Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:42 AM UTC

PDB ID	:	7COH / pdb_00007coh
Title	:	Dimeric Form of Bovine Heart Cytochrome c Oxidase in the Fully Oxidized State
Authors	:	Shinzawa-Itoh, K.; Muramoto, K.
Deposited on	:	2020-08-04
Resolution	:	1.30 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 ⓘ symbol.

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

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

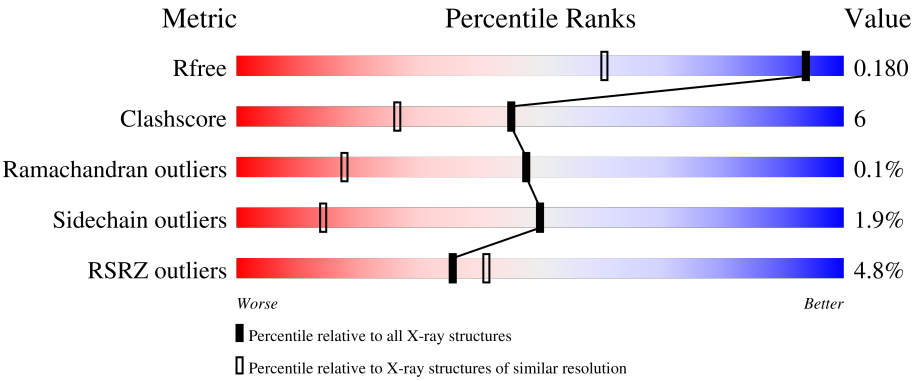
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 1.30 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	1553 (1.30-1.30)
Clashscore	190562	1595 (1.30-1.30)
Ramachandran outliers	187476	1551 (1.30-1.30)
Sidechain outliers	187428	1551 (1.30-1.30)
RSRZ outliers	180081	1549 (1.30-1.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	514	83% 15%
1	N	514	2% 88% 11%
2	B	227	9% 78% 17%
2	O	227	5% 81% 16%
3	C	261	2% 85% 14%

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Mol	Chain	Length	Quality of chain
3	P	261	85% 13%
4	D	147	90% 7%
4	Q	147	12% 87% 7%
5	E	109	93% 6%
5	R	109	92% 6%
6	F	98	3% 79% 11% 7%
6	S	98	3% 85% 7%
7	G	85	9% 73% 11% 15%
7	T	85	9% 69% 12% 15%
8	H	85	11% 75% 12% 12%
8	U	85	12% 75% 8% 5% 12%
9	I	73	14% 82% 12%
9	V	73	11% 77% 15%
10	J	59	10% 81% 12% 5%
10	W	59	10% 85% 10% 5%
11	K	56	4% 80% 5% 12%
11	X	56	11% 79% 7% 12%
12	L	47	6% 83% 9% 6%
12	Y	47	2% 85% 9% 6%
13	M	46	4% 76% 9% 13%
13	Z	46	11% 80% 7% 13%

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	LFA	C	612	-	-	-	X
22	LFA	C	615	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	LFA	P	614	-	-	-	X
22	LFA	P	615	-	-	-	X
22	LFA	P	623	-	-	-	X
22	LFA	P	624	-	-	-	X
23	EDO	C	807	-	-	-	X

2 Entry composition (i)

There are 29 unique types of molecules in this entry. The entry contains 33049 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 Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	513	Total	C	N	O	S	0	15	0
			4130	2757	636	696	41			
1	N	513	Total	C	N	O	S	0	15	0
			4130	2757	636	696	41			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	227	Total	C	N	O	S	0	5	0
			1870	1216	288	347	19			
2	O	227	Total	C	N	O	S	0	5	0
			1870	1216	288	347	19			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	258	Total	C	N	O	S	0	9	0
			2171	1449	342	364	16			
3	P	258	Total	C	N	O	S	0	9	0
			2172	1449	343	364	16			

- Molecule 4 is a protein called Cytochrome c oxidase subunit 4 isoform 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	143	Total	C	N	O	S	0	1	0
			1192	776	195	217	4			
4	Q	137	Total	C	N	O	S	0	1	0
			1148	749	188	207	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	102	Total	C	N	O	S	0	0	0
			825	528	139	156	2			
5	R	102	Total	C	N	O	S	0	0	0
			825	528	139	156	2			

- Molecule 6 is a protein called Cytochrome c oxidase subunit 5B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	91	Total	C	N	O	S	0	2	0
			709	441	124	138	6			
6	S	91	Total	C	N	O	S	0	2	0
			709	441	124	138	6			

- Molecule 7 is a protein called Cytochrome c oxidase subunit 6A2, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	72	Total	C	N	O	S	0	1	0
			606	396	114	95	1			
7	T	72	Total	C	N	O	S	0	1	0
			606	396	114	95	1			

- Molecule 8 is a protein called Cytochrome c oxidase subunit 6B1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	75	Total	C	N	O	S	0	0	0
			628	395	114	114	5			
8	U	75	Total	C	N	O	S	0	0	0
			628	395	114	114	5			

- Molecule 9 is a protein called Cytochrome c oxidase subunit 6C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	70	Total	C	N	O	S	0	0	0
			575	375	103	93	4			
9	V	70	Total	C	N	O	S	0	0	0
			575	375	103	93	4			

- Molecule 10 is a protein called Cytochrome c oxidase subunit 7A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	56	Total	C	N	O	S	0	0	0
			441	285	73	80	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	W	56	Total	C	N	O	S	0	0	0
			441	285	73	80	3			

- Molecule 11 is a protein called Cytochrome c oxidase subunit 7B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	49	Total	C	N	O	S	0	0	0
			384	250	65	67	2			
11	X	49	Total	C	N	O	S	0	0	0
			384	250	65	67	2			

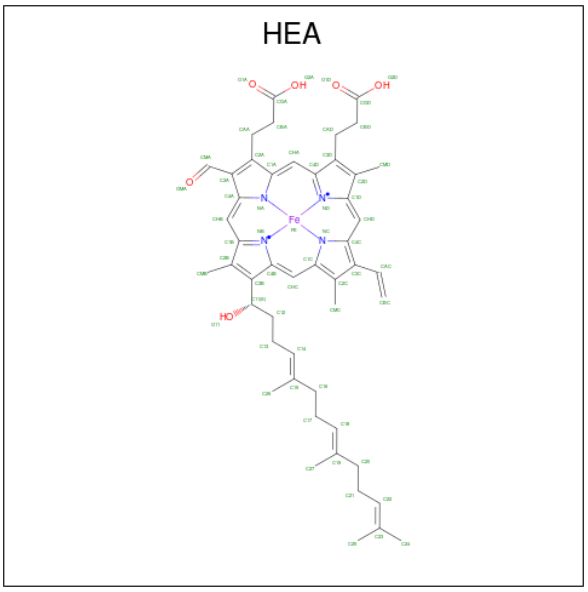
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	44	Total	C	N	O	S	0	0	0
			360	242	59	57	2			
12	Y	44	Total	C	N	O	S	0	0	0
			360	242	59	57	2			

- Molecule 13 is a protein called Cytochrome c oxidase subunit 8B.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	40	Total	C	N	O	0	0	0
			311	208	48	55			
13	Z	40	Total	C	N	O	0	0	0
			311	208	48	55			

- Molecule 14 is HEME-A (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	A	1	Total	C	Fe	N	O	0	1
			69	58	1	4	6		
14	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
14	N	1	Total	C	Fe	N	O	0	1
			69	58	1	4	6		
14	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		

- Molecule 15 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	1	Total	Cu	0	0
			1	1		
15	N	1	Total	Cu	0	0
			1	1		

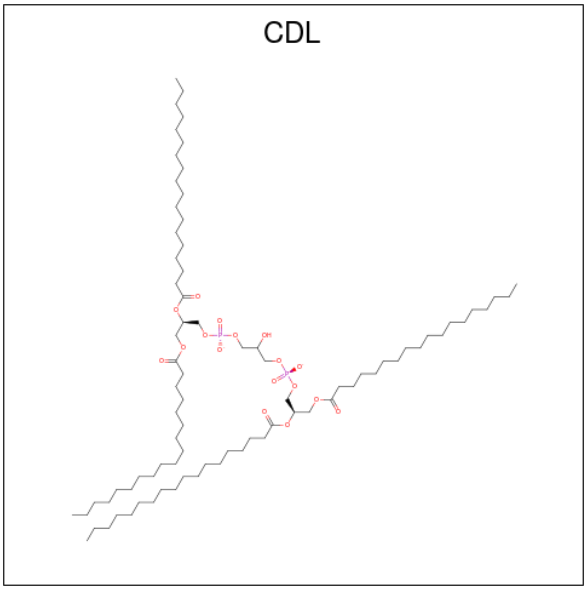
- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	1	Total	Mg	0	0
			1	1		
16	N	1	Total	Mg	0	0
			1	1		

- Molecule 17 is SODIUM ION (CCD ID: NA) (formula: Na).

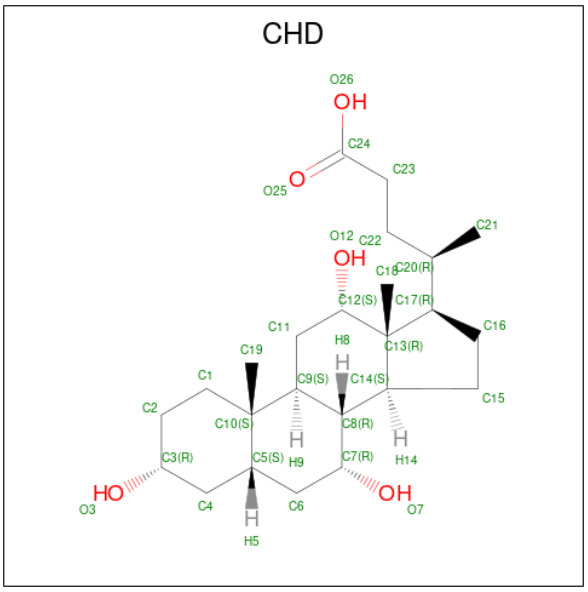
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total Na 1 1	0	0
17	N	1	Total Na 1 1	0	0

- Molecule 18 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



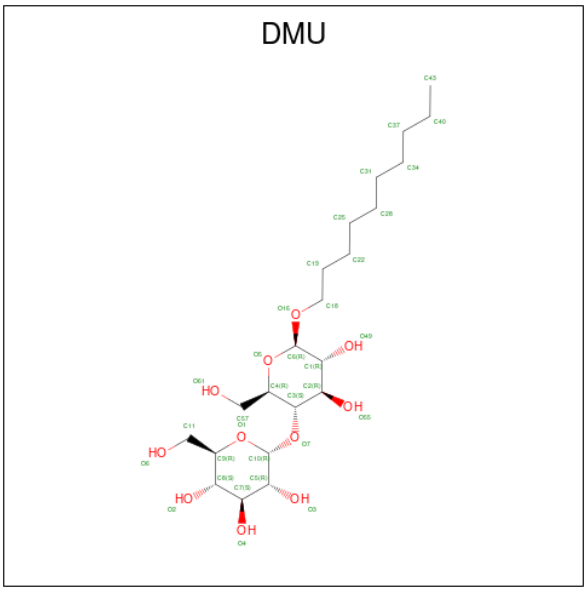
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total C O P 94 75 17 2	0	0
18	A	1	Total C O P 64 45 17 2	0	0
18	C	1	Total C O P 87 68 17 2	0	0
18	N	1	Total C O P 94 75 17 2	0	0
18	N	1	Total C O P 64 45 17 2	0	0
18	P	1	Total C O P 87 68 17 2	0	0

- Molecule 19 is CHOLIC ACID (CCD ID: CHD) (formula: $C_{24}H_{40}O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	A	1	Total C O 29 24 5	0	0
19	C	1	Total C O 29 24 5	0	0
19	G	1	Total C O 29 24 5	0	0
19	N	1	Total C O 29 24 5	0	0
19	P	1	Total C O 29 24 5	0	0
19	T	1	Total C O 29 24 5	0	0

- Molecule 20 is DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: DMU) (formula: $C_{22}H_{42}O_{11}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	A	1	Total C O 33 22 11	0	0
20	A	1	Total C 7 7	0	0
20	A	1	Total C O 33 22 11	0	0
20	A	1	Total C O 33 22 11	0	0
20	B	1	Total C O 11 10 1	0	0
20	B	1	Total C O 11 10 1	0	0
20	B	1	Total C O 22 16 6	0	0
20	C	1	Total C O 33 22 11	0	0
20	C	1	Total C O 33 22 11	0	1
20	C	1	Total C 7 7	0	0
20	C	1	Total C O 22 16 6	0	0
20	C	1	Total C O 33 22 11	0	0
20	C	1	Total C O 33 22 11	0	0
20	C	1	Total C O 11 10 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	G	1	Total C O 22 16 6	0	0
20	G	1	Total C O 11 10 1	0	0
20	G	1	Total C O 22 16 6	0	0
20	J	1	Total C O 11 10 1	0	0
20	J	1	Total C O 33 22 11	0	0
20	L	1	Total C O 22 16 6	0	0
20	M	1	Total C 8 8	0	0
20	N	1	Total C O 33 22 11	0	0
20	N	1	Total C 7 7	0	0
20	N	1	Total C O 33 22 11	0	0
20	N	1	Total C O 33 22 11	0	0
20	O	1	Total C O 11 10 1	0	0
20	O	1	Total C O 11 10 1	0	0
20	O	1	Total C O 22 16 6	0	0
20	P	1	Total C O 33 22 11	0	0
20	P	1	Total C O 33 22 11	0	1
20	P	1	Total C 7 7	0	0
20	P	1	Total C O 22 16 6	0	0
20	P	1	Total C O 33 22 11	0	0
20	P	1	Total C O 33 22 11	0	0
20	P	1	Total C O 11 10 1	0	0

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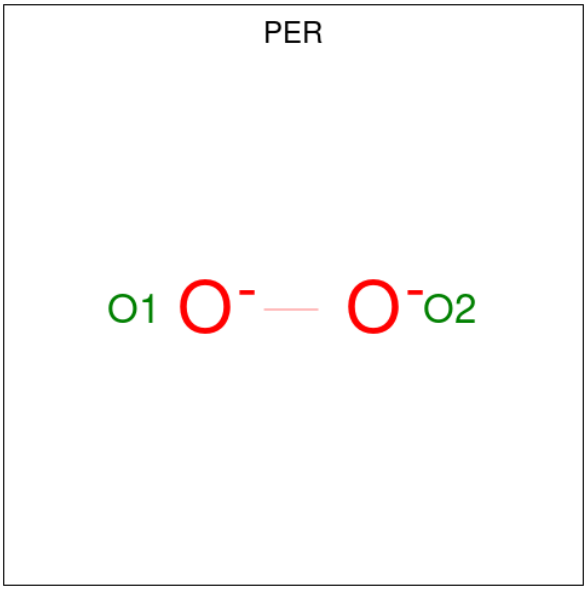
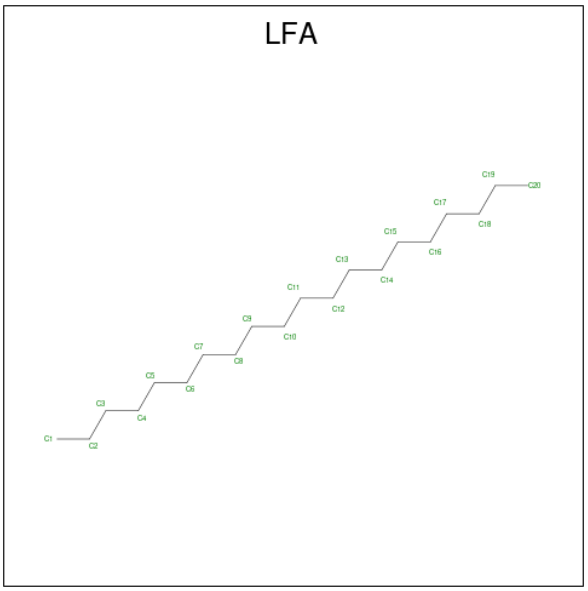
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	T	1	Total C O 22 16 6	0	0
20	T	1	Total C O 11 10 1	0	0
20	T	1	Total C O 22 16 6	0	0
20	W	1	Total C O 11 10 1	0	0
20	W	1	Total C O 33 22 11	0	0
20	Y	1	Total C O 22 16 6	0	0
20	Z	1	Total C 8 8	0	0

- Molecule 21 is PEROXIDE ION (CCD ID: PER) (formula: O_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	A	1	Total O 2 2	0	0
21	N	1	Total O 2 2	0	0

