80,96,96	0
22	CLA	BB	612	65/65	0.89	0.08	82,89,92,95	0
22	CLA	BC	510	65/65	0.89	0.11	79,83,92,92	0
22	CLA	AC	508	65/65	0.89	0.09	80,86,99,101	0
26	BCR	AB	618	40/40	0.89	0.07	75,78,82,83	0
35	CA	BK	101	1/1	0.89	0.06	90,90,90,90	0
26	BCR	AB	619	40/40	0.89	0.08	62,70,82,83	0
30	LMG	AB	622	49/55	0.90	0.08	64,73,80,83	0
22	CLA	BC	501	65/65	0.90	0.07	76,80,87,88	0
22	CLA	AB	612	65/65	0.90	0.09	63,75,81,83	0
26	BCR	AC	515	40/40	0.90	0.07	69,75,80,81	0
22	CLA	BC	504	65/65	0.90	0.09	87,92,102,102	0
23	PHO	BD	403	64/64	0.90	0.10	77,88,92,93	0
22	CLA	BB	610	65/65	0.90	0.08	60,70,77,81	0
22	CLA	BB	611	65/65	0.90	0.08	67,74,81,85	0
26	BCR	AT	102	40/40	0.90	0.09	72,79,91,91	0
22	CLA	AD	404	65/65	0.90	0.08	80,83,102,103	0
22	CLA	BA	407	65/65	0.90	0.09	72,76,103,104	0
30	LMG	BB	624	49/55	0.90	0.08	68,72,78,79	0
26	BCR	BB	622	40/40	0.90	0.07	67,71,79,80	0
22	CLA	BC	509	65/65	0.90	0.09	73,83,93,94	0
22	CLA	AA	404	65/65	0.90	0.09	63,72,97,99	0
26	BCR	AA	409	40/40	0.90	0.09	59,67,70,71	0
26	BCR	AB	617	40/40	0.90	0.07	56,67,75,76	0
22	CLA	BB	606	65/65	0.90	0.08	58,61,74,76	0
22	CLA	BB	613	65/65	0.91	0.09	69,77,82,84	0
22	CLA	AB	613	65/65	0.91	0.08	65,69,84,87	0
22	CLA	AB	610	65/65	0.91	0.08	60,67,79,80	0
31	CL	BA	415	1/1	0.91	0.06	81,81,81,81	0
22	CLA	BA	405	65/65	0.91	0.08	72,76,104,105	0
23	PHO	AD	403	64/64	0.91	0.08	39,56,70,72	0
23	PHO	BA	406	64/64	0.91	0.07	54,61,70,74	0
22	CLA	AC	505	65/65	0.91	0.07	69,73,77,79	0

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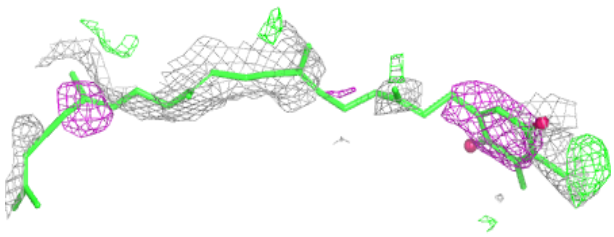
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
34	HEM	BE	101	43/43	0.91	0.12	93,95,104,107	0
22	CLA	BC	502	65/65	0.91	0.08	81,85,101,103	0
22	CLA	AB	603	65/65	0.91	0.08	54,60,72,74	0
22	CLA	AC	501	65/65	0.92	0.08	78,83,85,86	0
22	CLA	BB	605	65/65	0.92	0.09	77,82,86,89	0
22	CLA	AB	611	65/65	0.92	0.07	62,68,71,73	0
22	CLA	BB	616	65/65	0.92	0.07	49,54,79,82	0
22	CLA	AB	607	65/65	0.92	0.07	50,55,74,74	0
22	CLA	AA	406	65/65	0.92	0.08	54,60,89,90	0
26	BCR	BA	410	40/40	0.92	0.07	61,74,82,83	0
22	CLA	BA	403	65/65	0.93	0.08	57,64,71,75	0
22	CLA	BB	614	65/65	0.93	0.08	59,68,75,77	0
22	CLA	BB	615	65/65	0.93	0.08	60,72,77,81	0
22	CLA	AB	602	65/65	0.93	0.07	81,85,88,90	0
22	CLA	AB	605	65/65	0.93	0.08	68,76,84,85	0
22	CLA	AD	402	65/65	0.93	0.08	47,58,69,71	0
26	BCR	BB	621	40/40	0.93	0.07	57,69,82,83	0
26	BCR	AC	514	40/40	0.93	0.07	56,66,73,74	0
26	BCR	BC	514	40/40	0.93	0.08	81,83,87,87	0
34	HEM	AE	101	43/43	0.93	0.11	85,92,103,106	0
24	PL9	BD	405	55/55	0.93	0.07	63,70,76,78	0
22	CLA	AC	503	65/65	0.93	0.10	78,86,92,95	0
23	PHO	AA	405	64/64	0.93	0.07	40,64,67,69	0
22	CLA	BB	607	65/65	0.94	0.06	53,64,86,87	0
22	CLA	BB	608	65/65	0.94	0.07	45,53,76,78	0
22	CLA	BD	402	65/65	0.94	0.07	50,57,79,83	0
22	CLA	BA	404	65/65	0.94	0.07	55,60,68,70	0
22	CLA	AA	402	65/65	0.94	0.07	51,58,66,69	0
22	CLA	AC	502	65/65	0.94	0.07	50,58,81,84	0
22	CLA	AC	509	65/65	0.94	0.08	59,74,86,89	0
22	CLA	AC	510	65/65	0.94	0.07	48,56,70,72	0
35	CA	AO	301	1/1	0.94	0.04	87,87,87,87	0
22	CLA	AA	403	65/65	0.94	0.07	41,48,56,60	0
24	PL9	AD	405	55/55	0.94	0.07	52,67,71,73	0
33	BCT	BD	401	4/4	0.96	0.05	84,86,87,88	0
34	HEM	AV	201	43/43	0.96	0.07	60,63,66,67	0
33	BCT	AD	401	4/4	0.97	0.04	90,91,91,92	0
34	HEM	BV	201	43/43	0.97	0.07	58,67,76,79	0
35	CA	AK	101	1/1	0.97	0.07	95,95,95,95	0
21	FE2	AA	401	1/1	0.98	0.05	69,69,69,69	0
21	FE2	BA	402	1/1	0.99	0.06	81,81,81,81	0

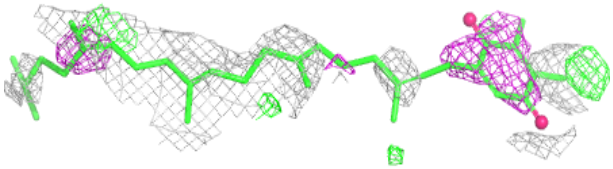
The following is a graphical depiction of the model fit to experimental electron density of all

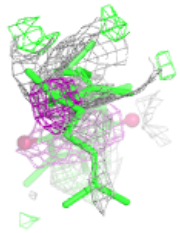
instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around PL9 AJ 101:

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

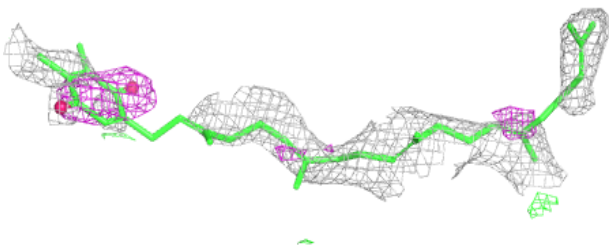


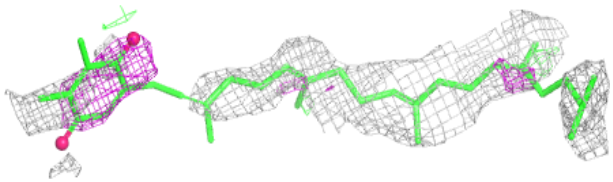


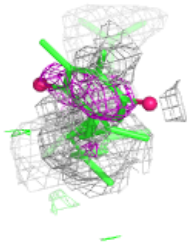


Electron density around PL9 BJ 101:

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

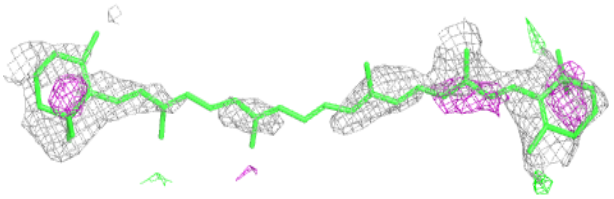


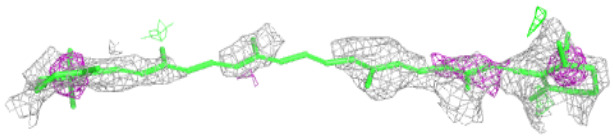


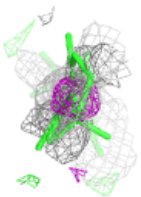


Electron density around BCR BJ 102:

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

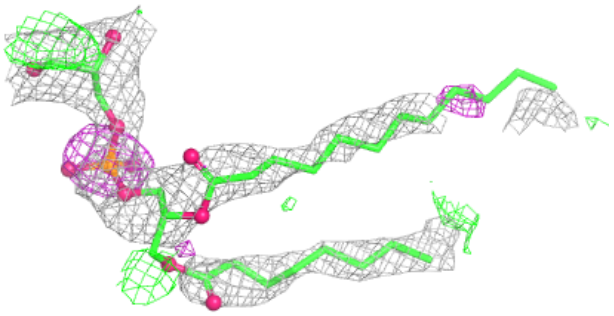


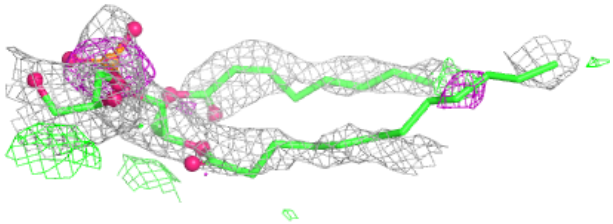


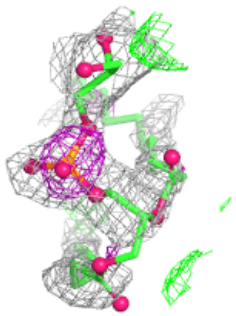


Electron density around LHG AC 521:

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

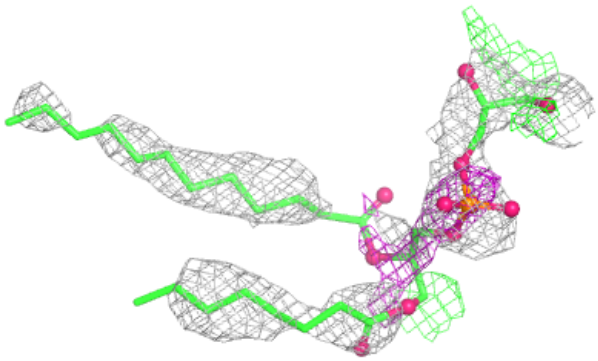


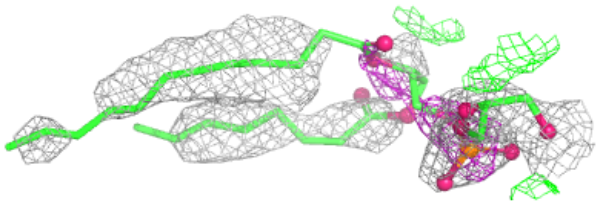


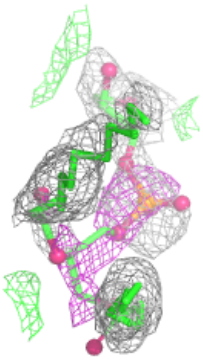


Electron density around LHG BC 521:

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

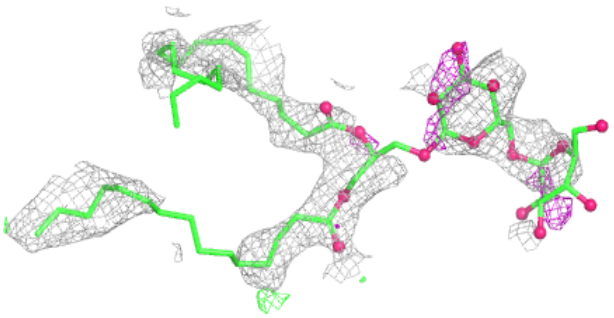


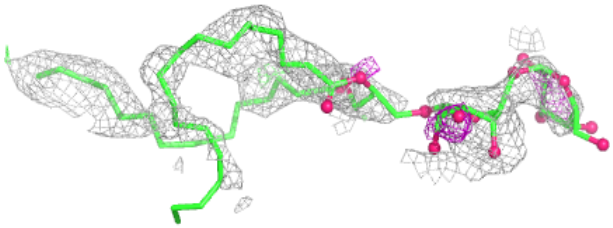




Electron density around DGD BD 410:

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

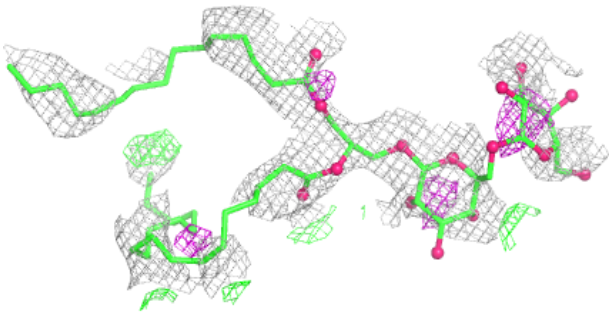


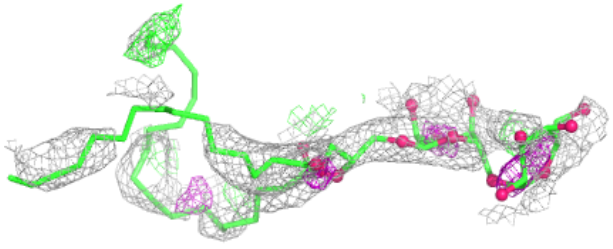




Electron density around DGD AD 410:

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

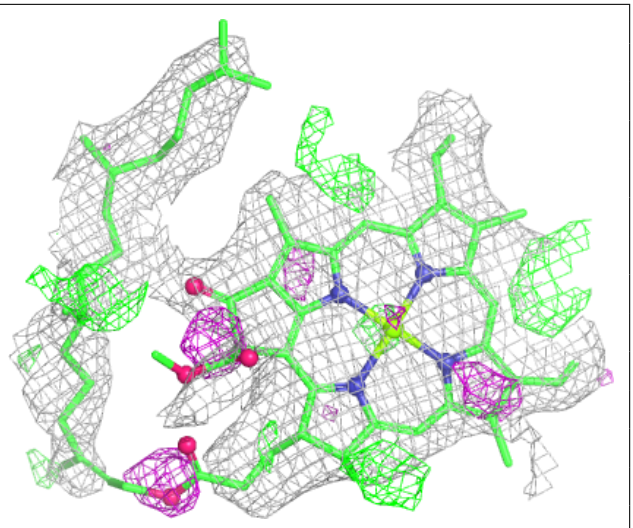


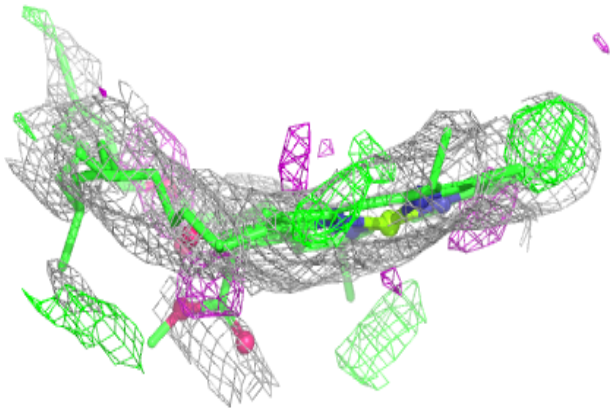


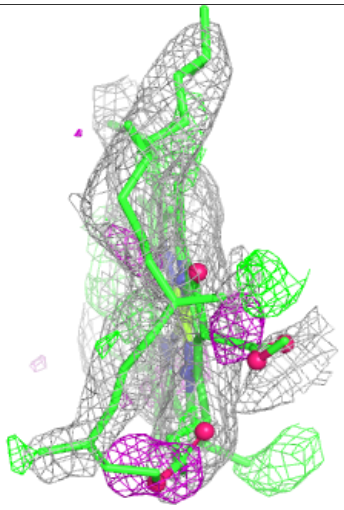


Electron density around CLA BB 604:

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

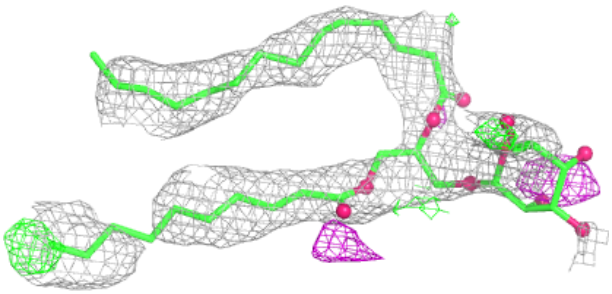


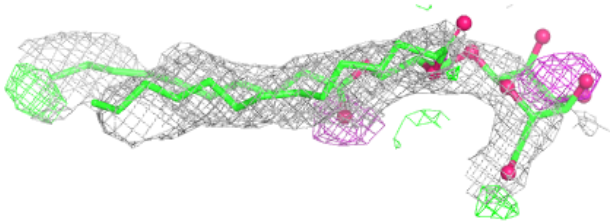


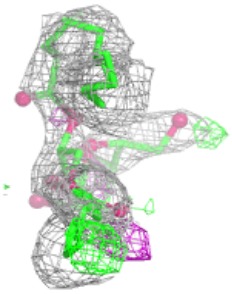


Electron density around LMG AI 101:

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

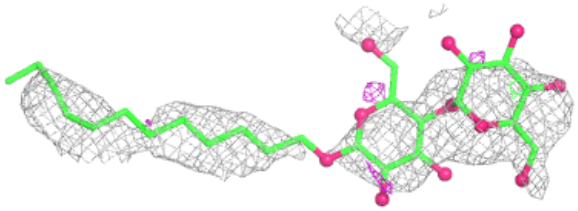


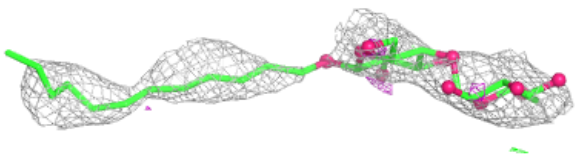


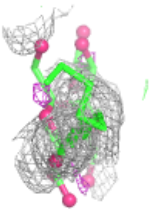


Electron density around LMT BI 102:

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

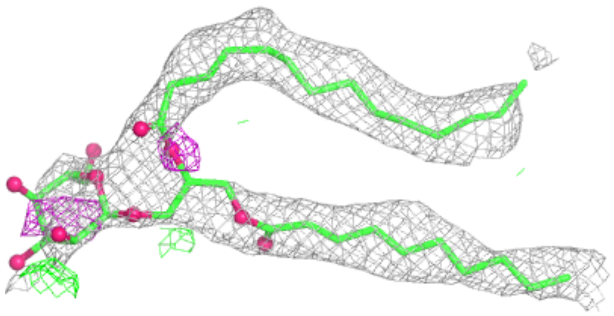


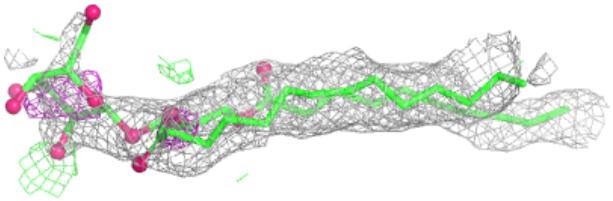


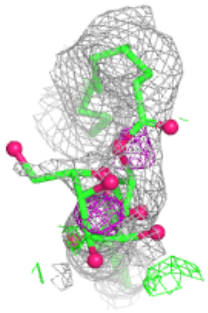


Electron density around LMG BI 101:

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

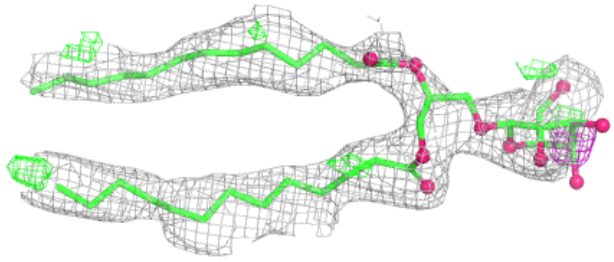


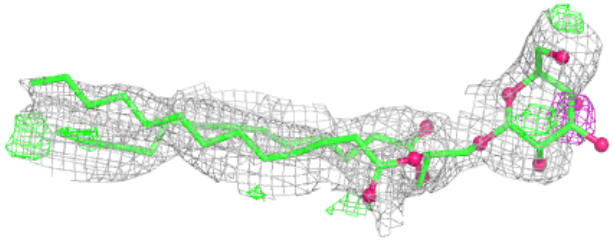


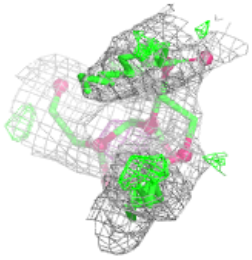


Electron density around LMG AC 520:

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

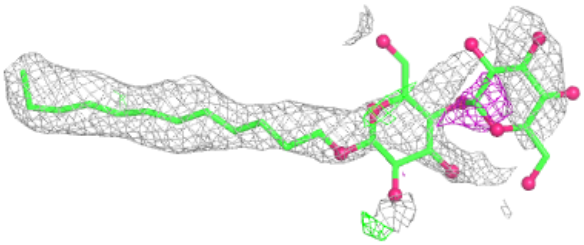


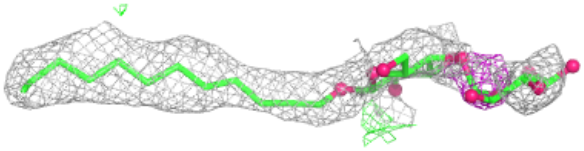


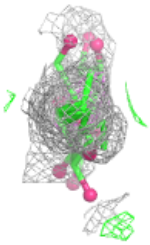


Electron density around LMT AB 627:

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

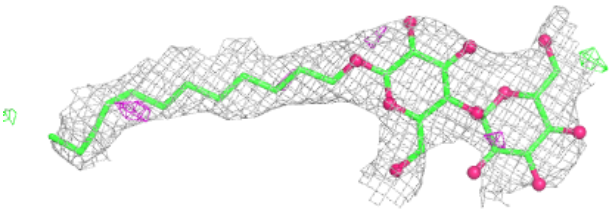


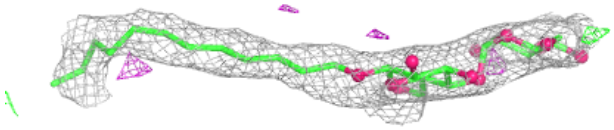


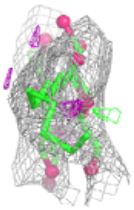


Electron density around LMT AI 102:

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

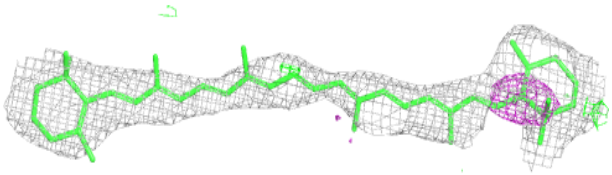




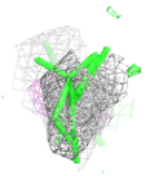


Electron density around BCR AJ 102:

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

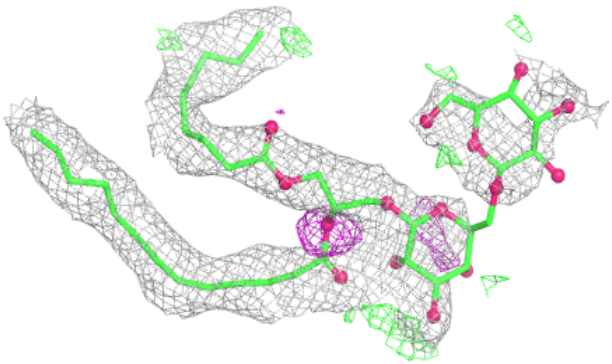


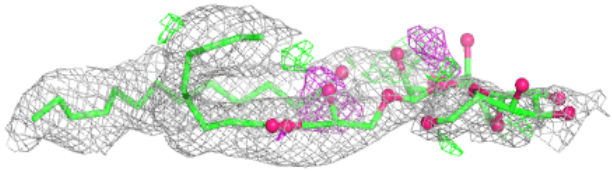


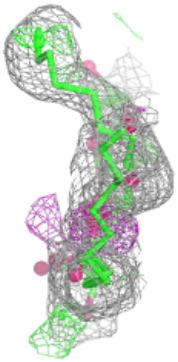


Electron density around DGD BB 602:

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

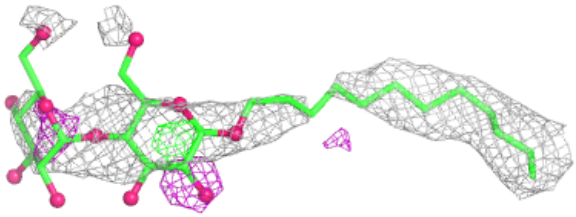


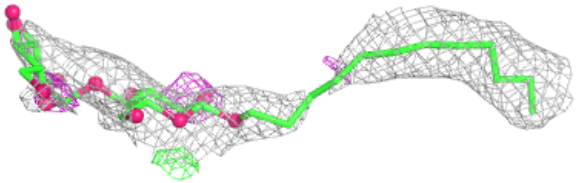


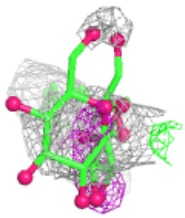


Electron density around LMT AB 624:

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

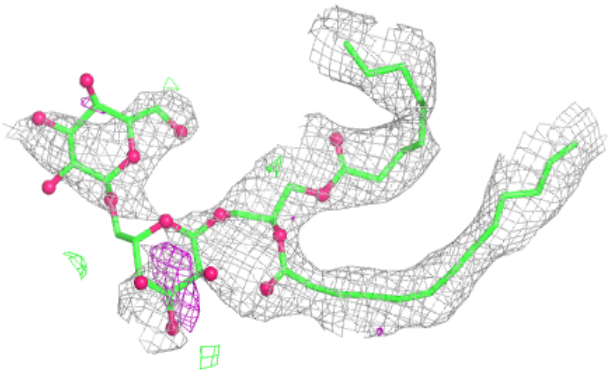


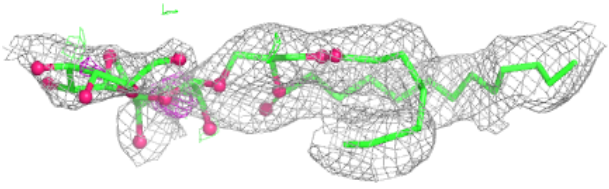


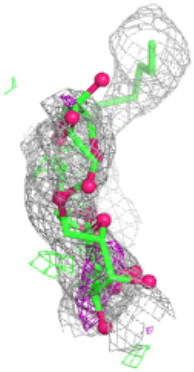


Electron density around DGD AB 626:

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

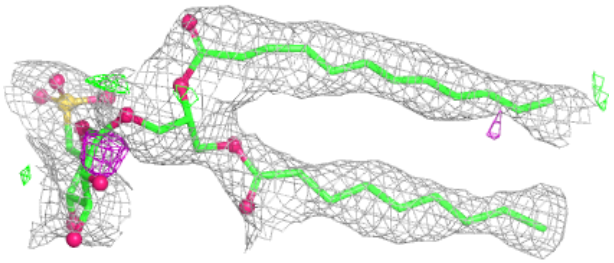


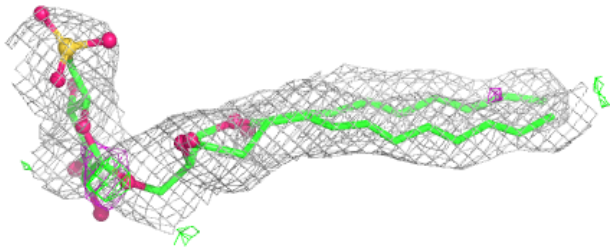


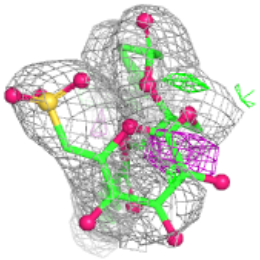


Electron density around SQD AD 409:

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

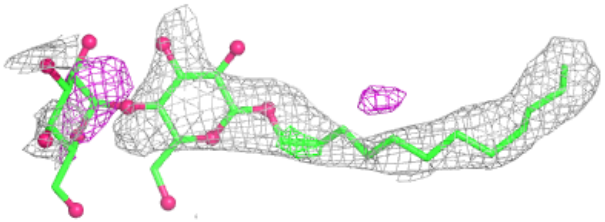


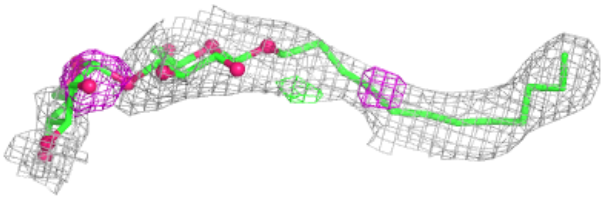


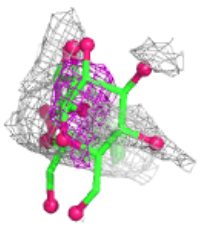


Electron density around LMT BB 625:

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

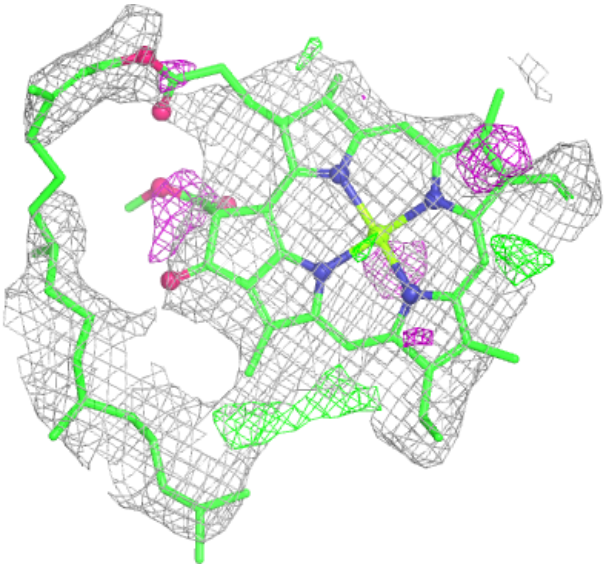


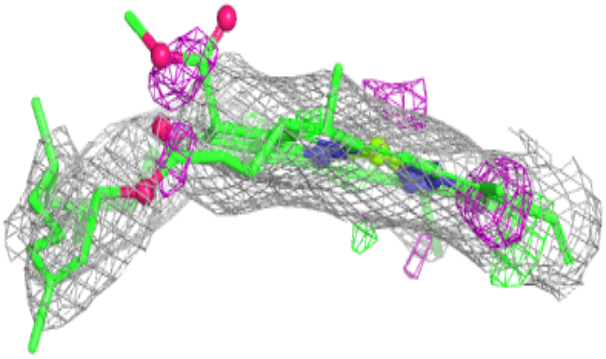


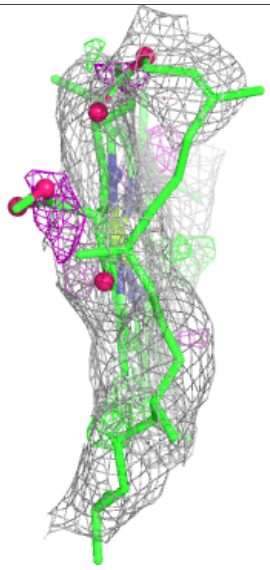


Electron density around CLA AB 601:

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

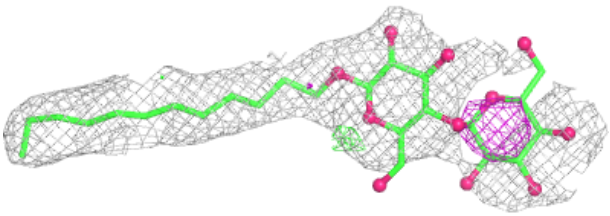


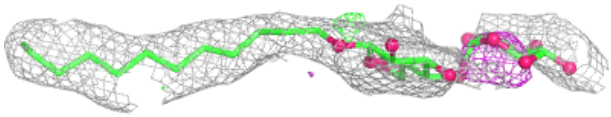


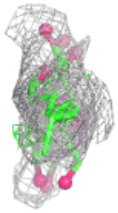


Electron density around LMT BB 603:

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

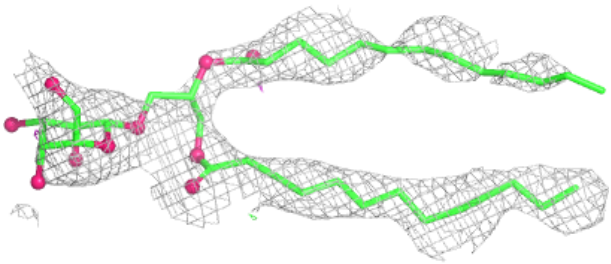


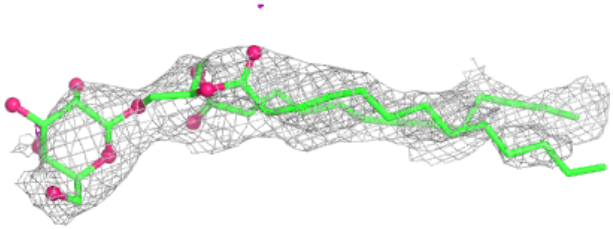


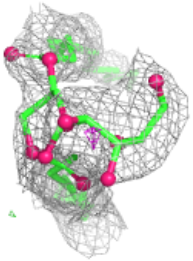


Electron density around LMG BC 520:

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

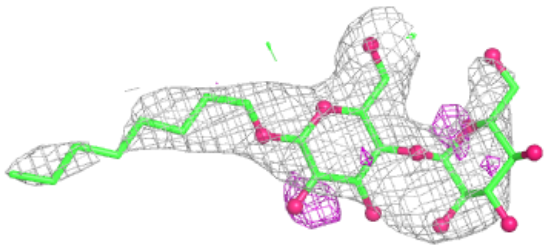


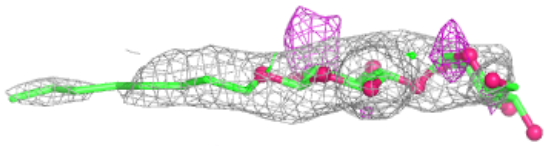


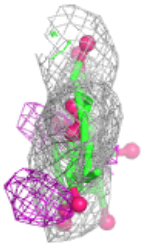


Electron density around LMT BD 411:

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

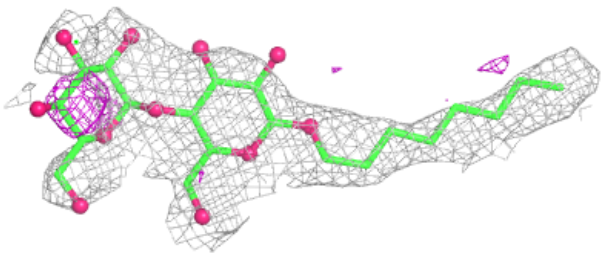


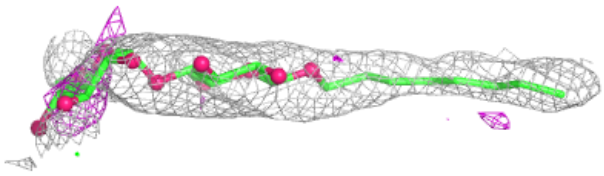


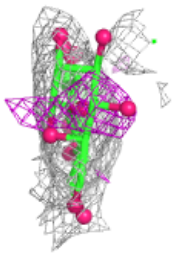


Electron density around LMT AD 411:

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

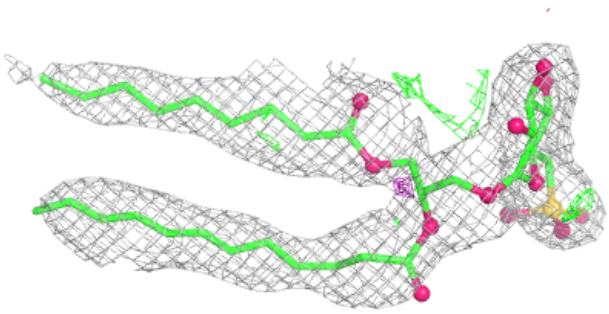


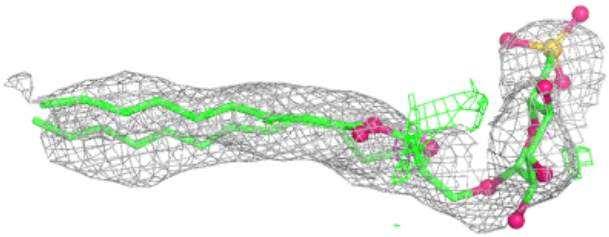


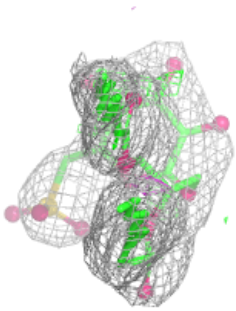


Electron density around SQD BD 409:

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

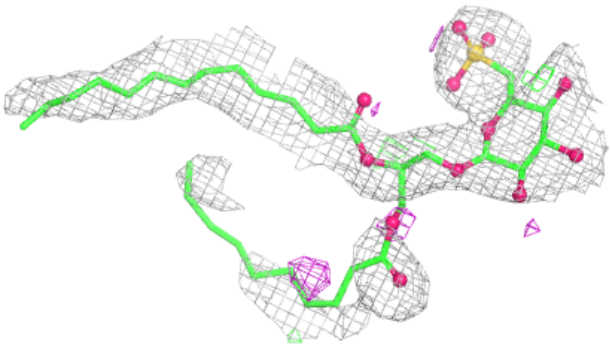


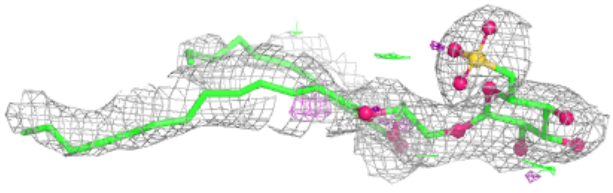


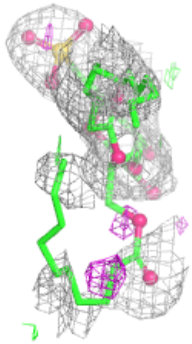


Electron density around SQD BF 101:

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

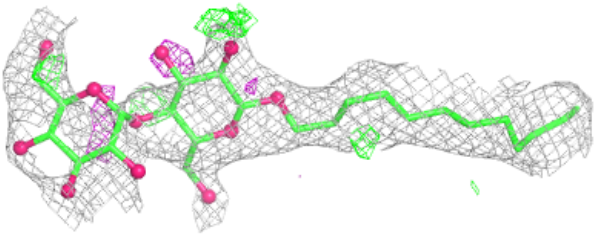


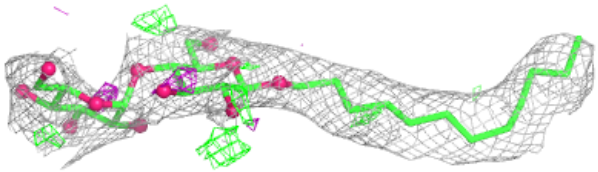


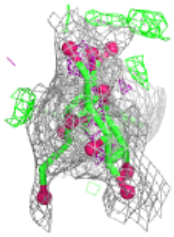


Electron density around LMT AT 101:

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

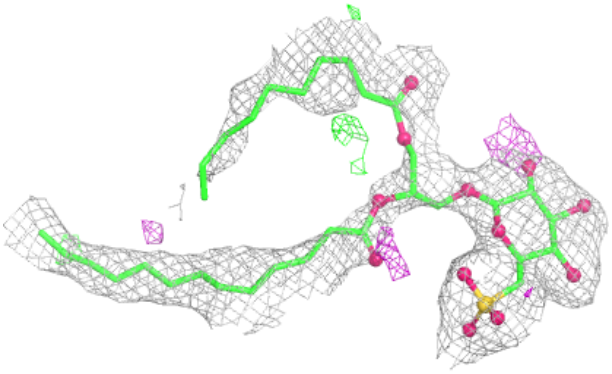


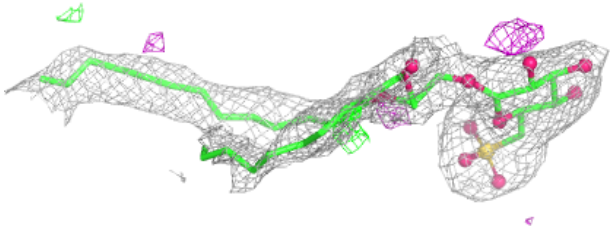


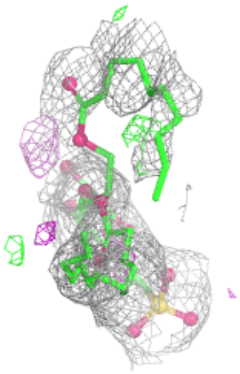


Electron density around SQD AF 101:

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

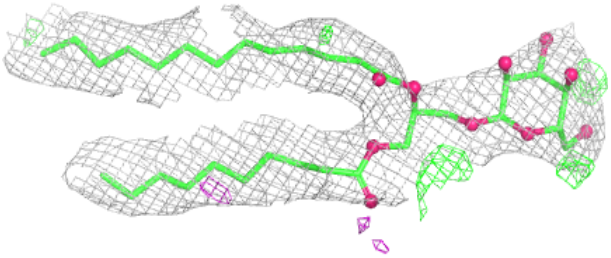


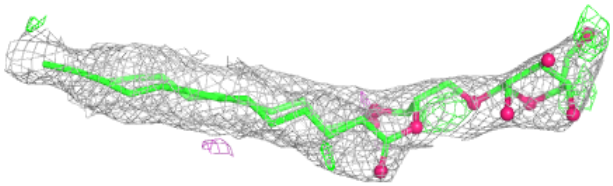


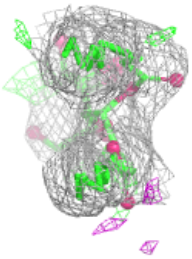


Electron density around LMG AM 101:

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

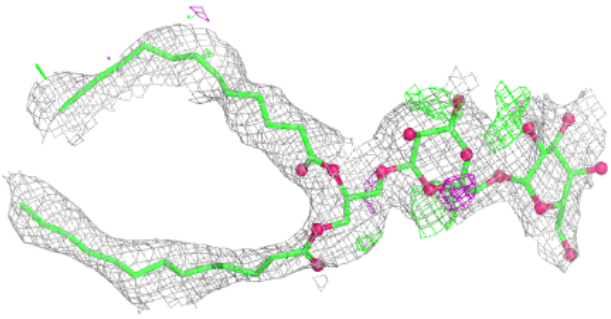


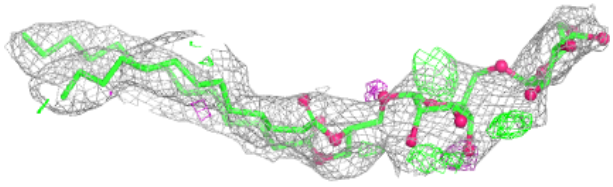


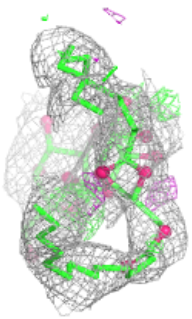


Electron density around DGD AA 410:

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

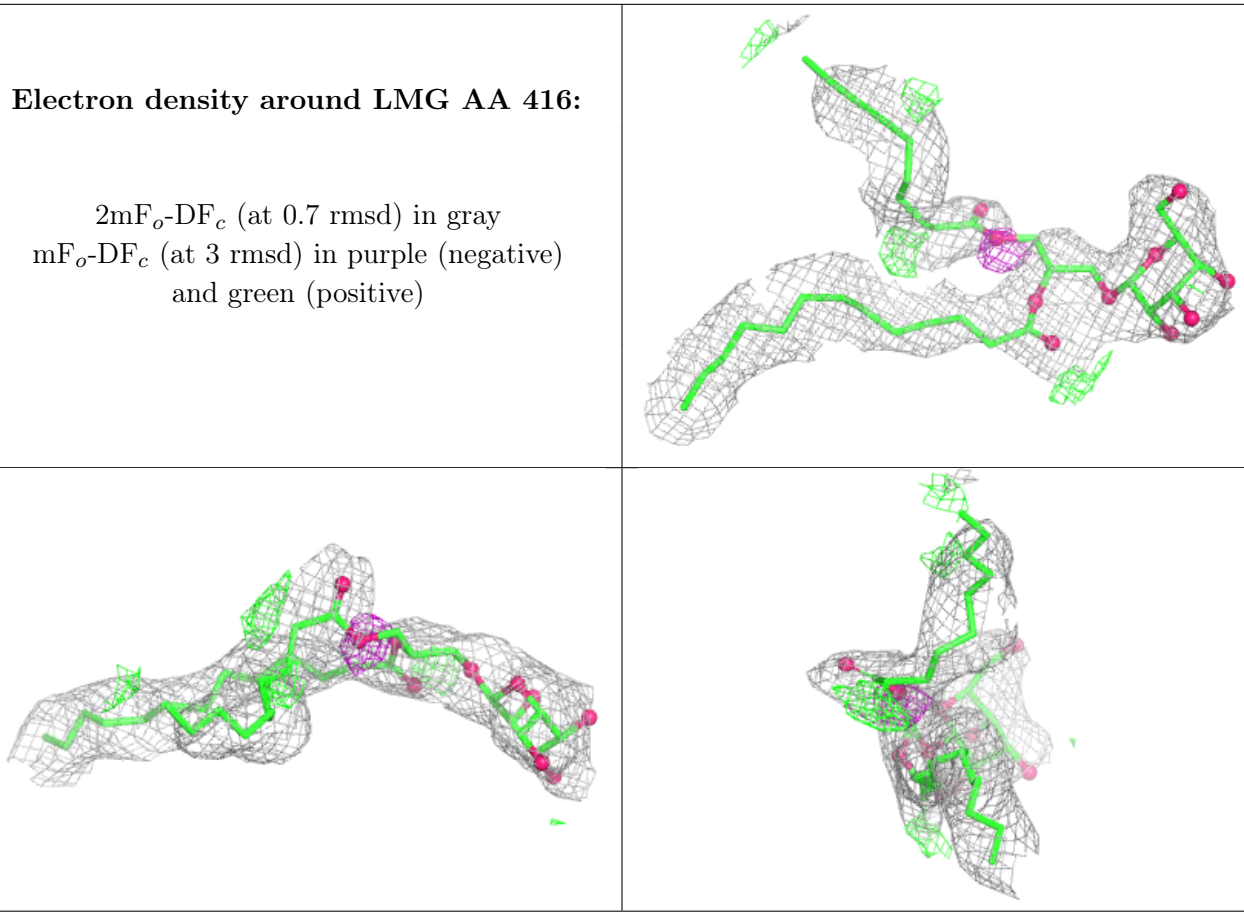






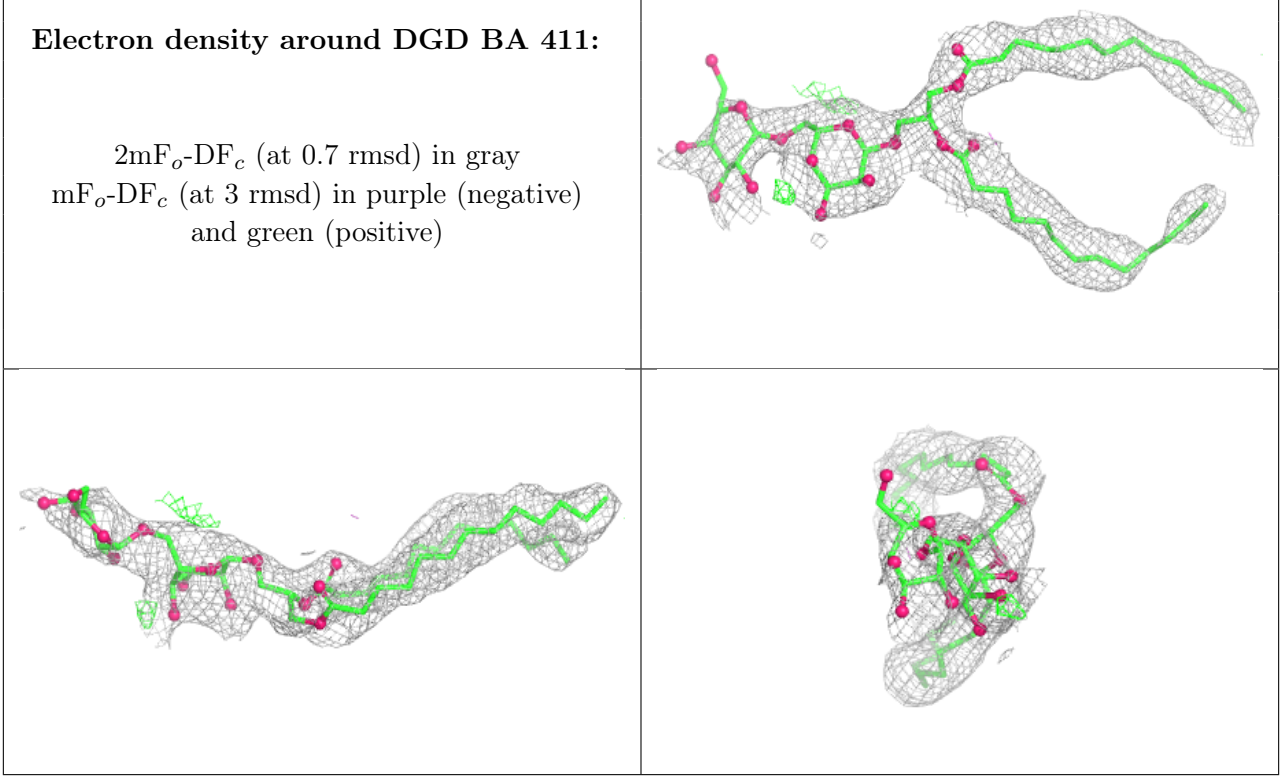
Electron density around LMG AA 416:

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



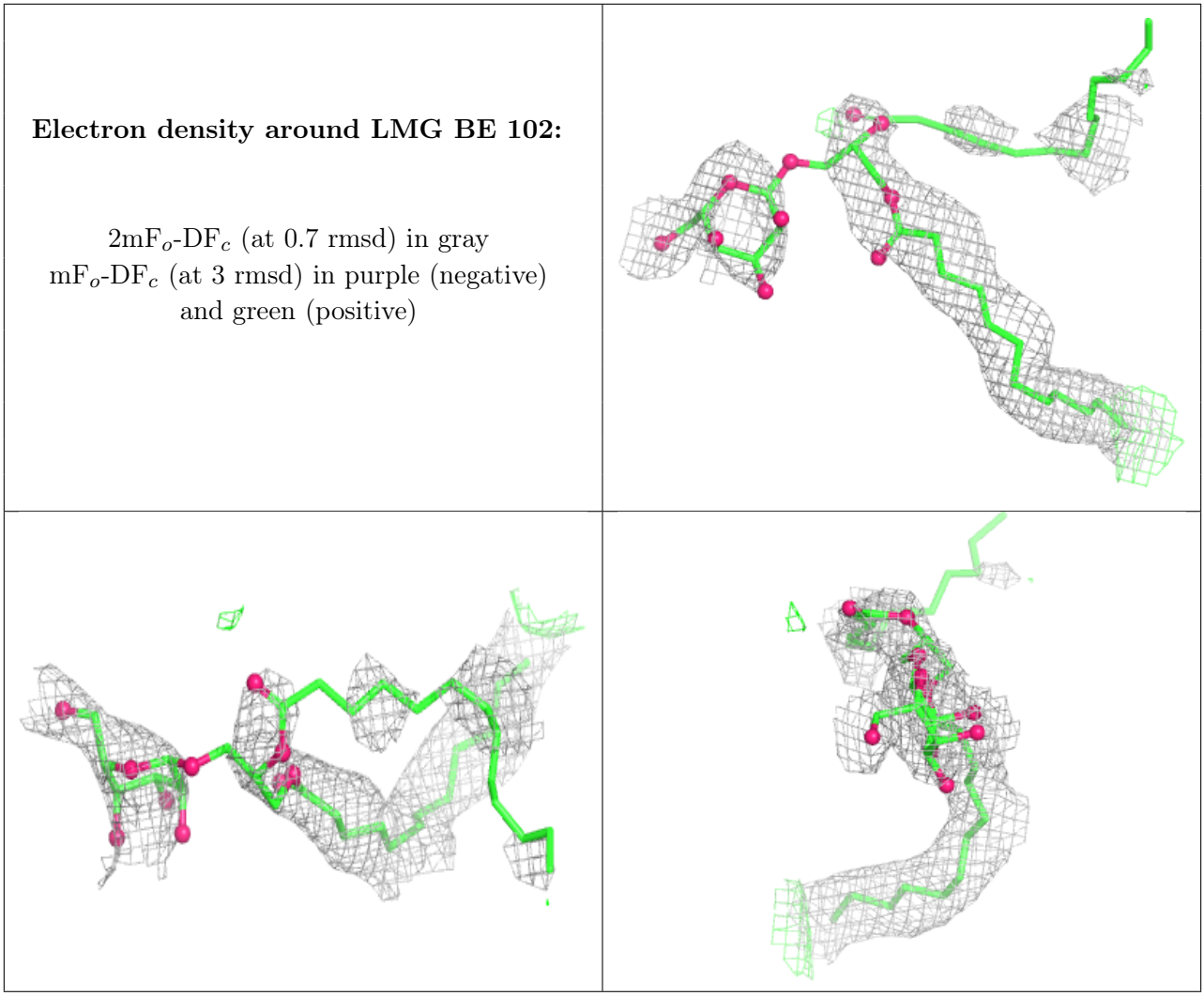
Electron density around DGD BA 411:

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



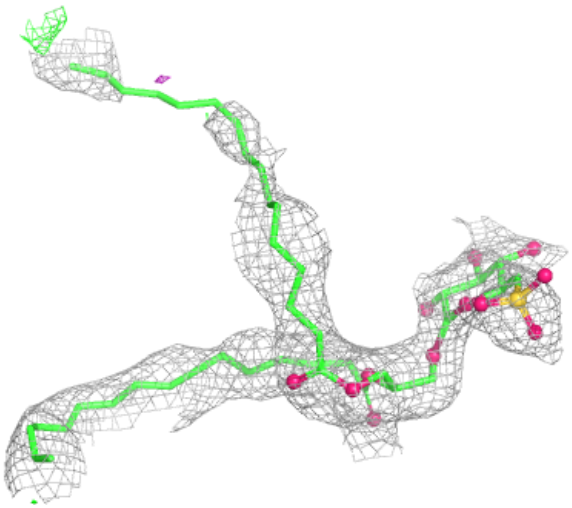
Electron density around LMG BE 102:

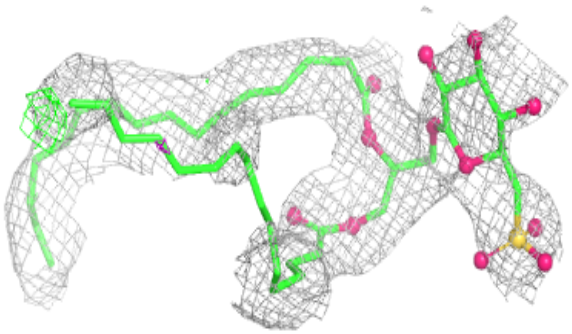
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around SQD BA 401:

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

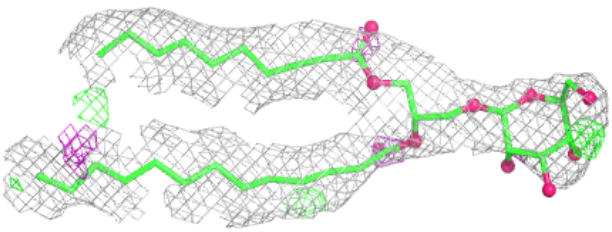


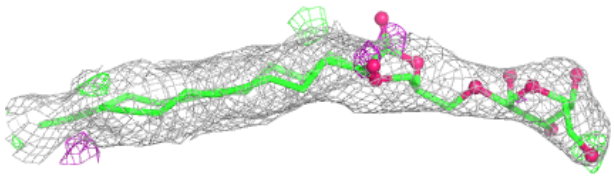


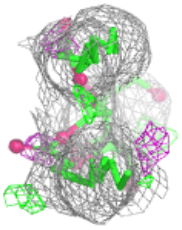


Electron density around LMG BM 102:

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

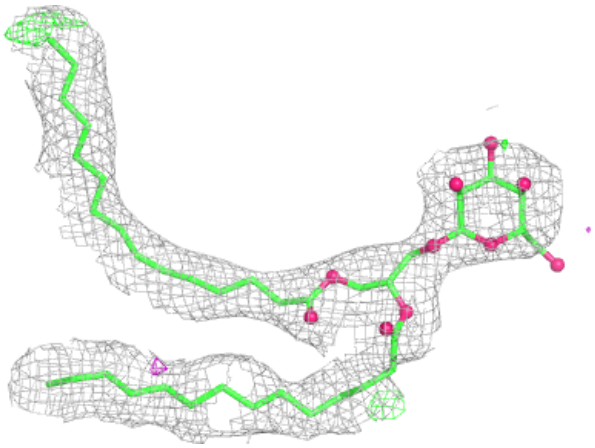


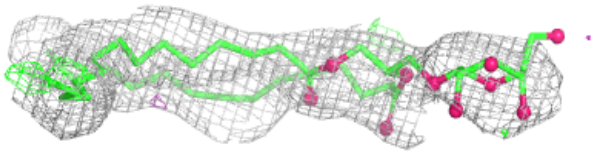


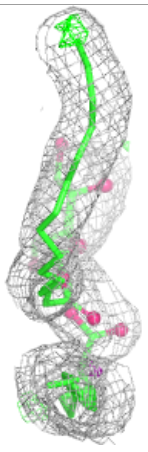


Electron density around LMG AC 519:

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

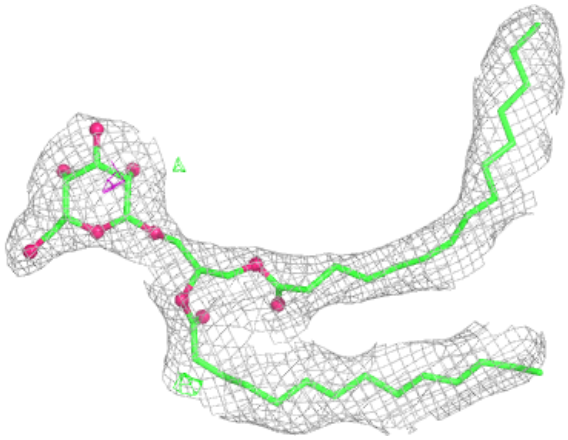


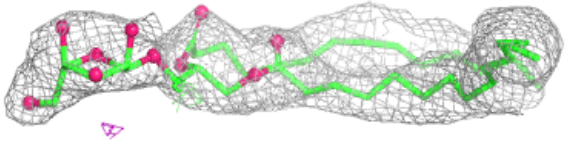


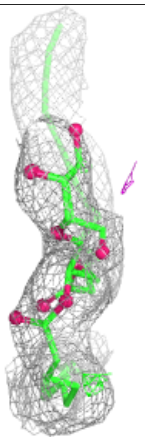


Electron density around LMG BC 519:

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

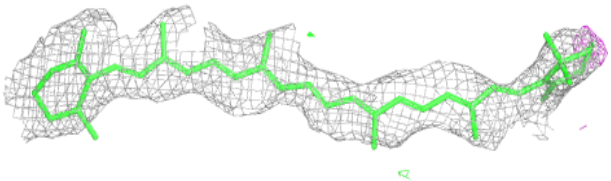


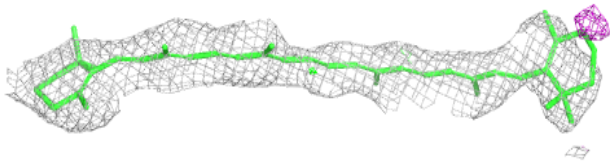


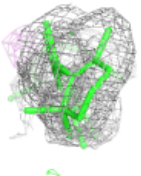


Electron density around BCR BZ 101:

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

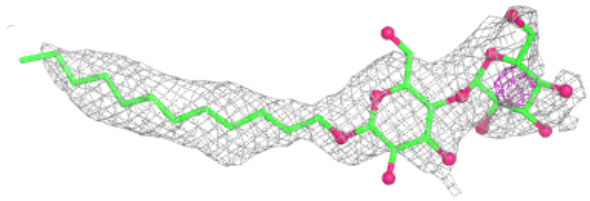


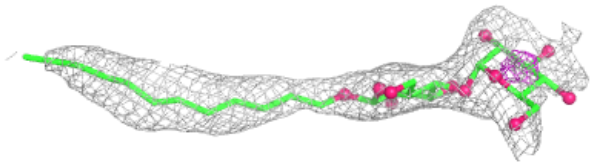


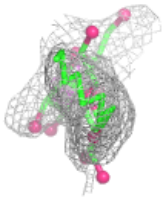


Electron density around LMT AB 625:

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

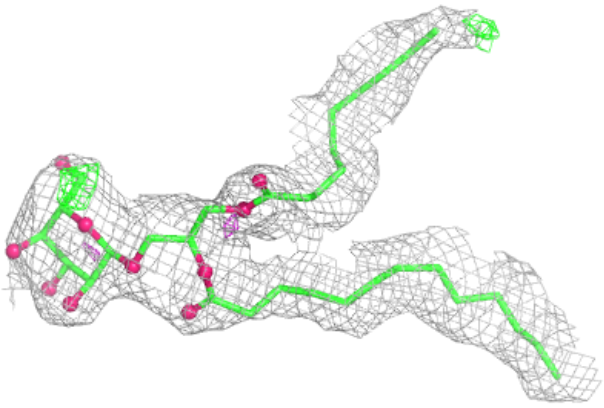


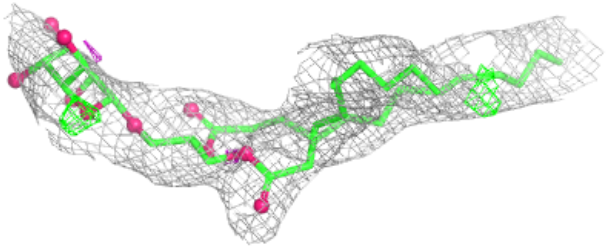


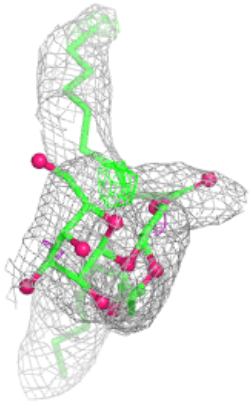


Electron density around LMG AB 623:

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

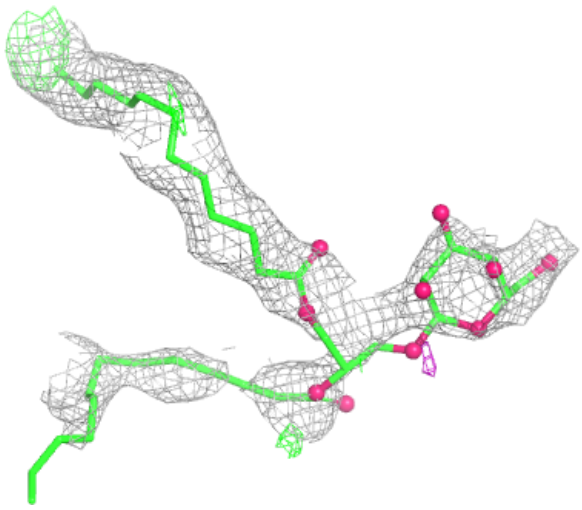


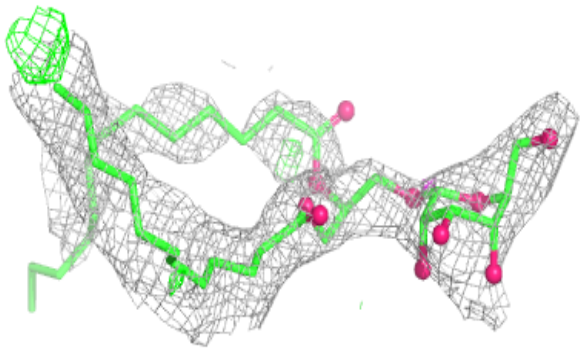


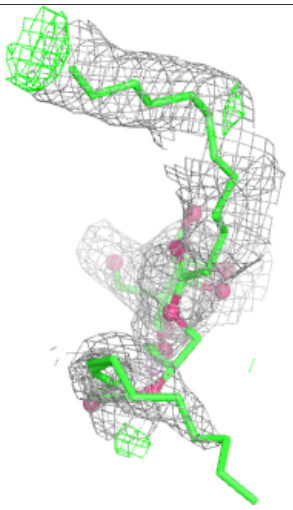


Electron density around LMG AE 102:

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

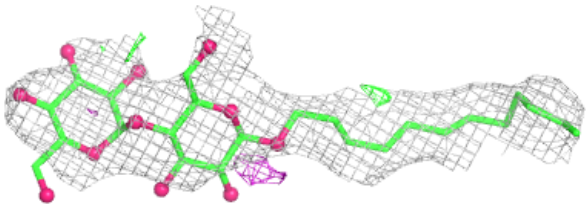


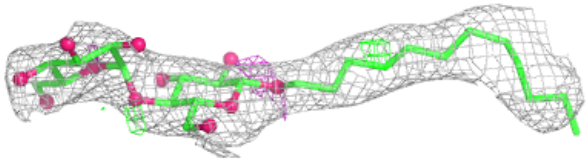


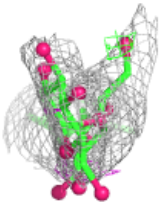


Electron density around LMT BT 101:

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

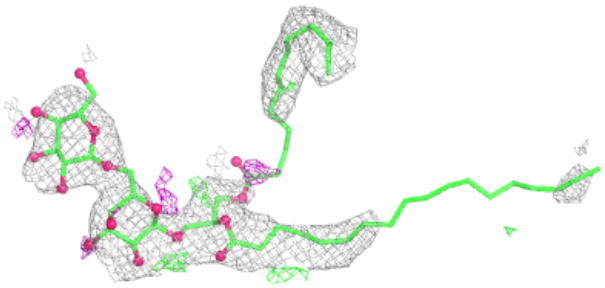


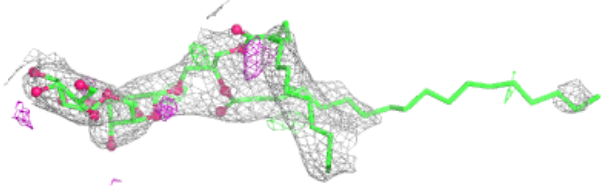


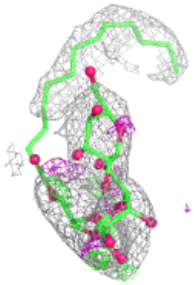


Electron density around DGD BC 517:

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

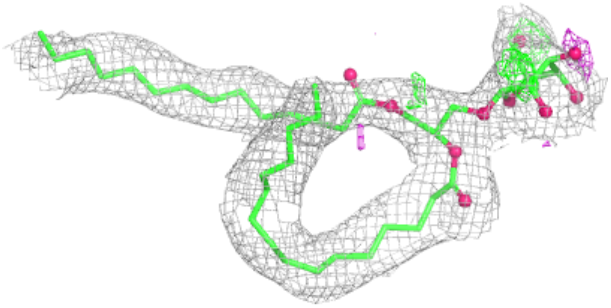


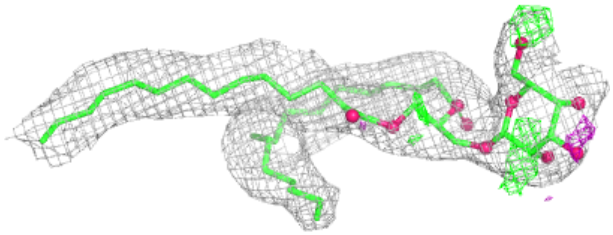


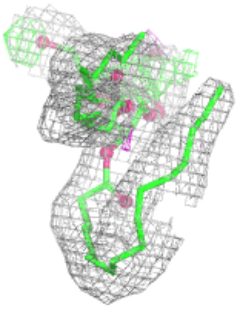


Electron density around LMG BB 623:

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

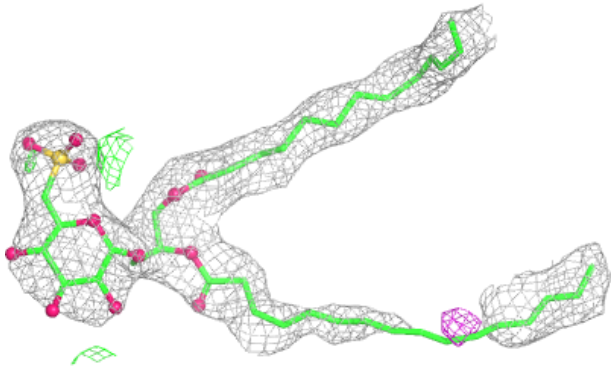


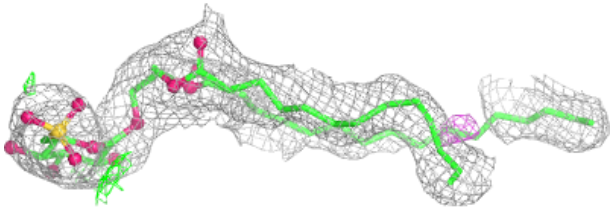


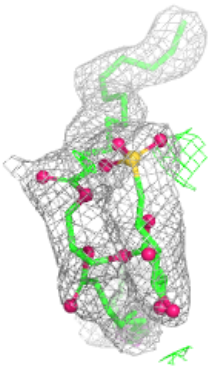


Electron density around SQD BA 413:

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

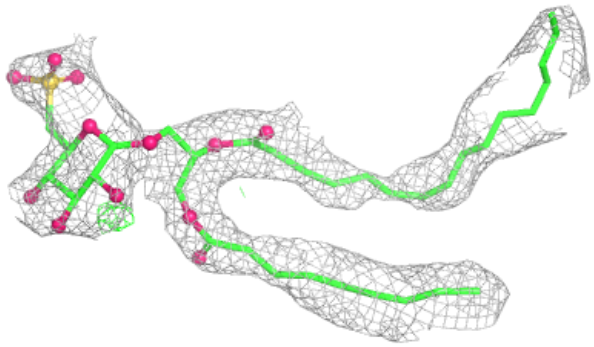


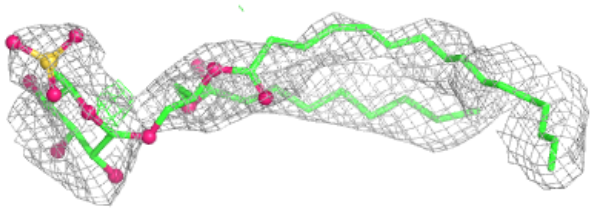


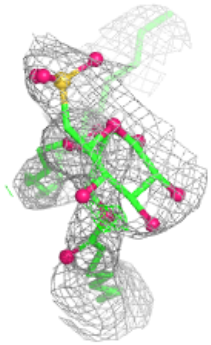


Electron density around SQD BL 101:

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

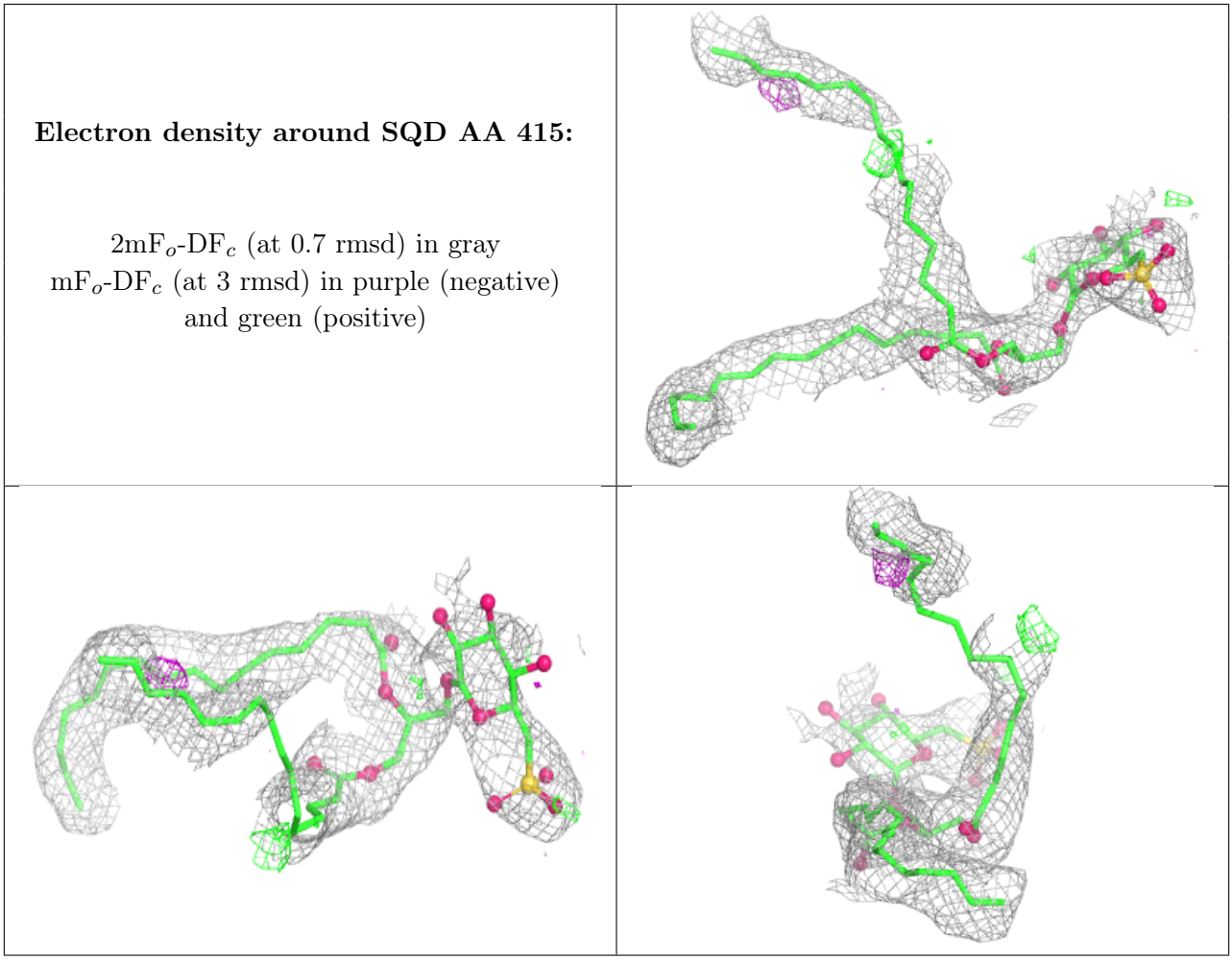






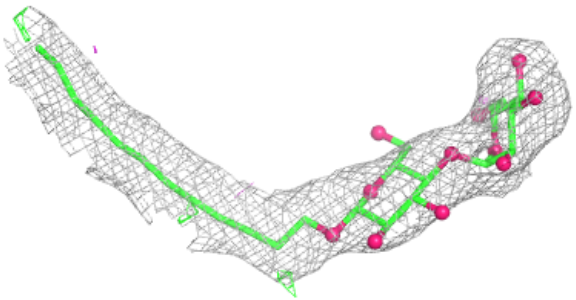
Electron density around SQD AA 415:

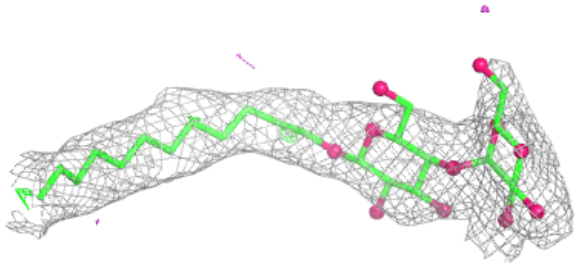
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

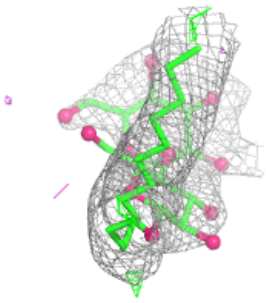


Electron density around LMT BM 101:

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

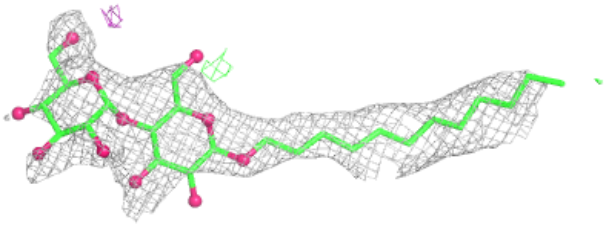


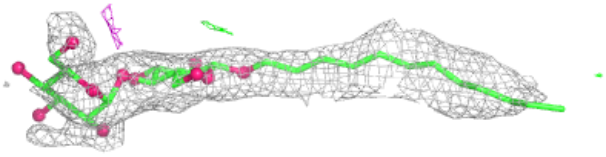


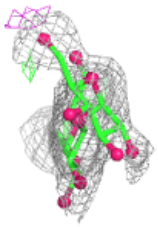


Electron density around LMT BB 626:

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

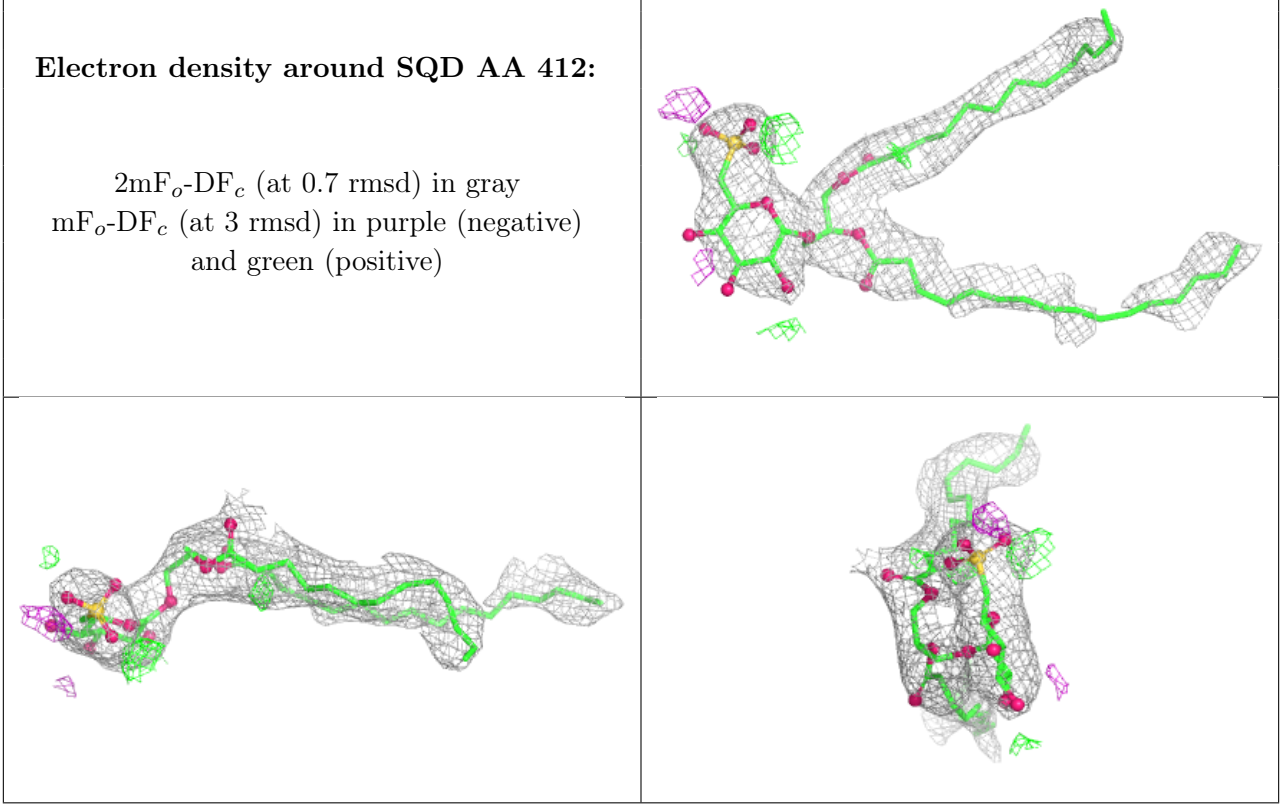






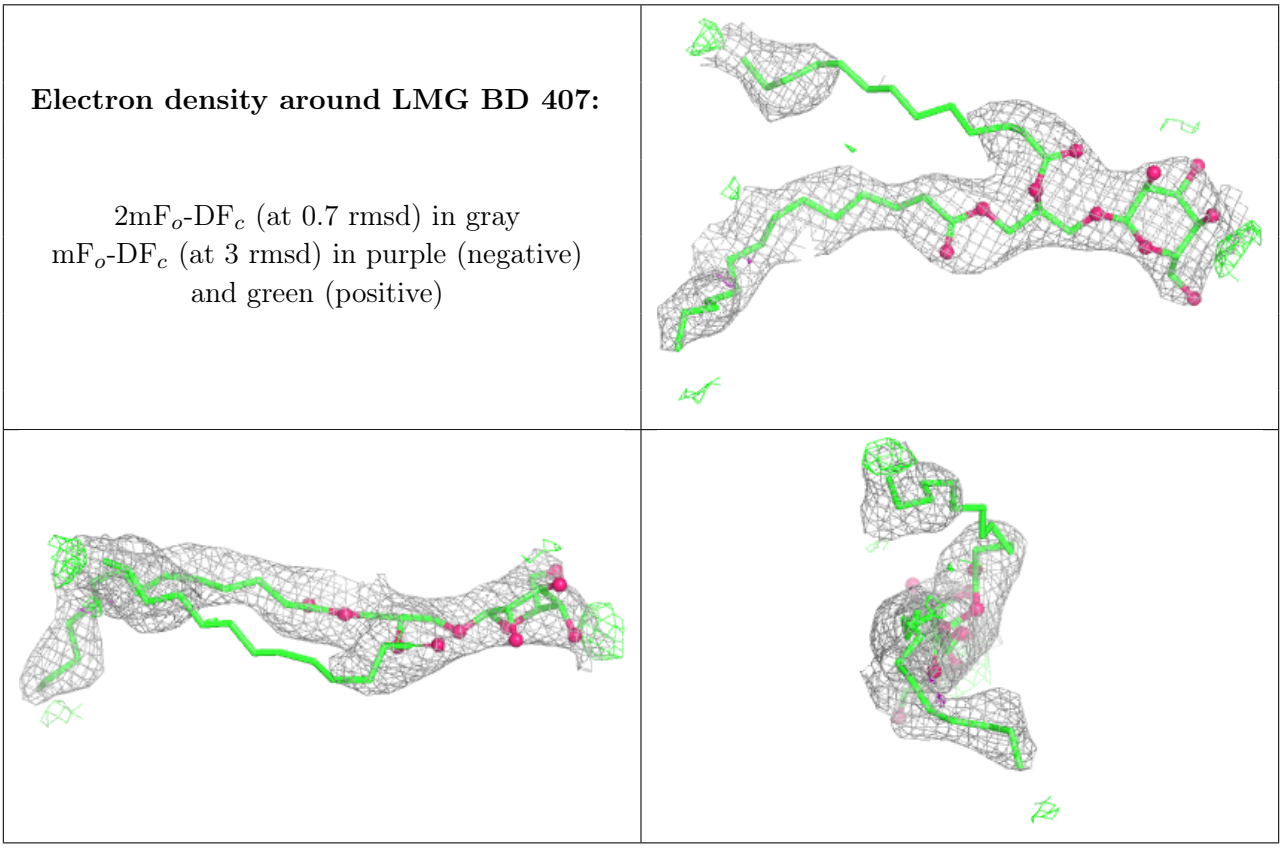
Electron density around SQD AA 412:

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



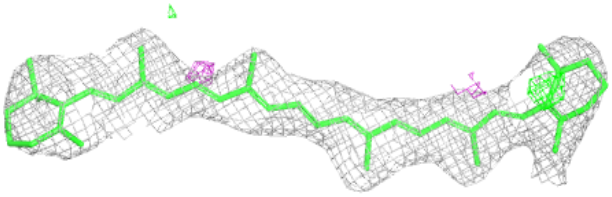
Electron density around LMG BD 407:

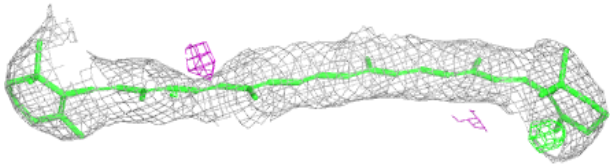
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

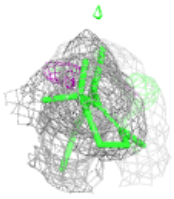


Electron density around BCR BC 515:

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

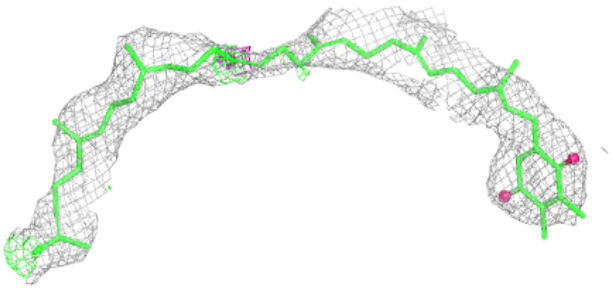


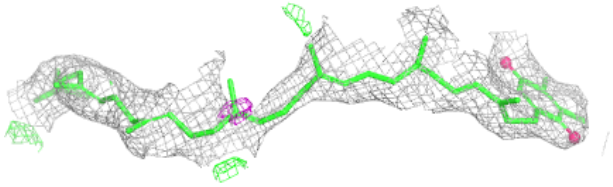


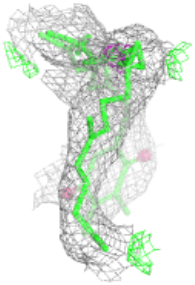


Electron density around PL9 AA 407:

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

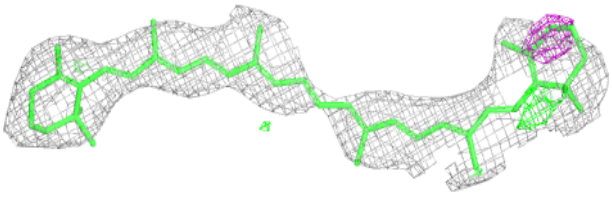


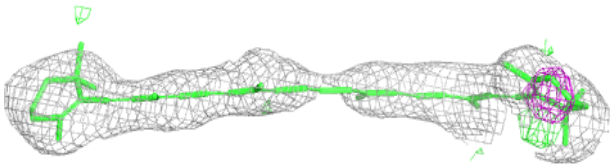


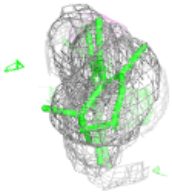


Electron density around BCR AK 102:

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

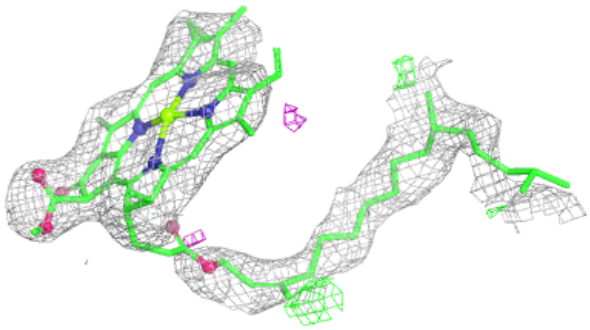


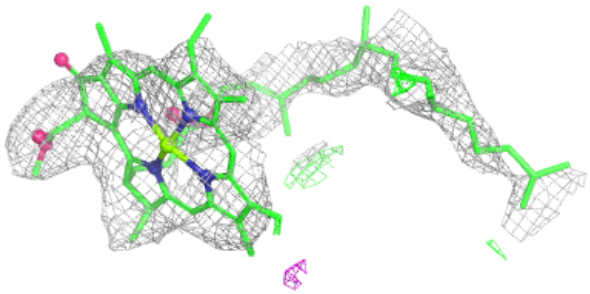


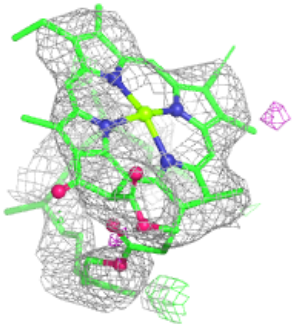


Electron density around CLA AC 513:

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

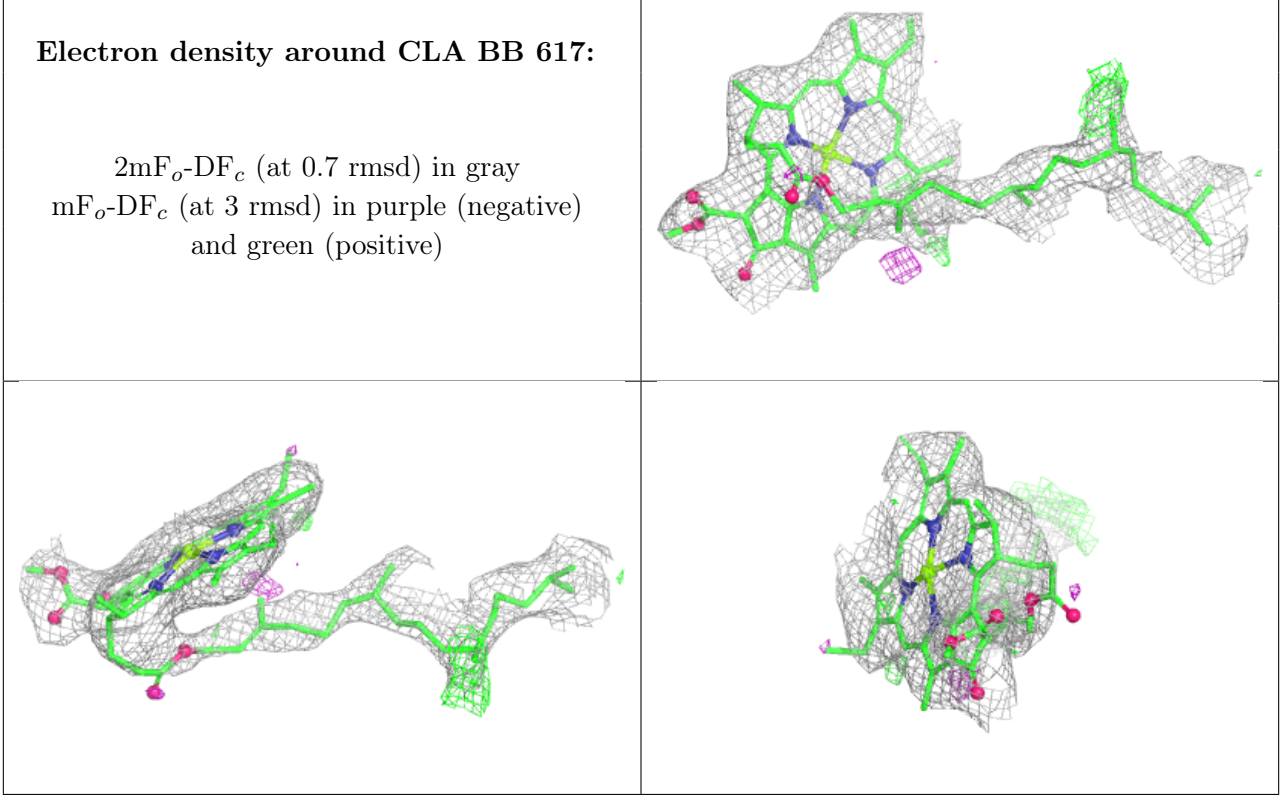






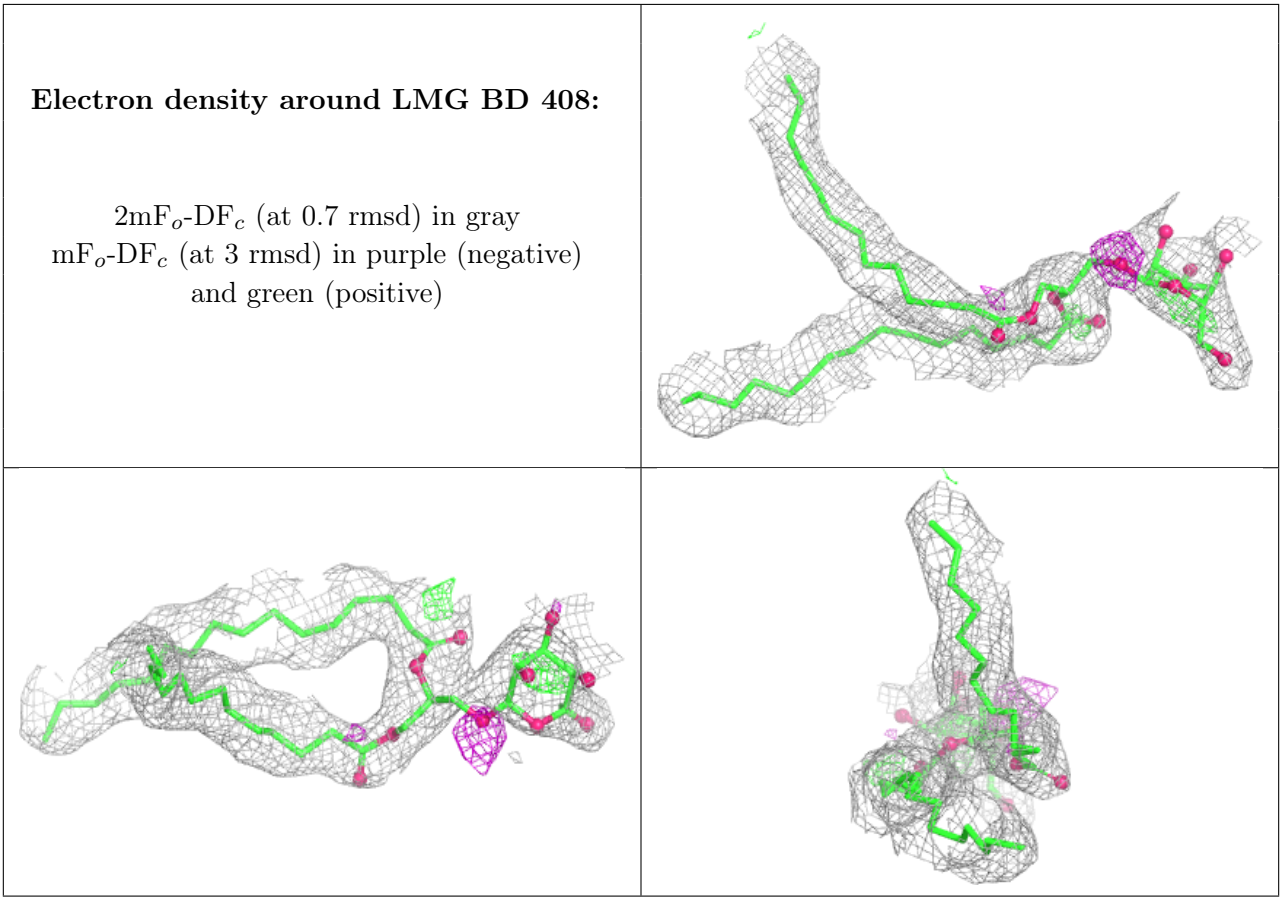
Electron density around CLA BB 617:

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



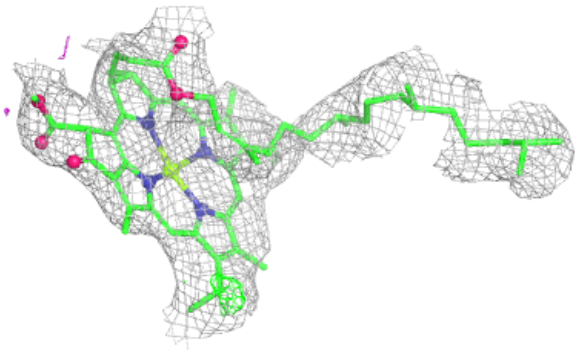
Electron density around LMG BD 408:

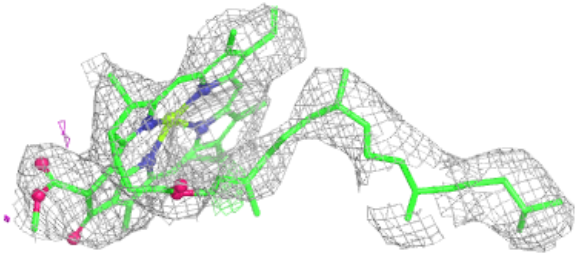
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

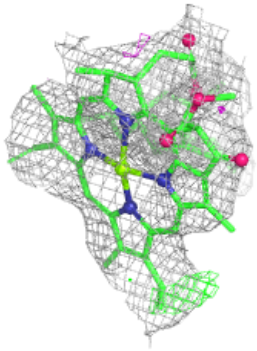


Electron density around CLA BC 505:

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

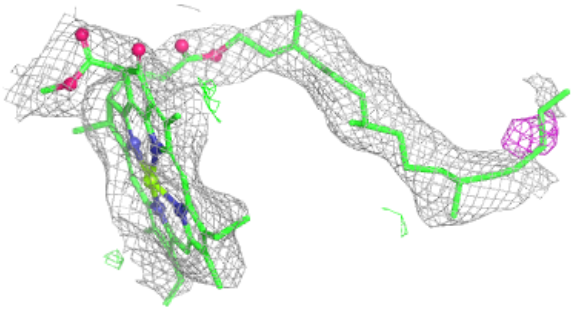


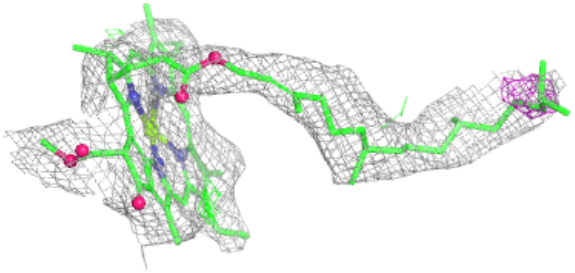


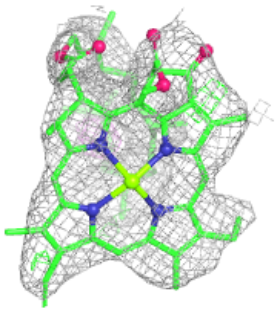


Electron density around CLA BC 508:

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

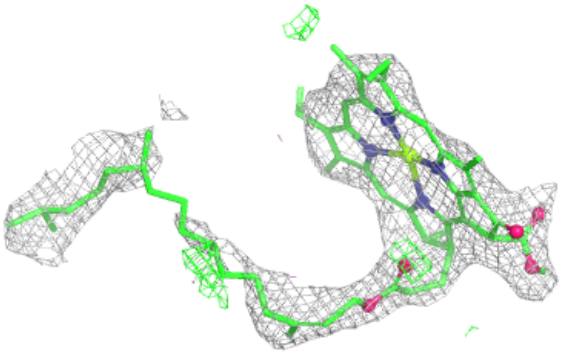


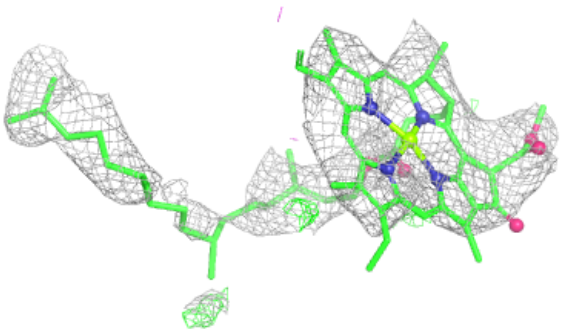


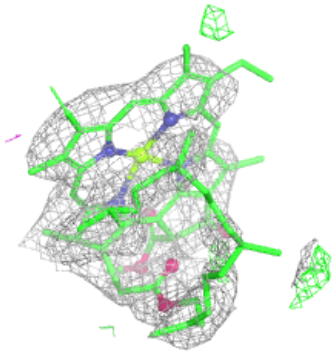


Electron density around CLA BC 513:

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

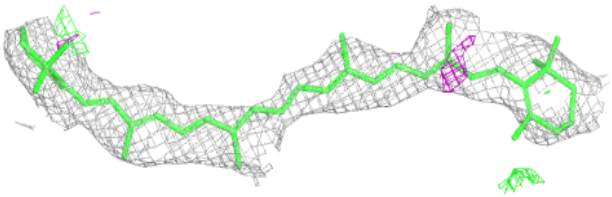


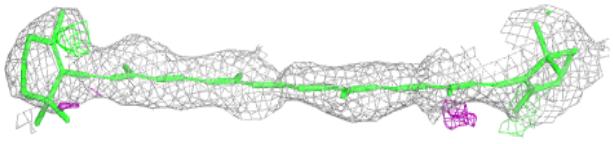


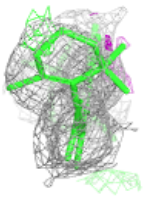


Electron density around BCR BX 101:

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

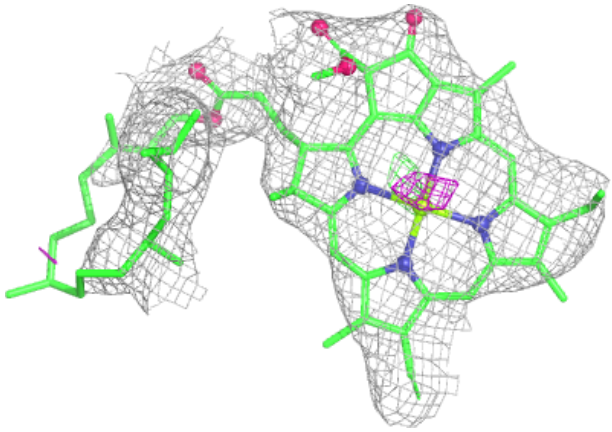


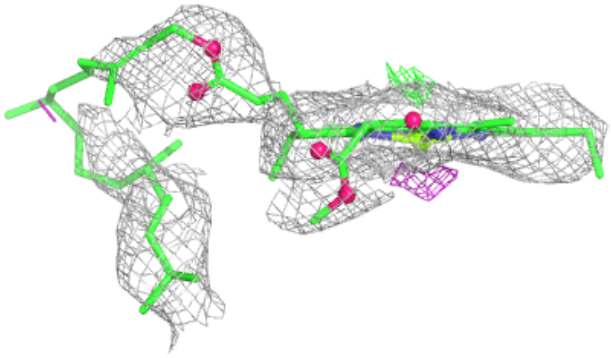


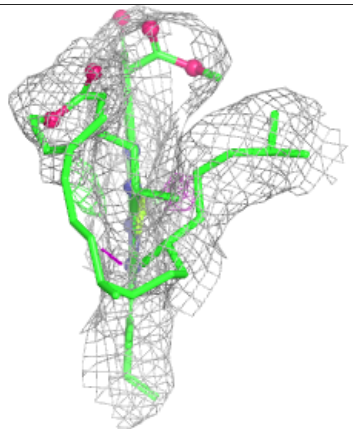


Electron density around CLA BC 512:

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

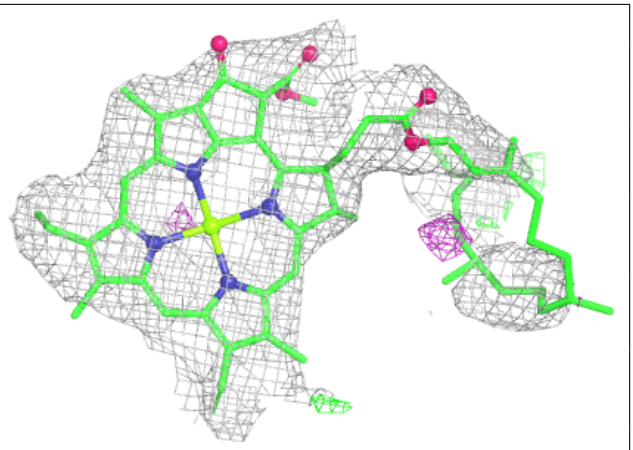


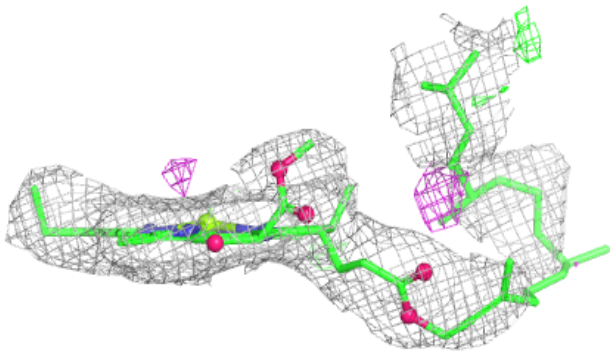




Electron density around CLA AC 512:

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

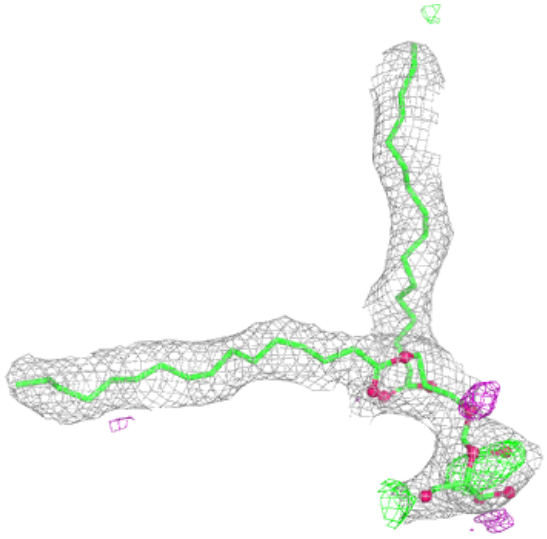


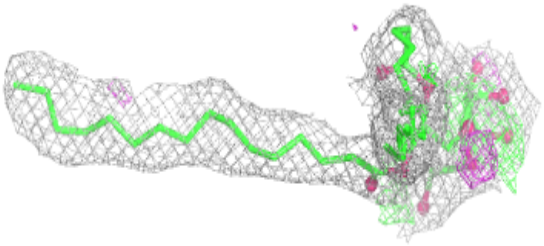


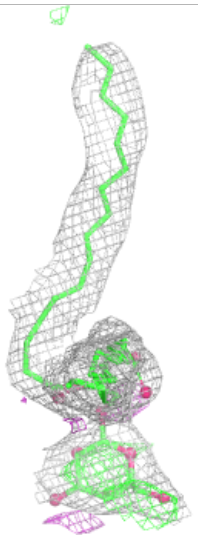


Electron density around LMG AA 413:

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

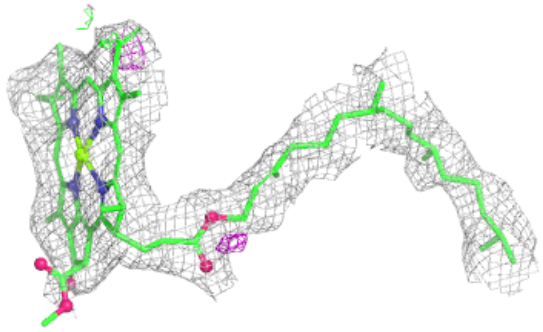


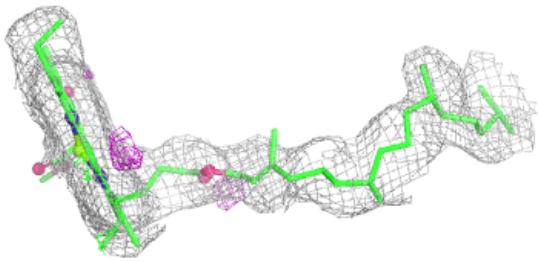


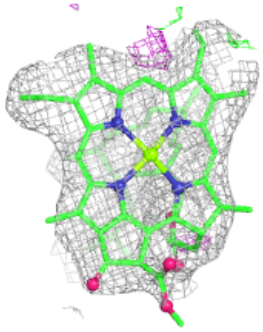


Electron density around CLA BD 404:

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

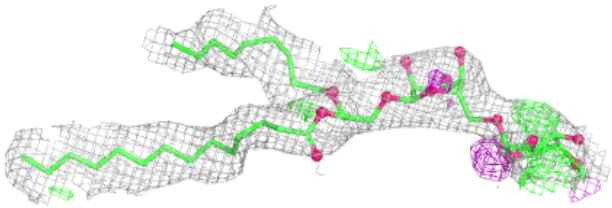


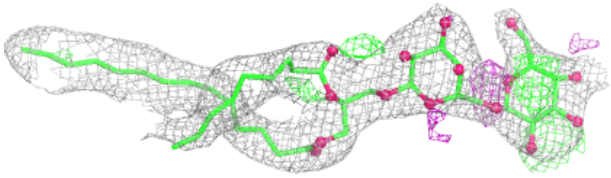


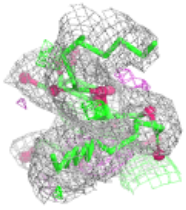


Electron density around DGD AC 516:

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

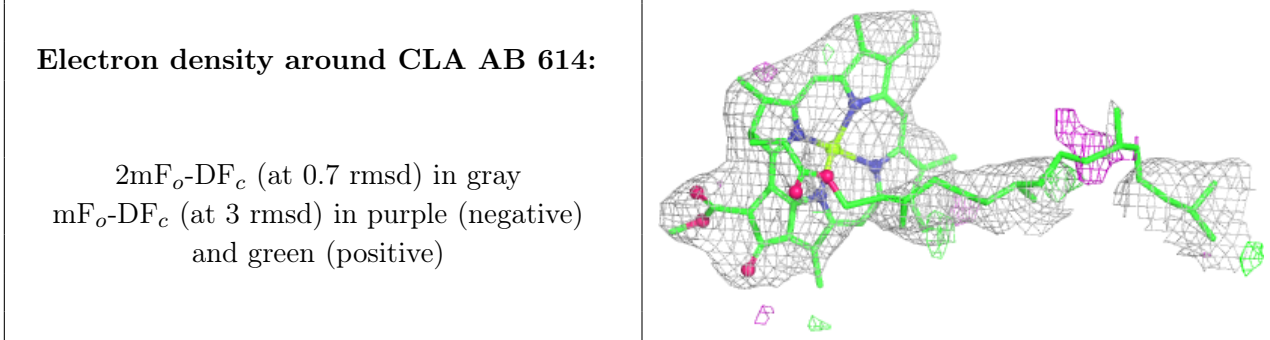


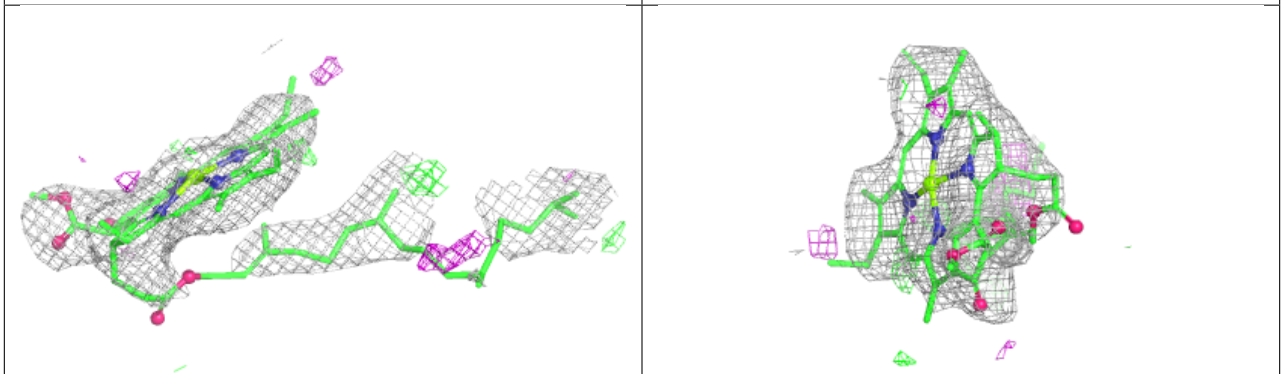




Electron density around CLA AB 614:

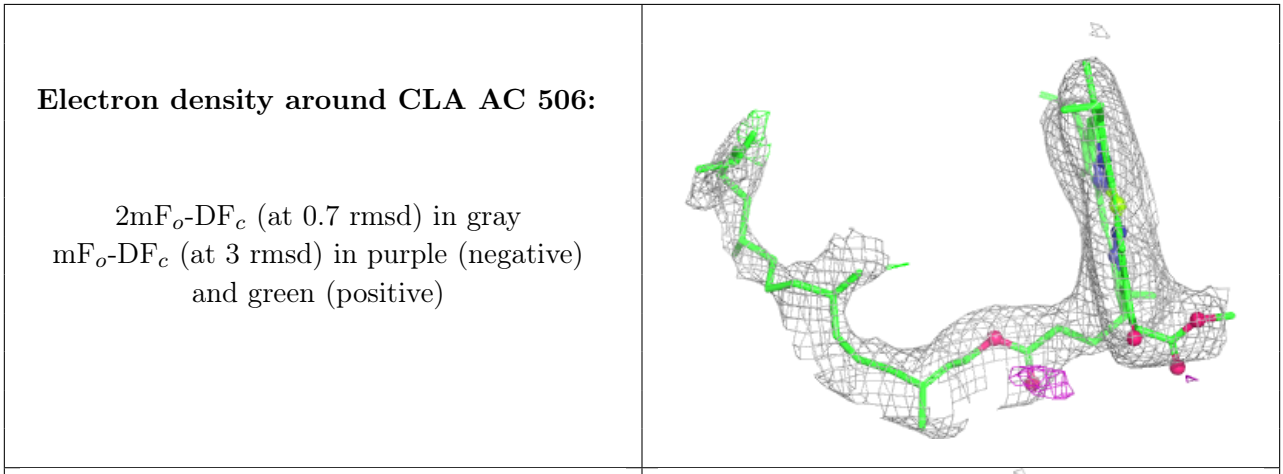
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

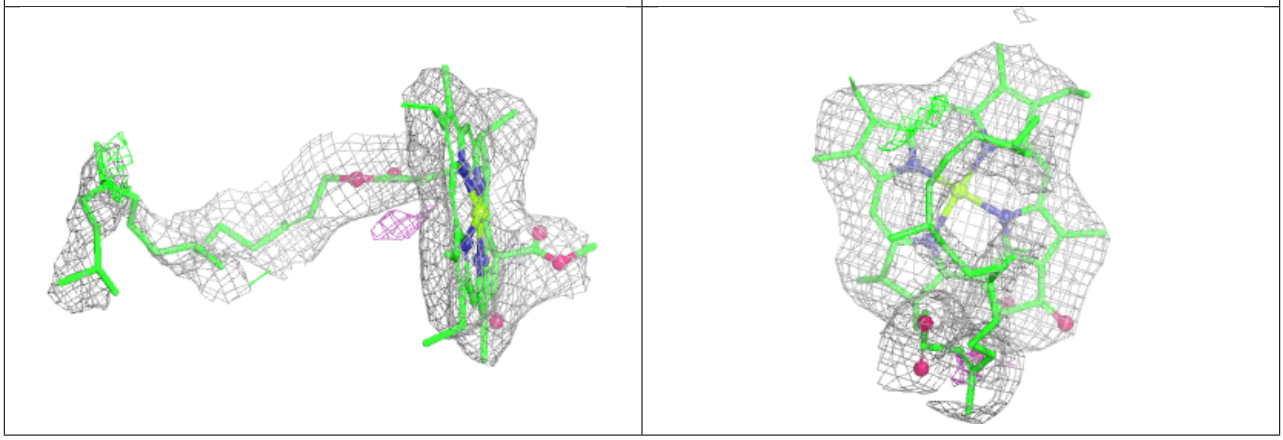




Electron density around CLA AC 506:

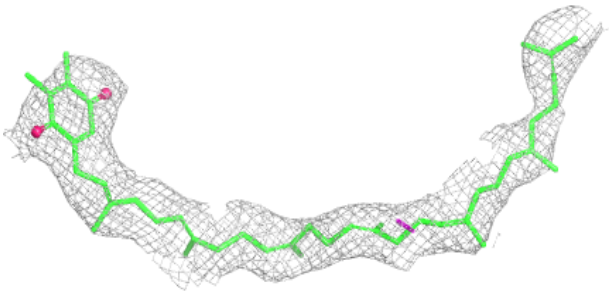
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

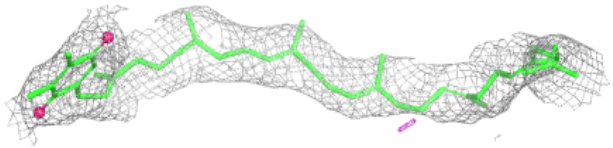


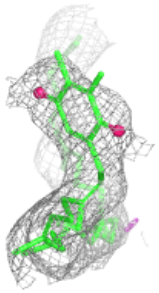


Electron density around PL9 BA 408:

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

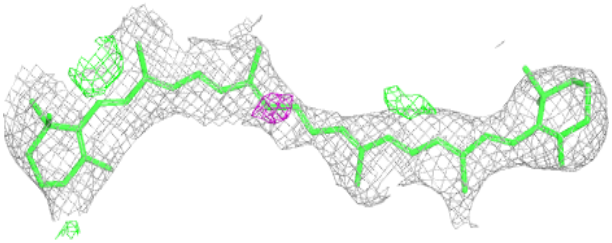


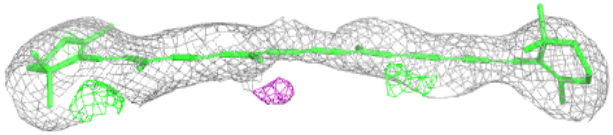


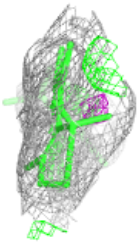


Electron density around BCR BK 102:

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

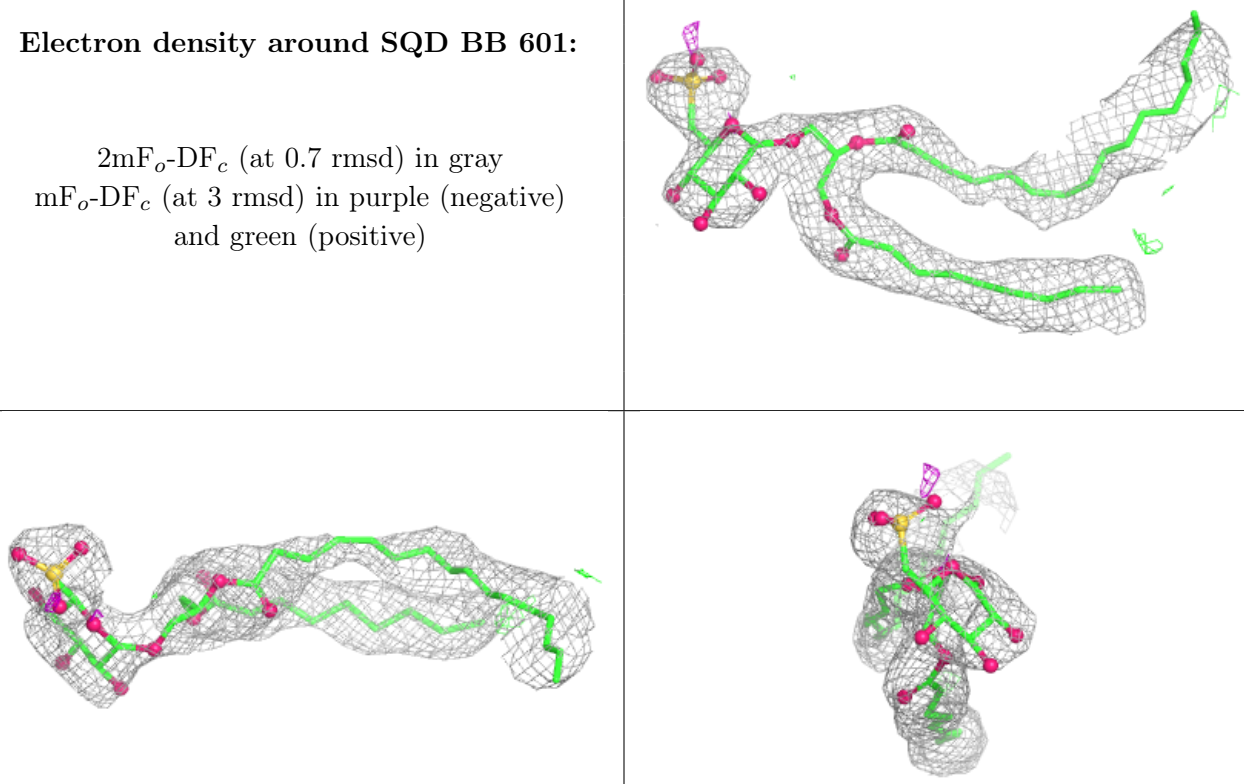






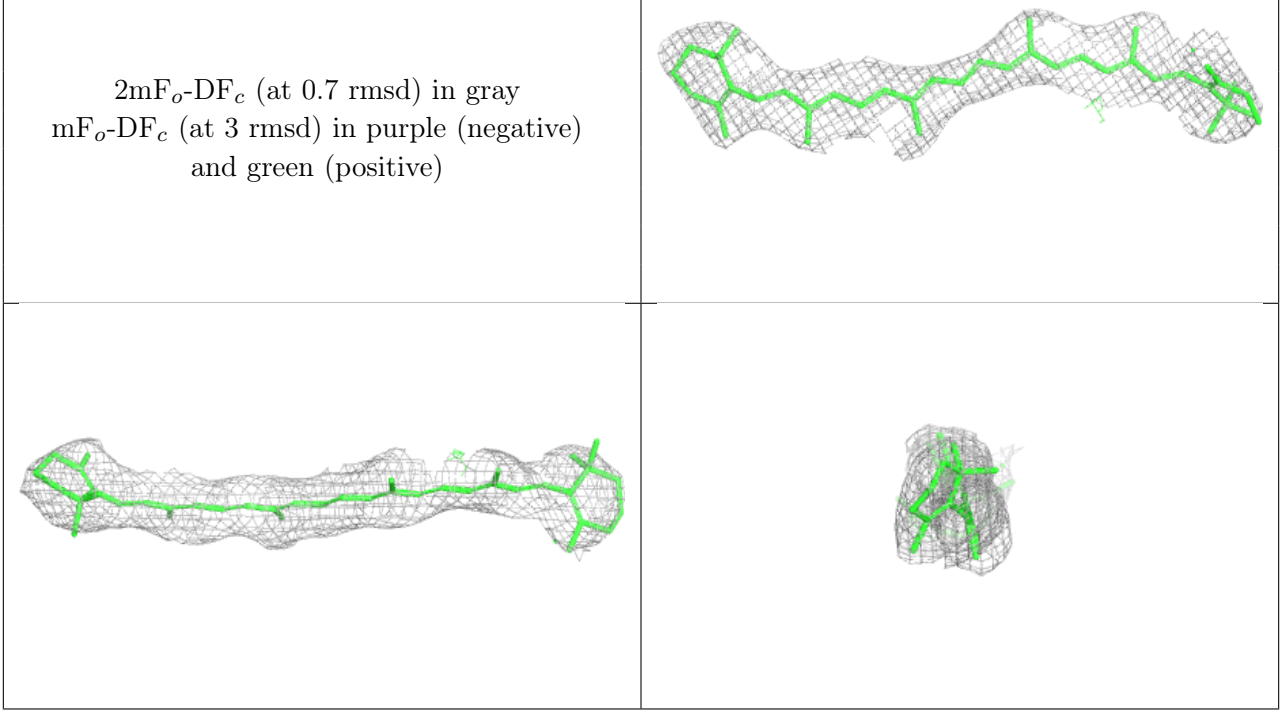
Electron density around SQD BB 601:

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



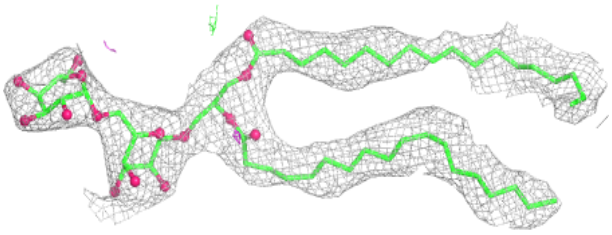
Electron density around BCR AZ 101:

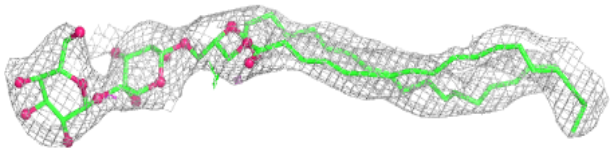
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

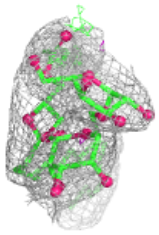


Electron density around DGD BC 518:

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

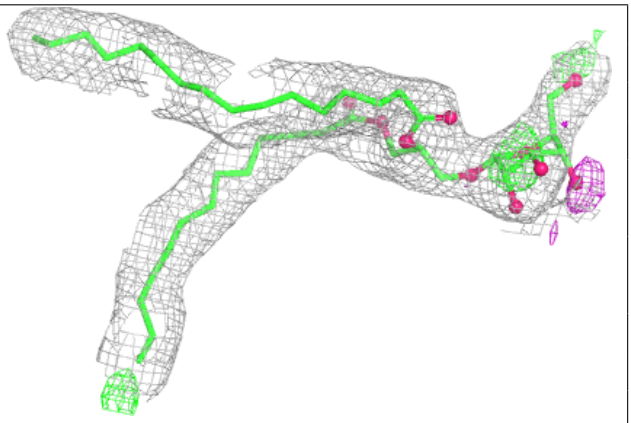


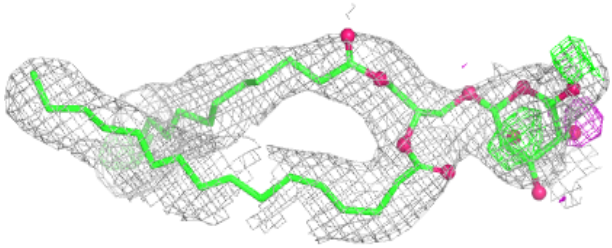


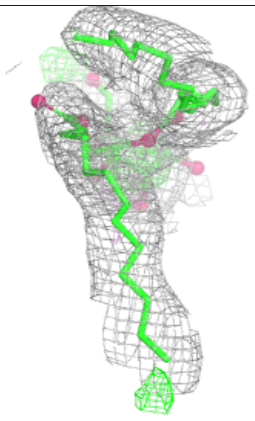


Electron density around LMG AD 408:

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

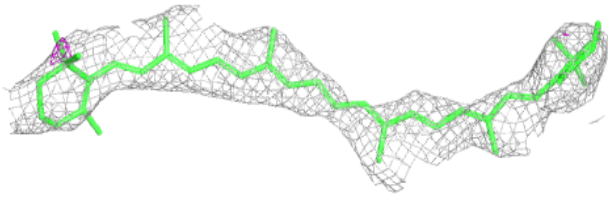


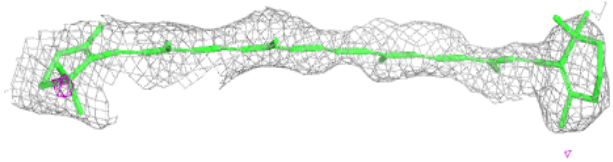


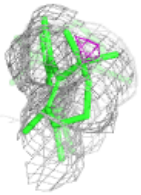


Electron density around BCR AH 101:

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

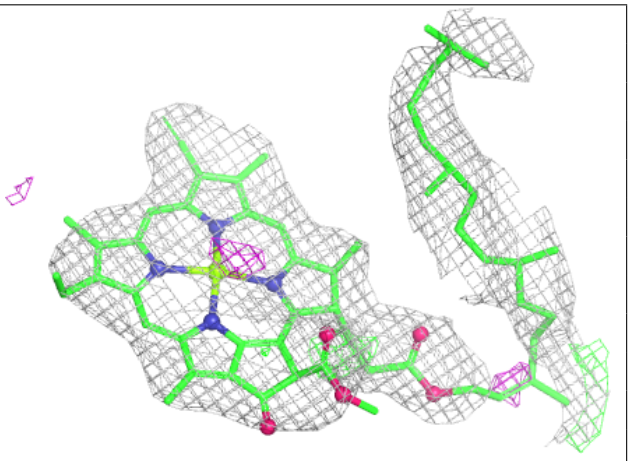


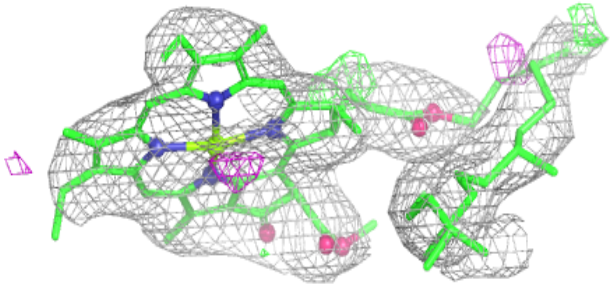


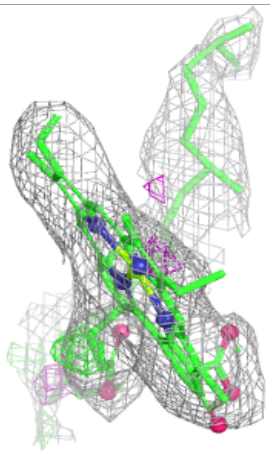


Electron density around CLA BB 619:

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

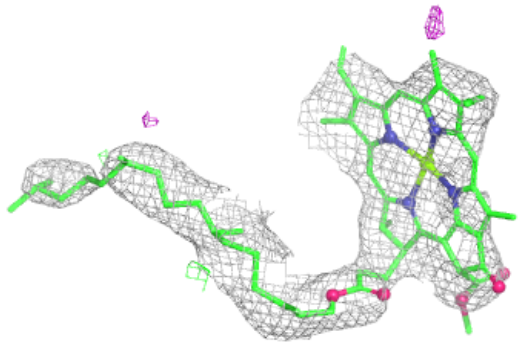


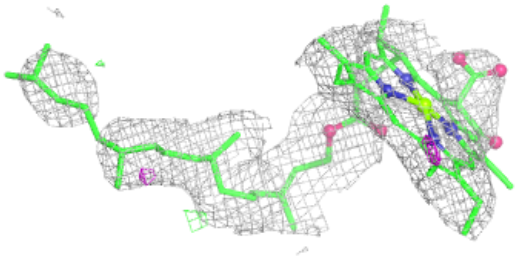


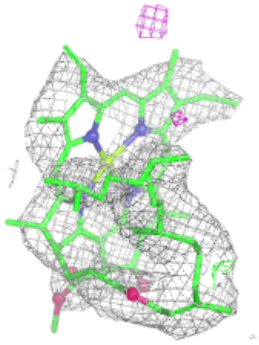


Electron density around CLA BC 511:

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

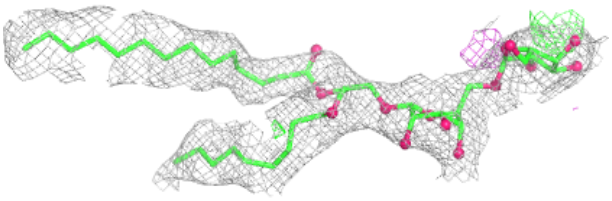


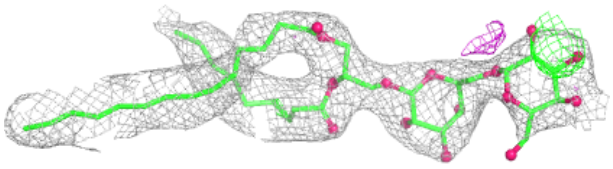


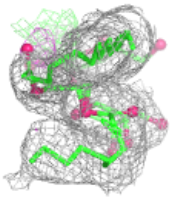


Electron density around DGD BC 516:

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

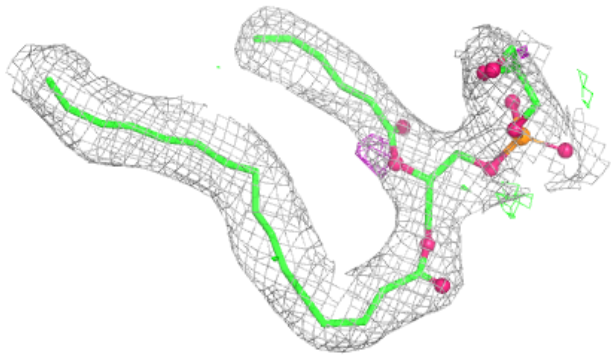


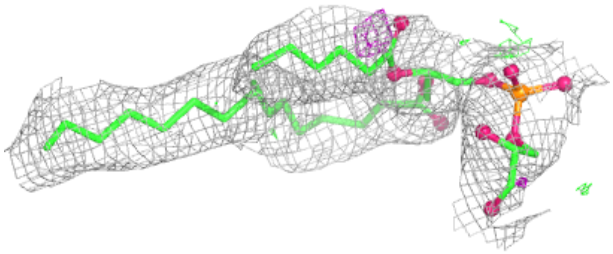




Electron density around LHG AA 411:

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

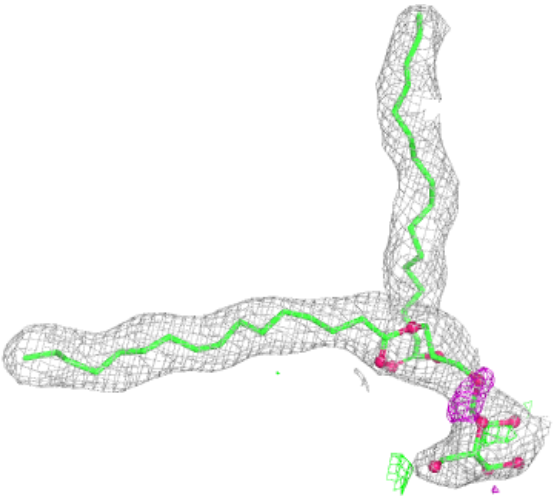


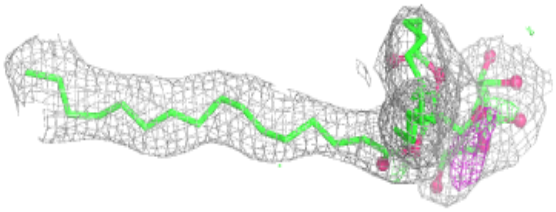




Electron density around LMG BA 414:

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

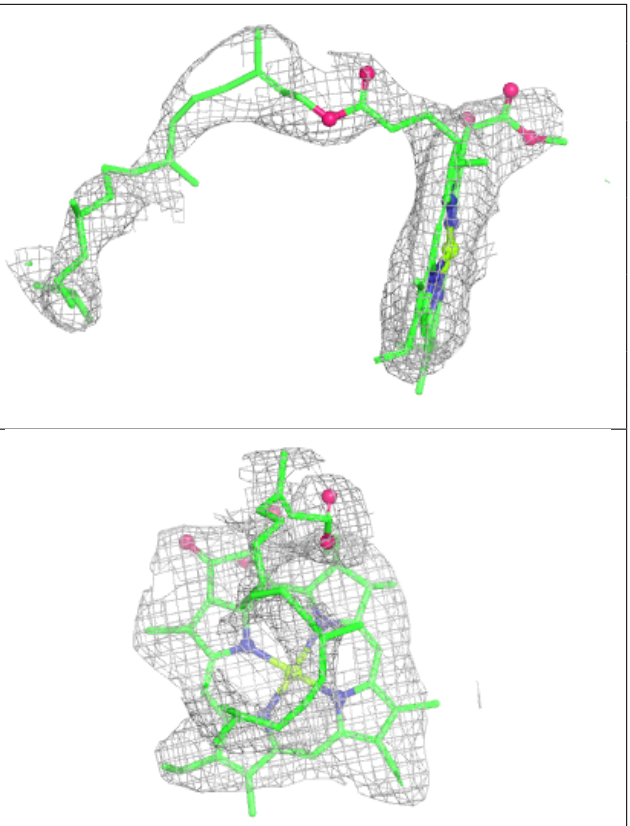






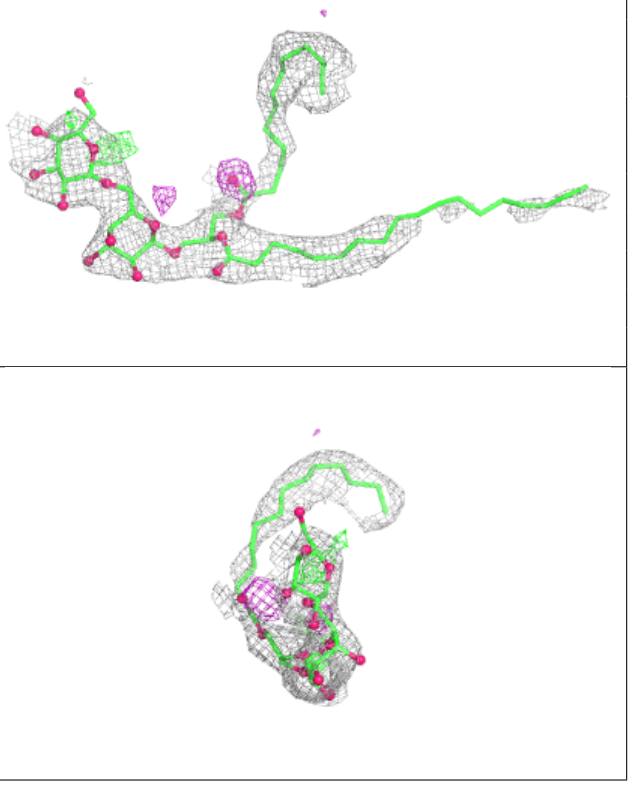
Electron density around CLA BC 506:

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



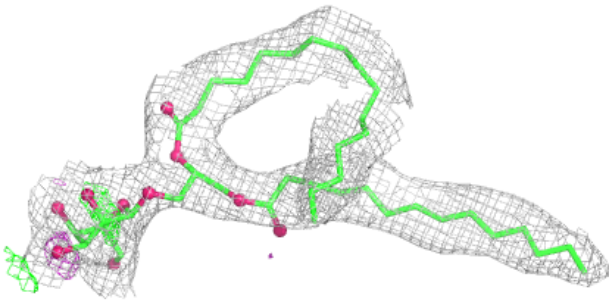
Electron density around DGD AC 517:

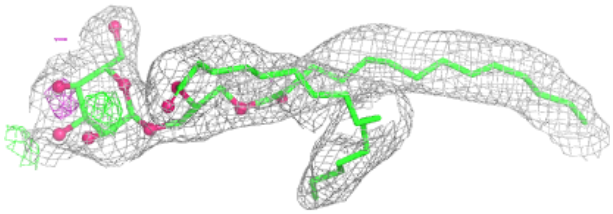
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

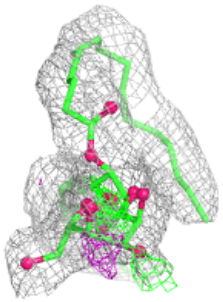


Electron density around LMG AB 621:

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

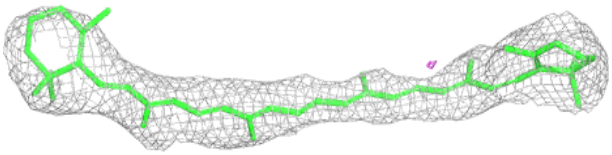


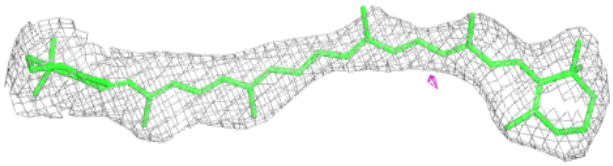


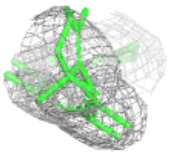


Electron density around BCR BD 406:

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

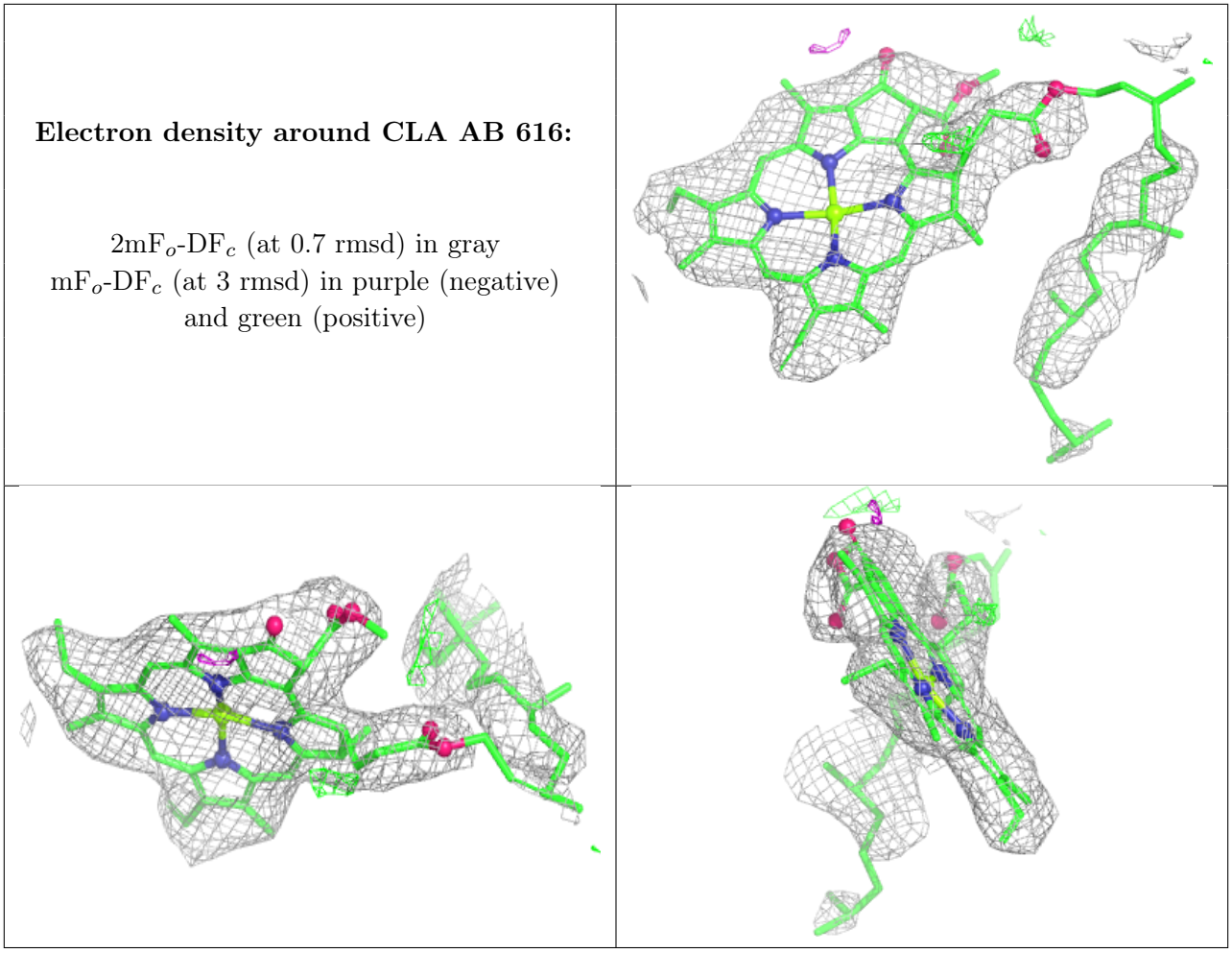






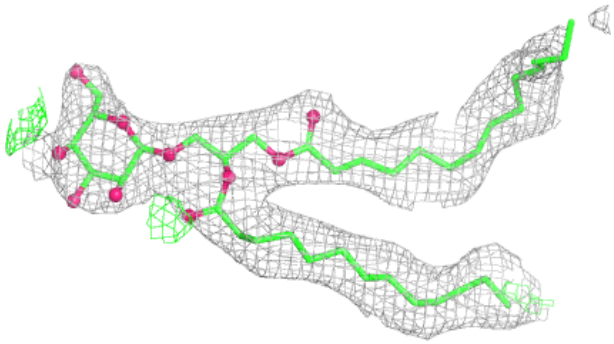
Electron density around CLA AB 616:

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

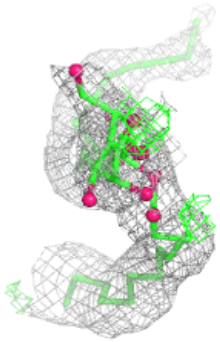


Electron density around LMG AD 407:

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

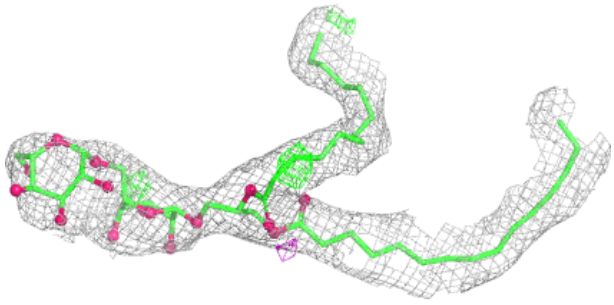


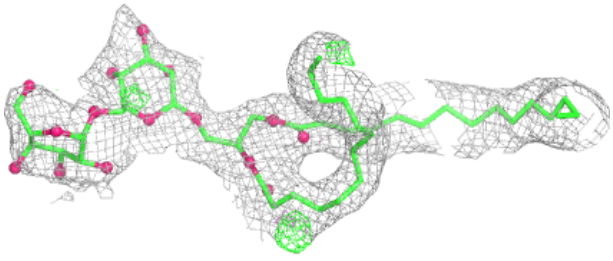


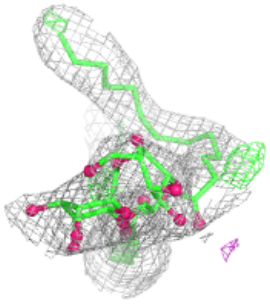


Electron density around DGD BH 101:

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

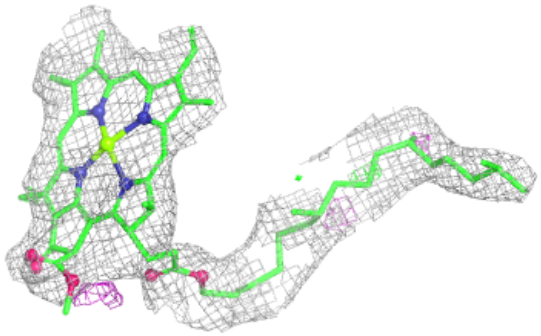


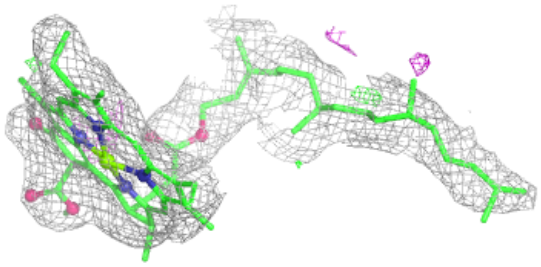


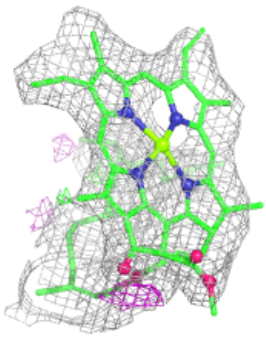


Electron density around CLA AC 511:

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

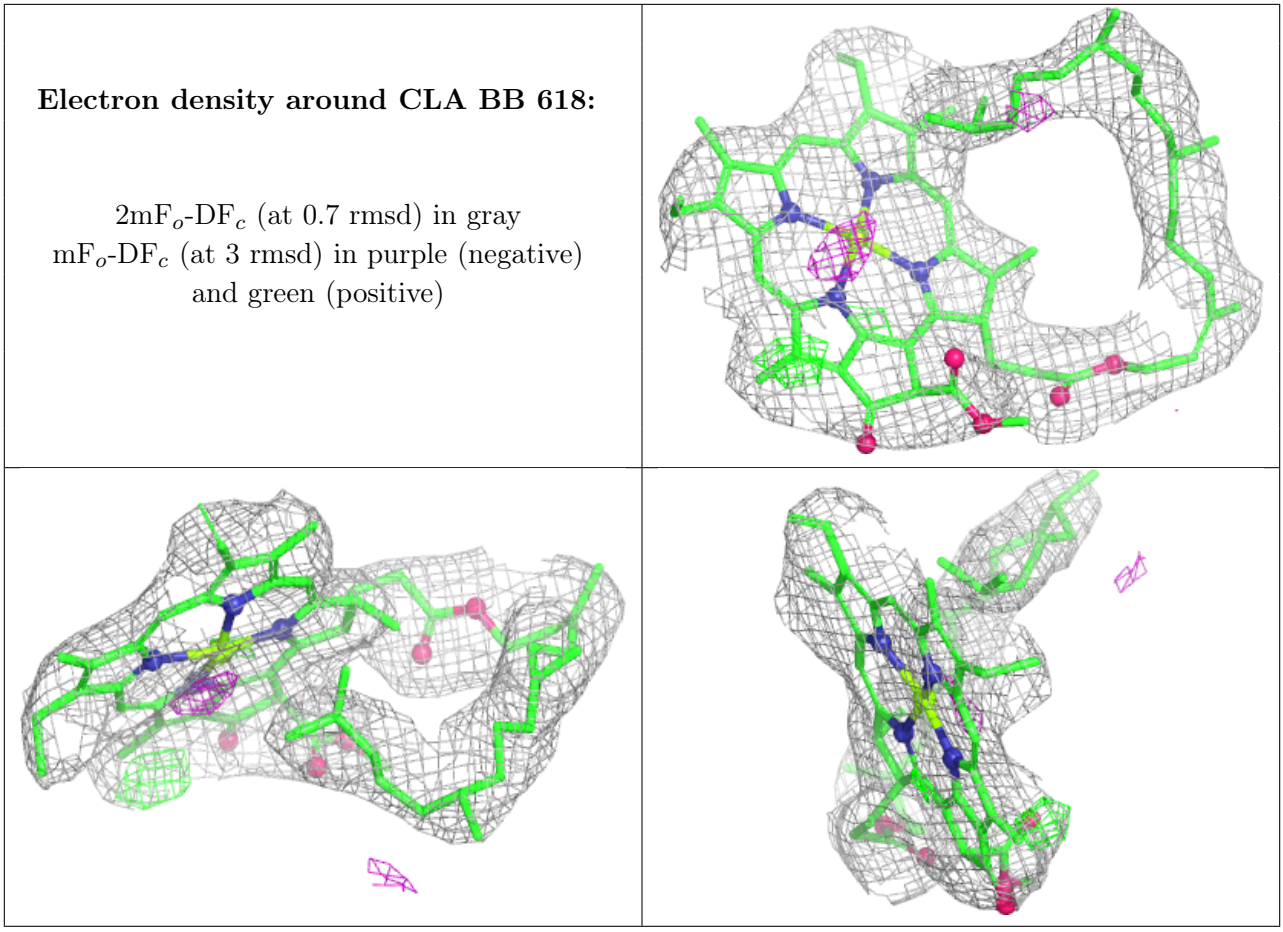






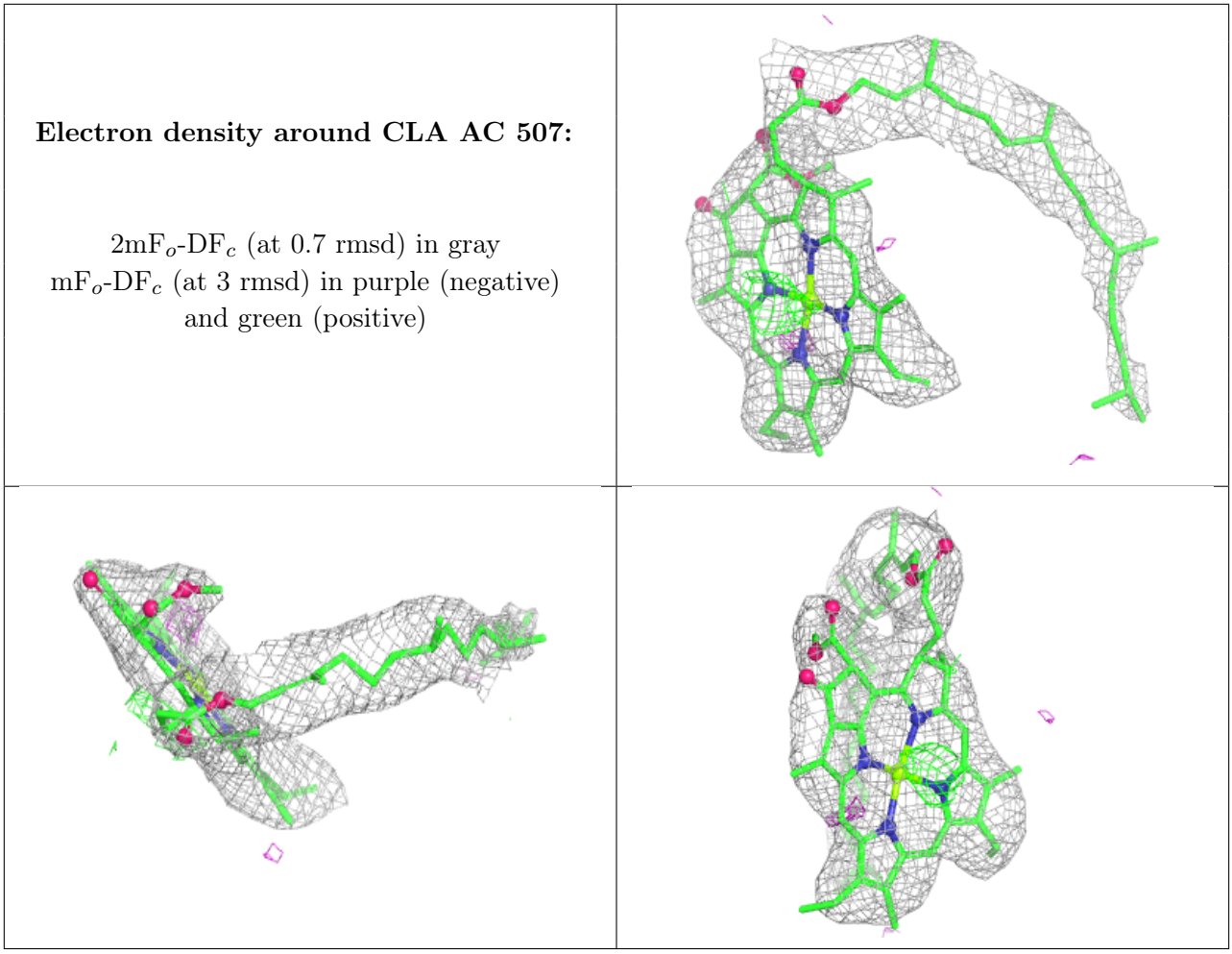
Electron density around CLA BB 618:

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



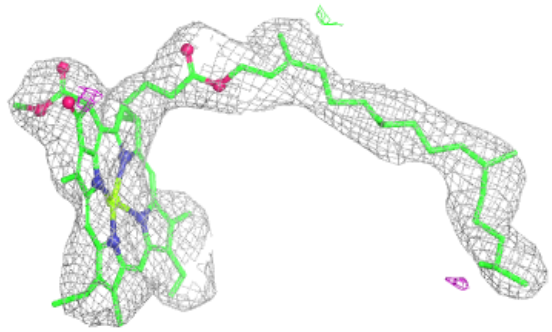
Electron density around CLA AC 507:

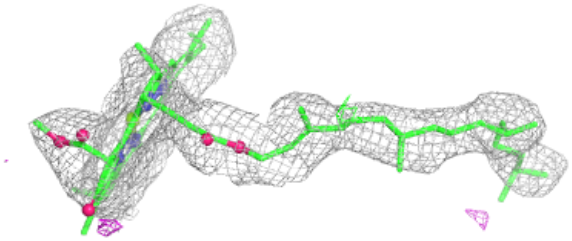
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

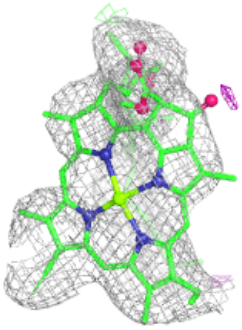


Electron density around CLA AB 609:

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

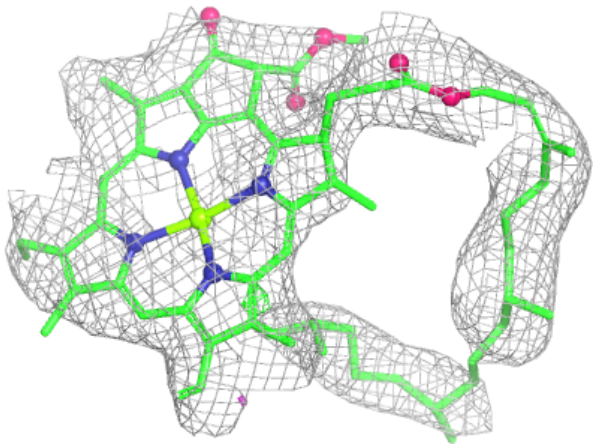


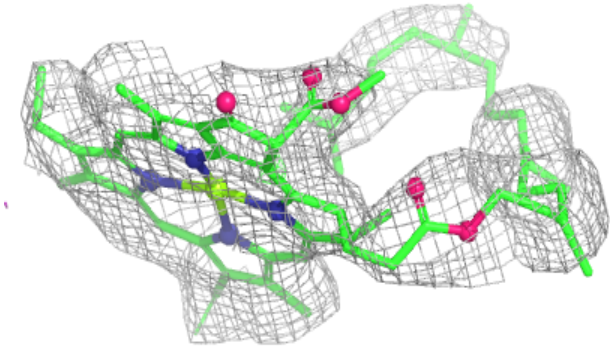


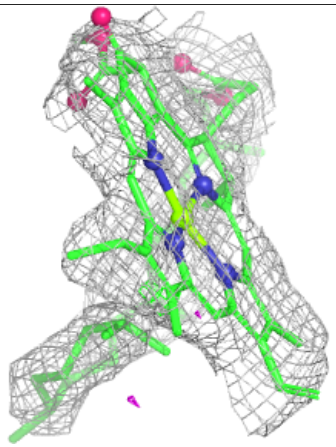


Electron density around CLA AB 615:

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

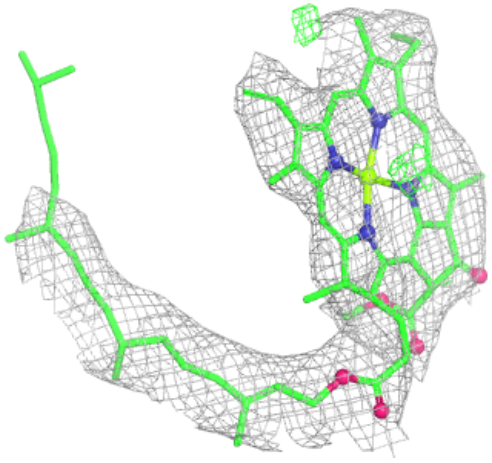


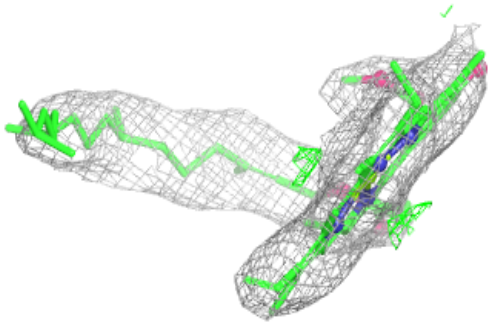


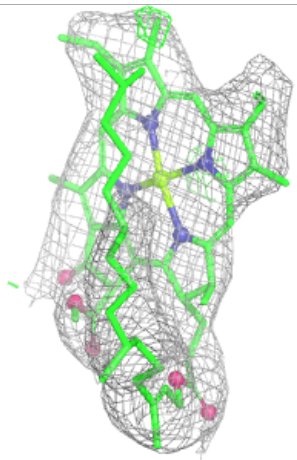


Electron density around CLA BC 507:

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

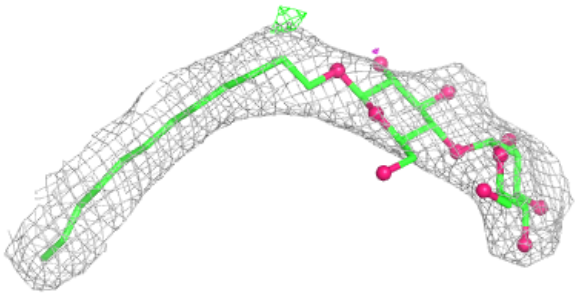


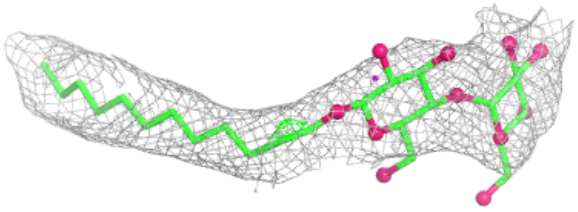


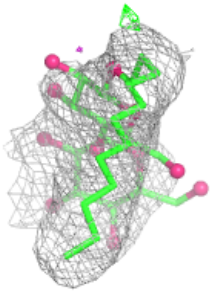


Electron density around LMT AM 102:

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

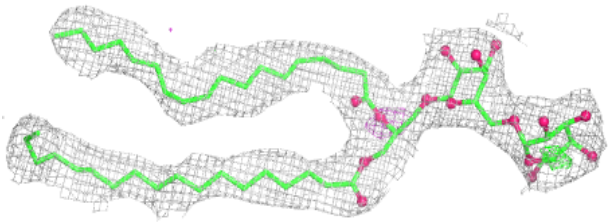


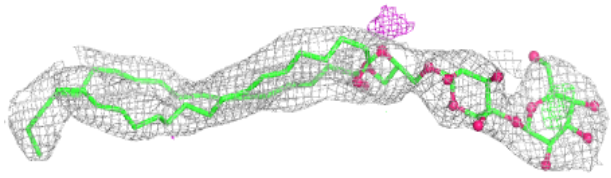


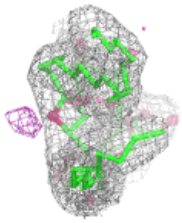


Electron density around DGD AC 518:

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

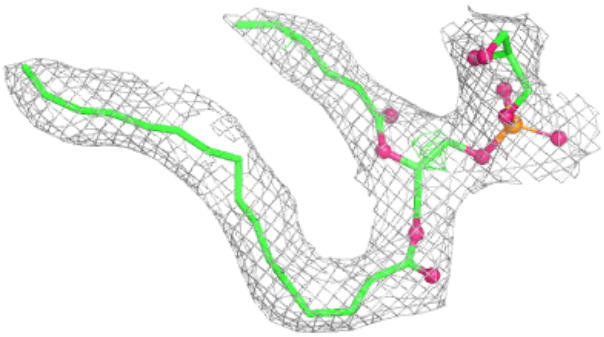


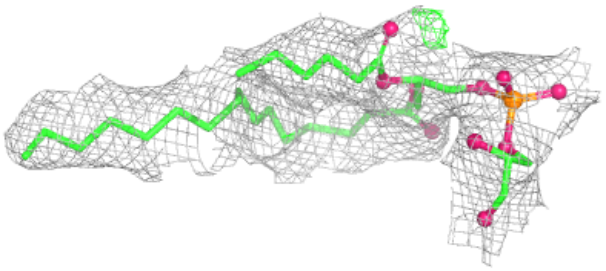


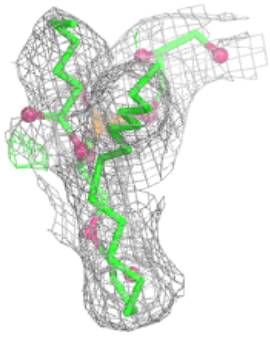


Electron density around LHG BA 412:

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

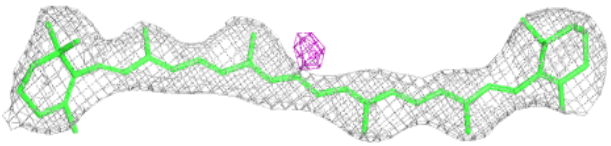


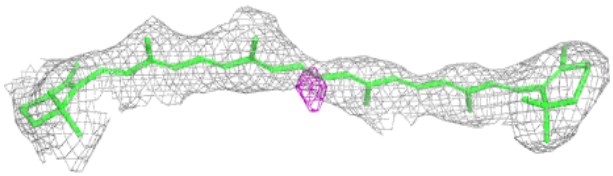


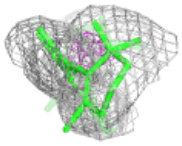


Electron density around BCR AB 620:

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



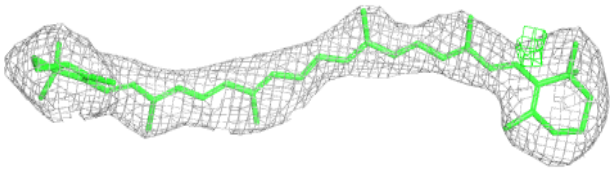


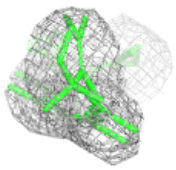


Electron density around BCR AD 406:

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

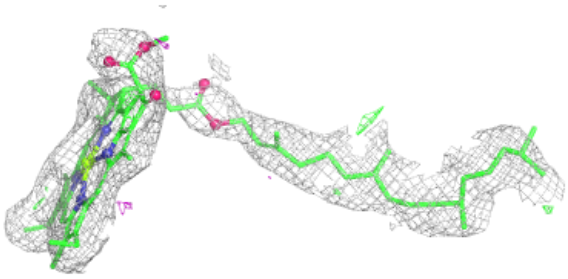


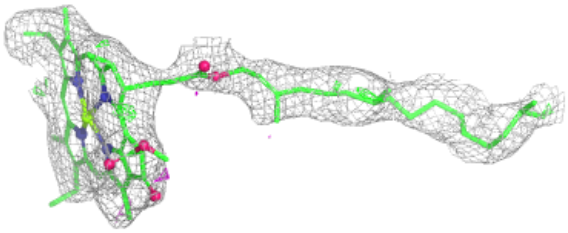


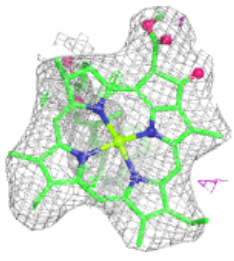


Electron density around CLA AB 604:

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

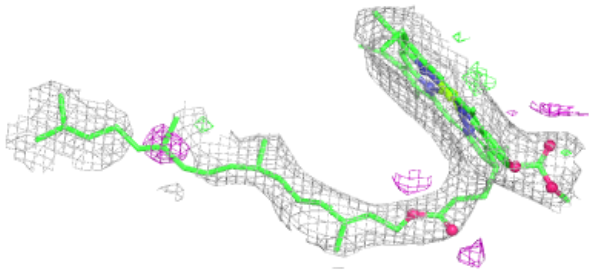


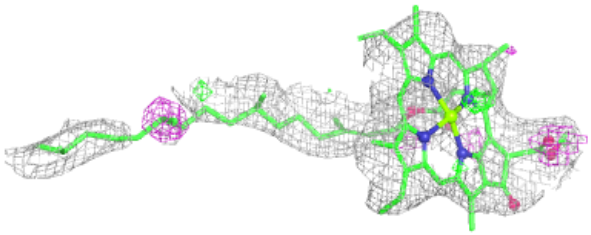


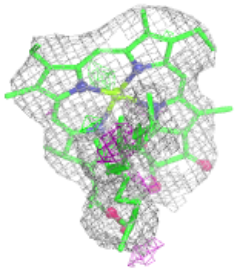


Electron density around CLA AC 504:

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

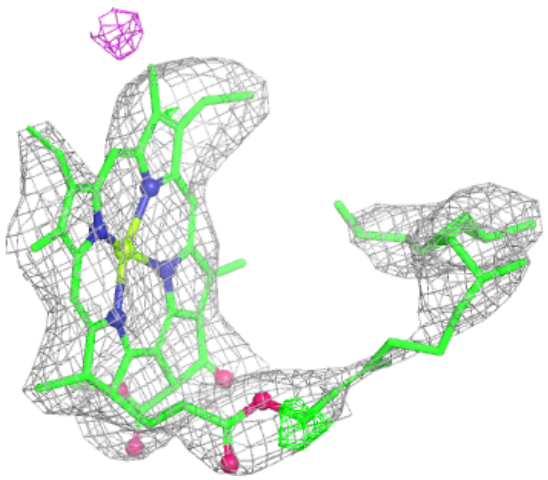


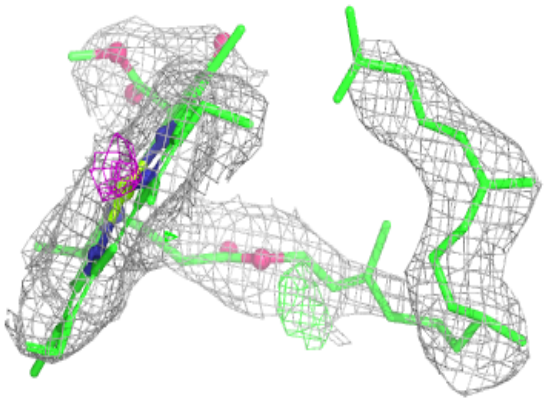


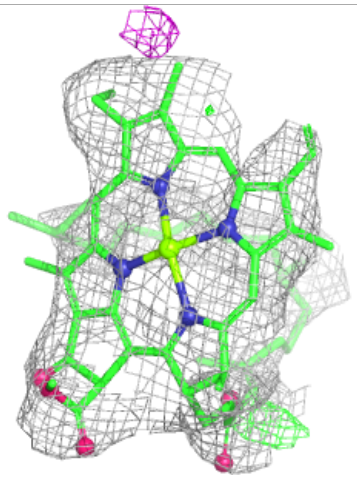


Electron density around CLA BC 503:

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

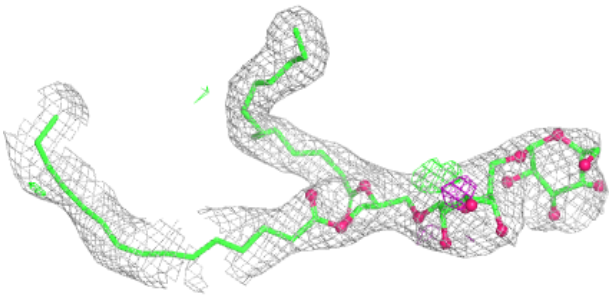


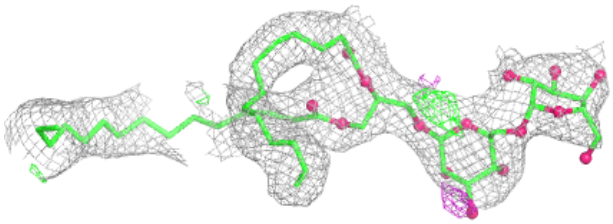


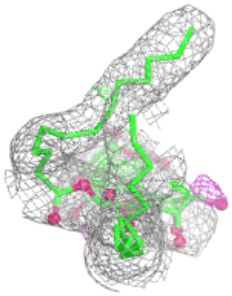


Electron density around DGD AH 102:

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

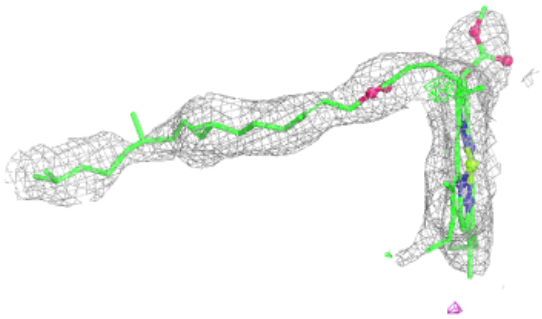


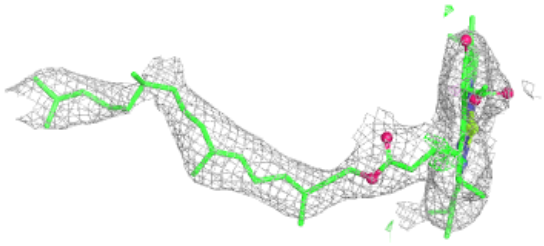


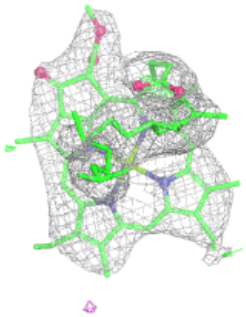


Electron density around CLA AB 606:

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

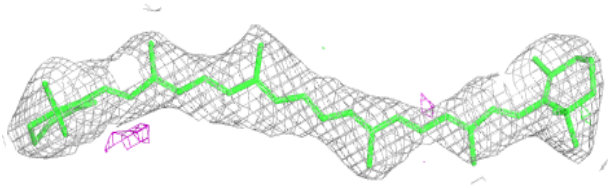


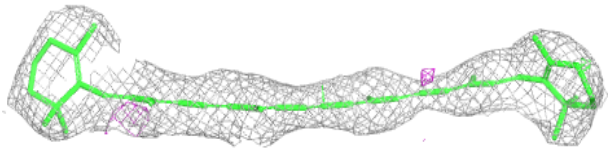


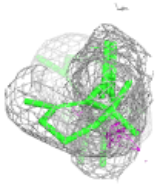


Electron density around BCR BB 620:

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

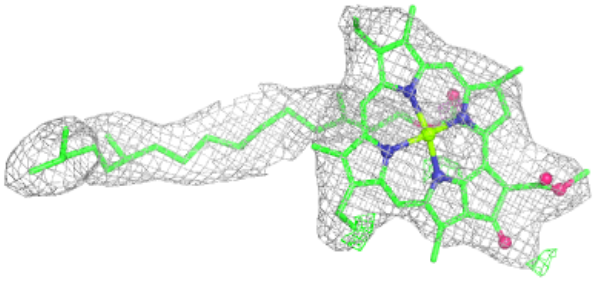


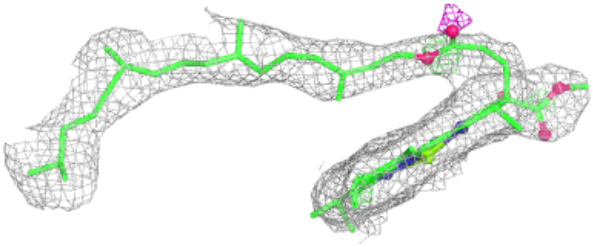


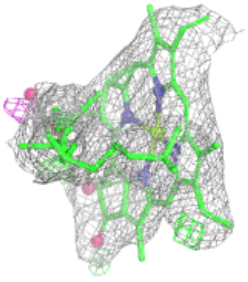


Electron density around CLA AB 608:

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

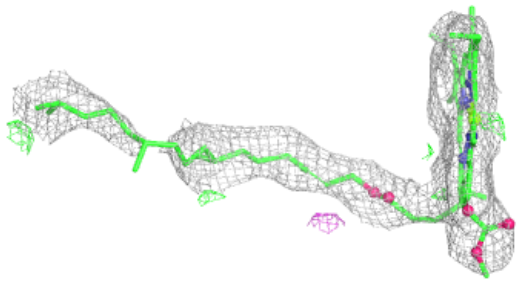


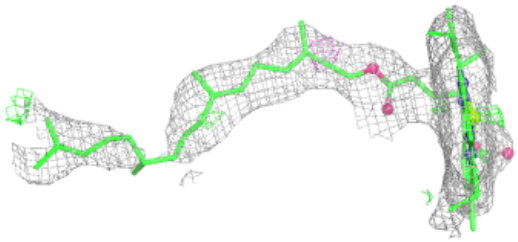


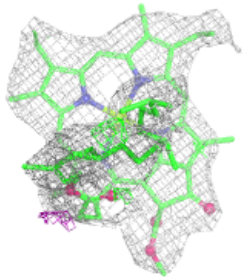


Electron density around CLA BB 609:

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

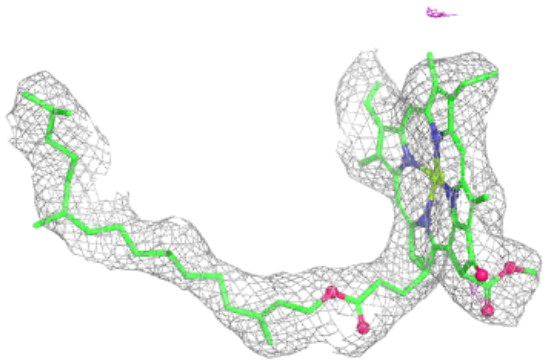


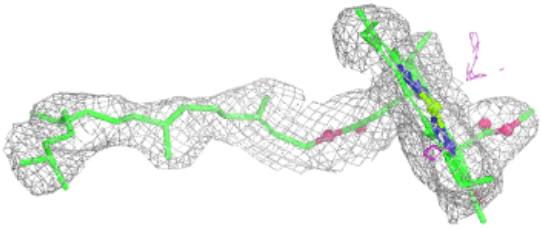


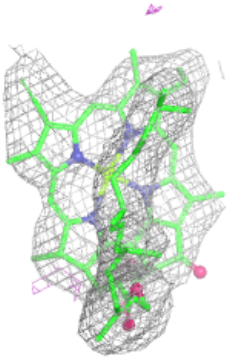


Electron density around CLA BB 612:

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

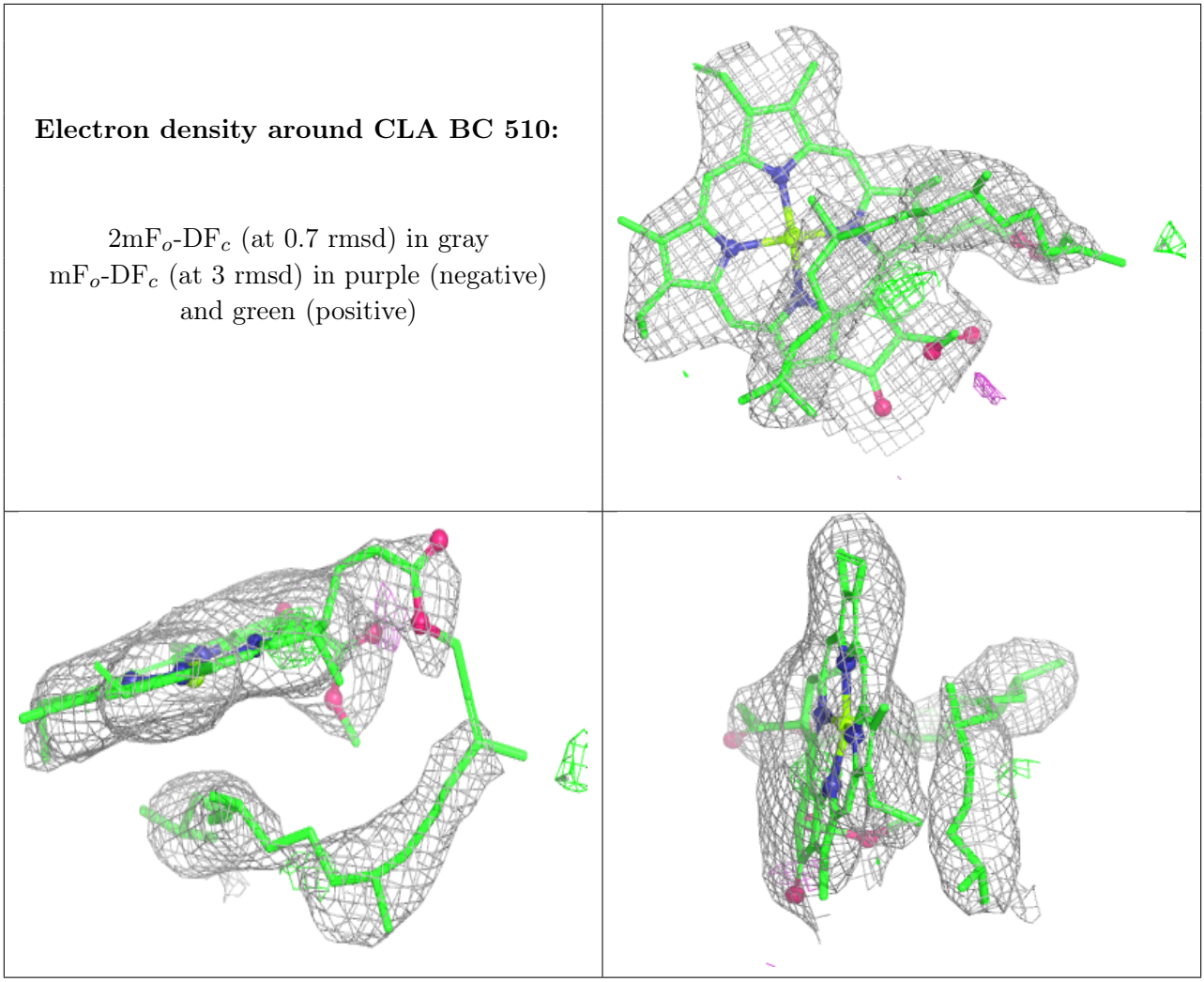






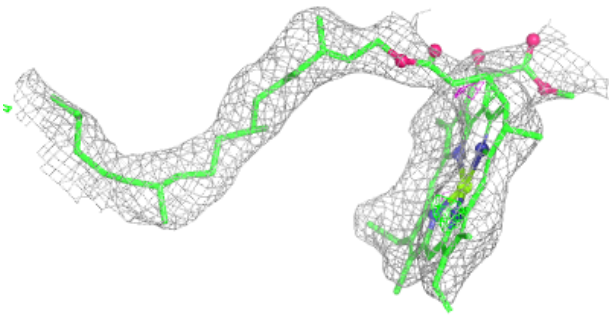
Electron density around CLA BC 510:

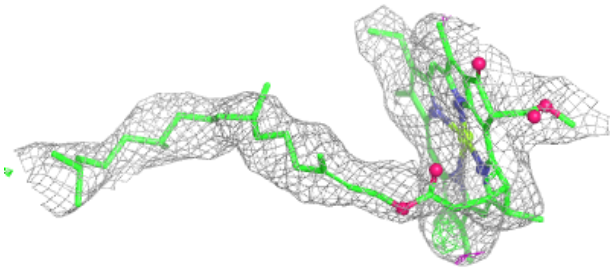
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

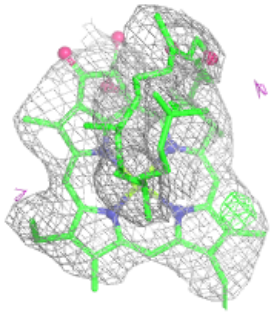


Electron density around CLA AC 508:

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

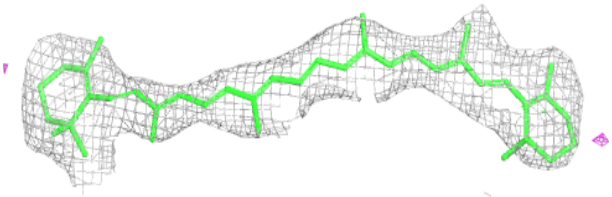


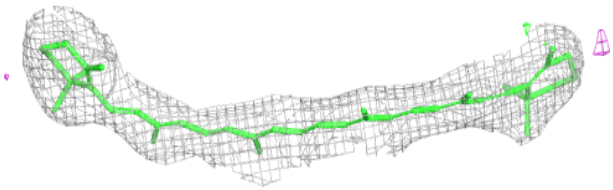


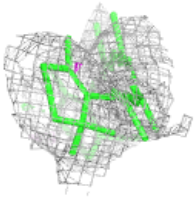


Electron density around BCR AB 618:

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

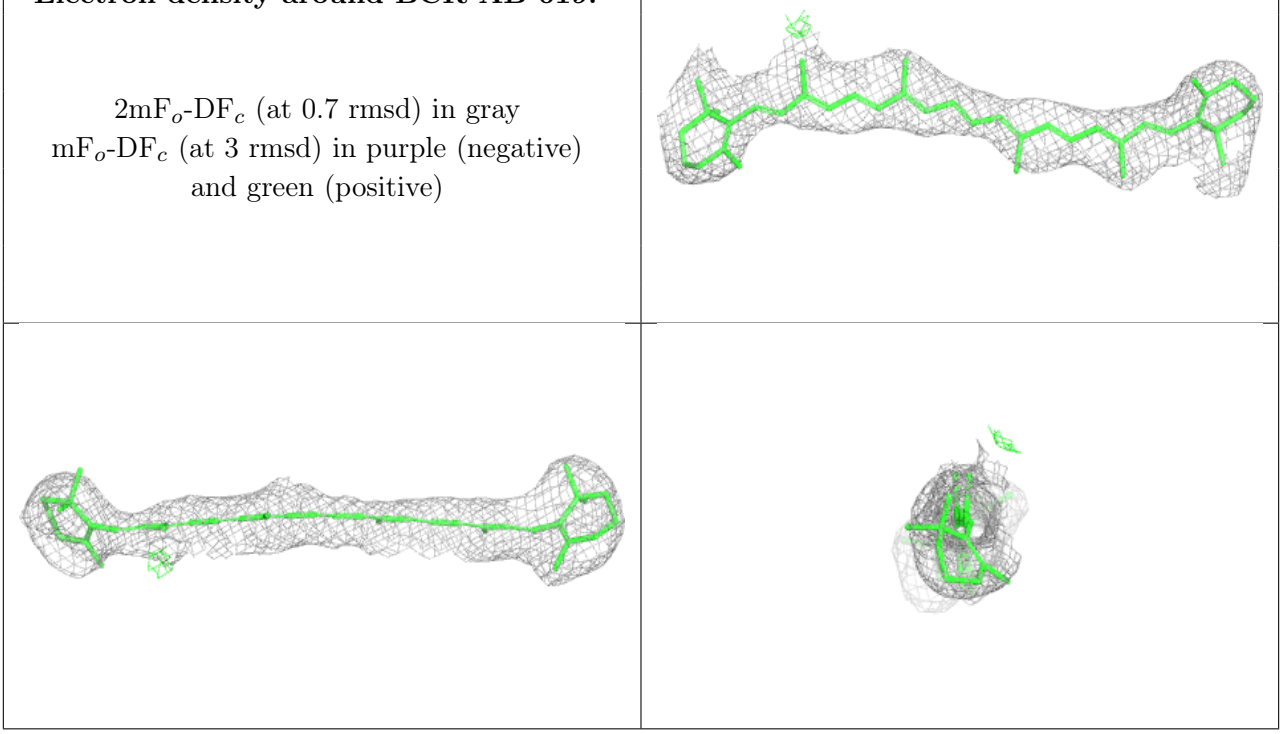






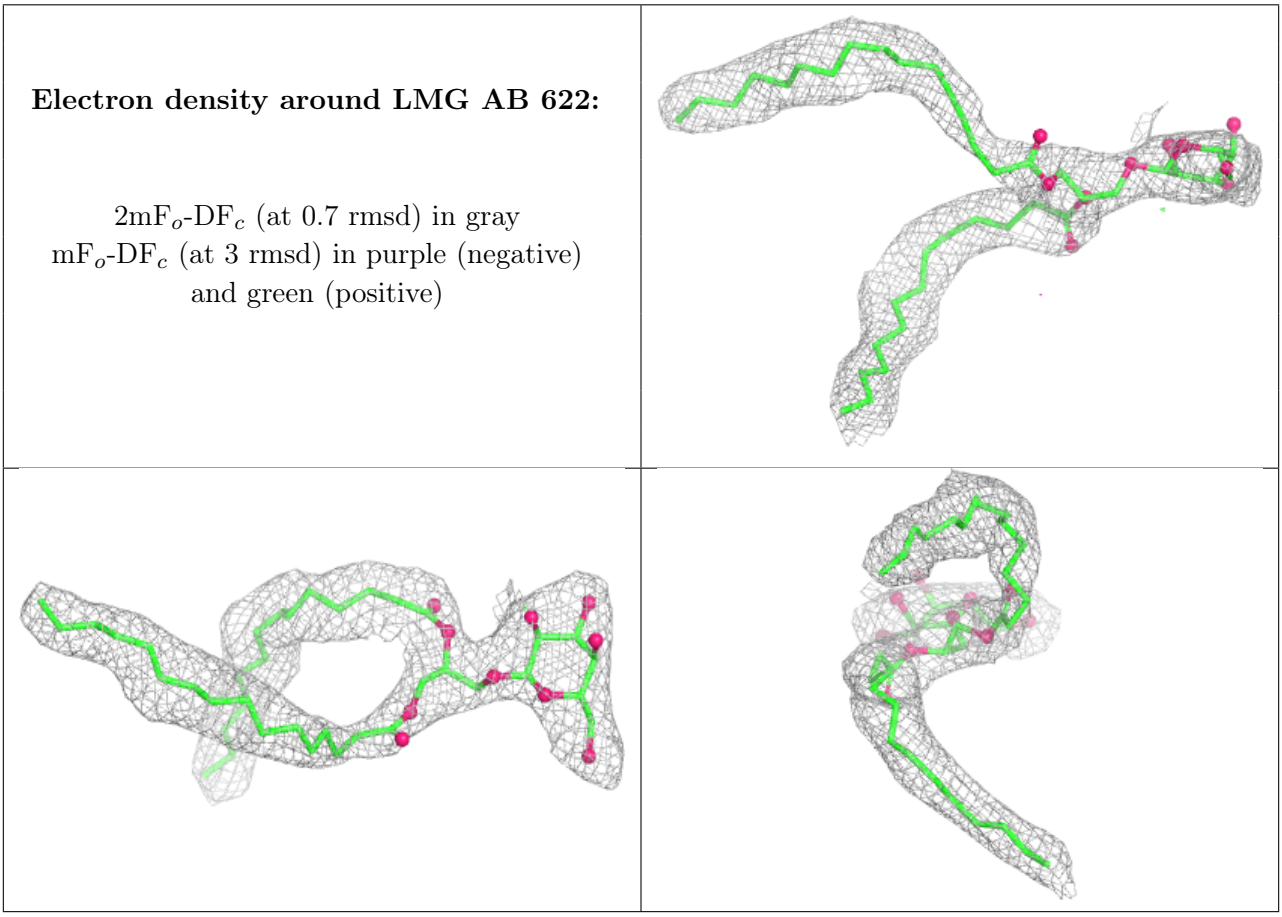
Electron density around BCR AB 619:

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



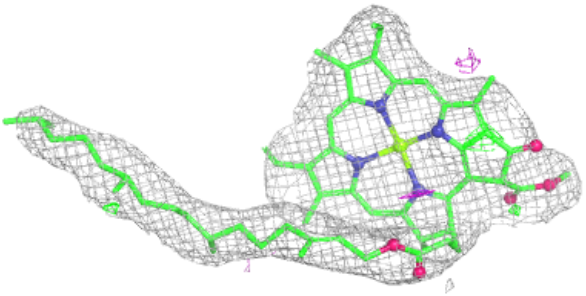
Electron density around LMG AB 622:

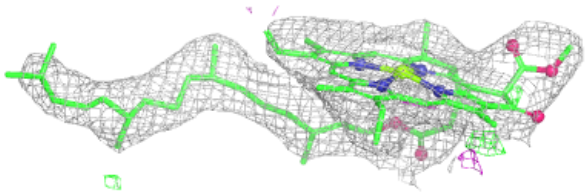
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

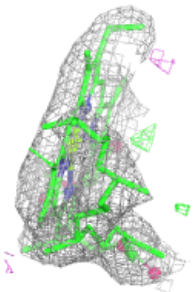


Electron density around CLA BC 501:

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

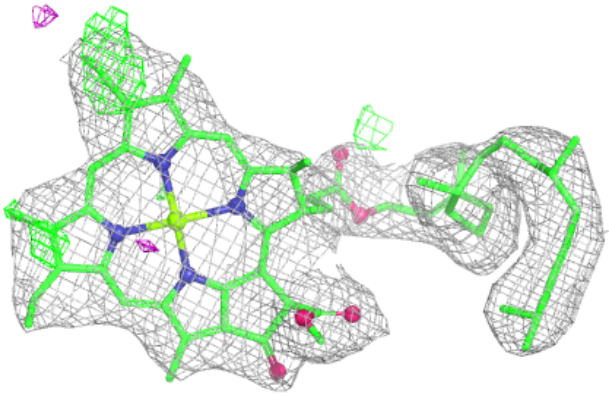


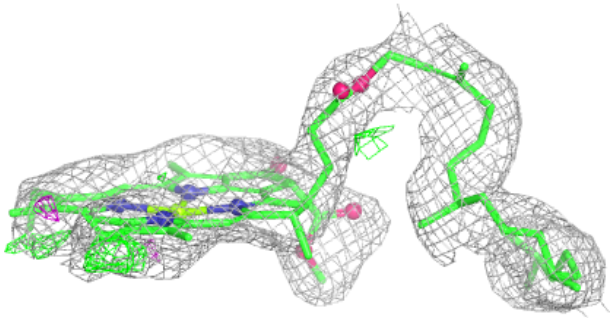


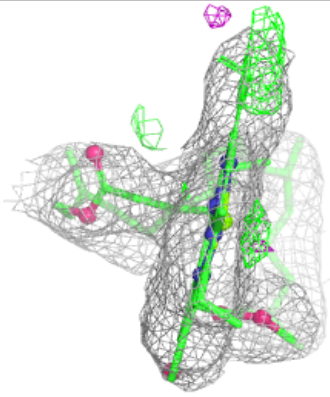


Electron density around CLA AB 612:

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



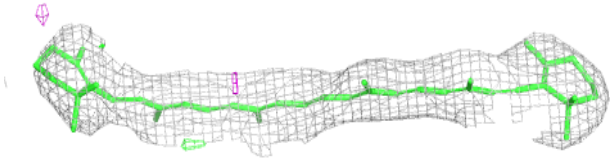


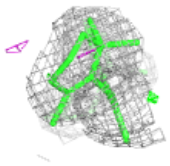


Electron density around BCR AC 515:

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

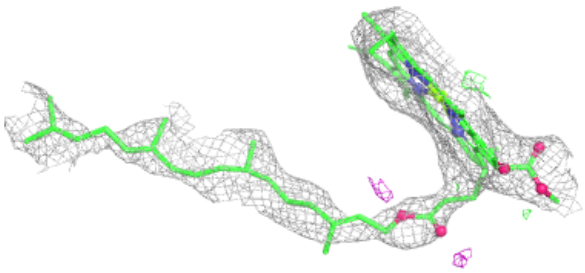


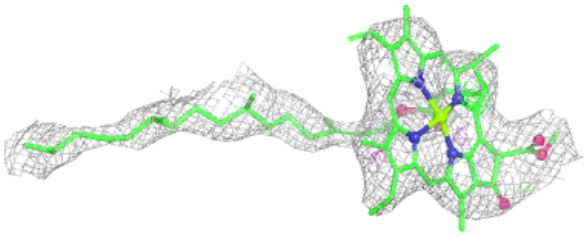


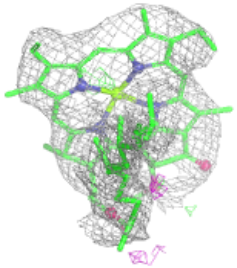


Electron density around CLA BC 504:

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

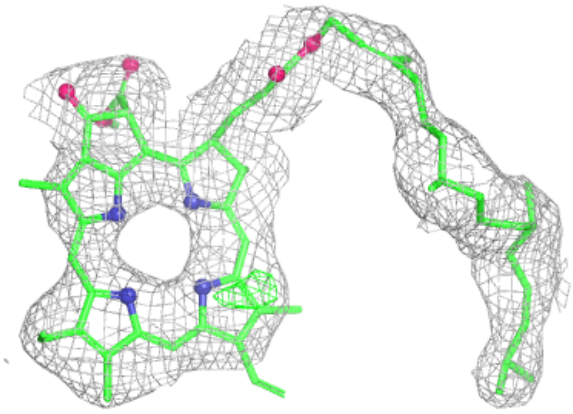


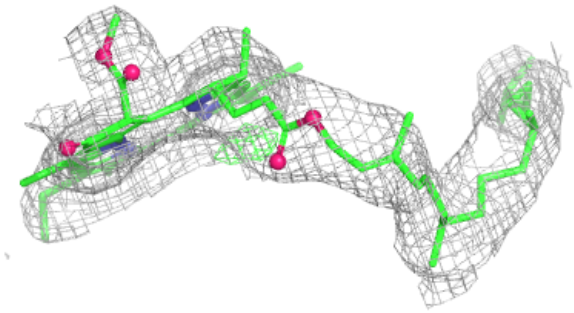


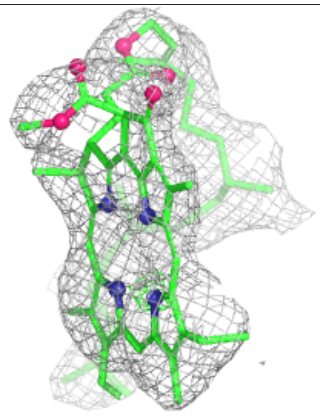


Electron density around PHO BD 403:

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

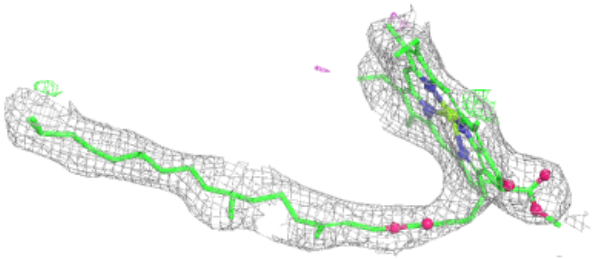


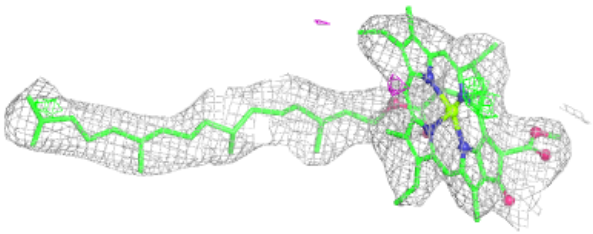


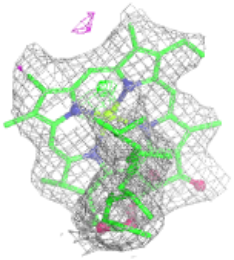


Electron density around CLA BB 610:

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

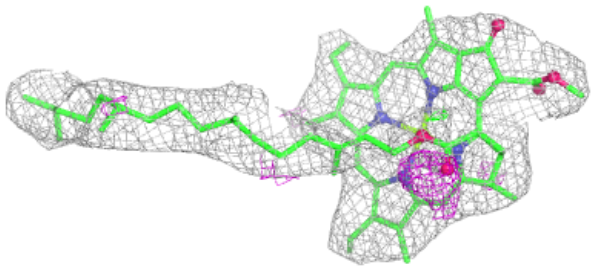


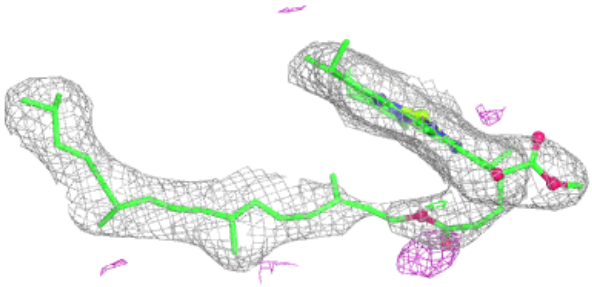


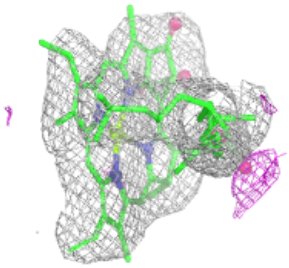


Electron density around CLA BB 611:

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

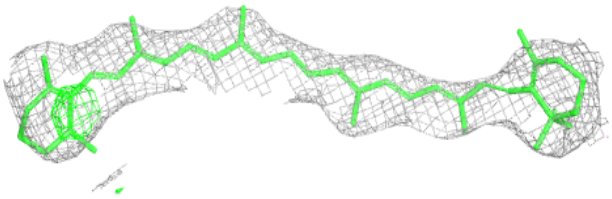


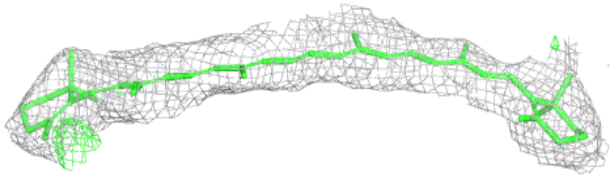


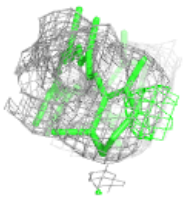


Electron density around BCR AT 102:

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

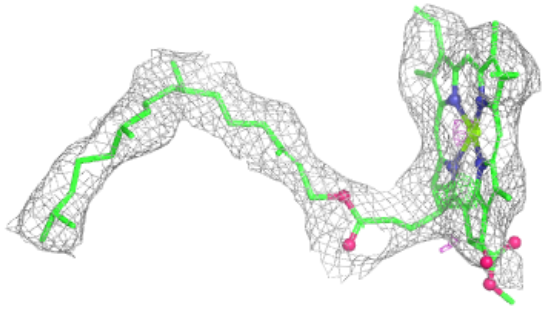


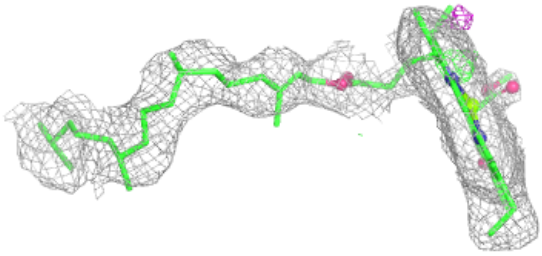


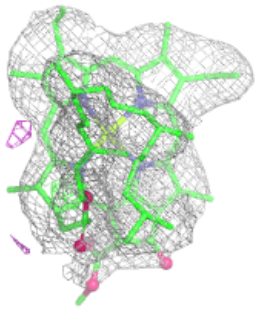


Electron density around CLA AD 404:

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

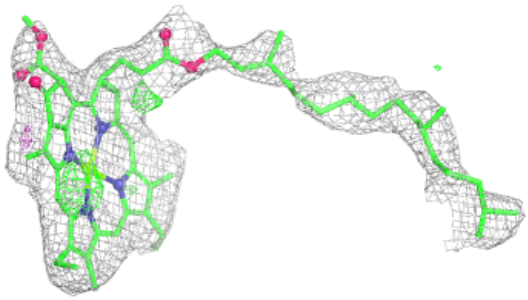


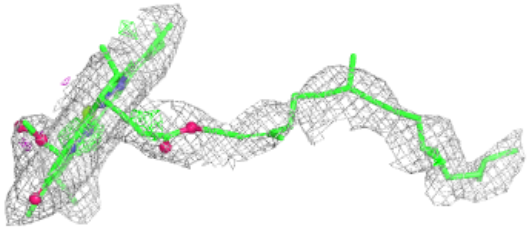


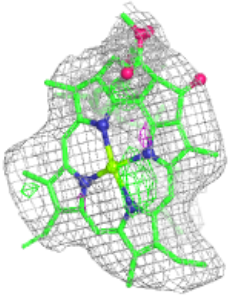


Electron density around CLA BA 407:

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

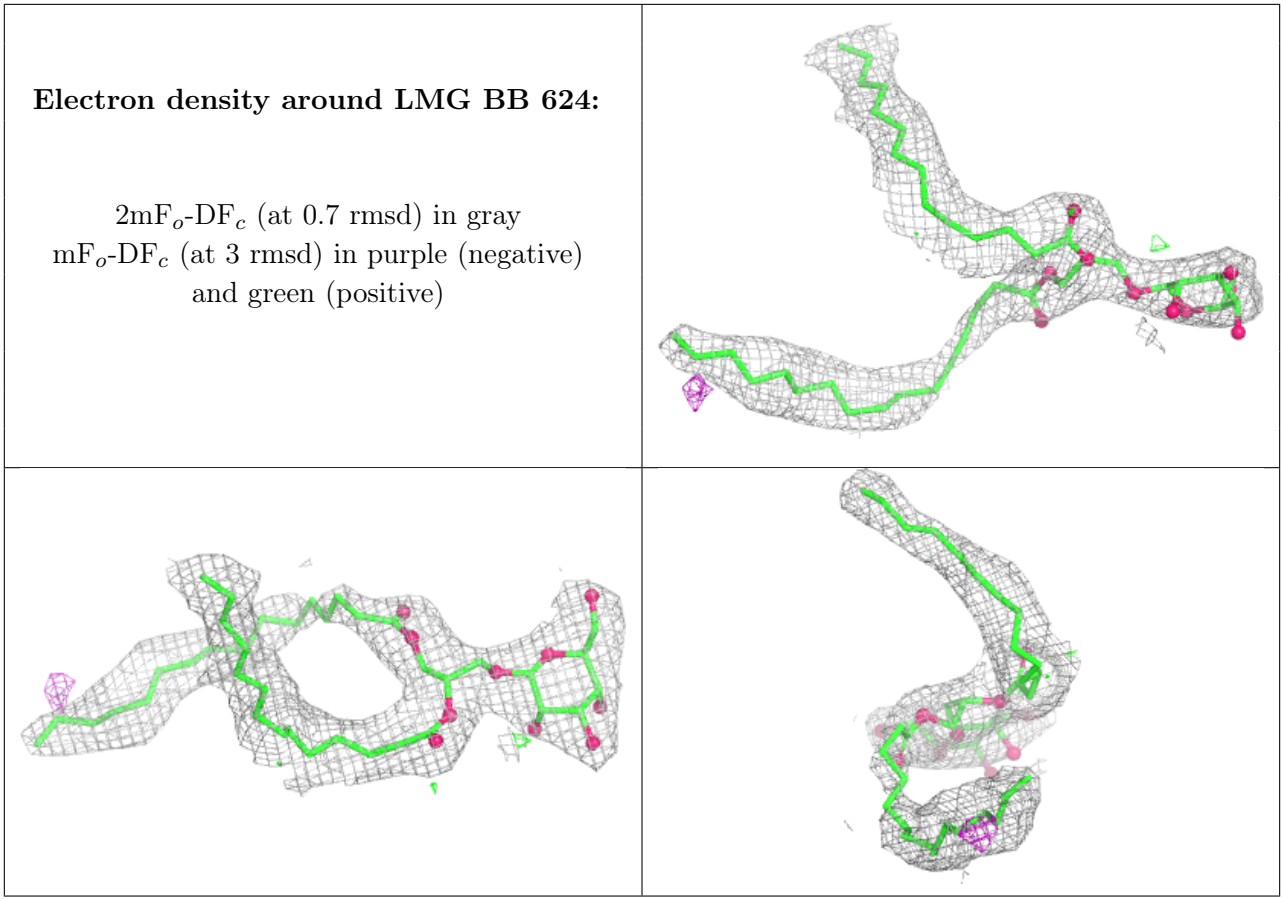






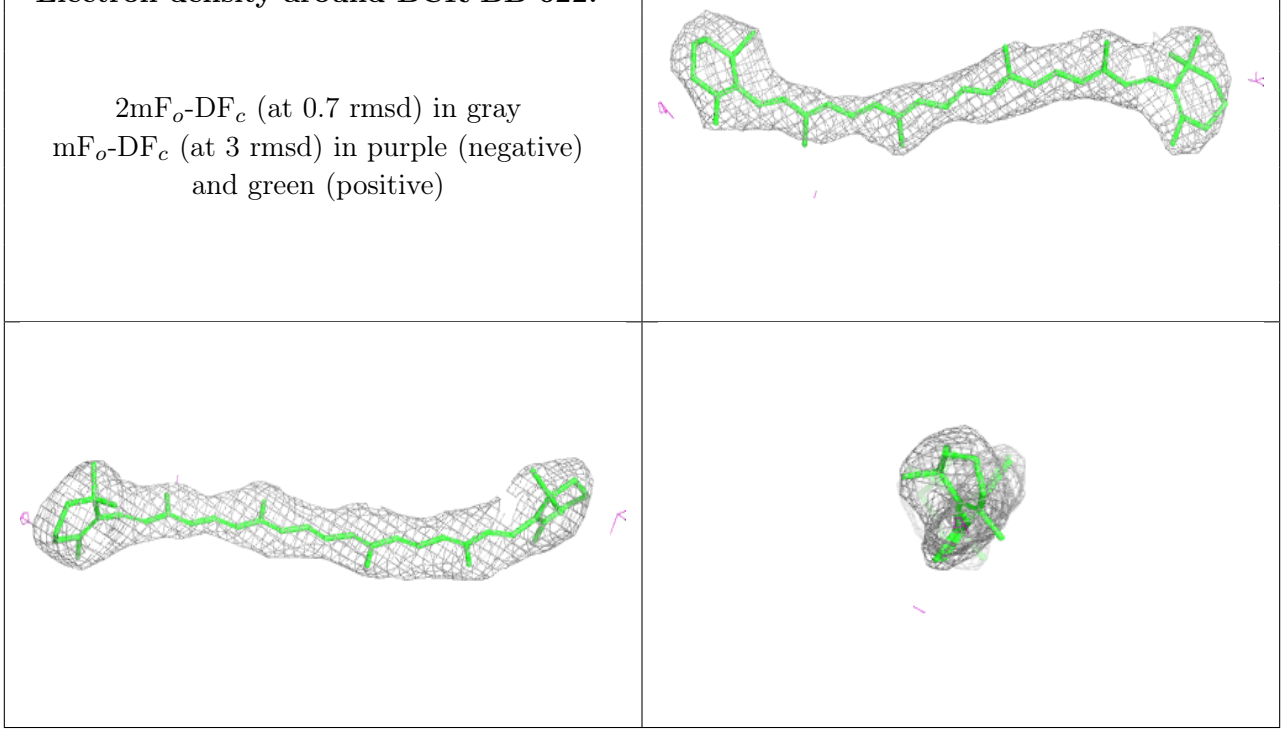
Electron density around LMG BB 624:

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



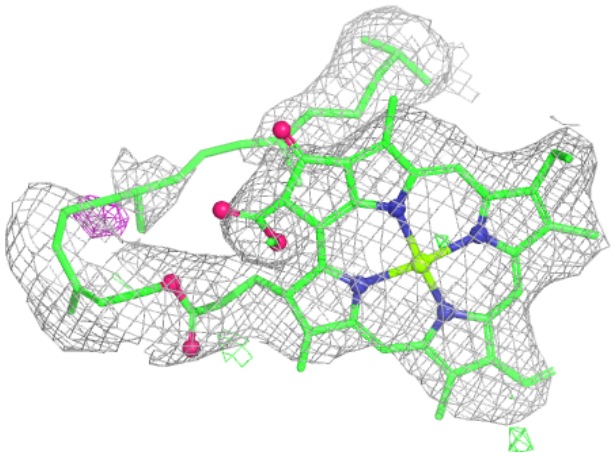
Electron density around BCR BB 622:

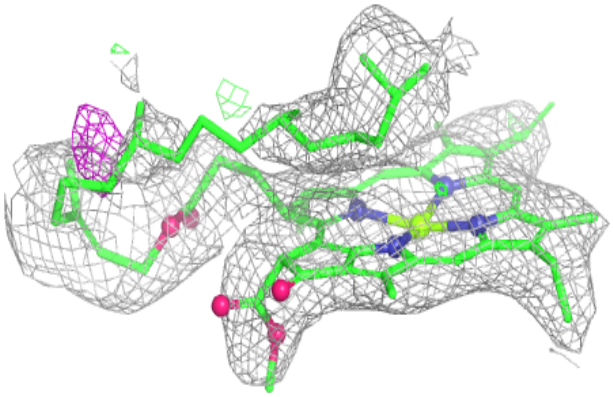
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

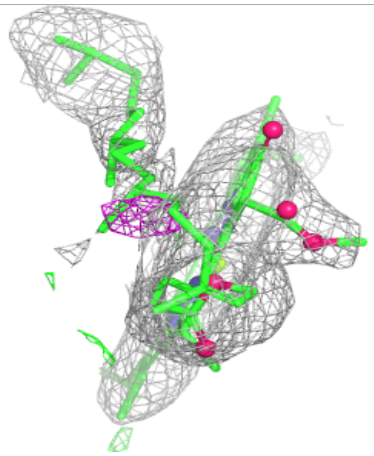


Electron density around CLA BC 509:

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

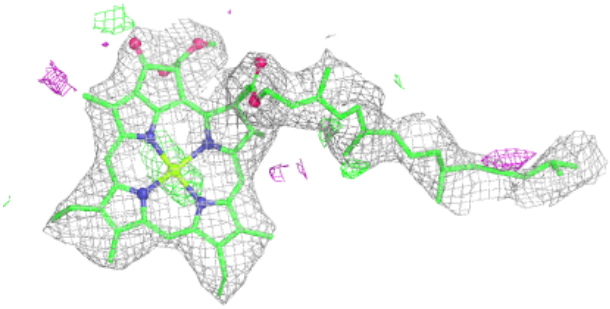


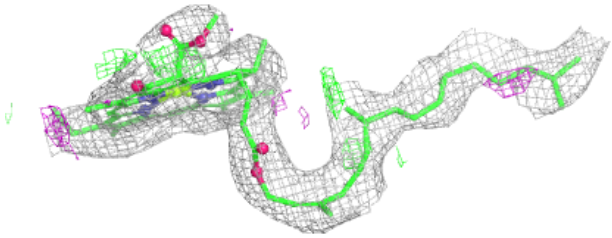


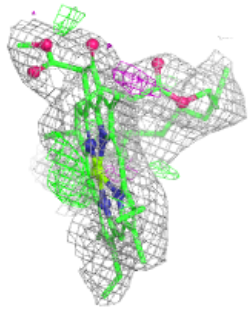


Electron density around CLA AA 404:

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

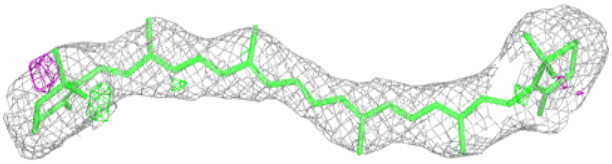


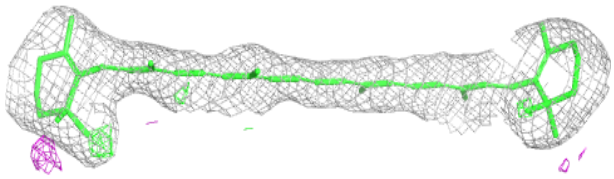


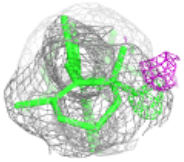


Electron density around BCR AA 409:

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

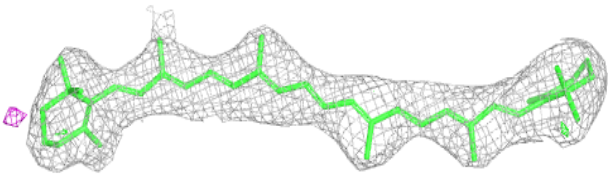


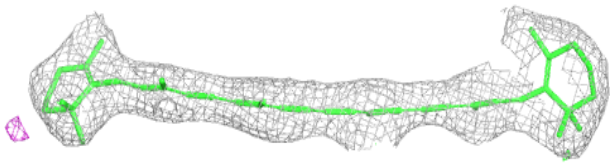


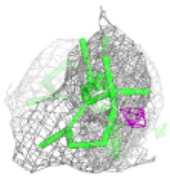


Electron density around BCR AB 617:

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

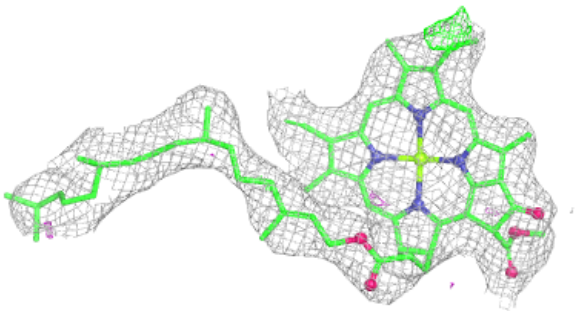


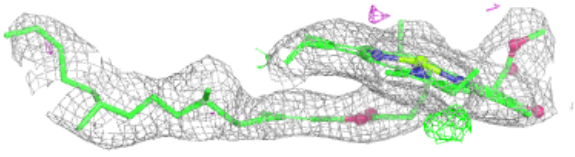


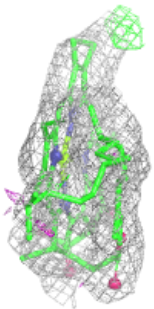


Electron density around CLA BB 606:

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

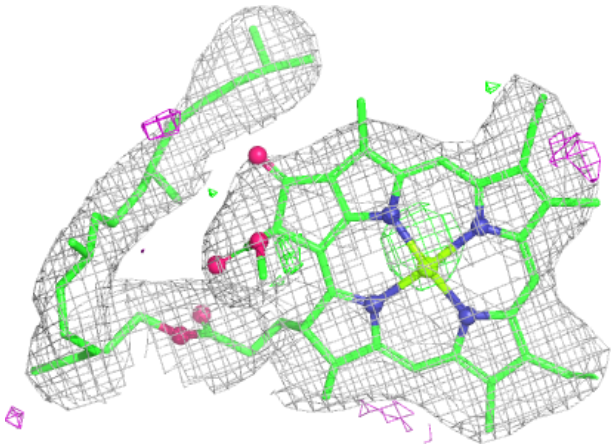


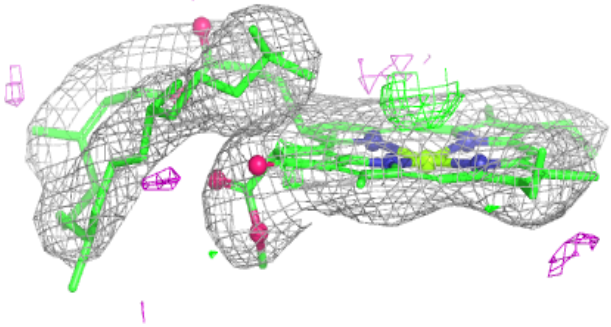


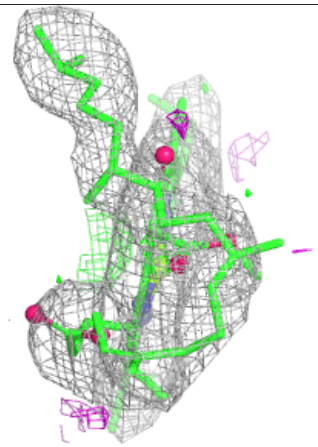


Electron density around CLA BB 613:

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

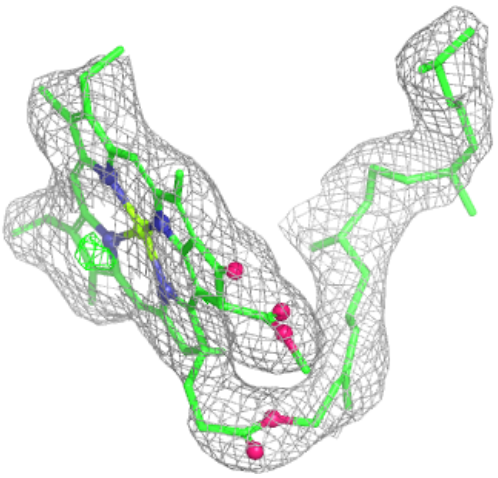


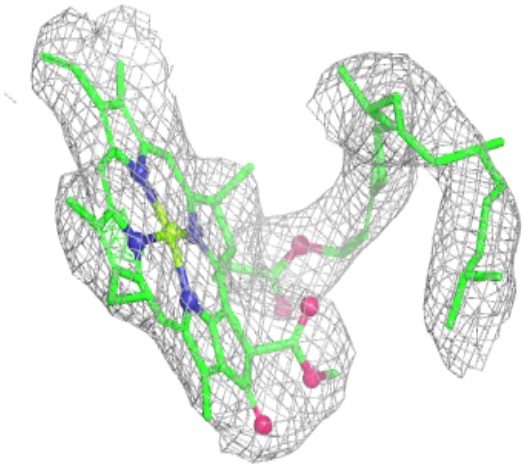


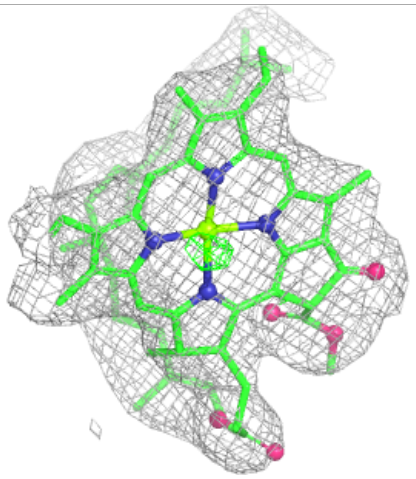


Electron density around CLA AB 613:

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

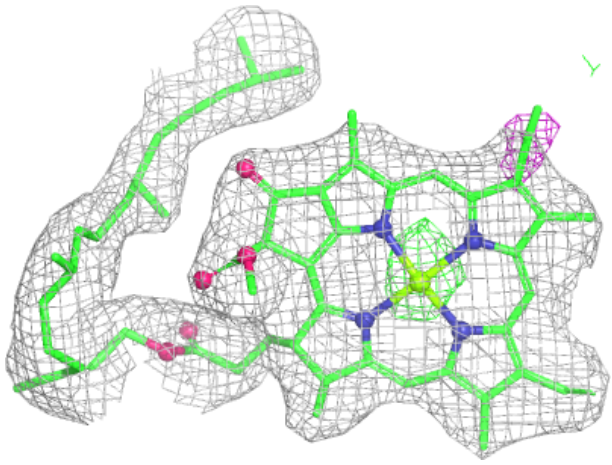


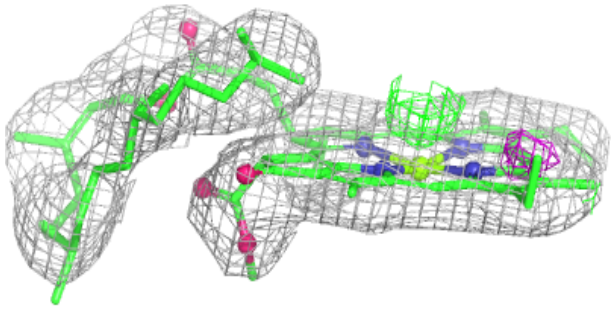




Electron density around CLA AB 610:

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

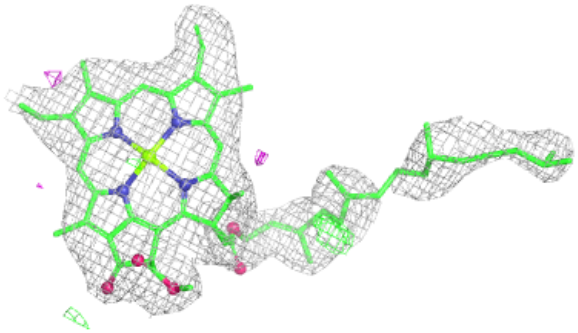


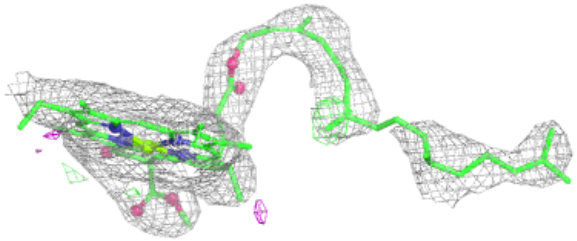


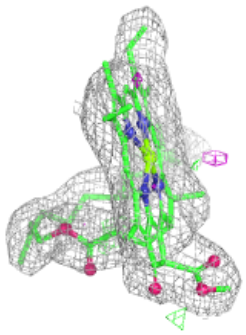


Electron density around CLA BA 405:

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

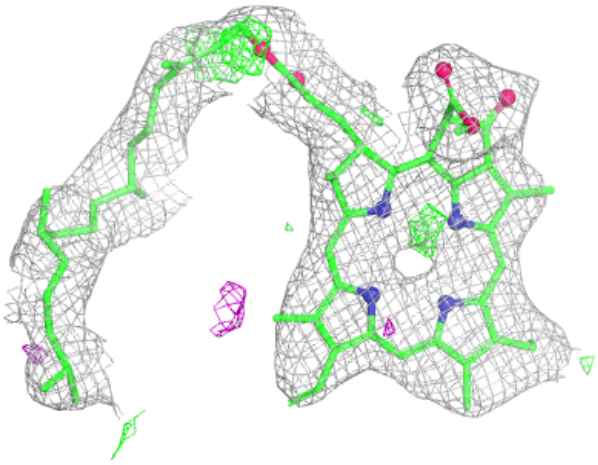


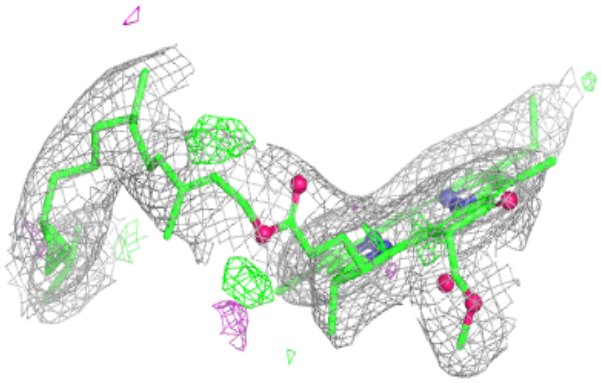




Electron density around PHO AD 403:

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

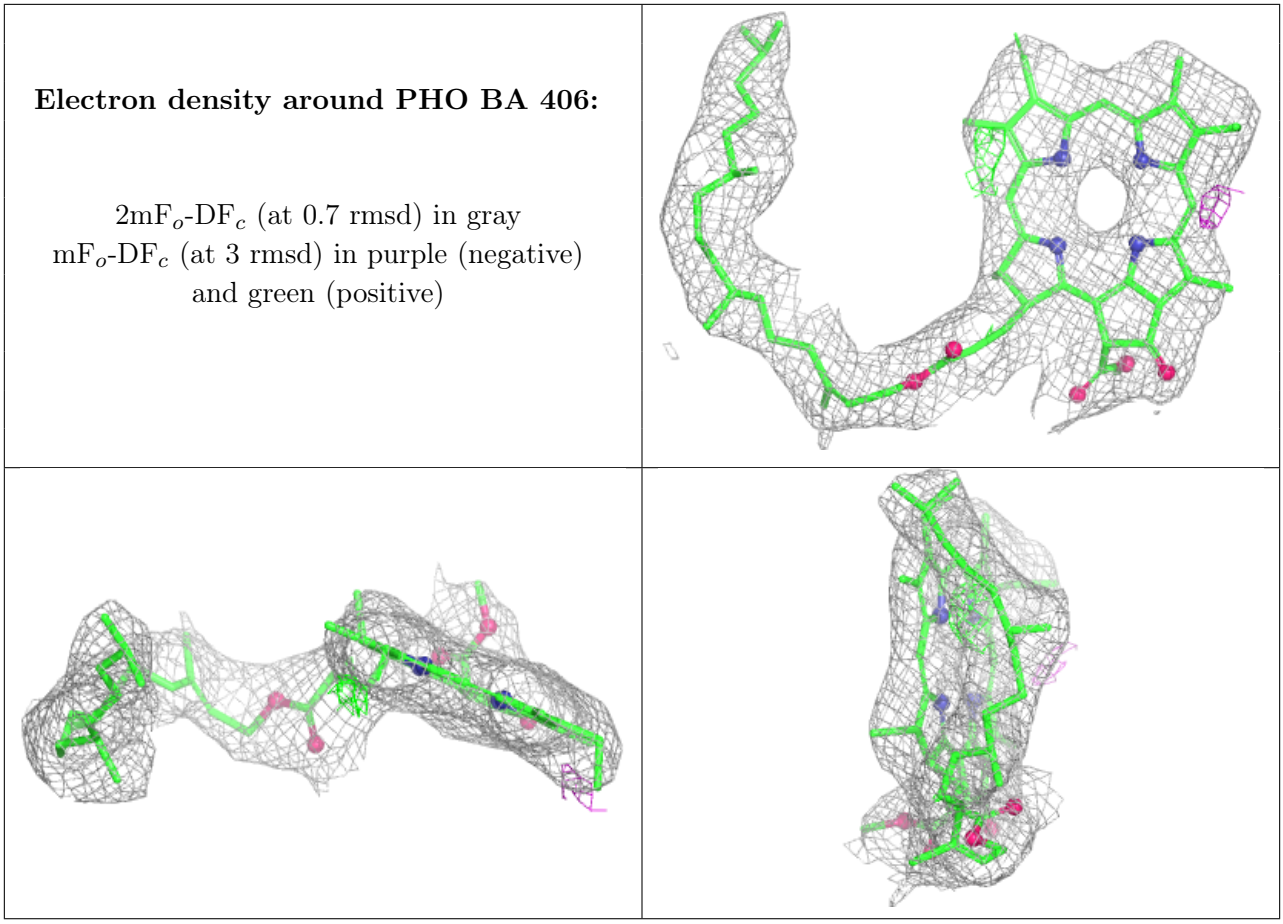






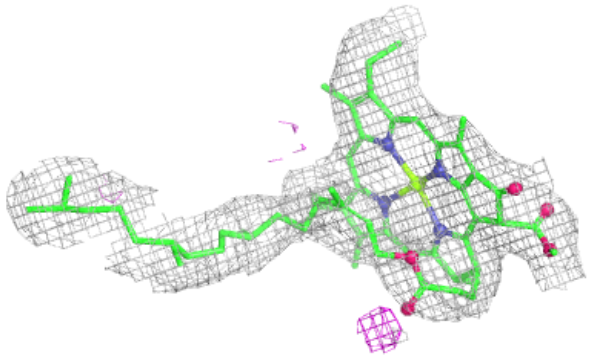
Electron density around PHO BA 406:

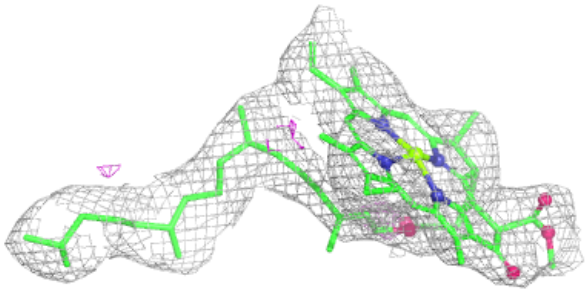
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

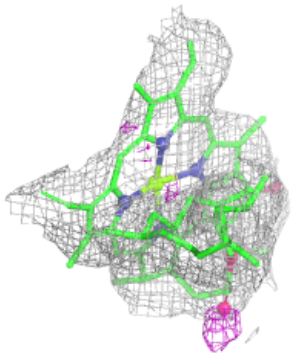


Electron density around CLA AC 505:

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

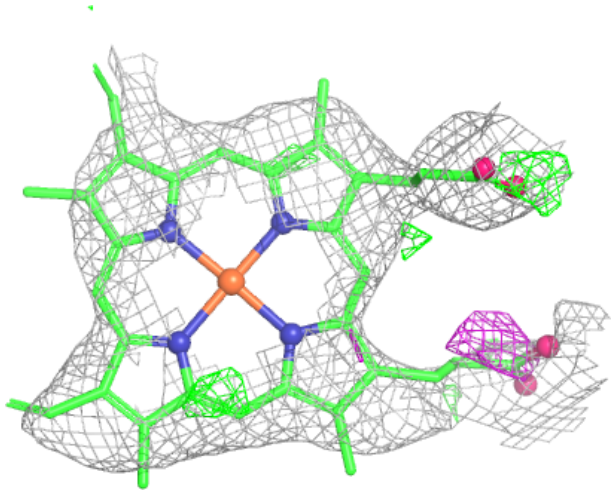


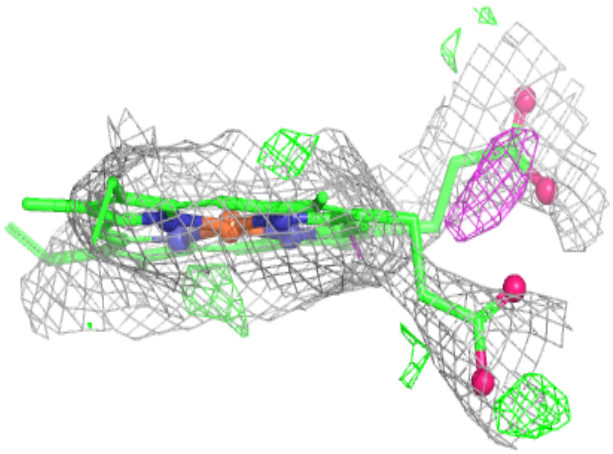


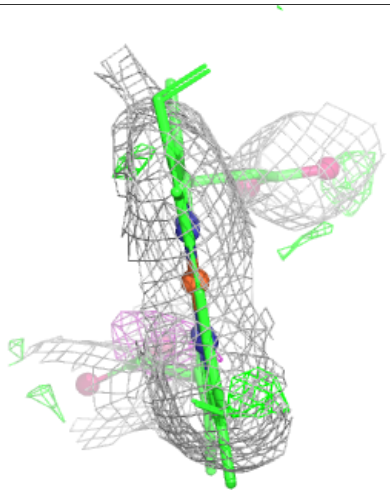


Electron density around HEM BE 101:

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

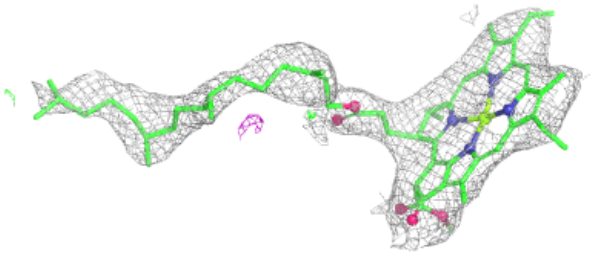


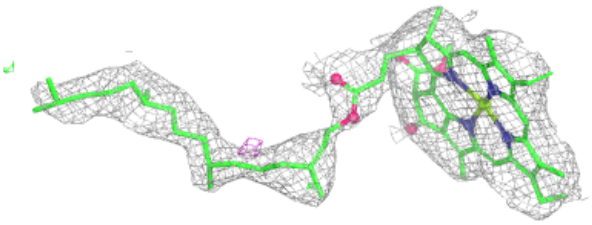


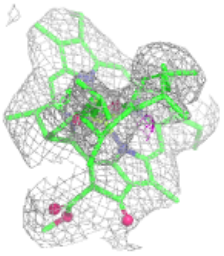


Electron density around CLA BC 502:

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

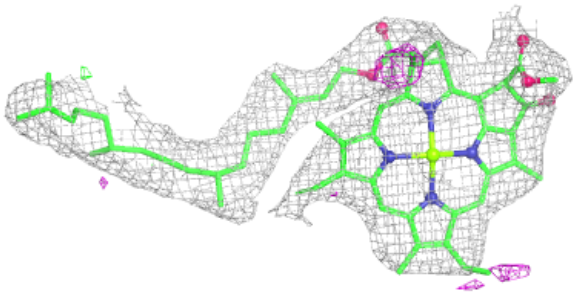


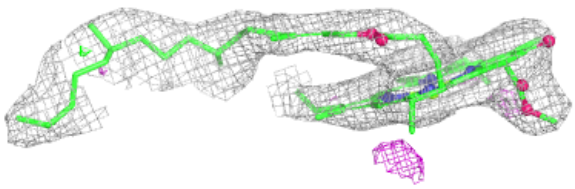


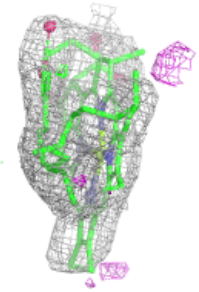


Electron density around CLA AB 603:

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

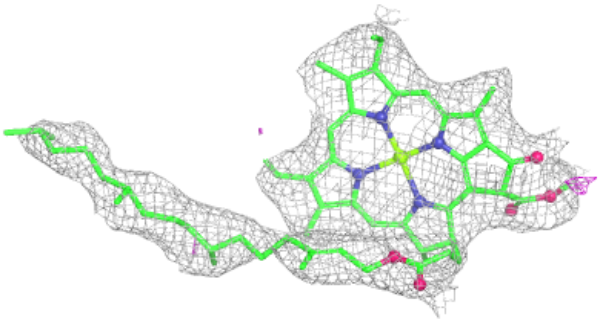


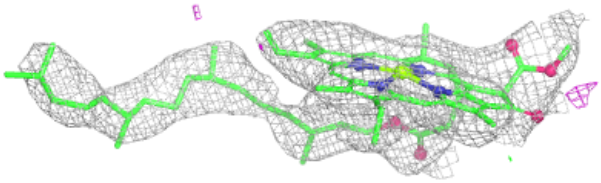


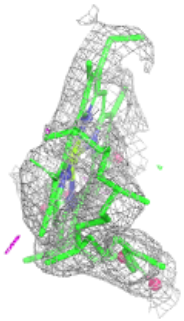


Electron density around CLA AC 501:

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

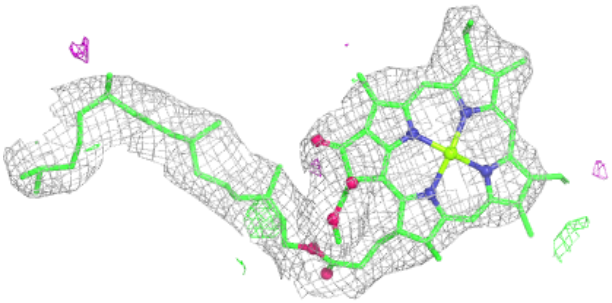


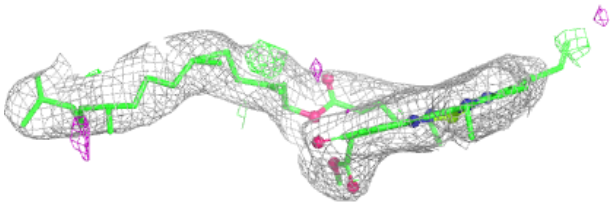


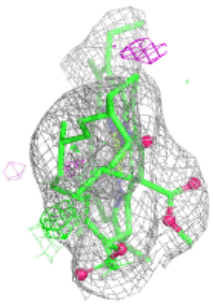


Electron density around CLA BB 605:

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

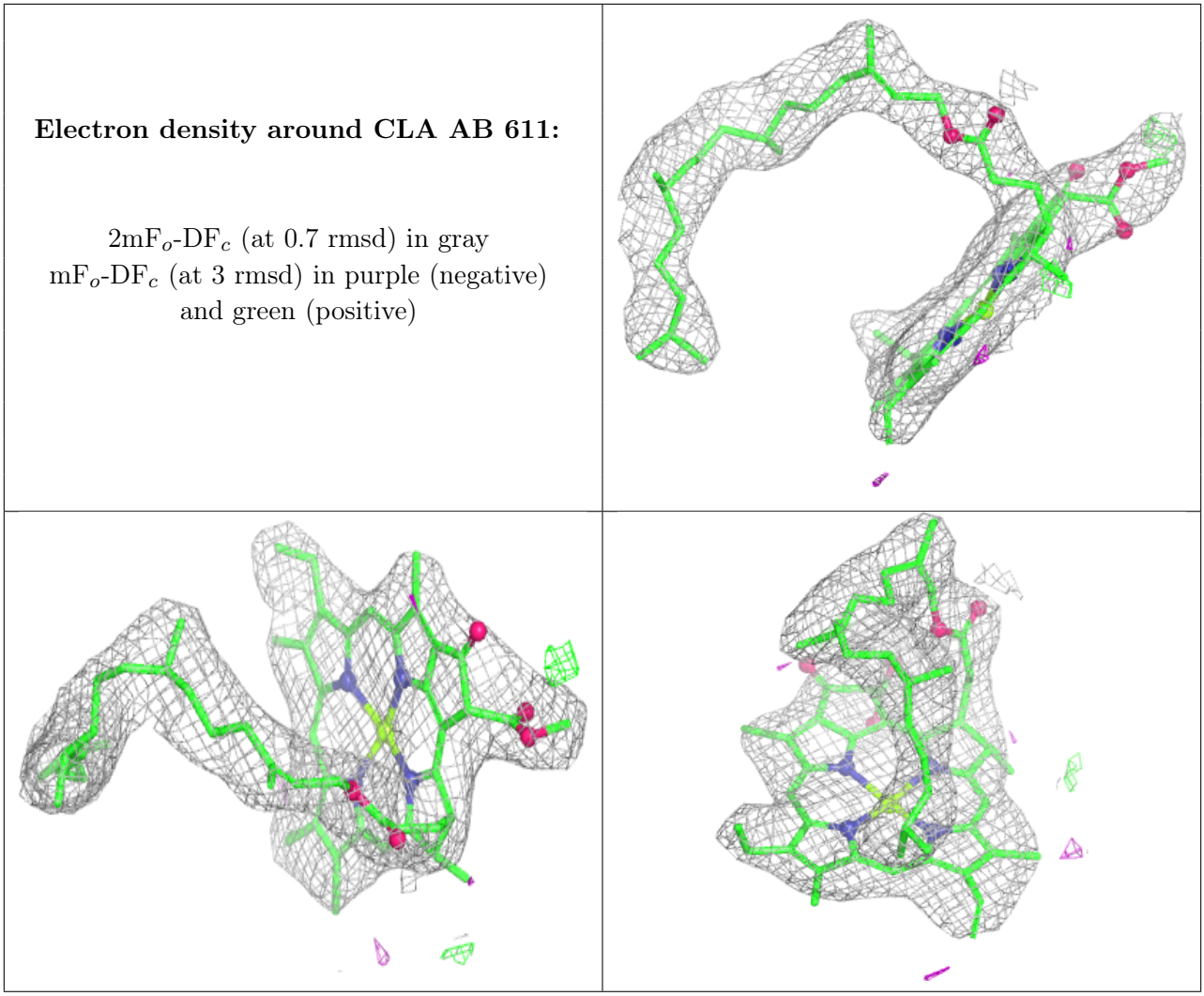






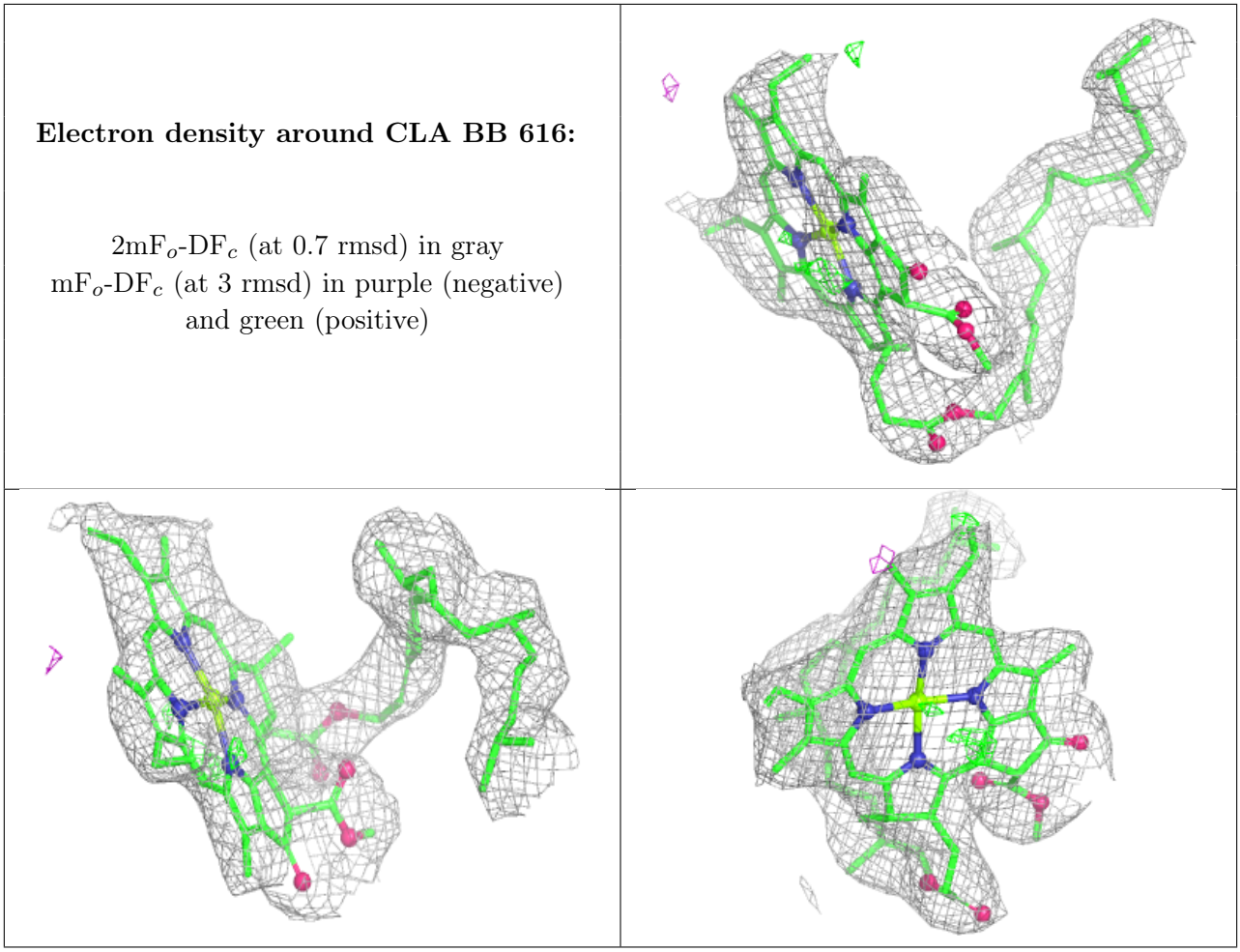
Electron density around CLA AB 611:

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



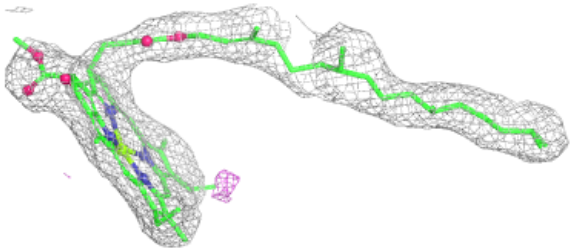
Electron density around CLA BB 616:

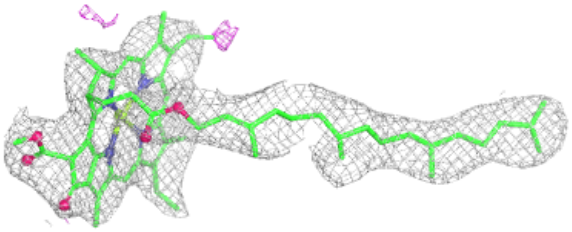
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

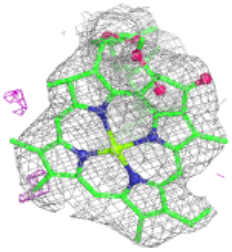


Electron density around CLA AB 607:

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

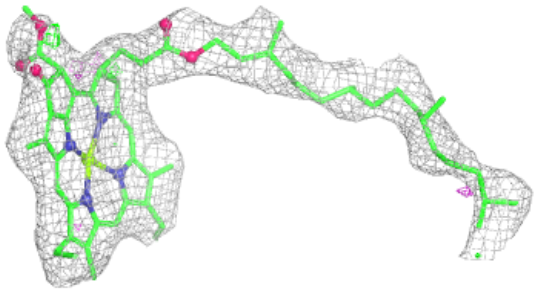


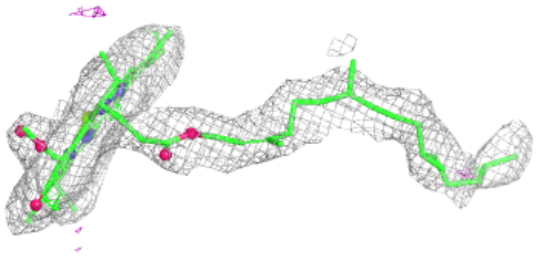


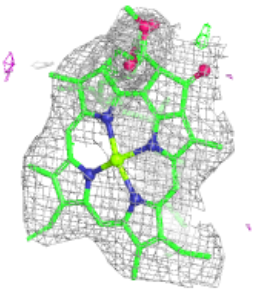


Electron density around CLA AA 406:

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

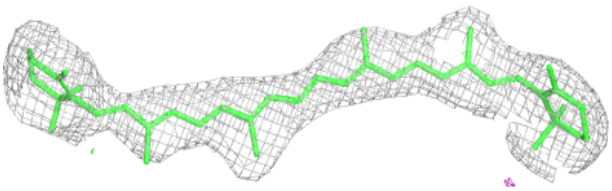


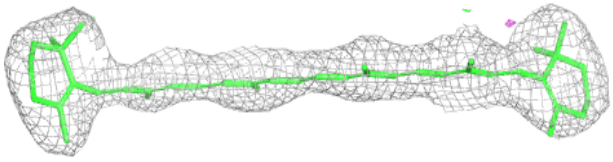


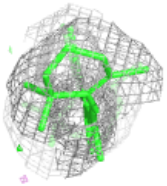


Electron density around BCR BA 410:

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

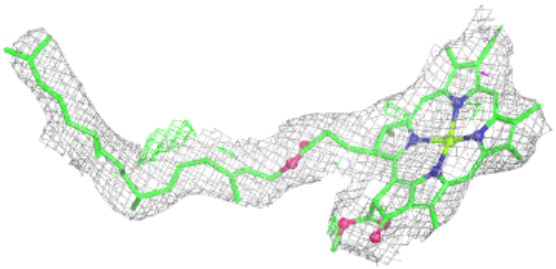


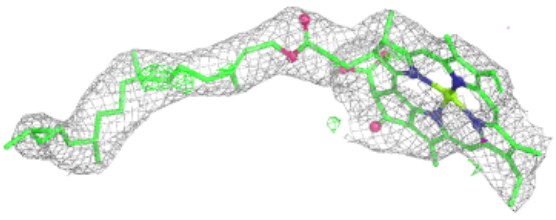


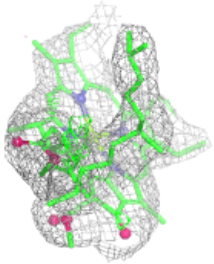


Electron density around CLA BA 403:

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

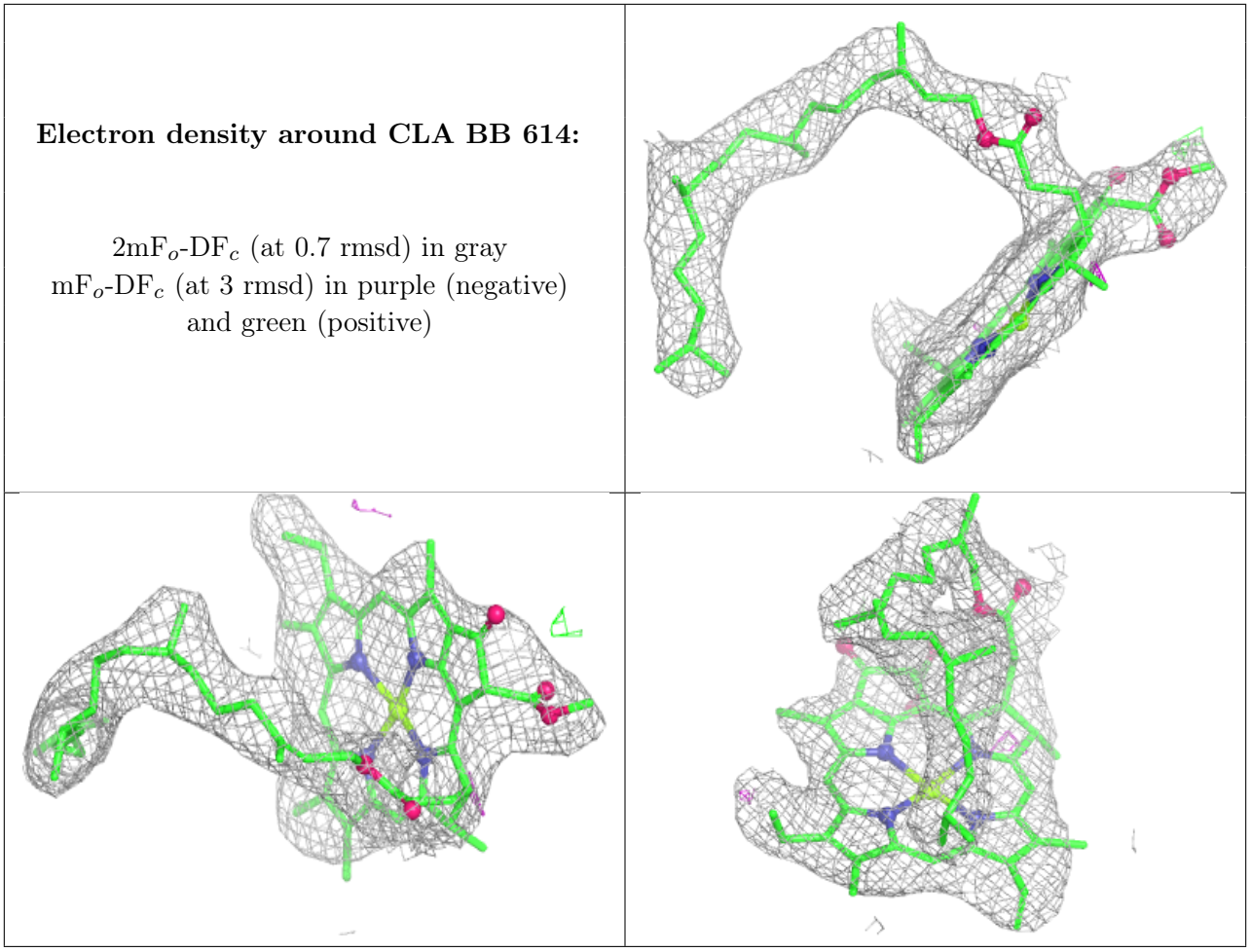






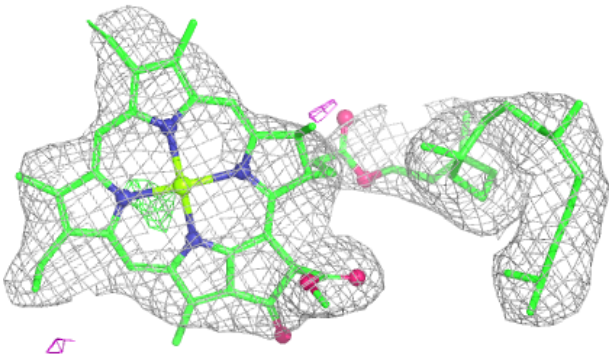
Electron density around CLA BB 614:

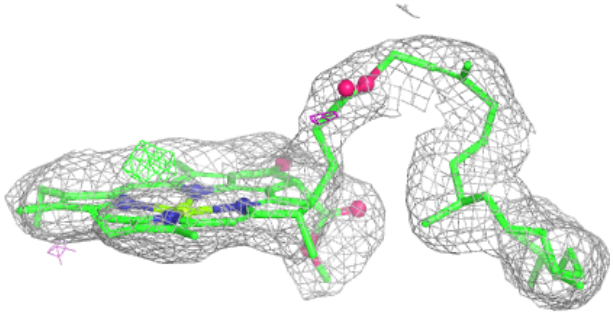
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

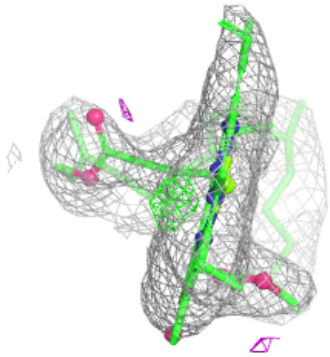


Electron density around CLA BB 615:

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

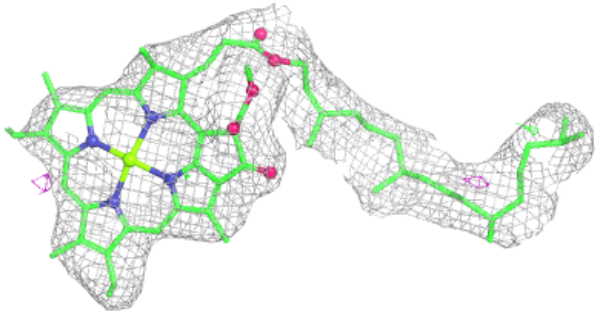


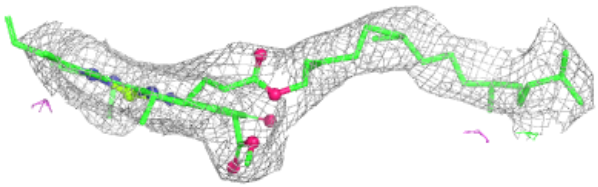


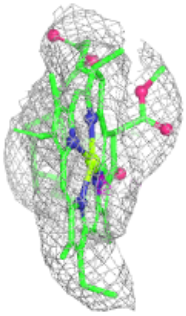


Electron density around CLA AB 602:

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

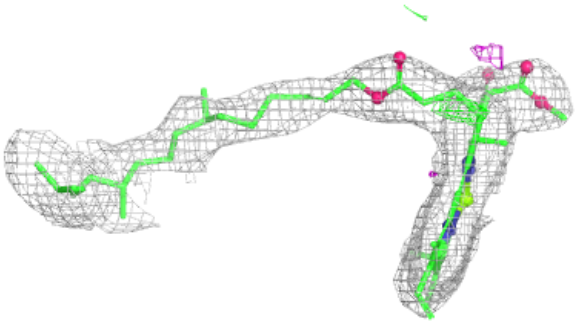


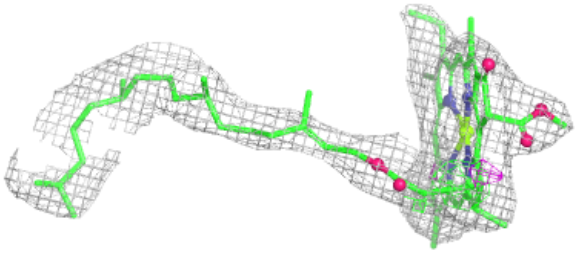


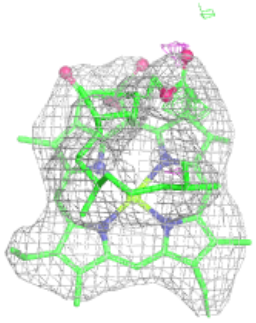


Electron density around CLA AB 605:

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

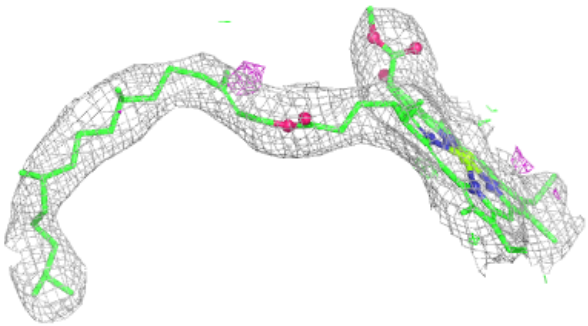


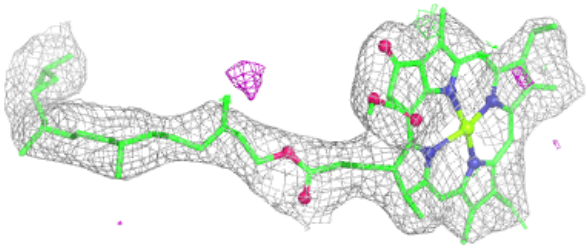


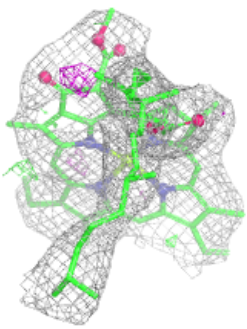


Electron density around CLA AD 402:

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

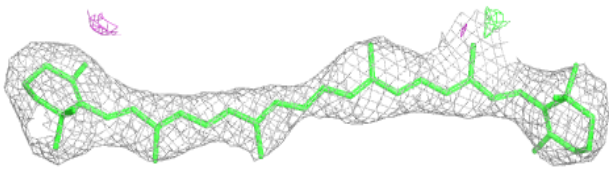


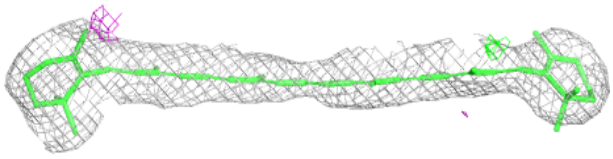


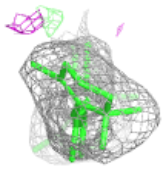


Electron density around BCR BB 621:

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

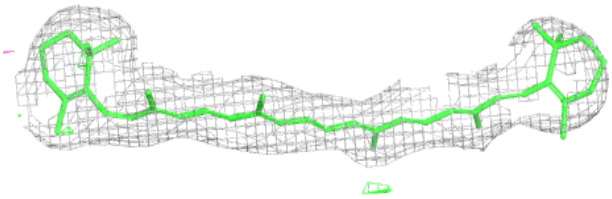


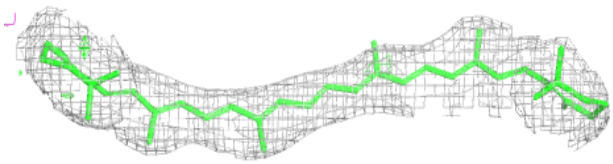


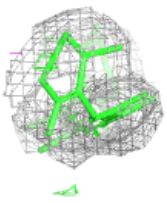


Electron density around BCR AC 514:

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

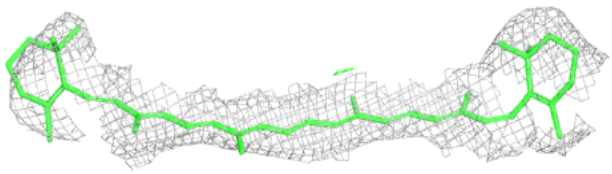


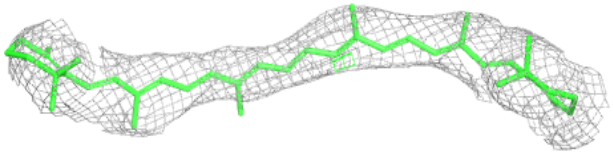


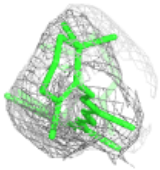


Electron density around BCR BC 514:

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

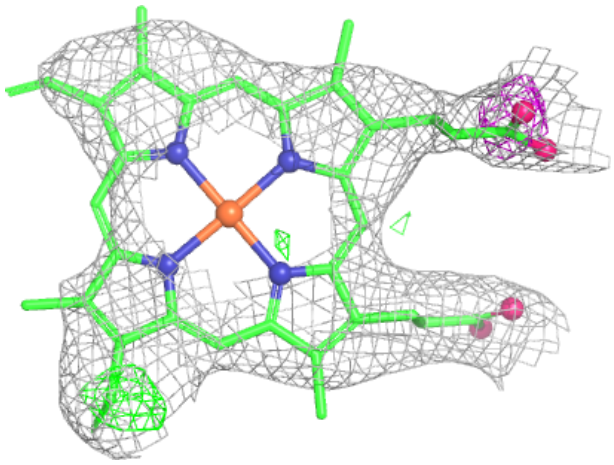


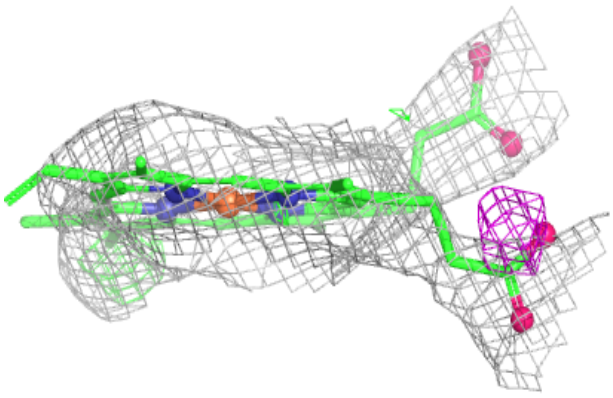


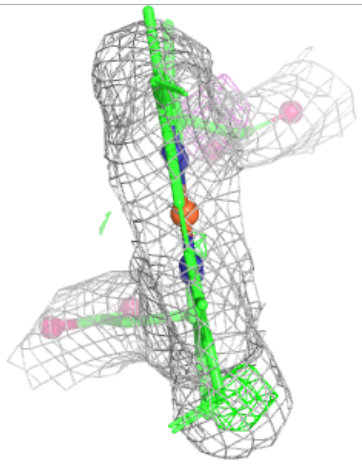


Electron density around HEM AE 101:

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

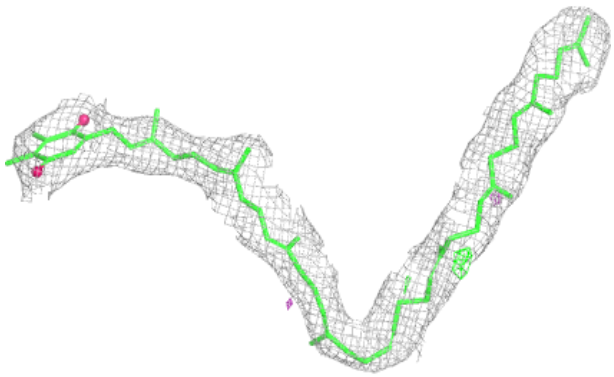


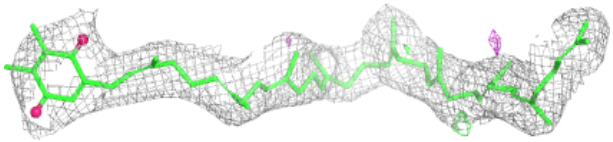




Electron density around PL9 BD 405:

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

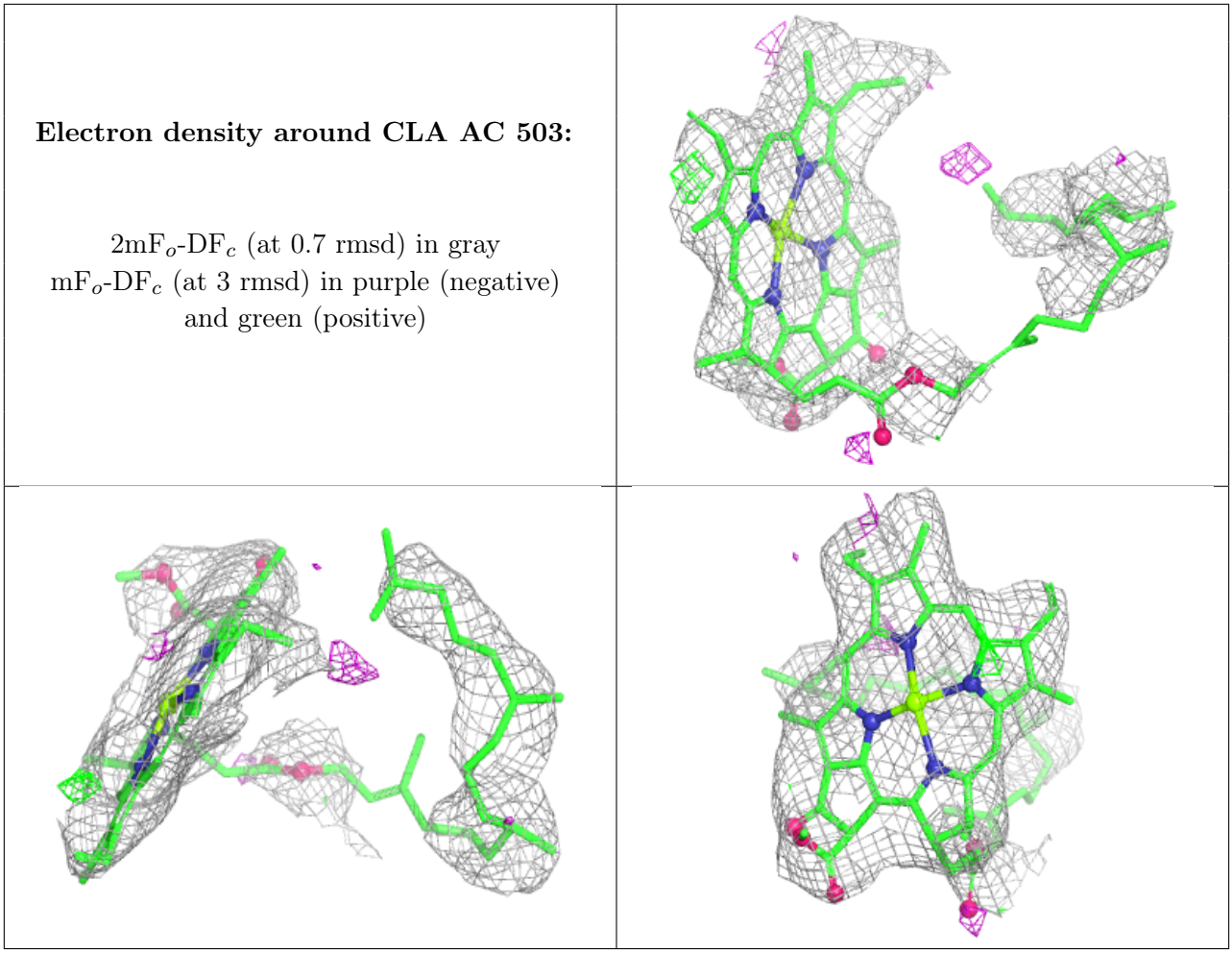






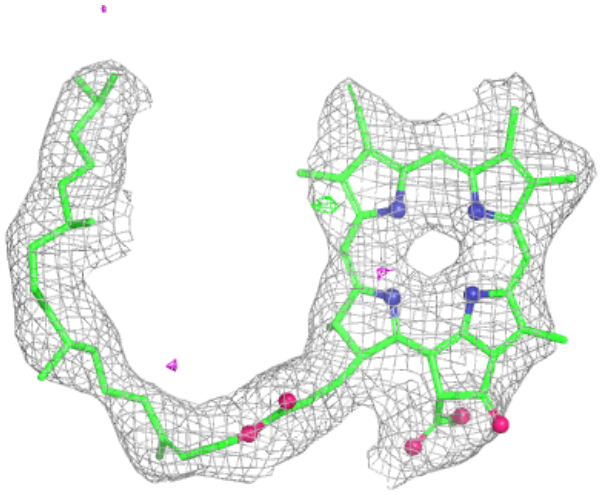
Electron density around CLA AC 503:

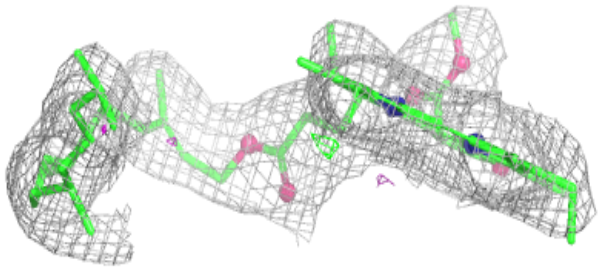
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

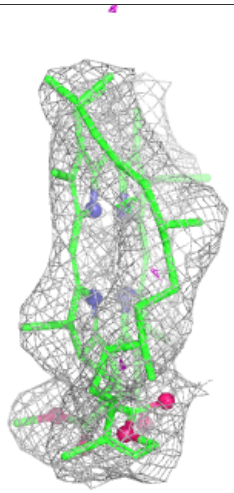


Electron density around PHO AA 405:

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

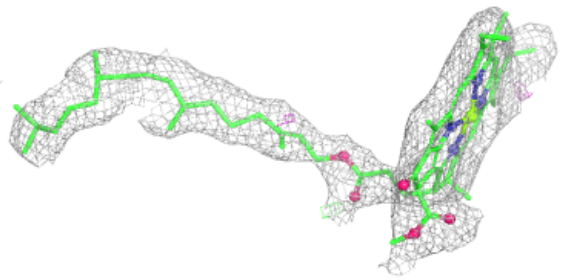


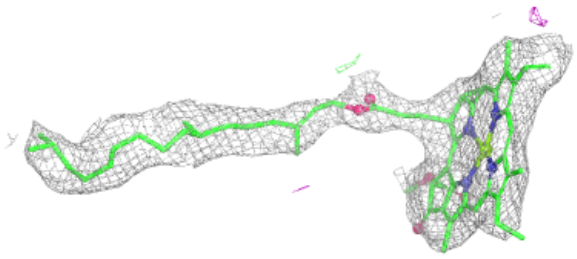


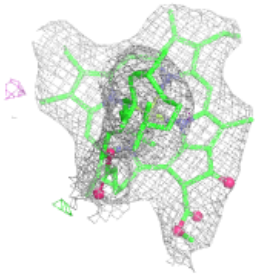


Electron density around CLA BB 607:

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

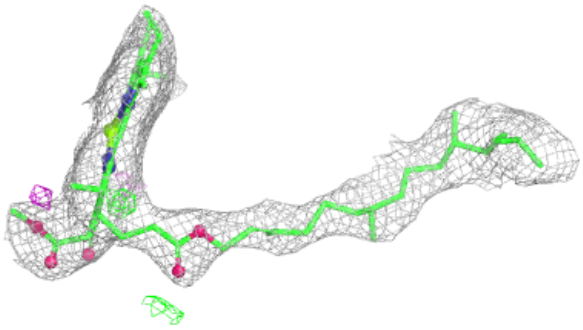


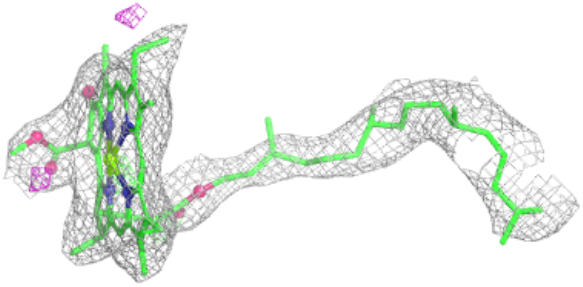


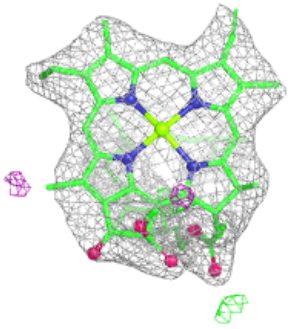


Electron density around CLA BB 608:

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

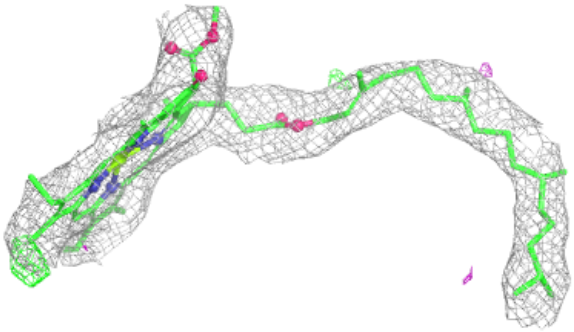


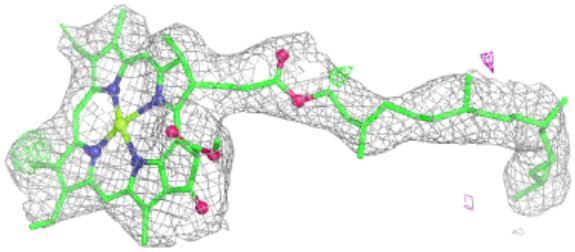


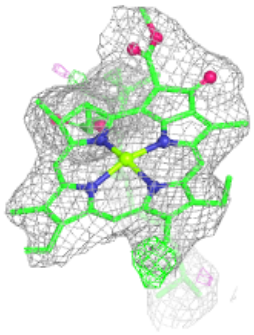


Electron density around CLA BD 402:

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

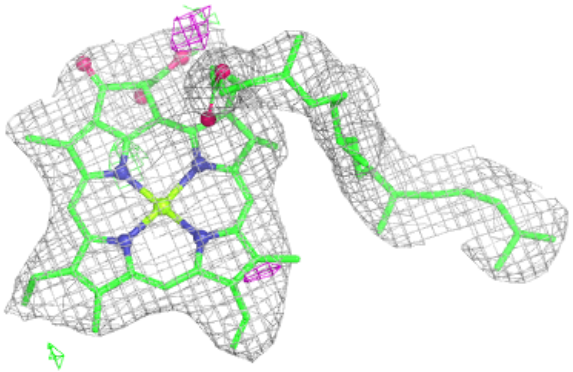


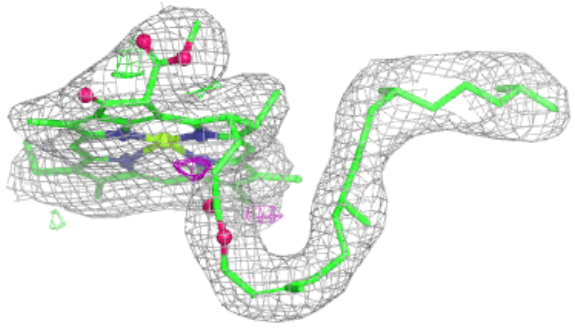


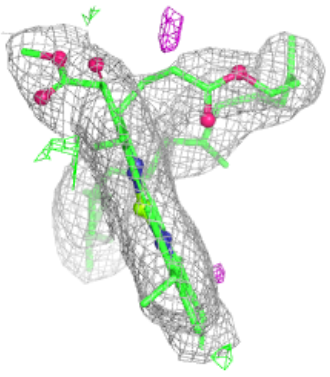


Electron density around CLA BA 404:

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

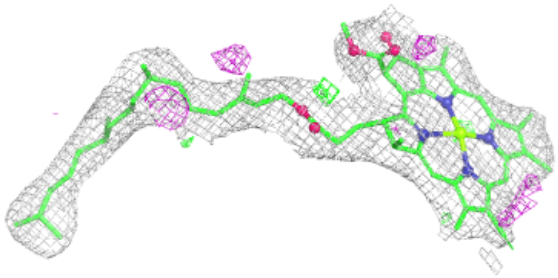


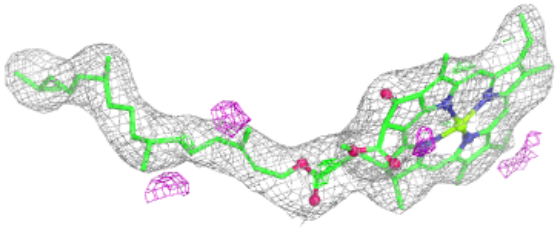


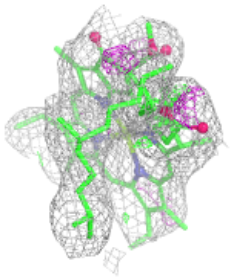


Electron density around CLA AA 402:

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

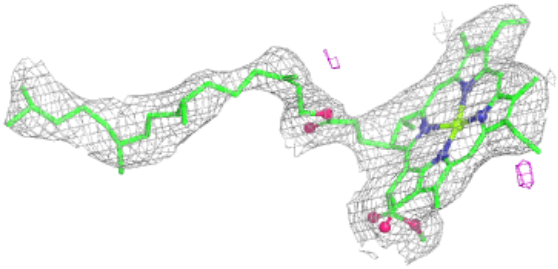


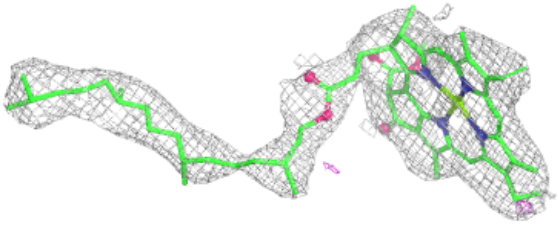


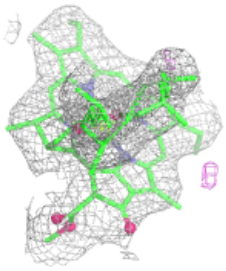


Electron density around CLA AC 502:

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

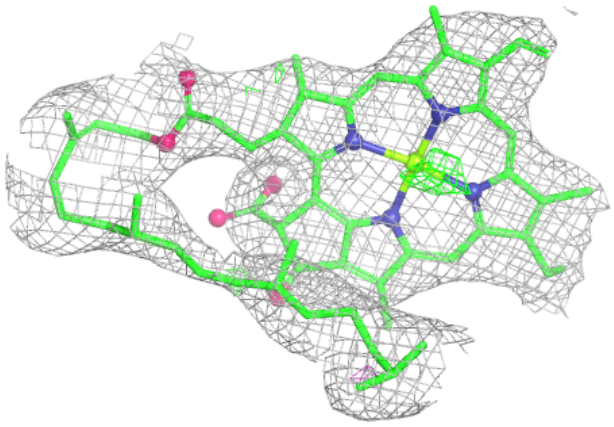


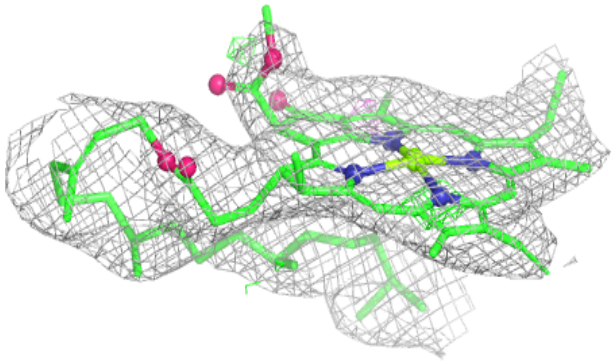


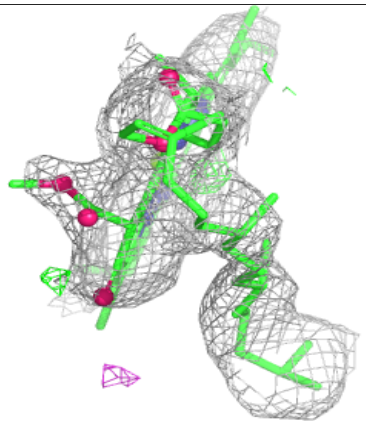


Electron density around CLA AC 509:

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

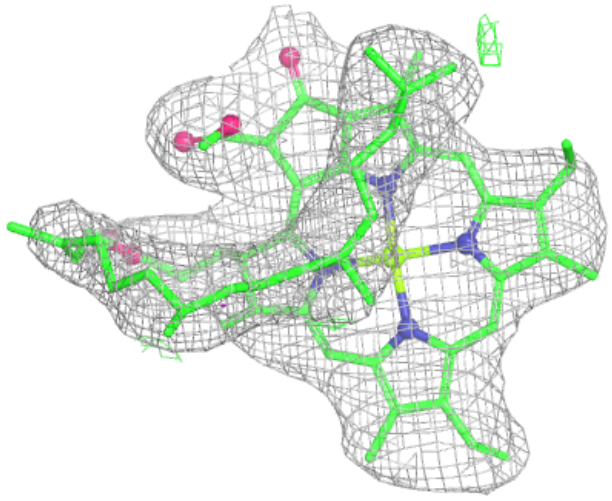


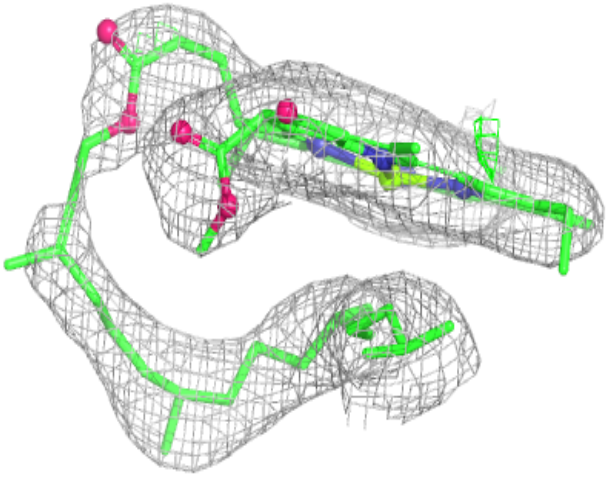


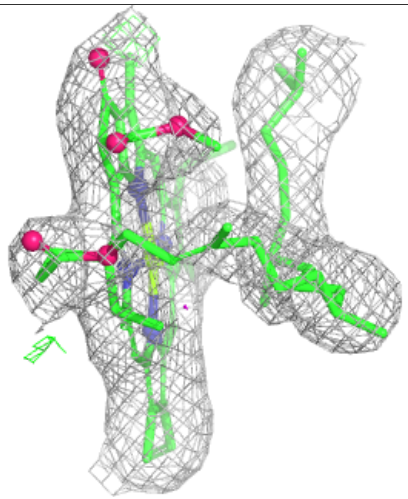


Electron density around CLA AC 510:

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

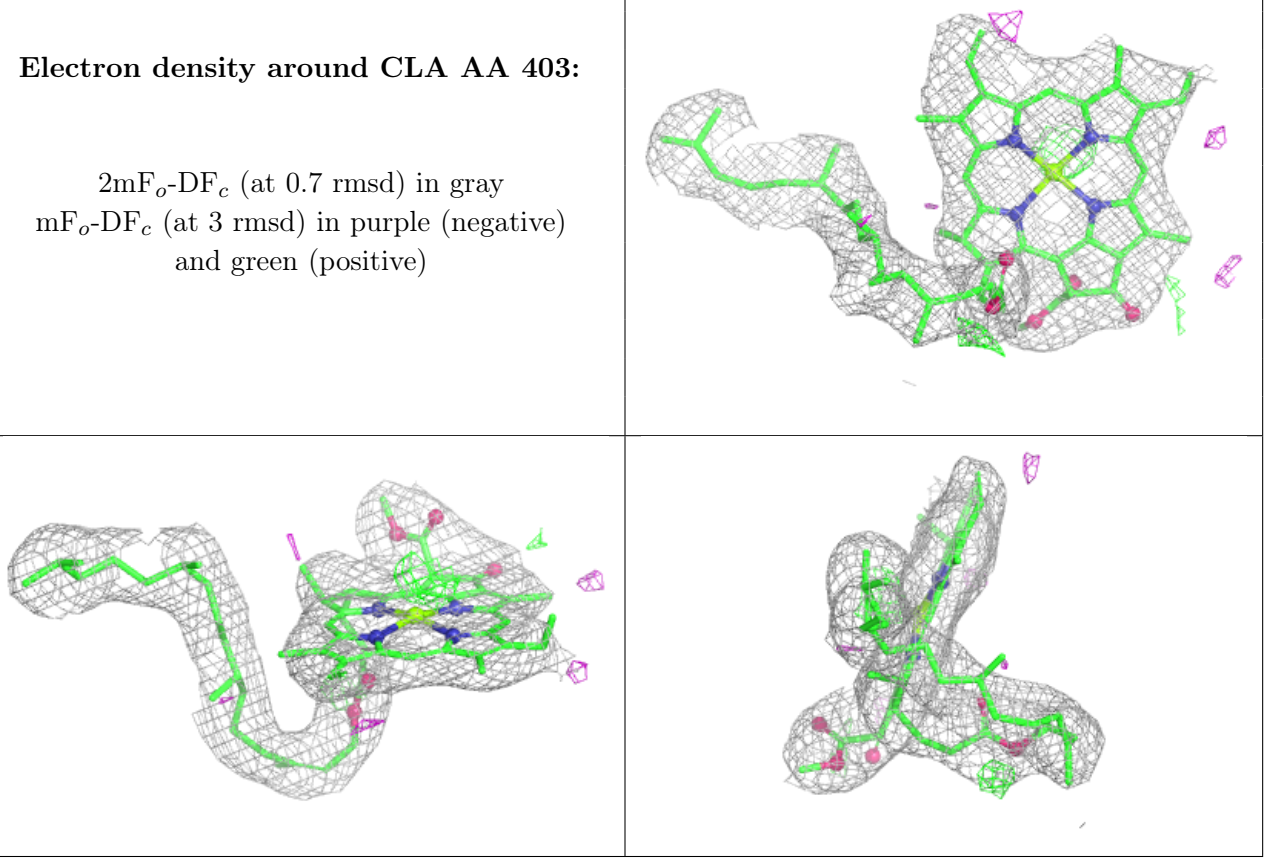






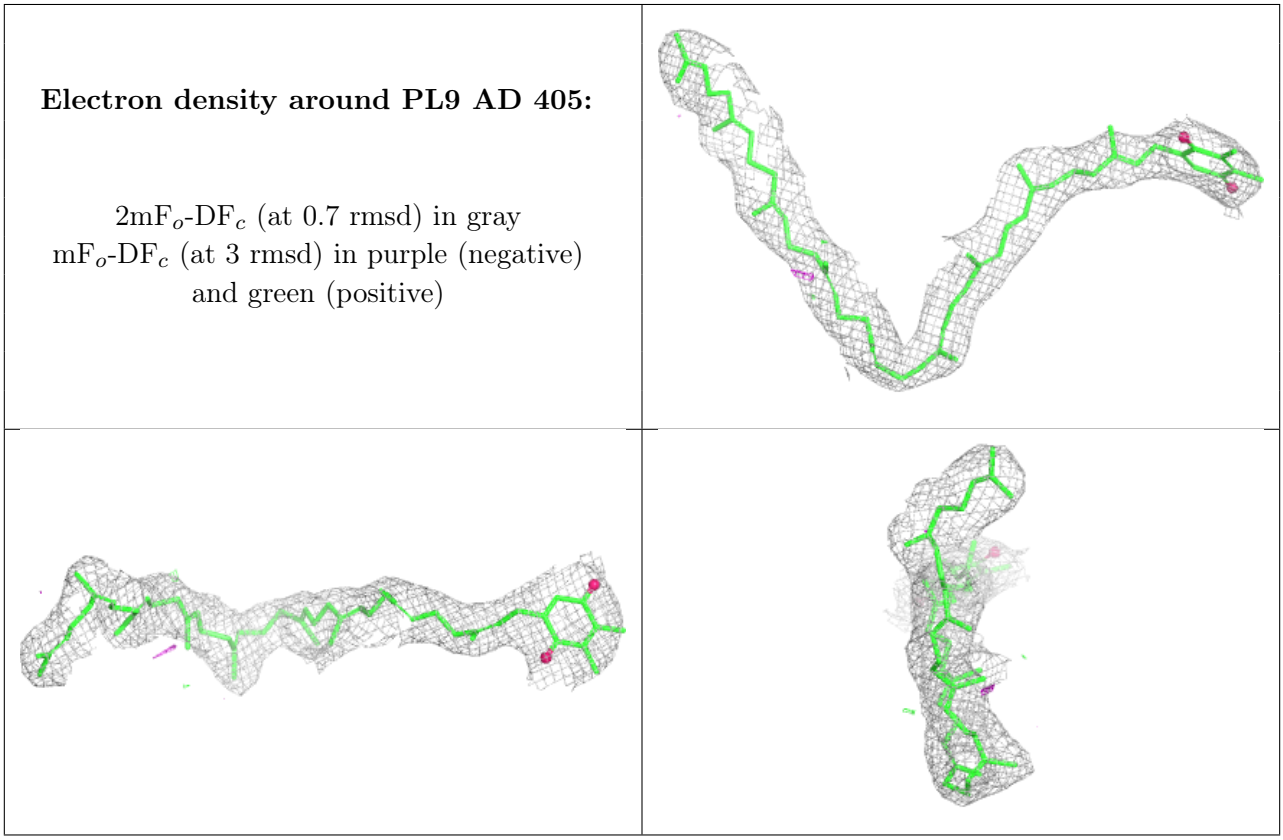
Electron density around CLA AA 403:

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



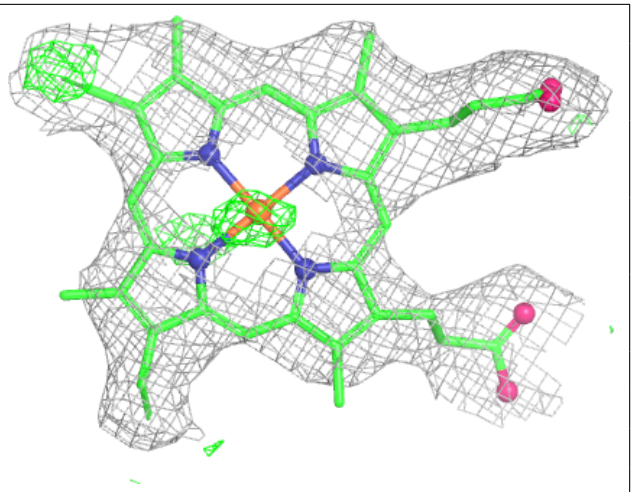
Electron density around PL9 AD 405:

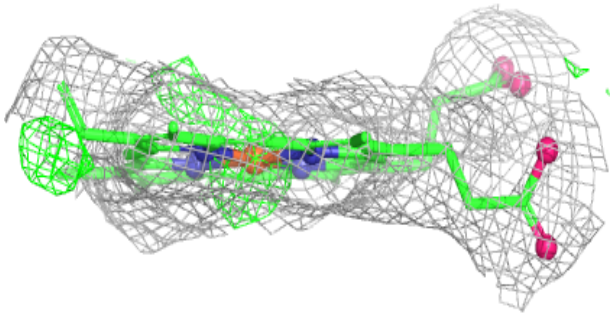
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

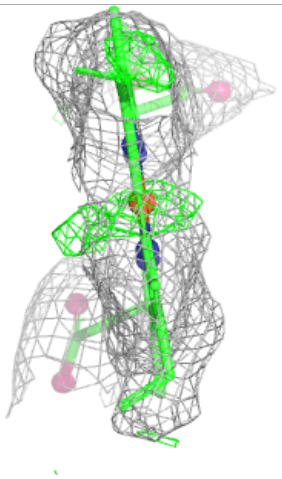


Electron density around HEM AV 201:

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

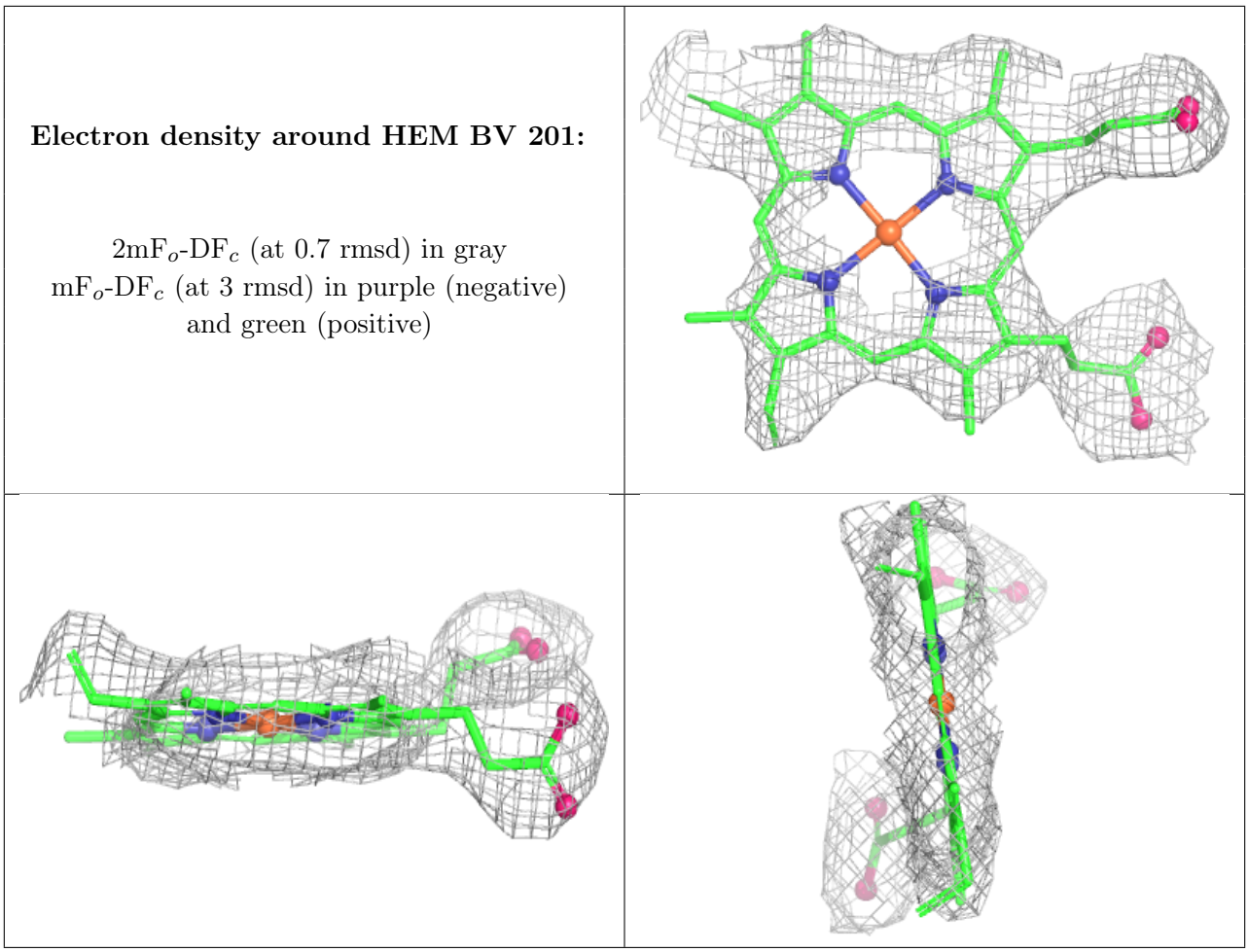






Electron density around HEM BV 201:

$2mF_o$-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

There are no such residues in this entry.