- Molecule 22 is EICOSANE (CCD ID: LFA) (formula: $C_{20}H_{42}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	A	1	Total C 14 14	0	0
22	A	1	Total C 14 14	0	0
22	C	1	Total C 11 11	0	0
22	C	1	Total C 6 6	0	0
22	C	1	Total C 15 15	0	0
22	C	1	Total C 11 11	0	0
22	C	1	Total C 14 14	0	0
22	C	1	Total C 11 11	0	0
22	C	1	Total C 15 15	0	0
22	C	1	Total C 13 13	0	0
22	C	1	Total C 18 18	0	1
22	G	1	Total C 17 17	0	0
22	G	1	Total C 11 11	0	0
22	N	1	Total C 14 14	0	0

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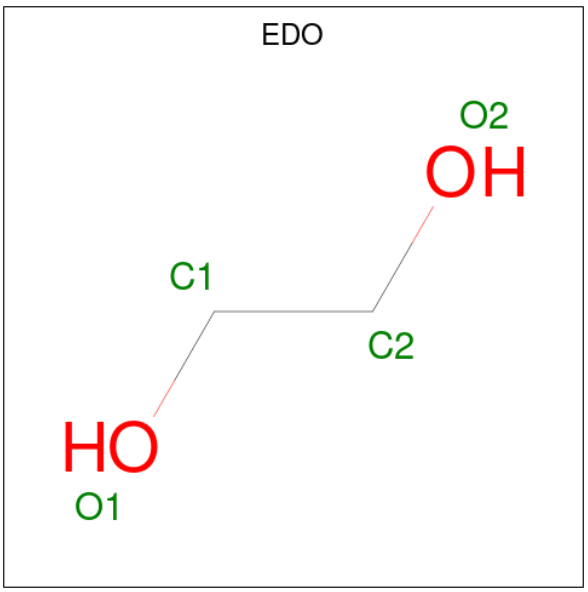
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	N	1	Total C 14 14	0	0
22	P	1	Total C 11 11	0	0
22	P	1	Total C 6 6	0	0
22	P	1	Total C 15 15	0	0
22	P	1	Total C 11 11	0	0
22	P	1	Total C 14 14	0	0
22	P	1	Total C 11 11	0	0
22	P	1	Total C 15 15	0	0
22	P	1	Total C 13 13	0	0
22	P	1	Total C 18 18	0	1
22	T	1	Total C 17 17	0	0
22	T	1	Total C 11 11	0	0

- Molecule 23 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	A	1	Total C O 4 2 2	0	0
23	A	1	Total C O 4 2 2	0	0
23	A	1	Total C O 4 2 2	0	0
23	A	1	Total C O 4 2 2	0	0
23	B	1	Total C O 4 2 2	0	0
23	C	1	Total C O 4 2 2	0	0
23	C	1	Total C O 4 2 2	0	0
23	C	1	Total C O 4 2 2	0	0
23	E	1	Total C O 4 2 2	0	0
23	E	1	Total C O 4 2 2	0	0
23	E	1	Total C O 4 2 2	0	0
23	F	1	Total C O 4 2 2	0	0
23	F	1	Total C O 4 2 2	0	0
23	G	1	Total C O 4 2 2	0	0
23	N	1	Total C O 4 2 2	0	0
23	N	1	Total C O 4 2 2	0	0
23	N	1	Total C O 4 2 2	0	0
23	N	1	Total C O 4 2 2	0	0
23	N	1	Total C O 4 2 2	0	0
23	O	1	Total C O 4 2 2	0	0
23	P	1	Total C O 4 2 2	0	0
23	P	1	Total C O 4 2 2	0	0

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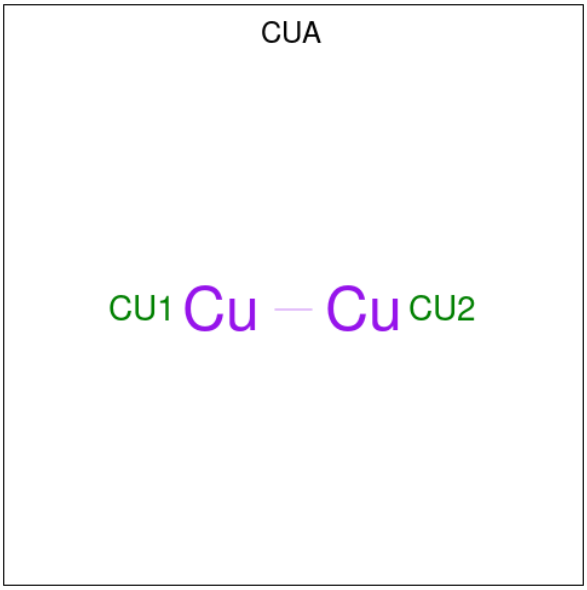
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	P	1	Total C O 4 2 2	0	0
23	R	1	Total C O 4 2 2	0	0
23	R	1	Total C O 4 2 2	0	0
23	R	1	Total C O 4 2 2	0	0
23	S	1	Total C O 4 2 2	0	0
23	S	1	Total C O 4 2 2	0	0
23	T	1	Total C O 4 2 2	0	0

- Molecule 24 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu_2).

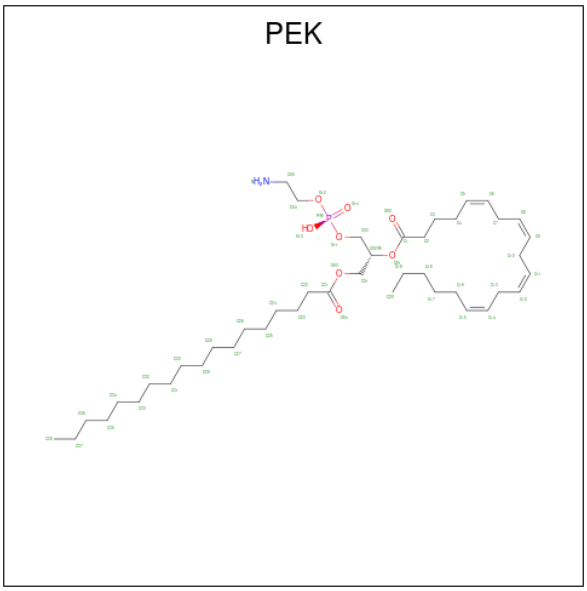


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	B	1	Total Cu 2 2	0	0
24	O	1	Total Cu 2 2	0	0

- Molecule 25 is UNKNOWN ATOM OR ION (CCD ID: UNX) (formula: X).

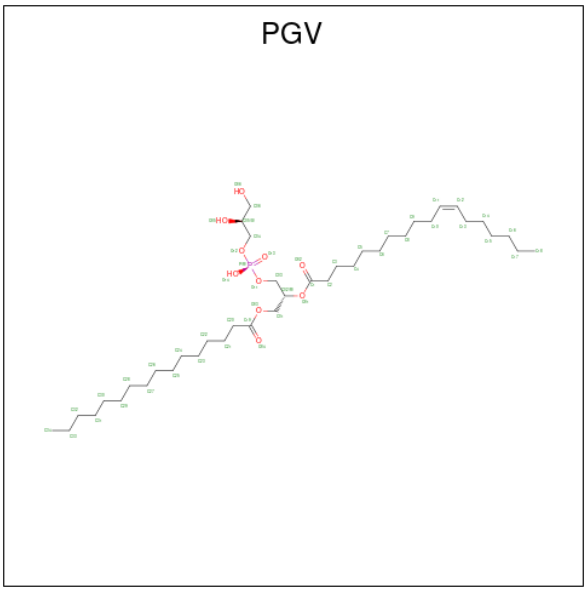
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	C	1	Total X 1 1	0	0
25	P	1	Total X 1 1	0	0

- Molecule 26 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (CCD ID: PEK) (formula: $C_{43}H_{78}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	C	1	Total C N O P 53 43 1 8 1	0	0
26	P	1	Total C N O P 53 43 1 8 1	0	0

- Molecule 27 is (1R)-2-{[{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: $C_{40}H_{77}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	C	1	Total C O P 51 40 10 1	0	0
27	C	1	Total C O P 51 40 10 1	0	0
27	P	1	Total C O P 51 40 10 1	0	0
27	P	1	Total C O P 51 40 10 1	0	0

- Molecule 28 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	F	1	Total Zn 1 1	0	0
28	S	1	Total Zn 1 1	0	0

- Molecule 29 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	1	Total O 1 1	0	0
29	A	2	Total O 2 2	0	0
29	A	2	Total O 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	3	Total O 3 3	0	0
29	A	6	Total O 6 6	0	0
29	A	4	Total O 4 4	0	0
29	A	3	Total O 3 3	0	0
29	A	4	Total O 4 4	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	11	Total O 11 11	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	3	Total O 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	2	Total O 2 2	0	0
29	A	3	Total O 3 3	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	2	Total O 2 2	0	0
29	A	1	Total O 1 1	0	0
29	A	4	Total O 4 4	0	0
29	A	1	Total O 1 1	0	0
29	A	3	Total O 3 3	0	0
29	A	2	Total O 2 2	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	2	Total O 2 2	0	0
29	A	1	Total O 1 1	0	0
29	A	2	Total O 2 2	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	2	Total O 2 2	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	3	Total O 3 3	0	0
29	A	1	Total O 2 2	0	1
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	2	Total O 2 2	0	0
29	A	2	Total O 2 2	0	0
29	A	2	Total O 2 2	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	2	Total O 2 2	0	0
29	A	7	Total O 7 7	0	0
29	A	5	Total O 5 5	0	0
29	A	1	Total O 1 1	0	0
29	A	8	Total O 8 8	0	0
29	A	1	Total O 1 1	0	0
29	A	8	Total O 8 8	0	0
29	A	2	Total O 2 2	0	0
29	A	1	Total O 1 1	0	0
29	A	2	Total O 3 3	0	1
29	A	3	Total O 4 4	0	1
29	A	2	Total O 3 3	0	1
29	A	2	Total O 2 2	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	2	Total O 2 2	0	0
29	A	2	Total O 2 2	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	1	Total O 1 1	0	0
29	A	2	Total O 2 2	0	0
29	A	1	Total O 1 1	0	0
29	A	2	Total O 3 3	0	1
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	2	Total O 2 2	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 2 2	0	1
29	A	1	Total O 1 1	0	0
29	A	2	Total O 3 3	0	1
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 2 2	0	1

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	2	Total O 2 2	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 2 2	0	1
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 2 2	0	1
29	A	1	Total O 1 1	0	0
29	A	1	Total O 2 2	0	1
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	2	Total O 2 2	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	2	Total O 2 2	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	2	Total O 2 2	0	0
29	A	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	2	Total O 2 2	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	2	Total O 2 2	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	3	Total O 3 3	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	B	3	Total O 3 3	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	3	Total O 3 3	0	0
29	B	1	Total O 1 1	0	0
29	B	2	Total O 2 2	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	2	Total O 2 2	0	0
29	B	1	Total O 1 1	0	0
29	B	3	Total O 3 3	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 2 2	0	1
29	B	2	Total O 2 2	0	0
29	B	4	Total O 4 4	0	0
29	B	2	Total O 2 2	0	0
29	B	1	Total O 1 1	0	0
29	B	2	Total O 2 2	0	0
29	B	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	2	Total O 2 2	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	2	Total O 2 2	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	B	1	Total O 1 1	0	0
29	B	2	Total O 2 2	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	2	Total O 2 2	0	0
29	B	6	Total O 7 7	0	1
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	3	Total O 3 3	0	0
29	B	2	Total O 2 2	0	0
29	B	2	Total O 2 2	0	0
29	B	2	Total O 2 2	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	C	2	Total O 2 2	0	0
29	C	1	Total O 1 1	0	0
29	C	1	Total O 1 1	0	0
29	C	1	Total O 1 1	0	0
29	C	1	Total O 1 1	0	0
29	C	1	Total O 1 1	0	0
29	C	4	Total O 4 4	0	0
29	C	1	Total O 1 1	0	0
29	C	1	Total O 1 1	0	0
29	C	1	Total O 1 1	0	0
29	C	1	Total O 2 2	0	1
29	C	1	Total O 1 1	0	0
29	C	2	Total O 2 2	0	0
29	C	1	Total O 1 1	0	0
29	C	1	Total O 1 1	0	0
29	C	1	Total O 1 1	0	0
29	C	1	Total O 1 1	0	0
29	C	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	C	1	Total O 1 1	0	0
29	C	1	Total O 1 1	0	0
29	C	1	Total O 1 1	0	0
29	C	1	Total O 1 1	0	0
29	C	2	Total O 2 2	0	0
29	C	1	Total O 1 1	0	0
29	C	1	Total O 1 1	0	0
29	C	1	Total O 1 1	0	0
29	C	2	Total O 2 2	0	0
29	C	1	Total O 1 1	0	0
29	C	1	Total O 1 1	0	0
29	C	1	Total O 1 1	0	0
29	C	1	Total O 1 1	0	0
29	C	1	Total O 1 1	0	0
29	C	1	Total O 1 1	0	0
29	C	1	Total O 1 1	0	0
29	C	1	Total O 1 1	0	0
29	C	2	Total O 2 2	0	0
29	C	1	Total O 1 1	0	0
29	C	1	Total O 1 1	0	0
29	C	1	Total O 1 1	0	0
29	C	2	Total O 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	C	1	Total O 1 1	0	0
29	C	1	Total O 1 1	0	0
29	C	2	Total O 2 2	0	0
29	C	1	Total O 1 1	0	0
29	C	2	Total O 2 2	0	0
29	C	1	Total O 1 1	0	0
29	C	1	Total O 1 1	0	0
29	C	1	Total O 1 1	0	0
29	C	1	Total O 1 1	0	0
29	C	1	Total O 1 1	0	0
29	C	1	Total O 1 1	0	0
29	C	1	Total O 1 1	0	0
29	C	1	Total O 1 1	0	0
29	C	1	Total O 1 1	0	0
29	C	1	Total O 1 1	0	0
29	C	1	Total O 1 1	0	0
29	C	2	Total O 2 2	0	0
29	C	1	Total O 1 1	0	0
29	C	1	Total O 1 1	0	0
29	C	1	Total O 1 1	0	0
29	C	1	Total O 1 1	0	0
29	C	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	C	1	Total O 1 1	0	0
29	C	1	Total O 1 1	0	0
29	C	1	Total O 1 1	0	0
29	C	1	Total O 1 1	0	0
29	C	1	Total O 1 1	0	0
29	C	1	Total O 1 1	0	0
29	C	1	Total O 1 1	0	0
29	C	1	Total O 1 1	0	0
29	C	1	Total O 1 1	0	0
29	C	1	Total O 1 1	0	0
29	C	2	Total O 2 2	0	0
29	C	1	Total O 1 1	0	0
29	C	1	Total O 1 1	0	0
29	C	1	Total O 1 1	0	0
29	C	1	Total O 1 1	0	0
29	C	1	Total O 1 1	0	0
29	C	1	Total O 1 1	0	0
29	C	1	Total O 1 1	0	0
29	C	1	Total O 1 1	0	0
29	C	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	C	1	Total O 1 1	0	0
29	C	1	Total O 1 1	0	0
29	C	1	Total O 1 1	0	0
29	C	1	Total O 1 1	0	0
29	C	1	Total O 1 1	0	0
29	C	1	Total O 1 1	0	0
29	D	2	Total O 2 2	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	2	Total O 2 2	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	2	Total O 2 2	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 2 2	0	1
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	2	Total O 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 2 2	0	1
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 2 2	0	1
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	2	Total O 2 2	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	2	Total O 2 2	0	0
29	D	1	Total O 2 2	0	1
29	D	2	Total O 3 3	0	1
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 2 2	0	1
29	D	1	Total O 1 1	0	0
29	D	2	Total O 2 2	0	0
29	D	2	Total O 2 2	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 2 2	0	1
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 2 2	0	1
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 2 2	0	1
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	2	Total O 2 2	0	0
29	D	4	Total O 4 4	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	3	Total O 3 3	0	0
29	D	2	Total O 2 2	0	0
29	D	1	Total O 1 1	0	0
29	D	2	Total O 2 2	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	2	Total O 2 2	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	2	Total O 2 2	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	2	Total O 2 2	0	0
29	E	2	Total O 2 2	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	2	Total O 2 2	0	0
29	E	2	Total O 2 2	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 2 2	0	1
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	2	Total O 2 2	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 2 2	0	1
29	E	1	Total O 1 1	0	0
29	E	1	Total O 2 2	0	1
29	E	1	Total O 2 2	0	1
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	E	2	Total O 2 2	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 2 2	0	1
29	E	1	Total O 1 1	0	0
29	E	1	Total O 2 2	0	1
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 2 2	0	1
29	E	1	Total O 1 1	0	0
29	E	2	Total O 2 2	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	2	Total O 2 2	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	3	Total O 3 3	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	2	Total O 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	3	Total O 3 3	0	0
29	E	1	Total O 1 1	0	0
29	E	6	Total O 6 6	0	0
29	E	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	2	Total O 2 2	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 2 2	0	1
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	2	Total O 2 2	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	2	Total O 4 4	0	2
29	F	2	Total O 2 2	0	0
29	F	1	Total O 1 1	0	0
29	F	2	Total O 2 2	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	F	1	Total O 1 1	0	0
29	F	1	Total O 2 2	0	1
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	2	Total O 3 3	0	1
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 2 2	0	1
29	F	1	Total O 1 1	0	0
29	F	2	Total O 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	2	Total O 2 2	0	0
29	F	4	Total O 4 4	0	0
29	F	7	Total O 7 7	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	F	1	Total O 1 1	0	0
29	F	2	Total O 2 2	0	0
29	F	1	Total O 1 1	0	0
29	F	2	Total O 3 3	0	1
29	G	1	Total O 1 1	0	0
29	G	1	Total O 1 1	0	0
29	G	1	Total O 1 1	0	0
29	G	1	Total O 1 1	0	0
29	G	1	Total O 1 1	0	0
29	G	1	Total O 1 1	0	0
29	G	1	Total O 1 1	0	0
29	G	1	Total O 1 1	0	0
29	G	1	Total O 1 1	0	0
29	G	1	Total O 1 1	0	0
29	G	1	Total O 1 1	0	0
29	G	1	Total O 1 1	0	0
29	G	1	Total O 1 1	0	0
29	G	1	Total O 1 1	0	0
29	G	1	Total O 1 1	0	0
29	G	1	Total O 1 1	0	0
29	G	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	G	1	Total O 1 1	0	0
29	G	1	Total O 1 1	0	0
29	G	1	Total O 1 1	0	0
29	G	1	Total O 1 1	0	0
29	G	1	Total O 2 2	0	1
29	G	1	Total O 1 1	0	0
29	G	1	Total O 1 1	0	0
29	G	1	Total O 1 1	0	0
29	G	1	Total O 1 1	0	0
29	G	1	Total O 1 1	0	0
29	G	1	Total O 1 1	0	0
29	G	1	Total O 1 1	0	0
29	G	1	Total O 1 1	0	0
29	G	1	Total O 1 1	0	0
29	G	1	Total O 1 1	0	0
29	G	1	Total O 1 1	0	0
29	G	1	Total O 1 1	0	0
29	G	1	Total O 1 1	0	0
29	G	1	Total O 1 1	0	0
29	G	1	Total O 1 1	0	0
29	G	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	G	1	Total O 1 1	0	0
29	G	1	Total O 1 1	0	0
29	G	1	Total O 1 1	0	0
29	G	1	Total O 1 1	0	0
29	H	1	Total O 1 1	0	0
29	H	1	Total O 1 1	0	0
29	H	2	Total O 2 2	0	0
29	H	1	Total O 1 1	0	0
29	H	1	Total O 1 1	0	0
29	H	1	Total O 1 1	0	0
29	H	1	Total O 1 1	0	0
29	H	1	Total O 1 1	0	0
29	H	1	Total O 1 1	0	0
29	H	1	Total O 1 1	0	0
29	H	1	Total O 1 1	0	0
29	H	1	Total O 1 1	0	0
29	H	1	Total O 1 1	0	0
29	H	1	Total O 1 1	0	0
29	H	2	Total O 2 2	0	0
29	H	2	Total O 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	H	1	Total O 1 1	0	0
29	H	1	Total O 1 1	0	0
29	H	1	Total O 1 1	0	0
29	H	1	Total O 1 1	0	0
29	H	1	Total O 1 1	0	0
29	H	1	Total O 1 1	0	0
29	H	1	Total O 1 1	0	0
29	H	1	Total O 1 1	0	0
29	H	1	Total O 1 1	0	0
29	H	1	Total O 1 1	0	0
29	H	1	Total O 1 1	0	0
29	H	1	Total O 1 1	0	0
29	H	1	Total O 1 1	0	0
29	H	1	Total O 1 1	0	0
29	H	1	Total O 1 1	0	0
29	H	1	Total O 1 1	0	0
29	H	1	Total O 1 1	0	0
29	H	1	Total O 1 1	0	0
29	H	1	Total O 1 1	0	0
29	H	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	H	1	Total O 1 1	0	0
29	H	1	Total O 1 1	0	0
29	H	1	Total O 1 1	0	0
29	H	1	Total O 1 1	0	0
29	H	1	Total O 1 1	0	0
29	H	1	Total O 1 1	0	0
29	H	1	Total O 1 1	0	0
29	H	1	Total O 1 1	0	0
29	H	1	Total O 1 1	0	0
29	H	1	Total O 1 1	0	0
29	H	1	Total O 1 1	0	0
29	H	1	Total O 1 1	0	0
29	H	1	Total O 1 1	0	0
29	H	1	Total O 1 1	0	0
29	H	1	Total O 1 1	0	0
29	H	1	Total O 1 1	0	0
29	H	1	Total O 1 1	0	0
29	H	1	Total O 1 1	0	0
29	I	1	Total O 1 1	0	0
29	I	1	Total O 1 1	0	0
29	I	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	I	1	Total O 1 1	0	0
29	I	1	Total O 1 1	0	0
29	I	1	Total O 1 1	0	0
29	I	1	Total O 1 1	0	0
29	I	1	Total O 1 1	0	0
29	I	1	Total O 1 1	0	0
29	I	1	Total O 1 1	0	0
29	I	1	Total O 1 1	0	0
29	I	1	Total O 1 1	0	0
29	I	1	Total O 1 1	0	0
29	I	1	Total O 1 1	0	0
29	I	1	Total O 1 1	0	0
29	I	1	Total O 1 1	0	0
29	I	1	Total O 1 1	0	0
29	I	1	Total O 1 1	0	0
29	I	1	Total O 1 1	0	0
29	I	1	Total O 1 1	0	0
29	I	1	Total O 1 1	0	0
29	I	1	Total O 1 1	0	0
29	I	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	I	1	Total O 1 1	0	0
29	I	2	Total O 2 2	0	0
29	I	1	Total O 1 1	0	0
29	I	1	Total O 1 1	0	0
29	I	1	Total O 1 1	0	0
29	I	1	Total O 1 1	0	0
29	I	1	Total O 1 1	0	0
29	I	1	Total O 1 1	0	0
29	I	1	Total O 1 1	0	0
29	I	1	Total O 1 1	0	0
29	I	1	Total O 1 1	0	0
29	I	1	Total O 1 1	0	0
29	I	1	Total O 1 1	0	0
29	I	1	Total O 1 1	0	0
29	I	1	Total O 1 1	0	0
29	J	1	Total O 1 1	0	0
29	J	1	Total O 1 1	0	0
29	J	1	Total O 1 1	0	0
29	J	1	Total O 1 1	0	0
29	J	1	Total O 1 1	0	0
29	J	1	Total O 1 1	0	0
29	J	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	J	1	Total O 1 1	0	0
29	J	2	Total O 2 2	0	0
29	J	1	Total O 1 1	0	0
29	J	1	Total O 1 1	0	0
29	J	1	Total O 1 1	0	0
29	J	1	Total O 1 1	0	0
29	J	1	Total O 1 1	0	0
29	J	1	Total O 1 1	0	0
29	J	1	Total O 1 1	0	0
29	J	1	Total O 1 1	0	0
29	J	1	Total O 1 1	0	0
29	J	1	Total O 1 1	0	0
29	J	1	Total O 1 1	0	0
29	J	1	Total O 1 1	0	0
29	K	1	Total O 1 1	0	0
29	K	1	Total O 1 1	0	0
29	K	1	Total O 1 1	0	0
29	K	1	Total O 1 1	0	0
29	K	1	Total O 1 1	0	0
29	K	1	Total O 1 1	0	0
29	K	1	Total O 1 1	0	0
29	K	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	K	1	Total O 1 1	0	0
29	K	1	Total O 1 1	0	0
29	K	1	Total O 1 1	0	0
29	K	1	Total O 1 1	0	0
29	K	1	Total O 1 1	0	0
29	K	1	Total O 1 1	0	0
29	K	1	Total O 1 1	0	0
29	K	1	Total O 1 1	0	0
29	K	1	Total O 1 1	0	0
29	K	1	Total O 1 1	0	0
29	K	1	Total O 1 1	0	0
29	K	1	Total O 1 1	0	0
29	L	1	Total O 1 1	0	0
29	L	1	Total O 1 1	0	0
29	L	1	Total O 1 1	0	0
29	L	1	Total O 1 1	0	0
29	L	1	Total O 1 1	0	0
29	L	1	Total O 1 1	0	0
29	L	1	Total O 1 1	0	0
29	L	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	L	1	Total O 1 1	0	0
29	L	1	Total O 1 1	0	0
29	L	1	Total O 1 1	0	0
29	L	1	Total O 1 1	0	0
29	L	1	Total O 1 1	0	0
29	L	1	Total O 1 1	0	0
29	L	1	Total O 2 2	0	1
29	L	1	Total O 1 1	0	0
29	L	1	Total O 2 2	0	1
29	L	1	Total O 1 1	0	0
29	L	1	Total O 1 1	0	0
29	L	1	Total O 1 1	0	0
29	L	1	Total O 1 1	0	0
29	L	1	Total O 1 1	0	0
29	L	1	Total O 1 1	0	0
29	L	1	Total O 1 1	0	0
29	M	1	Total O 1 1	0	0
29	M	1	Total O 1 1	0	0
29	M	1	Total O 1 1	0	0
29	M	1	Total O 1 1	0	0
29	M	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	M	1	Total O 1 1	0	0
29	M	1	Total O 1 1	0	0
29	M	1	Total O 1 1	0	0
29	M	1	Total O 1 1	0	0
29	M	1	Total O 1 1	0	0
29	M	1	Total O 1 1	0	0
29	M	1	Total O 1 1	0	0
29	M	1	Total O 1 1	0	0
29	M	1	Total O 1 1	0	0
29	M	1	Total O 1 1	0	0
29	M	1	Total O 1 1	0	0
29	M	1	Total O 1 1	0	0
29	M	1	Total O 1 1	0	0
29	M	1	Total O 1 1	0	0
29	M	1	Total O 1 1	0	0
29	M	1	Total O 1 1	0	0
29	M	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	2	Total O 2 2	0	0
29	N	2	Total O 2 2	0	0
29	N	3	Total O 3 3	0	0
29	N	6	Total O 6 6	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	N	4	Total O 4 4	0	0
29	N	3	Total O 3 3	0	0
29	N	4	Total O 4 4	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	11	Total O 11 11	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	2	Total O 2 2	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	3	Total O 3 3	0	0
29	N	1	Total O 1 1	0	0
29	N	2	Total O 2 2	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	2	Total O 2 2	0	0
29	N	3	Total O 3 3	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	2	Total O 2 2	0	0
29	N	4	Total O 4 4	0	0
29	N	1	Total O 1 1	0	0
29	N	3	Total O 3 3	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	2	Total O 2 2	0	0
29	N	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	2	Total O 2 2	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	3	Total O 3 3	0	0
29	N	1	Total O 2 2	0	1
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	2	Total O 2 2	0	0
29	N	2	Total O 2 2	0	0
29	N	2	Total O 2 2	0	0
29	N	1	Total O 1 1	0	0
29	N	3	Total O 3 3	0	0
29	N	7	Total O 7 7	0	0
29	N	5	Total O 5 5	0	0
29	N	1	Total O 1 1	0	0
29	N	8	Total O 8 8	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	N	1	Total O 1 1	0	0
29	N	8	Total O 8 8	0	0
29	N	2	Total O 2 2	0	0
29	N	1	Total O 1 1	0	0
29	N	2	Total O 3 3	0	1
29	N	2	Total O 3 3	0	1
29	N	2	Total O 2 2	0	0
29	N	1	Total O 1 1	0	0
29	N	2	Total O 2 2	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	2	Total O 2 2	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	2	Total O 2 2	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	2	Total O 2 2	0	0
29	N	2	Total O 2 2	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	3	Total O 3 3	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 2 2	0	1
29	N	1	Total O 2 2	0	1
29	N	1	Total O 2 2	0	1
29	N	1	Total O 2 2	0	1
29	N	1	Total O 2 2	0	1
29	N	2	Total O 4 4	0	2
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	2	Total O 2 2	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	2	Total O 2 2	0	0
29	N	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	2	Total O 2 2	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	3	Total O 3 3	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	3	Total O 3 3	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	3	Total O 3 3	0	0
29	O	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	O	2	Total O 2 2	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	2	Total O 2 2	0	0
29	O	2	Total O 2 2	0	0
29	O	3	Total O 3 3	0	0
29	O	1	Total O 1 1	0	0
29	O	3	Total O 3 3	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 2 2	0	1
29	O	2	Total O 2 2	0	0
29	O	4	Total O 4 4	0	0
29	O	2	Total O 2 2	0	0
29	O	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	2	Total O 2 2	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	2	Total O 2 2	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	2	Total O 2 2	0	0
29	O	5	Total O 5 5	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	2	Total O 2 2	0	0
29	O	3	Total O 3 3	0	0
29	O	2	Total O 2 2	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	P	2	Total O 2 2	0	0
29	P	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	4	Total O 4 4	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 2 2	0	1
29	P	1	Total O 1 1	0	0
29	P	2	Total O 2 2	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	2	Total O 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	2	Total O 2 2	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	2	Total O 2 2	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	2	Total O 2 2	0	0
29	P	1	Total O 1 1	0	0
29	P	2	Total O 2 2	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	2	Total O 2 2	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	3	Total O 3 3	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	Q	2	Total O 2 2	0	0
29	Q	1	Total O 1 1	0	0
29	Q	1	Total O 1 1	0	0
29	Q	1	Total O 1 1	0	0
29	Q	1	Total O 1 1	0	0
29	Q	1	Total O 1 1	0	0
29	Q	1	Total O 1 1	0	0
29	Q	1	Total O 1 1	0	0
29	Q	2	Total O 2 2	0	0
29	Q	1	Total O 1 1	0	0
29	Q	2	Total O 2 2	0	0
29	Q	1	Total O 1 1	0	0
29	Q	1	Total O 1 1	0	0
29	Q	1	Total O 1 1	0	0
29	Q	1	Total O 1 1	0	0
29	Q	1	Total O 1 1	0	0
29	Q	1	Total O 1 1	0	0
29	Q	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	Q	1	Total O 1 1	0	0
29	Q	1	Total O 1 1	0	0
29	Q	1	Total O 1 1	0	0
29	Q	1	Total O 1 1	0	0
29	Q	1	Total O 1 1	0	0
29	Q	1	Total O 1 1	0	0
29	Q	1	Total O 1 1	0	0
29	Q	1	Total O 1 1	0	0
29	Q	1	Total O 1 1	0	0
29	Q	1	Total O 1 1	0	0
29	Q	1	Total O 1 1	0	0
29	Q	1	Total O 1 1	0	0
29	Q	1	Total O 1 1	0	0
29	Q	1	Total O 1 1	0	0
29	Q	1	Total O 1 1	0	0
29	Q	1	Total O 1 1	0	0
29	Q	1	Total O 1 1	0	0
29	Q	1	Total O 1 1	0	0
29	Q	1	Total O 1 1	0	0
29	Q	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	Q	1	Total O 1 1	0	0
29	Q	1	Total O 2 2	0	1
29	Q	1	Total O 2 2	0	1
29	Q	1	Total O 2 2	0	1
29	Q	1	Total O 2 2	0	1
29	Q	1	Total O 1 1	0	0
29	Q	1	Total O 1 1	0	0
29	Q	1	Total O 1 1	0	0
29	Q	4	Total O 4 4	0	0
29	Q	1	Total O 1 1	0	0
29	Q	1	Total O 1 1	0	0
29	Q	1	Total O 1 1	0	0
29	Q	1	Total O 1 1	0	0
29	Q	3	Total O 3 3	0	0
29	Q	2	Total O 2 2	0	0
29	Q	3	Total O 3 3	0	0
29	Q	1	Total O 1 1	0	0
29	Q	1	Total O 1 1	0	0
29	Q	2	Total O 2 2	0	0
29	Q	1	Total O 1 1	0	0
29	Q	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	Q	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	2	Total O 2 2	0	0
29	R	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	3	Total O 3 3	0	0
29	R	1	Total O 1 1	0	0
29	R	2	Total O 2 2	0	0
29	R	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	R	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	R	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	1	Total O 2 2	0	1
29	R	1	Total O 2 2	0	1
29	R	2	Total O 4 4	0	2
29	R	1	Total O 2 2	0	1
29	R	1	Total O 2 2	0	1
29	R	1	Total O 2 2	0	1
29	R	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	R	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	3	Total O 3 3	0	0
29	R	2	Total O 2 2	0	0
29	R	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	3	Total O 3 3	0	0
29	R	1	Total O 1 1	0	0
29	R	6	Total O 6 6	0	0
29	R	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
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29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	2	Total O 2 2	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 2 2	0	1
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	2	Total O 2 2	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	2	Total O 4 4	0	2

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	2	Total O 2 2	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	2	Total O 2 2	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 2 2	0	1
29	S	1	Total O 2 2	0	1
29	S	2	Total O 4 4	0	2
29	S	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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29	S	1	Total O 1 1	0	0
29	S	8	Total O 8 8	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	T	1	Total O 1 1	0	0
29	T	1	Total O 1 1	0	0
29	T	1	Total O 1 1	0	0
29	T	1	Total O 1 1	0	0
29	T	1	Total O 1 1	0	0
29	T	1	Total O 1 1	0	0
29	T	1	Total O 1 1	0	0
29	T	1	Total O 1 1	0	0
29	T	1	Total O 1 1	0	0
29	T	1	Total O 1 1	0	0
29	T	1	Total O 1 1	0	0
29	T	1	Total O 1 1	0	0
29	T	1	Total O 1 1	0	0
29	T	1	Total O 1 1	0	0
29	T	1	Total O 1 1	0	0
29	T	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	T	1	Total O 1 1	0	0
29	T	1	Total O 1 1	0	0
29	T	1	Total O 1 1	0	0
29	T	1	Total O 1 1	0	0
29	T	1	Total O 2 2	0	1
29	T	1	Total O 1 1	0	0
29	T	1	Total O 1 1	0	0
29	T	1	Total O 1 1	0	0
29	T	1	Total O 1 1	0	0
29	T	1	Total O 1 1	0	0
29	T	1	Total O 1 1	0	0
29	T	1	Total O 1 1	0	0
29	T	1	Total O 1 1	0	0
29	T	1	Total O 1 1	0	0
29	T	1	Total O 1 1	0	0
29	T	1	Total O 1 1	0	0
29	T	1	Total O 1 1	0	0
29	T	1	Total O 1 1	0	0
29	T	1	Total O 1 1	0	0
29	T	1	Total O 1 1	0	0
29	T	1	Total O 1 1	0	0
29	U	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	U	1	Total O 1 1	0	0
29	U	1	Total O 1 1	0	0
29	U	2	Total O 2 2	0	0
29	U	1	Total O 1 1	0	0
29	U	1	Total O 1 1	0	0
29	U	1	Total O 1 1	0	0
29	U	1	Total O 1 1	0	0
29	U	1	Total O 1 1	0	0
29	U	1	Total O 1 1	0	0
29	U	1	Total O 1 1	0	0
29	U	1	Total O 1 1	0	0
29	U	1	Total O 1 1	0	0
29	U	1	Total O 1 1	0	0
29	U	1	Total O 1 1	0	0
29	U	1	Total O 1 1	0	0
29	U	1	Total O 1 1	0	0
29	U	1	Total O 1 1	0	0
29	U	2	Total O 2 2	0	0
29	U	1	Total O 1 1	0	0
29	U	2	Total O 2 2	0	0
29	U	1	Total O 1 1	0	0
29	U	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	U	1	Total O 1 1	0	0
29	U	1	Total O 1 1	0	0
29	U	1	Total O 1 1	0	0
29	U	1	Total O 1 1	0	0
29	U	1	Total O 1 1	0	0
29	U	1	Total O 1 1	0	0
29	U	1	Total O 1 1	0	0
29	U	1	Total O 1 1	0	0
29	U	1	Total O 1 1	0	0
29	U	1	Total O 1 1	0	0
29	U	1	Total O 1 1	0	0
29	U	1	Total O 1 1	0	0
29	U	1	Total O 1 1	0	0
29	U	1	Total O 1 1	0	0
29	U	1	Total O 1 1	0	0
29	U	1	Total O 1 1	0	0
29	U	1	Total O 1 1	0	0
29	U	1	Total O 1 1	0	0
29	U	1	Total O 1 1	0	0
29	U	1	Total O 1 1	0	0
29	U	2	Total O 2 2	0	0
29	U	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	U	1	Total O 1 1	0	0
29	U	1	Total O 1 1	0	0
29	U	1	Total O 1 1	0	0
29	V	1	Total O 1 1	0	0
29	V	1	Total O 1 1	0	0
29	V	1	Total O 1 1	0	0
29	V	1	Total O 1 1	0	0
29	V	1	Total O 1 1	0	0
29	V	1	Total O 1 1	0	0
29	V	1	Total O 1 1	0	0
29	V	1	Total O 1 1	0	0
29	V	1	Total O 1 1	0	0
29	V	1	Total O 1 1	0	0
29	V	1	Total O 1 1	0	0
29	V	1	Total O 1 1	0	0
29	V	1	Total O 1 1	0	0
29	V	1	Total O 1 1	0	0
29	V	1	Total O 1 1	0	0
29	V	1	Total O 1 1	0	0
29	V	1	Total O 1 1	0	0
29	V	1	Total O 1 1	0	0
29	V	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	V	1	Total O 1 1	0	0
29	V	1	Total O 1 1	0	0
29	V	1	Total O 1 1	0	0
29	W	1	Total O 1 1	0	0
29	W	1	Total O 1 1	0	0
29	W	1	Total O 1 1	0	0
29	W	1	Total O 1 1	0	0
29	W	1	Total O 1 1	0	0
29	W	1	Total O 1 1	0	0
29	W	1	Total O 1 1	0	0
29	W	1	Total O 1 1	0	0
29	W	1	Total O 1 1	0	0
29	W	1	Total O 1 1	0	0
29	W	1	Total O 1 1	0	0
29	W	1	Total O 1 1	0	0
29	W	1	Total O 1 1	0	0
29	W	1	Total O 1 1	0	0
29	W	1	Total O 1 1	0	0
29	W	1	Total O 1 1	0	0
29	X	1	Total O 1 1	0	0
29	X	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	X	1	Total O 1 1	0	0
29	X	1	Total O 1 1	0	0
29	X	1	Total O 1 1	0	0
29	X	1	Total O 1 1	0	0
29	X	1	Total O 1 1	0	0
29	X	1	Total O 1 1	0	0
29	X	1	Total O 1 1	0	0
29	X	1	Total O 1 1	0	0
29	X	1	Total O 1 1	0	0
29	X	1	Total O 1 1	0	0
29	X	1	Total O 1 1	0	0
29	X	1	Total O 1 1	0	0
29	X	1	Total O 1 1	0	0
29	X	1	Total O 1 1	0	0
29	X	1	Total O 1 1	0	0
29	X	1	Total O 1 1	0	0
29	X	1	Total O 1 1	0	0
29	X	1	Total O 1 1	0	0
29	Y	1	Total O 1 1	0	0
29	Y	1	Total O 1 1	0	0
29	Y	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	Y	1	Total O 1 1	0	0
29	Y	1	Total O 1 1	0	0
29	Y	1	Total O 1 1	0	0
29	Y	1	Total O 1 1	0	0
29	Y	1	Total O 1 1	0	0
29	Y	1	Total O 1 1	0	0
29	Y	1	Total O 1 1	0	0
29	Y	1	Total O 1 1	0	0
29	Y	1	Total O 1 1	0	0
29	Y	1	Total O 1 1	0	0
29	Y	1	Total O 1 1	0	0
29	Y	1	Total O 1 1	0	0
29	Y	1	Total O 1 1	0	0
29	Y	2	Total O 4 4	0	2
29	Y	1	Total O 1 1	0	0
29	Y	1	Total O 1 1	0	0
29	Y	1	Total O 1 1	0	0
29	Y	3	Total O 3 3	0	0
29	Y	1	Total O 1 1	0	0
29	Z	1	Total O 1 1	0	0
29	Z	1	Total O 1 1	0	0

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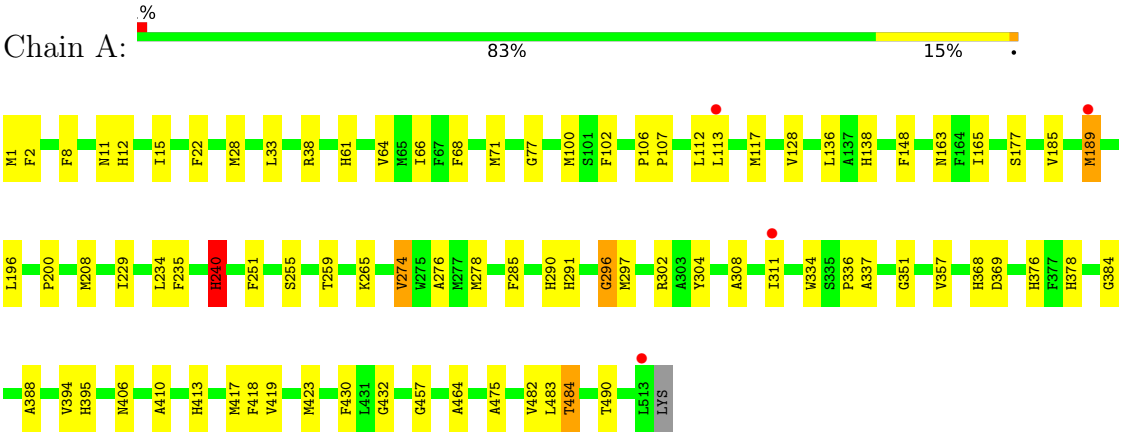
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	Z	1	Total O 1 1	0	0
29	Z	1	Total O 1 1	0	0
29	Z	1	Total O 1 1	0	0
29	Z	1	Total O 1 1	0	0
29	Z	1	Total O 1 1	0	0
29	Z	1	Total O 1 1	0	0
29	Z	1	Total O 1 1	0	0
29	Z	1	Total O 1 1	0	0
29	Z	1	Total O 1 1	0	0
29	Z	1	Total O 1 1	0	0
29	Z	1	Total O 1 1	0	0
29	Z	1	Total O 1 1	0	0
29	Z	1	Total O 1 1	0	0
29	Z	1	Total O 1 1	0	0
29	Z	1	Total O 1 1	0	0
29	Z	1	Total O 1 1	0	0

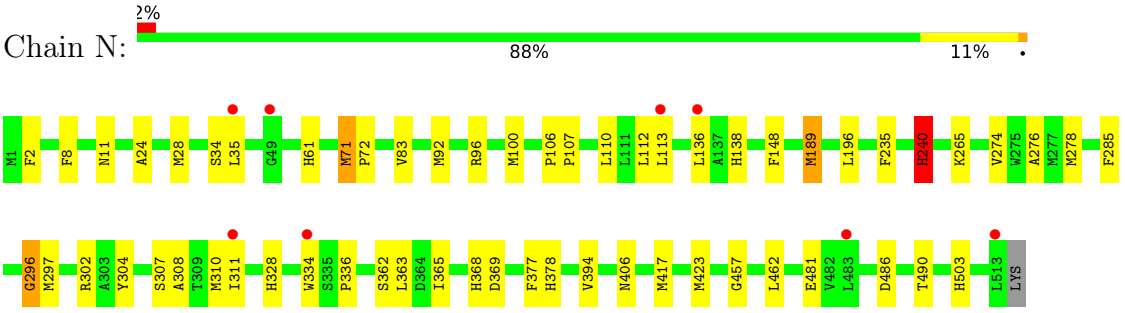
3 Residue-property plots (i)

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

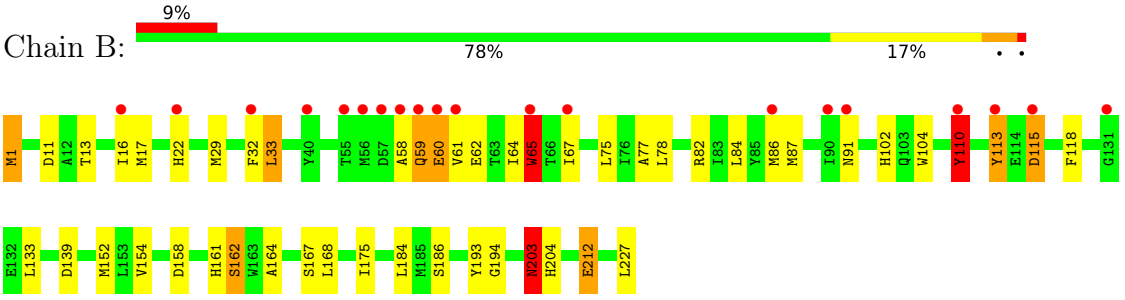
• Molecule 1: Cytochrome c oxidase subunit 1



• Molecule 1: Cytochrome c oxidase subunit 1

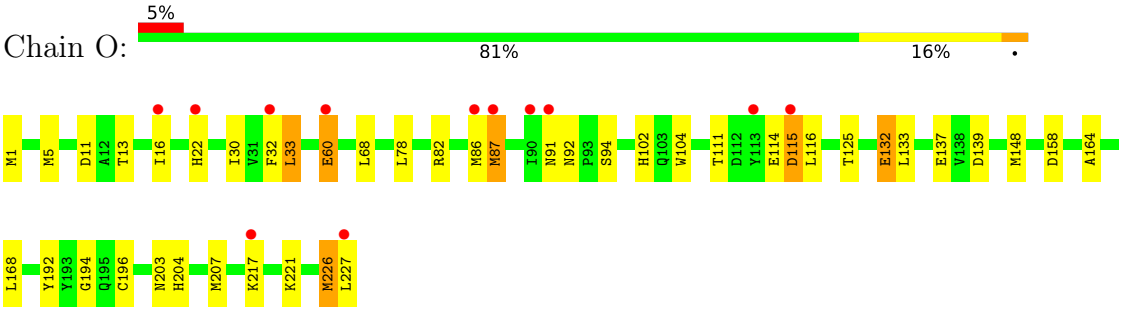


• Molecule 2: Cytochrome c oxidase subunit 2



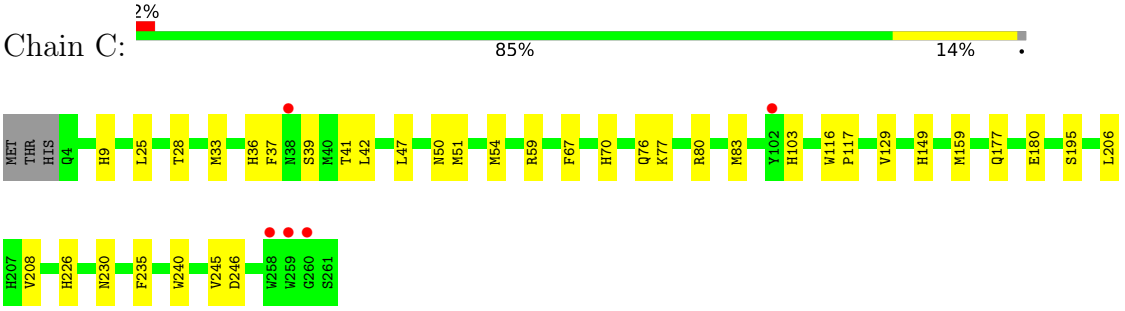
• Molecule 2: Cytochrome c oxidase subunit 2

Chain O:



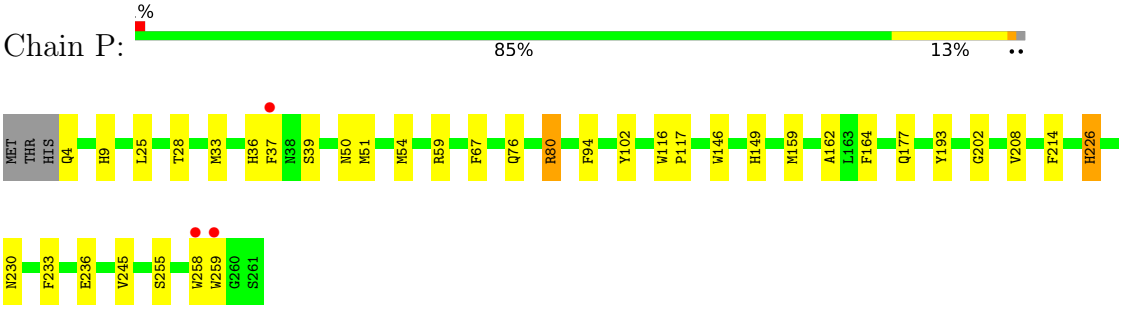
• Molecule 3: Cytochrome c oxidase subunit 3

Chain C:



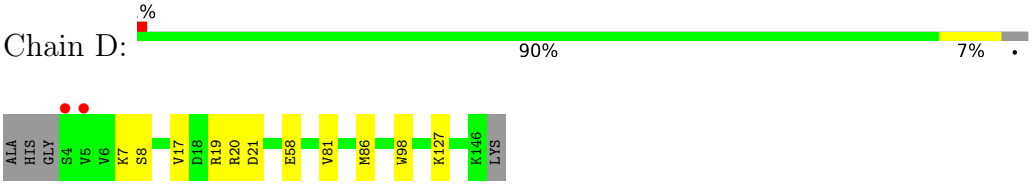
• Molecule 3: Cytochrome c oxidase subunit 3

Chain P:



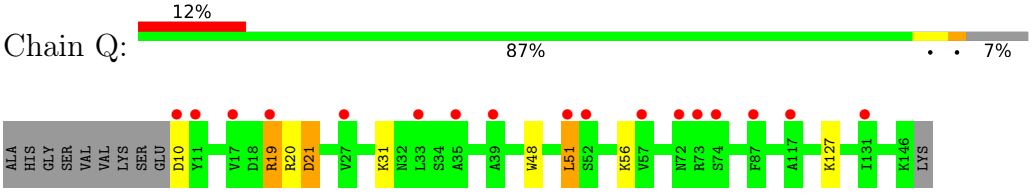
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

Chain D:



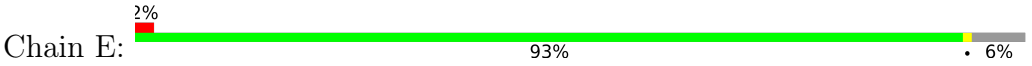
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

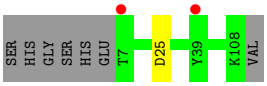
Chain Q:



• Molecule 5: Cytochrome c oxidase subunit 5A

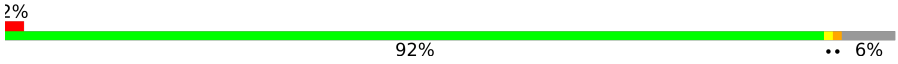
Chain E:

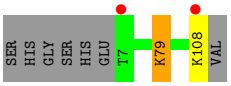




• Molecule 5: Cytochrome c oxidase subunit 5A

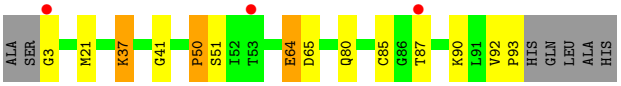
Chain R:





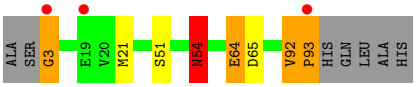
• Molecule 6: Cytochrome c oxidase subunit 5B

Chain F:



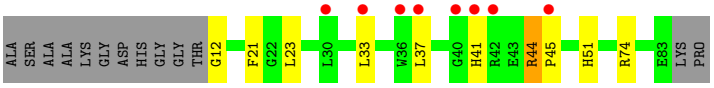
• Molecule 6: Cytochrome c oxidase subunit 5B

Chain S:



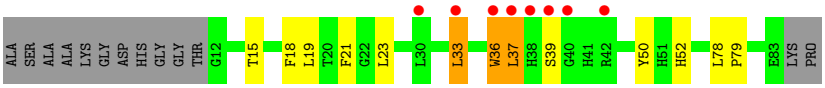
• Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain G:



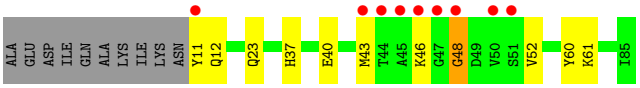
• Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain T:



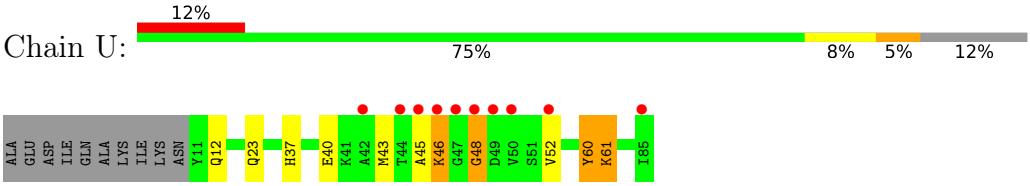
• Molecule 8: Cytochrome c oxidase subunit 6B1

Chain H:



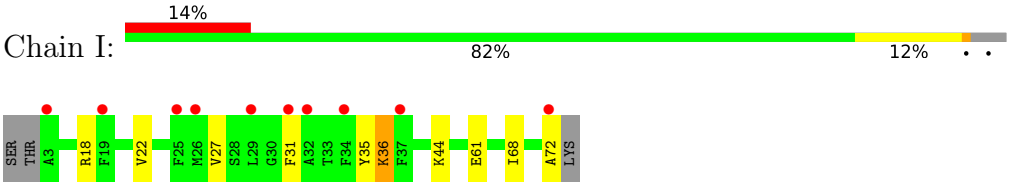
• Molecule 8: Cytochrome c oxidase subunit 6B1

Chain U:



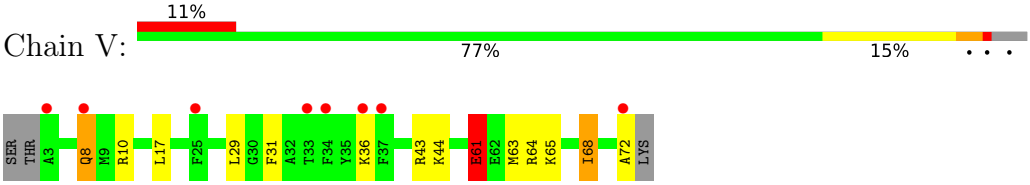
• Molecule 9: Cytochrome c oxidase subunit 6C

Chain I:



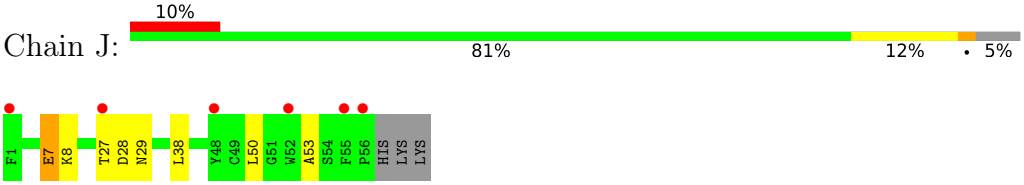
• Molecule 9: Cytochrome c oxidase subunit 6C

Chain V:



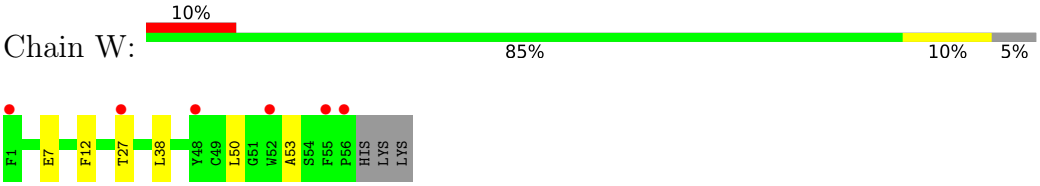
• Molecule 10: Cytochrome c oxidase subunit 7A1

Chain J:



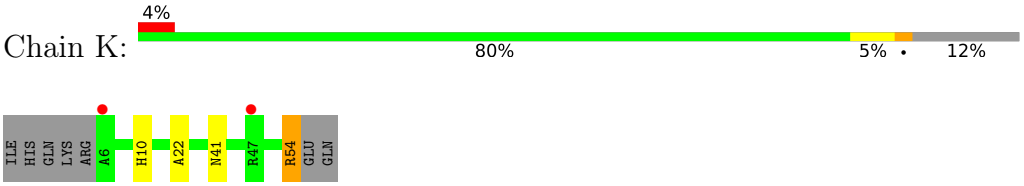
• Molecule 10: Cytochrome c oxidase subunit 7A1

Chain W:



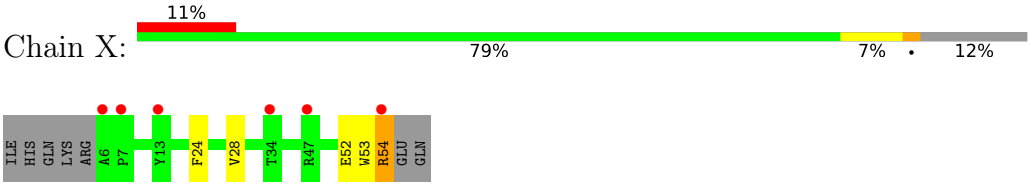
• Molecule 11: Cytochrome c oxidase subunit 7B

Chain K:



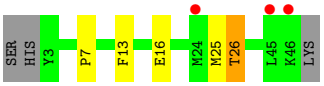
• Molecule 11: Cytochrome c oxidase subunit 7B

Chain X:



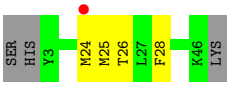
• Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

Chain L:



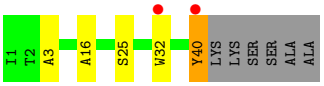
• Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

Chain Y:



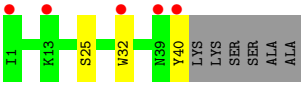
• Molecule 13: Cytochrome c oxidase subunit 8B

Chain M:



• Molecule 13: Cytochrome c oxidase subunit 8B

Chain Z:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	182.00Å 204.19Å 177.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.30 40.00 – 1.30	Depositor EDS
% Data completeness (in resolution range)	99.6 (40.00-1.30) 99.6 (40.00-1.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.50 (at 1.30Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.148 , 0.170 0.161 , 0.180	Depositor DCC
R_{free} test set	79184 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	19.3	Xtriage
Anisotropy	0.571	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 51.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.001 for l,-k,h	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	33049	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.42% 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: EDO, FME, PEK, CDL, LFA, MG, NA, ZN, PGV, HEA, CU, CUA, CHD, PER, DMU, UNX

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.52	35/4259 (0.8%)	1.64	34/5816 (0.6%)
1	N	1.36	19/4259 (0.4%)	1.44	14/5816 (0.2%)
2	B	1.61	16/1908 (0.8%)	1.60	26/2598 (1.0%)
2	O	1.20	4/1908 (0.2%)	1.35	9/2598 (0.3%)
3	C	1.38	7/2258 (0.3%)	1.45	5/3084 (0.2%)
3	P	1.31	6/2258 (0.3%)	1.41	9/3084 (0.3%)
4	D	1.17	3/1226 (0.2%)	1.29	4/1657 (0.2%)
4	Q	1.05	0/1182	1.31	1/1598 (0.1%)
5	E	1.09	0/843	1.29	1/1145 (0.1%)
5	R	1.08	0/843	1.30	0/1145
6	F	1.28	2/724 (0.3%)	1.36	3/983 (0.3%)
6	S	1.26	2/724 (0.3%)	1.33	8/983 (0.8%)
7	G	1.12	1/633 (0.2%)	1.27	2/864 (0.2%)
7	T	1.15	0/633	1.33	2/864 (0.2%)
8	H	1.21	1/648 (0.2%)	1.35	1/877 (0.1%)
8	U	1.15	1/648 (0.2%)	1.36	3/877 (0.3%)
9	I	1.17	3/588 (0.5%)	1.49	4/781 (0.5%)
9	V	1.18	1/588 (0.2%)	1.45	1/781 (0.1%)
10	J	1.06	0/451	1.32	2/610 (0.3%)
10	W	1.05	0/451	1.28	1/610 (0.2%)
11	K	1.19	1/398 (0.3%)	1.51	1/546 (0.2%)
11	X	1.16	0/398	1.31	2/546 (0.4%)
12	L	1.27	0/372	1.44	4/500 (0.8%)
12	Y	1.14	0/372	1.24	2/500 (0.4%)
13	M	1.20	0/321	1.46	4/440 (0.9%)
13	Z	1.13	0/321	1.36	0/440
All	All	1.31	102/29214 (0.3%)	1.43	143/39743 (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	A	0	4
1	N	0	3
2	B	0	5
6	S	0	1
11	K	0	1
All	All	0	14

All (102) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	110	TYR	CE1-CZ	22.92	1.93	1.38
2	B	162	SER	C-O	-18.95	1.00	1.23
2	B	110	TYR	CG-CD1	17.21	1.75	1.39
2	B	212	GLU	C-N	11.88	1.50	1.33
2	B	110	TYR	CG-CD2	11.74	1.64	1.39
3	C	9	HIS	CE1-NE2	11.64	1.44	1.32
1	N	481	GLU	CD-OE2	10.64	1.45	1.25
8	U	61	LYS	C-O	9.77	1.35	1.24
3	P	9	HIS	CE1-NE2	9.17	1.41	1.32
1	N	189	MET	CB-CG	8.15	1.76	1.52
1	A	235	PHE	C-O	7.85	1.33	1.24
1	A	376	HIS	C-O	7.50	1.32	1.24
1	A	368	HIS	CE1-NE2	7.42	1.40	1.32
1	A	483	LEU	CA-C	7.09	1.56	1.52
1	A	77	GLY	C-O	7.03	1.33	1.23
4	D	7	LYS	C-O	6.90	1.32	1.23
3	P	226	HIS	CE1-NE2	6.85	1.39	1.32
2	B	110	TYR	CE2-CZ	6.81	1.54	1.38
1	A	22	PHE	C-O	6.80	1.31	1.24
2	B	152	MET	CB-CG	-6.79	1.32	1.52
2	B	102	HIS	CE1-NE2	6.79	1.39	1.32
2	B	204	HIS	CE1-NE2	6.77	1.39	1.32
1	N	378	HIS	CG-ND1	6.71	1.45	1.38
2	B	212	GLU	CA-C	6.70	1.62	1.53
3	C	36	HIS	CE1-NE2	6.66	1.39	1.32
2	B	161	HIS	CE1-NE2	6.65	1.39	1.32
2	B	115	ASP	CG-OD2	6.63	1.38	1.25
2	O	204	HIS	CE1-NE2	6.63	1.39	1.32
1	N	138	HIS	CE1-NE2	6.62	1.39	1.32
1	N	368	HIS	CE1-NE2	6.61	1.39	1.32
1	A	64	VAL	C-O	6.58	1.31	1.24
3	P	76	GLN	C-O	6.57	1.31	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	58	GLU	CD-OE1	6.56	1.37	1.25
9	I	72	ALA	C-O	6.39	1.36	1.23
1	N	503	HIS	CE1-NE2	6.26	1.38	1.32
1	A	475	ALA	C-O	6.21	1.31	1.24
1	N	328	HIS	CE1-NE2	6.16	1.38	1.32
6	S	92	VAL	C-O	-6.15	1.16	1.24
1	N	235	PHE	C-O	6.08	1.31	1.24
1	N	189	MET	CG-SD	-6.06	1.65	1.80
9	I	61	GLU	CD-OE2	-6.03	1.13	1.25
1	A	406	ASN	C-O	6.01	1.31	1.24
1	A	68	PHE	C-O	5.86	1.31	1.23
2	O	132	GLU	CD-OE2	5.85	1.36	1.25
3	P	36	HIS	CE1-NE2	5.83	1.38	1.32
1	A	464	ALA	C-O	5.75	1.30	1.24
9	I	18	ARG	C-O	5.71	1.30	1.24
1	A	66	ILE	C-O	5.71	1.29	1.24
1	N	92	MET	CB-CG	5.69	1.69	1.52
1	A	100	MET	C-O	5.68	1.31	1.24
2	B	212	GLU	C-O	-5.63	1.17	1.23
3	C	103	HIS	ND1-CE1	5.61	1.38	1.32
1	N	100	MET	C-O	5.60	1.30	1.24
1	A	419	VAL	C-O	5.57	1.30	1.24
1	A	33	LEU	C-O	5.56	1.30	1.24
1	A	276	ALA	C-O	5.54	1.30	1.24
1	A	61	HIS	CE1-NE2	5.52	1.38	1.32
6	F	90	LYS	C-O	5.51	1.30	1.23
6	S	64	GLU	C-N	-5.49	1.26	1.33
1	A	395	HIS	C-O	5.47	1.30	1.24
1	A	432	GLY	C-O	5.46	1.30	1.23
1	N	71	MET	CG-SD	5.43	1.94	1.80
1	A	430	PHE	C-O	5.43	1.30	1.24
1	N	486	ASP	CG-OD1	5.41	1.35	1.25
1	A	163	ASN	C-O	5.41	1.30	1.24
1	N	11	ASN	C-O	5.39	1.30	1.24
1	N	83	VAL	CA-CB	5.37	1.57	1.54
2	O	102	HIS	CE1-NE2	5.37	1.38	1.32
6	F	3	GLY	C-O	5.37	1.34	1.23
2	O	86	MET	C-O	5.33	1.30	1.24
1	N	276	ALA	C-O	5.33	1.30	1.24
1	A	12	HIS	CG-CD2	5.32	1.41	1.35
2	B	186	SER	CA-CB	-5.30	1.45	1.53
9	V	61	GLU	C-O	5.30	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	413	HIS	C-O	5.29	1.30	1.24
1	A	8	PHE	C-O	5.26	1.30	1.24
7	G	51	HIS	CE1-NE2	5.25	1.37	1.32
1	A	384	GLY	C-O	5.24	1.30	1.23
1	A	357	VAL	C-O	5.24	1.30	1.24
1	A	12	HIS	ND1-CE1	5.23	1.37	1.32
3	C	70	HIS	CD2-NE2	5.21	1.43	1.37
3	P	255	SER	C-O	5.18	1.30	1.24
8	H	11	TYR	N-CA	5.17	1.56	1.46
1	A	413	HIS	CG-ND1	-5.17	1.32	1.38
1	N	71	MET	SD-CE	-5.14	1.66	1.79
2	B	113	TYR	C-O	-5.14	1.17	1.24
4	D	8	SER	C-O	-5.13	1.18	1.24
1	A	189	MET	CG-SD	-5.11	1.68	1.80
1	A	11	ASN	C-O	5.10	1.30	1.24
3	C	235	PHE	C-O	5.09	1.30	1.24
3	C	226	HIS	CE1-NE2	5.09	1.37	1.32
1	A	378	HIS	CG-ND1	5.06	1.43	1.38
1	A	15	ILE	C-O	5.06	1.29	1.24
3	C	83	MET	C-O	5.05	1.30	1.24
1	A	378	HIS	C-O	5.05	1.30	1.24
11	K	10	HIS	CE1-NE2	5.04	1.37	1.32
3	P	76	GLN	CD-OE1	5.04	1.33	1.23
2	B	154	VAL	C-N	-5.03	1.26	1.33
1	N	61	HIS	CE1-NE2	5.01	1.37	1.32
1	N	406	ASN	C-O	5.01	1.30	1.24
1	A	177	SER	CA-CB	-5.01	1.45	1.53
1	A	410	ALA	C-O	5.00	1.30	1.24

All (143) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	K	54	ARG	CA-C-O	-18.22	89.82	120.80
2	B	110	TYR	CB-CG-CD1	-12.43	102.16	120.80
2	B	64	ILE	CA-C-N	10.83	135.21	120.38
2	B	64	ILE	C-N-CA	10.83	135.21	120.38
1	N	71	MET	CG-SD-CE	-10.73	77.29	100.90
2	B	110	TYR	OH-CZ-CE2	-10.52	88.34	119.90
9	I	72	ALA	CA-C-O	-10.13	103.58	120.80
2	O	82	ARG	NE-CZ-NH2	-9.75	110.43	119.20
8	U	61	LYS	O-C-N	9.67	132.15	122.09
1	A	378	HIS	CG-CD2-NE2	9.15	116.35	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	115	ASP	CB-CA-C	9.07	126.19	112.03
1	A	196	LEU	O-C-N	9.05	131.71	122.12
9	V	72	ALA	CA-C-O	-8.87	105.72	120.80
1	N	240	HIS	CA-CB-CG	-8.79	105.02	113.80
2	B	110	TYR	CD1-CG-CD2	8.75	131.23	118.10
1	A	240	HIS	CA-CB-CG	-8.72	105.08	113.80
2	B	212	GLU	CA-C-N	-8.72	109.03	121.50
2	B	212	GLU	C-N-CA	-8.72	109.03	121.50
4	D	20	ARG	NE-CZ-NH2	8.70	127.03	119.20
2	B	82	ARG	NE-CZ-NH2	-8.65	111.42	119.20
2	B	110	TYR	CD1-CE1-CZ	-8.63	104.06	119.60
1	A	71	MET	CG-SD-CE	-8.56	82.06	100.90
1	A	368	HIS	CG-CD2-NE2	8.28	115.48	107.20
2	B	158	ASP	CA-CB-CG	8.27	120.87	112.60
2	B	65	TRP	CA-CB-CG	8.25	129.27	113.60
2	B	65	TRP	CB-CA-C	-8.13	96.86	110.68
4	D	58	GLU	CB-CG-CD	8.11	126.38	112.60
2	O	139	ASP	CA-CB-CG	8.11	120.71	112.60
2	B	82	ARG	CG-CD-NE	-7.98	94.44	112.00
2	B	184	LEU	N-CA-CB	-7.76	97.38	110.80
1	N	240	HIS	N-CA-CB	7.71	119.52	110.42
4	D	20	ARG	NE-CZ-NH1	-7.67	113.83	121.50
1	A	240	HIS	N-CA-CB	7.49	119.26	110.42
1	N	481	GLU	CG-CD-OE2	-6.97	102.37	118.40
1	N	61	HIS	CG-CD2-NE2	6.93	114.13	107.20
8	U	61	LYS	CA-C-O	-6.88	113.54	120.90
3	P	76	GLN	CG-CD-NE2	-6.85	106.12	116.40
12	L	25	MET	CA-C-N	6.71	129.17	120.44
12	L	25	MET	C-N-CA	6.71	129.17	120.44
1	A	61	HIS	CG-CD2-NE2	6.67	113.88	107.20
1	A	368	HIS	CE1-NE2-CD2	-6.59	102.41	109.00
4	D	21	ASP	CA-CB-CG	6.54	119.14	112.60
1	N	377	PHE	CA-CB-CG	6.50	120.30	113.80
1	N	310	MET	CG-SD-CE	-6.43	86.76	100.90
1	A	8	PHE	CA-CB-CG	6.35	120.15	113.80
1	A	106	PRO	CB-CA-C	6.32	118.63	110.92
3	P	80	ARG	CG-CD-NE	-6.28	98.18	112.00
5	E	25	ASP	CA-CB-CG	6.25	118.85	112.60
11	X	54	ARG	CA-C-O	-6.21	110.24	120.80
2	O	82	ARG	CG-CD-NE	-6.19	98.39	112.00
7	T	18	PHE	CA-CB-CG	6.16	119.96	113.80
1	A	482	VAL	O-C-N	6.16	129.16	122.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	S	93	PRO	CB-CA-C	6.15	121.78	110.10
6	F	64	GLU	CA-C-N	-6.12	114.25	125.02
6	F	64	GLU	C-N-CA	-6.12	114.25	125.02
2	B	203	ASN	OD1-CG-ND2	-6.07	116.53	122.60
3	P	233	PHE	CA-CB-CG	-6.07	107.73	113.80
6	S	92	VAL	O-C-N	-6.07	114.19	121.10
1	A	388	ALA	CA-C-N	6.06	128.20	120.56
1	A	388	ALA	C-N-CA	6.06	128.20	120.56
1	A	484	THR	CA-CB-OG1	-6.05	100.52	109.60
2	B	59	GLN	CB-CG-CD	6.02	122.83	112.60
12	L	16	GLU	CB-CG-CD	5.99	122.78	112.60
1	N	196	LEU	O-C-N	5.91	128.39	122.12
10	J	7	GLU	CB-CA-C	5.90	120.88	110.85
2	O	11	ASP	CA-CB-CG	5.90	118.50	112.60
7	G	44	ARG	CA-C-N	5.85	126.31	119.99
7	G	44	ARG	C-N-CA	5.85	126.31	119.99
3	P	193	TYR	CA-C-N	5.84	126.43	120.00
3	P	193	TYR	C-N-CA	5.84	126.43	120.00
2	B	212	GLU	N-CA-C	5.84	120.85	107.48
1	A	274	VAL	O-C-N	5.77	127.90	121.90
13	M	3	ALA	O-C-N	5.75	129.57	123.42
3	C	76	GLN	CG-CD-NE2	-5.75	107.78	116.40
1	A	102	PHE	CA-CB-CG	-5.73	108.07	113.80
2	B	110	TYR	CE1-CZ-CE2	5.68	131.67	120.30
2	B	212	GLU	CB-CA-C	-5.68	103.14	111.77
1	A	337	ALA	CA-C-N	5.62	127.81	120.28
1	A	337	ALA	C-N-CA	5.62	127.81	120.28
2	B	212	GLU	CA-C-O	-5.58	109.92	120.69
1	A	196	LEU	CA-C-O	-5.57	114.65	120.55
1	A	378	HIS	CE1-NE2-CD2	-5.55	103.45	109.00
3	C	80	ARG	CG-CD-NE	-5.54	99.82	112.00
2	B	139	ASP	CA-CB-CG	5.53	118.13	112.60
1	A	64	VAL	N-CA-C	-5.52	105.34	110.53
1	A	200	PRO	O-C-N	5.52	129.34	122.22
6	S	64	GLU	CA-C-N	-5.51	115.46	125.66
6	S	64	GLU	C-N-CA	-5.51	115.46	125.66
1	A	189	MET	N-CA-CB	5.51	118.00	110.01
2	B	82	ARG	NH1-CZ-NH2	5.50	126.45	119.30
13	M	40	TYR	CA-C-O	-5.50	111.45	120.80
6	S	93	PRO	CA-C-O	-5.49	102.52	119.00
2	O	158	ASP	CA-CB-CG	5.49	118.09	112.60
1	A	378	HIS	CB-CG-CD2	5.47	138.32	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	8	PHE	CA-CB-CG	5.46	119.26	113.80
1	N	61	HIS	CE1-NE2-CD2	-5.46	103.54	109.00
6	S	54	ASN	OD1-CG-ND2	-5.45	117.15	122.60
1	A	15	ILE	CA-C-N	5.45	126.14	119.99
1	A	15	ILE	C-N-CA	5.45	126.14	119.99
8	U	12	GLN	N-CA-C	-5.44	104.68	112.13
3	C	195	SER	N-CA-C	-5.43	105.01	111.03
9	I	27	VAL	CA-C-O	-5.42	115.11	120.85
3	P	214	PHE	CA-CB-CG	5.40	119.20	113.80
2	B	11	ASP	CA-CB-CG	5.39	118.00	112.60
2	O	115	ASP	CB-CA-C	5.39	120.09	111.73
1	A	235	PHE	CA-CB-CG	-5.39	108.41	113.80
8	H	12	GLN	N-CA-C	-5.38	104.75	112.13
6	F	50	PRO	N-CA-CB	5.36	108.01	103.35
12	Y	25	MET	CA-C-N	5.34	127.75	120.54
12	Y	25	MET	C-N-CA	5.34	127.75	120.54
2	B	167	SER	N-CA-CB	5.33	119.23	110.39
1	N	96	ARG	CB-CA-C	5.32	119.73	110.79
3	C	206	LEU	N-CA-C	-5.31	105.39	111.07
2	O	192	TYR	CB-CA-C	5.30	119.30	109.70
10	J	28	ASP	CA-CB-CG	5.29	117.89	112.60
2	B	167	SER	CA-CB-OG	-5.29	100.52	111.10
12	L	26	THR	N-CA-C	-5.28	105.42	111.07
1	A	351	GLY	O-C-N	-5.28	117.13	122.19
13	M	16	ALA	CA-C-N	5.27	127.20	120.56
13	M	16	ALA	C-N-CA	5.27	127.20	120.56
1	A	255	SER	O-C-N	5.26	127.57	122.09
3	P	94	PHE	CA-C-N	5.26	127.33	120.28
3	P	94	PHE	C-N-CA	5.26	127.33	120.28
6	S	3	GLY	CA-C-N	5.25	131.70	121.41
6	S	3	GLY	C-N-CA	5.25	131.70	121.41
1	A	185	VAL	O-C-N	5.24	126.95	121.87
1	A	378	HIS	ND1-CG-CD2	-5.23	100.87	106.10
4	Q	21	ASP	CA-CB-CG	5.21	117.81	112.60
3	C	129	VAL	N-CA-CB	5.19	113.77	110.50
1	N	106	PRO	CB-CA-C	5.18	117.24	110.92
1	N	83	VAL	O-C-N	5.18	123.73	120.42
11	X	53	TRP	N-CA-C	-5.17	107.63	114.04
9	I	22	VAL	CA-C-N	5.14	125.69	119.98
9	I	22	VAL	C-N-CA	5.14	125.69	119.98
10	W	7	GLU	CB-CA-C	5.14	119.32	110.79
1	A	251	PHE	O-C-N	5.08	127.50	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	165	ILE	O-C-N	5.07	126.88	121.91
2	O	125	THR	O-C-N	5.07	127.49	122.12
1	N	285	PHE	CA-C-O	-5.07	113.15	119.18
7	T	36	TRP	N-CA-C	-5.06	107.26	112.93
1	A	259	THR	O-C-N	5.04	127.26	122.07
2	O	221	LYS	N-CA-C	-5.03	105.88	111.36
3	P	76	GLN	CG-CD-OE1	5.00	130.81	120.80

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
1	A	296	GLY	Mainchain
1	A	304	TYR	Sidechain
1	A	38	ARG	Sidechain
2	B	110	TYR	Sidechain
2	B	113	TYR	Mainchain
2	B	162	SER	Mainchain
2	B	203	ASN	Sidechain
2	B	212	GLU	Mainchain
11	K	41	ASN	Sidechain
1	N	240	HIS	Sidechain
1	N	296	GLY	Mainchain
1	N	304	TYR	Sidechain
6	S	92	VAL	Mainchain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4130	0	4102	56	0
1	N	4130	0	4102	60	0
2	B	1870	0	1870	34	0
2	O	1870	0	1870	20	0
3	C	2171	0	2080	30	0
3	P	2172	0	2081	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1192	0	1178	5	0
4	Q	1148	0	1131	6	0
5	E	825	0	823	0	0
5	R	825	0	823	2	0
6	F	709	0	691	12	0
6	S	709	0	691	6	0
7	G	606	0	577	5	0
7	T	606	0	577	9	0
8	H	628	0	580	13	0
8	U	628	0	580	13	0
9	I	575	0	584	6	0
9	V	575	0	584	9	0
10	J	441	0	439	8	0
10	W	441	0	439	6	0
11	K	384	0	366	1	0
11	X	384	0	366	2	0
12	L	360	0	360	4	0
12	Y	360	0	360	4	0
13	M	311	0	321	3	0
13	Z	311	0	321	3	0
14	A	129	0	88	8	0
14	N	129	0	88	9	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	N	1	0	0	0	0
18	A	158	0	213	10	0
18	C	87	0	124	15	0
18	N	158	0	213	8	0
18	P	87	0	124	13	0
19	A	29	0	39	0	0
19	C	29	0	39	0	0
19	G	29	0	39	1	0
19	N	29	0	39	0	0
19	P	29	0	39	1	0
19	T	29	0	39	1	0
20	A	106	0	138	6	0
20	B	44	0	73	0	0
20	C	172	0	230	2	0
20	G	55	0	81	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	J	44	0	61	6	0
20	L	22	0	31	0	0
20	M	8	0	15	0	0
20	N	106	0	138	2	0
20	O	44	0	73	2	0
20	P	172	0	231	3	0
20	T	55	0	83	1	0
20	W	44	0	61	7	0
20	Y	22	0	31	0	0
20	Z	8	0	15	0	0
21	A	2	0	0	1	0
21	N	2	0	0	1	0
22	A	28	0	54	17	0
22	C	114	0	219	7	0
22	G	28	0	54	1	0
22	N	28	0	54	9	0
22	P	114	0	219	4	0
22	T	28	0	54	4	0
23	A	16	0	24	0	0
23	B	4	0	6	0	0
23	C	12	0	18	0	0
23	E	12	0	18	0	0
23	F	8	0	12	0	0
23	G	4	0	6	0	0
23	N	20	0	30	0	0
23	O	4	0	6	0	0
23	P	12	0	18	0	0
23	R	12	0	18	0	0
23	S	8	0	12	0	0
23	T	4	0	6	0	0
24	B	2	0	0	0	0
24	O	2	0	0	0	0
25	C	1	0	0	0	0
25	P	1	0	0	1	0
26	C	53	0	77	5	0
26	P	53	0	77	3	0
27	C	102	0	152	3	0
27	P	102	0	152	1	0
28	F	1	0	0	0	0
28	S	1	0	0	0	0
29	A	254	0	0	11	0
29	B	179	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	C	101	0	0	1	0
29	D	147	0	0	0	0
29	E	117	0	0	0	0
29	F	107	0	0	1	0
29	G	43	0	0	1	0
29	H	59	0	0	2	0
29	I	39	0	0	1	0
29	J	21	0	0	0	0
29	K	20	0	0	0	0
29	L	27	0	0	1	0
29	M	21	0	0	0	0
29	N	236	0	0	7	0
29	O	147	0	0	0	0
29	P	102	0	0	5	0
29	Q	78	0	0	1	0
29	R	96	0	0	0	0
29	S	97	0	0	0	0
29	T	37	0	0	0	0
29	U	50	0	0	3	0
29	V	21	0	0	1	0
29	W	16	0	0	0	0
29	X	20	0	0	0	0
29	Y	27	0	0	1	0
29	Z	18	0	0	0	0
All	All	33049	0	31527	366	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 6.

All (366) 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)
2:B:110:TYR:CG	2:B:110:TYR:CD1	1.75	1.69
1:N:189:MET:CG	1:N:189:MET:CB	1.76	1.62
2:B:110:TYR:CZ	2:B:110:TYR:CE1	1.93	1.57
8:H:52:VAL:HG12	8:U:46:LYS:HG2	1.18	1.14
21:A:520:PER:O2	21:A:520:PER:O1	1.70	1.09
21:N:520:PER:O1	21:N:520:PER:O2	1.67	1.09
3:C:33[B]:MET:HE1	20:J:61:DMU:H12	1.34	1.08
3:C:245:VAL:C	3:C:246[B]:ASP:CA	2.32	1.01
1:N:136[B]:LEU:HD11	29:N:3268:HOH:O	1.64	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136[B]:LEU:HD11	29:A:3514:HOH:O	1.63	0.97
1:N:423[B]:MET:HE2	1:N:457:GLY:HA2	1.48	0.95
1:N:297[B]:MET:SD	1:N:302:ARG:HG2	2.08	0.93
8:H:52:VAL:HG12	8:U:46:LYS:CG	1.99	0.92
1:A:423[B]:MET:HE2	1:A:457:GLY:HA2	1.51	0.92
2:B:110:TYR:CD1	2:B:110:TYR:CB	2.55	0.88
8:H:52:VAL:CG1	8:U:46:LYS:HG2	2.03	0.88
3:C:33[B]:MET:CE	20:J:61:DMU:H12	2.03	0.88
3:P:149:HIS:NE2	22:P:624:LFA:H11	1.89	0.88
1:N:417[B]:MET:HE2	29:N:2011:HOH:O	1.75	0.87
25:P:262:UNX:UNK	29:P:2021:HOH:O	1.52	0.86
18:C:270:CDL:HB61	18:C:270:CDL:HB21	1.58	0.86
1:A:28:MET:CE	14:A:515[A]:HEA:C27	2.57	0.82
1:A:423[B]:MET:HE2	1:A:457:GLY:CA	2.09	0.82
1:N:278[B]:MET:SD	22:N:627:LFA:H51	2.20	0.82
1:A:297[B]:MET:SD	1:A:302:ARG:HG2	2.20	0.82
3:P:33[B]:MET:CA	3:P:33[B]:MET:HE2	2.03	0.81
10:J:50:LEU:HB2	20:J:61:DMU:H20	1.62	0.81
1:A:113[A]:LEU:HD12	18:A:521:CDL:C87	2.10	0.81
1:A:297[B]:MET:HG2	1:A:302:ARG:HG3	1.62	0.81
1:N:189:MET:CB	1:N:189:MET:SD	2.70	0.79
18:A:521:CDL:O1	29:L:3766[B]:HOH:O	2.00	0.77
1:A:297[B]:MET:SD	1:A:302:ARG:CG	2.74	0.76
2:O:22[B]:HIS:CE1	9:V:44:LYS:HE2	2.20	0.76
1:N:297[B]:MET:SD	1:N:302:ARG:CG	2.73	0.76
7:T:33:LEU:HD22	7:T:37:LEU:HD22	1.66	0.75
1:A:28:MET:CE	14:A:515[A]:HEA:H271	2.16	0.75
1:A:484:THR:HG22	29:A:3347:HOH:O	1.86	0.75
1:A:113[A]:LEU:HD12	18:A:521:CDL:H873	1.68	0.74
1:N:28:MET:CE	14:N:515[A]:HEA:C27	2.65	0.74
1:A:297[B]:MET:CG	1:A:302:ARG:HG3	2.17	0.74
2:B:110:TYR:CD1	2:B:110:TYR:CZ	2.59	0.74
18:P:270:CDL:HB61	18:P:270:CDL:HB21	1.70	0.73
2:B:110:TYR:CG	2:B:110:TYR:CE1	2.62	0.73
2:B:1:FME:HE1	2:B:133:LEU:CD2	2.19	0.72
3:C:51[B]:MET:HE2	18:C:270:CDL:H861	1.71	0.72
3:P:4:GLN:N	29:P:3471:HOH:O	2.23	0.71
1:A:28:MET:HE1	14:A:515[A]:HEA:C27	2.18	0.71
18:C:270:CDL:HA62	18:C:270:CDL:H121	1.72	0.71
1:A:278[B]:MET:SD	22:A:627:LFA:H52	2.30	0.71
3:C:33[B]:MET:CA	3:C:33[B]:MET:HE2	1.97	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:13:THR:HB	2:B:168:LEU:HD23	1.73	0.70
1:N:423[B]:MET:HE2	1:N:457:GLY:CA	2.21	0.70
1:A:278[A]:MET:CE	22:A:628:LFA:H51	2.21	0.70
1:N:28:MET:CE	14:N:515[A]:HEA:H271	2.22	0.70
1:N:278[A]:MET:HE1	22:N:628:LFA:C5	2.21	0.69
3:C:180[B]:GLU:HG2	29:C:3893:HOH:O	1.91	0.69
2:B:1:FME:HE1	2:B:133:LEU:HD22	1.76	0.68
1:N:113[A]:LEU:HD12	18:N:521:CDL:H871	1.74	0.68
3:C:149:HIS:NE2	22:C:624:LFA:H11	2.09	0.67
18:P:270:CDL:HA62	18:P:270:CDL:H121	1.77	0.67
6:F:41:GLY:HA3	6:F:87[B]:THR:HG22	1.77	0.67
3:C:33[B]:MET:HE1	20:J:61:DMU:C25	2.14	0.67
1:N:28:MET:HE1	14:N:515[A]:HEA:C27	2.25	0.66
1:N:189:MET:CG	1:N:189:MET:CA	2.72	0.66
29:A:3305:HOH:O	3:C:77:LYS:HE3	1.96	0.66
2:B:16[A]:ILE:HD11	2:B:86:MET:HG2	1.76	0.65
1:N:297[B]:MET:HG2	1:N:302:ARG:HG3	1.78	0.65
1:N:278[A]:MET:CE	22:N:628:LFA:H51	2.26	0.65
29:A:3684:HOH:O	22:C:716[B]:LFA:H52	1.95	0.65
2:B:61:VAL:HG22	2:B:65:TRP:CZ3	2.32	0.65
3:P:33[B]:MET:HE1	20:W:61:DMU:H12	1.79	0.65
3:C:33[A]:MET:HE3	3:C:39:SER:OG	1.97	0.64
18:P:270:CDL:HB61	18:P:270:CDL:CB2	2.26	0.64
3:C:33[A]:MET:CE	3:C:42:LEU:H	2.11	0.64
1:A:28:MET:HE2	14:A:515[A]:HEA:H273	1.80	0.63
3:P:259:TRP:CD1	20:P:714:DMU:H31	2.17	0.63
2:B:110:TYR:HE1	2:B:118:PHE:CE2	2.17	0.63
9:V:61:GLU:OE1	9:V:64:ARG:NH2	2.31	0.63
8:U:37:HIS:HE1	29:U:3552:HOH:O	1.80	0.63
1:N:278[A]:MET:HE1	22:N:628:LFA:H51	1.81	0.62
29:A:3684:HOH:O	22:C:716[B]:LFA:C5	2.46	0.62
1:A:297[B]:MET:SD	1:A:302:ARG:HG3	2.40	0.62
1:A:113[B]:LEU:HD11	1:A:117[B]:MET:SD	2.39	0.62
3:C:33[A]:MET:HE2	3:C:42:LEU:H	1.64	0.62
2:O:16[A]:ILE:HD12	2:O:87[A]:MET:HG3	1.80	0.62
2:B:22[B]:HIS:CE1	9:I:44:LYS:HE2	2.35	0.62
1:N:274:VAL:HG12	1:N:278[A]:MET:HE2	1.82	0.62
3:P:50:ASN:ND2	3:P:54[A]:MET:HE2	2.14	0.61
1:A:278[A]:MET:HE1	22:A:628:LFA:C5	2.30	0.61
1:N:417[B]:MET:CE	29:N:2011:HOH:O	2.41	0.61
3:P:226:HIS:HE1	18:P:270:CDL:H111	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423[B]:MET:CE	1:A:457:GLY:N	2.63	0.61
1:N:278[A]:MET:SD	22:N:628:LFA:H51	2.41	0.61
1:A:278[A]:MET:HE1	22:A:628:LFA:H51	1.81	0.61
1:A:297[B]:MET:O	1:A:302:ARG:NE	2.29	0.61
1:N:278[A]:MET:HE1	22:N:628:LFA:H52	1.82	0.60
4:Q:48:TRP:O	4:Q:51:LEU:HB2	2.01	0.60
6:F:64:GLU:O	6:F:65:ASP:HB2	2.02	0.60
1:A:1:FME:HE2	1:A:1:FME:HA	1.83	0.60
6:F:37:LYS:HG2	29:F:3928:HOH:O	2.01	0.59
29:N:3540:HOH:O	4:Q:20:ARG:HG2	2.03	0.59
1:N:297[B]:MET:CG	1:N:302:ARG:HG3	2.32	0.59
20:A:744:DMU:H11	4:D:81:VAL:HG11	1.84	0.58
3:P:33[B]:MET:CE	20:W:61:DMU:H12	2.32	0.58
29:A:3932:HOH:O	6:F:37:LYS:HE3	2.03	0.58
29:N:3838[B]:HOH:O	4:Q:19:ARG:HD3	2.02	0.58
1:N:2:PHE:HE2	18:N:521:CDL:H712	1.69	0.58
8:H:43:MET:HE1	8:U:52:VAL:HG11	1.85	0.57
3:P:59:ARG:HB2	18:P:270:CDL:OA9	2.04	0.57
18:A:521:CDL:H842	18:A:521:CDL:C41	2.34	0.57
8:H:52:VAL:HG21	8:U:43:MET:HE1	1.87	0.57
1:N:28:MET:HE2	14:N:515[A]:HEA:H273	1.87	0.57
2:B:110:TYR:CD1	2:B:110:TYR:N	2.73	0.57
18:P:270:CDL:HA21	10:W:12:PHE:CZ	2.40	0.56
1:N:2:PHE:CE2	18:N:521:CDL:H712	2.40	0.56
9:V:61:GLU:OE1	9:V:64:ARG:NE	2.39	0.56
1:N:28:MET:CE	14:N:515[A]:HEA:H273	2.36	0.56
12:Y:26:THR:HG23	13:Z:25:SER:HB3	1.88	0.56
1:A:28:MET:HE2	14:A:515[A]:HEA:C27	2.36	0.56
6:S:64:GLU:O	6:S:65:ASP:HB2	2.04	0.56
8:U:37:HIS:CE1	29:U:3552:HOH:O	2.58	0.56
3:C:149:HIS:NE2	22:C:624:LFA:C1	2.69	0.55
4:Q:19:ARG:HD2	4:Q:21:ASP:OD1	2.07	0.55
8:H:46:LYS:CE	8:H:46:LYS:O	2.55	0.55
2:B:32[B]:PHE:CD2	9:I:31:PHE:CZ	2.95	0.55
22:C:625:LFA:H22	22:C:626:LFA:H71	1.88	0.55
2:B:16[B]:ILE:HG23	29:B:1078:HOH:O	2.05	0.55
2:B:29:MET:SD	9:I:36:LYS:NZ	2.76	0.55
1:A:112:LEU:C	1:A:112:LEU:HD23	2.32	0.55
18:A:521:CDL:H512	12:L:13:PHE:HB3	1.89	0.55
1:A:28:MET:HE1	14:A:515[A]:HEA:H271	1.85	0.55
1:A:278[B]:MET:HE1	22:A:627:LFA:H52	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113[A]:LEU:CD1	18:A:521:CDL:C87	2.83	0.54
1:A:28:MET:CE	14:A:515[A]:HEA:H273	2.37	0.54
26:P:264:PEK:H71	26:P:264:PEK:H32	1.89	0.54
1:N:308:ALA:HA	1:N:311[A]:ILE:HD12	1.88	0.54
1:N:423[B]:MET:HE3	1:N:457:GLY:N	2.22	0.54
1:N:365:ILE:HD11	29:N:3309:HOH:O	2.08	0.53
1:A:189:MET:HE3	22:A:627:LFA:H31	1.90	0.53
18:C:270:CDL:HB21	18:C:270:CDL:CB6	2.35	0.53
8:H:46:LYS:O	8:H:46:LYS:HE2	2.09	0.53
3:C:59:ARG:HG3	18:C:270:CDL:HA4	1.91	0.53
3:P:4:GLN:CA	29:P:3471:HOH:O	2.57	0.53
26:C:264:PEK:C11	26:C:264:PEK:H161	2.39	0.53
9:V:8:GLN:OE1	9:V:10:ARG:O	2.27	0.53
2:O:13:THR:HB	2:O:168:LEU:HD23	1.90	0.52
1:A:2:PHE:CE1	18:A:521:CDL:H712	2.44	0.52
12:Y:26:THR:HG23	13:Z:25:SER:CB	2.39	0.52
2:B:67:ILE:HD11	22:T:621:LFA:H61	1.92	0.52
1:N:28:MET:HE1	14:N:515[A]:HEA:H271	1.91	0.52
1:A:423[B]:MET:HE3	1:A:457:GLY:N	2.24	0.51
2:O:22[B]:HIS:CE1	9:V:44:LYS:CE	2.91	0.51
3:P:164:PHE:CD1	19:P:271:CHD:H192	2.45	0.51
3:P:226:HIS:CE1	18:P:270:CDL:H111	2.45	0.51
2:B:1:FME:HE1	2:B:133:LEU:HD21	1.93	0.51
1:A:112:LEU:HG	29:A:1053:HOH:O	2.10	0.51
3:P:116:TRP:HA	3:P:117:PRO:C	2.35	0.51
1:A:274:VAL:HG12	1:A:278[A]:MET:HE2	1.92	0.51
10:W:53:ALA:HB2	20:W:61:DMU:H10	1.93	0.51
3:C:33[B]:MET:HE2	3:C:33[B]:MET:N	2.25	0.50
3:P:67:PHE:CE2	18:P:270:CDL:O1	2.55	0.50
1:N:113[A]:LEU:CD1	18:N:521:CDL:H871	2.40	0.50
11:X:54:ARG:HD2	11:X:54:ARG:C	2.36	0.50
2:B:1:FME:HCN	2:B:193:TYR:HD1	1.76	0.50
26:C:264:PEK:H161	26:C:264:PEK:C12	2.42	0.50
1:N:278[B]:MET:HE1	22:N:627:LFA:H52	1.94	0.50
20:G:712:DMU:H19	1:N:307:SER:HB3	1.93	0.50
18:P:270:CDL:HA21	10:W:12:PHE:CE2	2.47	0.50
29:Q:4067:HOH:O	5:R:108:LYS:HD3	2.10	0.50
1:A:278[A]:MET:SD	22:A:628:LFA:H51	2.51	0.50
2:B:67:ILE:CD1	22:T:621:LFA:H61	2.41	0.50
4:D:86:MET:HE1	11:K:22:ALA:HB2	1.94	0.50
7:G:12:GLY:HA3	29:G:1207:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:32[B]:PHE:CD2	9:V:31:PHE:CZ	2.99	0.50
18:P:270:CDL:H751	10:W:27:THR:HG21	1.94	0.50
3:C:33[B]:MET:CE	20:J:61:DMU:C25	2.81	0.50
18:C:270:CDL:CA5	18:C:270:CDL:OA8	2.60	0.50
26:C:264:PEK:C38	27:C:266:PGV:H343	2.42	0.49
1:N:113[A]:LEU:HD12	18:N:521:CDL:C87	2.42	0.49
18:P:270:CDL:H121	18:P:270:CDL:CA6	2.40	0.49
12:Y:24:MET:HG3	29:Y:4051:HOH:O	2.11	0.49
1:N:110:LEU:HD21	20:W:61:DMU:H24	1.94	0.49
2:B:60:GLU:H	2:B:60:GLU:CD	2.19	0.49
3:C:33[A]:MET:HE1	3:C:41:THR:HB	1.93	0.49
2:O:60:GLU:CD	2:O:60:GLU:H	2.20	0.49
1:N:110:LEU:CD2	20:W:61:DMU:H24	2.42	0.49
22:A:628:LFA:C6	7:T:19:LEU:HD23	2.43	0.49
3:C:33[B]:MET:HG3	3:C:37:PHE:HB2	1.94	0.49
18:C:270:CDL:CA5	18:C:270:CDL:OB4	2.61	0.49
18:N:522:CDL:H1	18:N:522:CDL:OA3	2.13	0.49
1:A:418:PHE:CD1	20:A:744:DMU:H24	2.48	0.49
2:B:33:LEU:HD13	9:I:31:PHE:CD2	2.48	0.48
3:P:258:TRP:CE2	22:P:611:LFA:H32	2.48	0.48
1:A:285:PHE:CD2	22:A:627:LFA:H121	2.49	0.48
1:A:423[B]:MET:HE2	1:A:457:GLY:N	2.27	0.48
1:N:35:LEU:HD11	1:N:462:LEU:HB2	1.95	0.48
20:P:715[A]:DMU:O61	20:P:715[A]:DMU:H35	2.13	0.48
6:F:51:SER:O	6:F:93:PRO:HA	2.14	0.48
3:P:33[B]:MET:HG3	3:P:37:PHE:HB2	1.95	0.48
18:C:270:CDL:HB22	10:J:8:LYS:HE3	1.94	0.48
3:P:102:TYR:CE1	22:P:615:LFA:H91	2.49	0.48
1:A:278[B]:MET:CE	22:A:627:LFA:H52	2.43	0.48
14:A:516:HEA:HBC1	14:A:516:HEA:HMC3	1.95	0.48
3:C:50:ASN:ND2	3:C:54[A]:MET:HE2	2.28	0.48
1:N:336:PRO:HB2	1:N:394[B]:VAL:HG11	1.96	0.48
2:O:132:GLU:HB3	2:O:137:GLU:HG3	1.95	0.48
6:F:64:GLU:O	6:F:65:ASP:CB	2.59	0.48
1:N:112:LEU:HD23	1:N:112:LEU:C	2.39	0.48
2:O:30:ILE:HG12	20:O:731:DMU:H16	1.94	0.48
1:A:240:HIS:C	1:A:240:HIS:CD2	2.92	0.48
6:F:85:CYS:SG	6:F:87[B]:THR:OG1	2.70	0.48
1:N:423[B]:MET:CE	1:N:457:GLY:CA	2.92	0.47
8:H:37:HIS:HD2	8:H:40:GLU:OE2	1.97	0.47
1:N:297[B]:MET:SD	1:N:302:ARG:HG3	2.53	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:516:HEA:HBC1	14:N:516:HEA:HMC3	1.95	0.47
2:B:110:TYR:N	2:B:110:TYR:HD1	2.13	0.47
1:A:290:HIS:CD2	1:A:291:HIS:CD2	3.02	0.47
18:C:270:CDL:HB61	18:C:270:CDL:CB2	2.36	0.47
10:J:53:ALA:HB2	20:J:61:DMU:H10	1.97	0.47
1:N:297[B]:MET:O	1:N:302:ARG:NE	2.41	0.47
6:S:21[B]:MET:HE2	6:S:21[B]:MET:HB2	1.71	0.47
1:A:417[B]:MET:CE	29:A:1011:HOH:O	2.63	0.47
3:C:33[A]:MET:CE	3:C:41:THR:HB	2.45	0.47
8:H:43:MET:O	8:H:48:GLY:N	2.48	0.47
29:P:2107[B]:HOH:O	10:W:27:THR:HG22	2.14	0.47
3:C:51[B]:MET:HE2	18:C:270:CDL:C86	2.44	0.47
2:O:116:LEU:HD13	2:O:226:MET:HG3	1.96	0.47
8:U:37:HIS:HD2	8:U:40:GLU:OE2	1.98	0.47
3:P:33[B]:MET:HE2	3:P:33[B]:MET:N	2.30	0.47
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.50	0.46
18:C:270:CDL:H121	18:C:270:CDL:CA6	2.44	0.46
3:C:47:LEU:O	3:C:51[A]:MET:HG2	2.15	0.46
2:B:86:MET:HE2	2:B:86:MET:HB2	1.71	0.46
3:P:33[A]:MET:HG2	3:P:39:SER:O	2.16	0.46
1:N:240:HIS:C	1:N:240:HIS:CD2	2.93	0.46
6:F:41:GLY:HA3	6:F:87[B]:THR:CG2	2.44	0.46
18:A:522:CDL:OA3	18:A:522:CDL:H1	2.15	0.46
1:N:423[B]:MET:CE	1:N:457:GLY:N	2.79	0.46
1:A:148:PHE:HB3	3:C:28:THR:HB	1.97	0.46
1:A:308:ALA:O	1:A:311[B]:ILE:HG12	2.16	0.45
18:A:521:CDL:H722	18:A:521:CDL:H752	1.51	0.45
1:N:265:LYS:HB2	1:N:490:THR:HG21	1.97	0.45
1:N:362[A]:SER:HA	2:O:87[A]:MET:HE1	1.98	0.45
1:A:265:LYS:HB2	1:A:490:THR:HG21	1.97	0.45
1:A:417[B]:MET:HE2	29:A:1011:HOH:O	2.16	0.45
3:C:116:TRP:HA	3:C:117:PRO:C	2.40	0.45
6:S:54:ASN:HD22	6:S:54:ASN:C	2.25	0.45
22:A:628:LFA:H121	22:A:628:LFA:H81	1.99	0.45
26:P:264:PEK:H32	26:P:264:PEK:C7	2.46	0.45
7:T:36:TRP:HE3	7:T:39:SER:HB3	1.81	0.45
22:A:628:LFA:H61	7:T:19:LEU:HD23	1.98	0.45
2:O:33:LEU:HD13	9:V:31:PHE:CD2	2.51	0.45
13:M:32:TRP:CZ3	13:M:40:TYR:OH	2.68	0.45
2:B:16[B]:ILE:HG13	2:B:17:MET:N	2.31	0.45
2:B:84:LEU:O	2:B:87[B]:MET:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:71:MET:HB2	1:N:72:PRO:HD3	1.98	0.45
20:N:744:DMU:H36	20:N:744:DMU:O55	2.17	0.45
1:A:336:PRO:HB2	1:A:394[B]:VAL:HG11	1.98	0.44
3:P:50:ASN:HD22	3:P:51[A]:MET:HE2	1.82	0.44
22:A:627:LFA:H12	22:A:628:LFA:C1	2.47	0.44
9:I:35:TYR:CD1	9:I:35:TYR:C	2.95	0.44
8:U:43:MET:O	8:U:48:GLY:N	2.50	0.44
1:N:136[B]:LEU:CD1	29:N:3268:HOH:O	2.42	0.44
2:O:164:ALA:O	2:O:194:GLY:HA3	2.18	0.44
1:A:278[B]:MET:SD	22:A:627:LFA:C5	3.04	0.44
2:O:94:SER:OG	2:O:148:MET:HE2	2.17	0.44
20:A:526:DMU:H11	4:D:98:TRP:CE2	2.53	0.44
1:N:107:PRO:HB3	3:P:25:LEU:HB2	1.99	0.44
2:O:196:CYS:HB2	2:O:207:MET:HG3	2.00	0.44
5:R:79:LYS:HD2	5:R:79:LYS:N	2.32	0.44
1:A:334:TRP:CE3	20:A:743:DMU:H19	2.53	0.44
11:X:24:PHE:O	11:X:28:VAL:HG12	2.18	0.44
1:N:334:TRP:HB2	20:N:744:DMU:C57	2.48	0.44
18:P:270:CDL:CA5	18:P:270:CDL:OB4	2.65	0.44
3:P:202:GLY:HA3	26:P:264:PEK:H21	1.99	0.44
6:S:64:GLU:O	6:S:65:ASP:CB	2.65	0.44
3:C:208:VAL:HG22	3:C:245:VAL:CG1	2.47	0.43
20:O:742:DMU:H16	9:V:17:LEU:HD21	2.00	0.43
9:V:63:MET:HB3	9:V:68:ILE:HD11	2.00	0.43
1:N:148:PHE:HB3	3:P:28:THR:HB	1.98	0.43
3:P:51[B]:MET:HE3	18:P:270:CDL:H861	2.01	0.43
13:Z:32:TRP:CZ3	13:Z:40:TYR:OH	2.70	0.43
22:A:628:LFA:H92	7:T:23:LEU:HB2	1.99	0.43
2:B:67:ILE:HD11	22:T:621:LFA:C6	2.48	0.43
20:C:733:DMU:H25	10:J:38:LEU:HD23	2.00	0.43
4:D:127:LYS:HD2	29:I:1320:HOH:O	2.18	0.43
12:L:26:THR:HG23	13:M:25:SER:CB	2.47	0.43
4:D:17[B]:VAL:HG22	4:D:19:ARG:HG3	1.99	0.43
6:S:51:SER:O	6:S:93:PRO:HA	2.18	0.43
2:B:110:TYR:CE1	2:B:118:PHE:CE2	3.02	0.43
2:O:1:FME:HE1	2:O:133:LEU:HD22	2.00	0.43
1:A:278[A]:MET:HE1	22:A:628:LFA:H52	2.00	0.43
2:B:164:ALA:O	2:B:194:GLY:HA3	2.19	0.43
26:C:264:PEK:H382	27:C:266:PGV:H343	2.00	0.43
4:Q:127:LYS:HD2	29:V:2320:HOH:O	2.18	0.43
7:T:21:PHE:CD1	22:T:622:LFA:H62	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:24:ALA:HB2	14:N:515[B]:HEA:H253	1.99	0.42
18:C:270:CDL:OA3	18:C:270:CDL:H1	2.19	0.42
18:C:270:CDL:H751	10:J:27:THR:HG21	2.00	0.42
6:F:92:VAL:HG23	6:F:92:VAL:O	2.18	0.42
3:P:146:TRP:CD2	3:P:162:ALA:HB2	2.54	0.42
20:W:61:DMU:O55	20:W:61:DMU:O3	2.32	0.42
29:A:1275:HOH:O	12:L:7:PRO:HG3	2.18	0.42
3:P:208:VAL:HG22	3:P:245:VAL:CG1	2.50	0.42
1:A:334:TRP:HB2	20:A:744:DMU:C57	2.50	0.42
18:C:270:CDL:CB2	10:J:8:LYS:HE3	2.49	0.42
7:G:21:PHE:CD1	22:G:622:LFA:H62	2.54	0.42
1:N:71:MET:HB3	1:N:71:MET:HE2	1.96	0.42
20:A:744:DMU:H36	20:A:744:DMU:O55	2.19	0.42
8:H:37:HIS:HE1	29:H:3679:HOH:O	2.01	0.42
3:P:177:GLN:OE1	3:P:177:GLN:HA	2.19	0.42
3:C:54[A]:MET:HE1	27:C:267:PGV:H141	2.00	0.42
3:C:240:TRP:CE2	22:C:626:LFA:H51	2.55	0.42
12:L:26:THR:HG23	13:M:25:SER:HB3	2.01	0.42
7:G:41:HIS:HB3	7:G:74:ARG:NH1	2.34	0.42
2:O:111:THR:HA	2:O:114:GLU:O	2.20	0.42
2:O:114:GLU:HG3	2:O:227:LEU:HD21	2.01	0.42
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.55	0.42
9:I:68:ILE:HD13	9:I:68:ILE:HG21	1.85	0.42
3:P:28:THR:HG22	27:P:266:PGV:H182	2.02	0.42
8:U:60:TYR:CD1	8:U:60:TYR:C	2.98	0.42
7:G:23:LEU:HB2	22:N:628:LFA:H92	2.01	0.41
29:P:2093:HOH:O	6:S:3:GLY:HA3	2.18	0.41
1:N:189:MET:CB	1:N:189:MET:CE	2.98	0.41
18:N:521:CDL:H532	12:Y:28:PHE:CD1	2.55	0.41
1:A:107:PRO:HB3	3:C:25:LEU:HB2	2.02	0.41
1:N:278[B]:MET:HE1	22:N:627:LFA:C5	2.49	0.41
19:T:86:CHD:H212	19:T:86:CHD:H12	2.01	0.41
2:B:58:ALA:O	2:B:62:GLU:HG3	2.20	0.41
7:G:44:ARG:HA	7:G:45:PRO:HD3	1.88	0.41
2:O:5:MET:HE2	2:O:5:MET:HB3	1.86	0.41
1:A:208[B]:MET:HE1	1:A:234:LEU:HD11	2.03	0.41
3:C:177:GLN:HA	3:C:177:GLN:OE1	2.20	0.41
2:B:227:LEU:HD21	29:B:3750:HOH:O	2.18	0.41
18:A:521:CDL:H362	18:A:521:CDL:H711	2.02	0.41
1:N:296:GLY:HA2	8:U:23:GLN:OE1	2.21	0.41
14:N:516:HEA:HBC1	14:N:516:HEA:CMC	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:A:3684:HOH:O	22:C:716[B]:LFA:H51	2.16	0.41
26:C:264:PEK:H11	26:C:264:PEK:H42	2.03	0.41
2:O:1:FME:HE1	2:O:133:LEU:CD2	2.51	0.41
20:P:733:DMU:H25	10:W:38:LEU:HD23	2.03	0.41
4:Q:51:LEU:HB3	4:Q:56:LYS:HG3	2.02	0.41
1:A:208[B]:MET:HE1	1:A:234:LEU:CD1	2.51	0.41
6:F:50:PRO:HA	6:F:92:VAL:CG2	2.51	0.41
8:U:46:LYS:CD	8:U:46:LYS:O	2.69	0.41
2:B:77:ALA:CB	20:T:711:DMU:H19	2.51	0.40
3:P:80:ARG:NH2	3:P:236:GLU:OE1	2.48	0.40
1:A:296:GLY:HA2	8:H:23:GLN:OE1	2.21	0.40
22:A:628:LFA:H21	7:T:15:THR:HG23	2.03	0.40
19:G:86:CHD:H212	19:G:86:CHD:H12	2.02	0.40
8:H:37:HIS:CE1	29:H:3679:HOH:O	2.74	0.40
18:N:521:CDL:H801	18:N:521:CDL:C41	2.51	0.40
22:P:716[B]:LFA:C5	29:U:3543:HOH:O	2.69	0.40
20:C:733:DMU:C43	10:J:38:LEU:HD23	2.51	0.40
10:J:29:ASN:HD22	10:J:29:ASN:H	1.69	0.40
1:N:189:MET:CB	1:N:189:MET:HE2	2.52	0.40
7:T:78:LEU:HB3	7:T:79:PRO:HD2	2.03	0.40
3:C:67:PHE:CE2	18:C:270:CDL:O1	2.70	0.40
6:F:21[B]:MET:HE2	6:F:21[B]:MET:HB2	1.68	0.40
7:T:50:TYR:HB3	7:T:52:HIS:CE1	2.56	0.40
1:A:229:ILE:HD11	2:B:175:ILE:HD13	2.03	0.40
6:F:21[B]:MET:HB3	6:F:21[B]:MET:HE3	1.79	0.40
8:H:52:VAL:CB	8:U:46:LYS:HG2	2.50	0.40
20:W:61:DMU:O3	20:W:61:DMU:C2	2.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	526/514 (102%)	510 (97%)	16 (3%)	0	100	100
1	N	526/514 (102%)	510 (97%)	16 (3%)	0	100	100
2	B	230/227 (101%)	225 (98%)	5 (2%)	0	100	100
2	O	230/227 (101%)	226 (98%)	4 (2%)	0	100	100
3	C	265/261 (102%)	261 (98%)	4 (2%)	0	100	100
3	P	265/261 (102%)	260 (98%)	5 (2%)	0	100	100
4	D	142/147 (97%)	139 (98%)	3 (2%)	0	100	100
4	Q	136/147 (92%)	133 (98%)	3 (2%)	0	100	100
5	E	100/109 (92%)	100 (100%)	0	0	100	100
5	R	100/109 (92%)	100 (100%)	0	0	100	100
6	F	91/98 (93%)	91 (100%)	0	0	100	100
6	S	91/98 (93%)	90 (99%)	1 (1%)	0	100	100
7	G	71/85 (84%)	68 (96%)	3 (4%)	0	100	100
7	T	71/85 (84%)	68 (96%)	3 (4%)	0	100	100
8	H	73/85 (86%)	70 (96%)	2 (3%)	1 (1%)	9	1
8	U	73/85 (86%)	69 (94%)	2 (3%)	2 (3%)	4	0
9	I	68/73 (93%)	67 (98%)	1 (2%)	0	100	100
9	V	68/73 (93%)	67 (98%)	1 (2%)	0	100	100
10	J	54/59 (92%)	54 (100%)	0	0	100	100
10	W	54/59 (92%)	54 (100%)	0	0	100	100
11	K	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
11	X	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
12	L	42/47 (89%)	40 (95%)	2 (5%)	0	100	100
12	Y	42/47 (89%)	41 (98%)	1 (2%)	0	100	100
13	M	38/46 (83%)	38 (100%)	0	0	100	100
13	Z	38/46 (83%)	38 (100%)	0	0	100	100
All	All	3488/3614 (96%)	3411 (98%)	74 (2%)	3 (0%)	48	18

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	U	45	ALA
8	H	48	GLY
8	U	48	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	440/426 (103%)	437 (99%)	3 (1%)	76 50
1	N	440/426 (103%)	438 (100%)	2 (0%)	81 60
2	B	215/210 (102%)	207 (96%)	8 (4%)	30 3
2	O	215/210 (102%)	204 (95%)	11 (5%)	21 1
3	C	232/226 (103%)	230 (99%)	2 (1%)	70 42
3	P	232/226 (103%)	230 (99%)	2 (1%)	70 42
4	D	128/129 (99%)	128 (100%)	0	100 100
4	Q	122/129 (95%)	118 (97%)	4 (3%)	33 4
5	E	89/95 (94%)	89 (100%)	0	100 100
5	R	89/95 (94%)	88 (99%)	1 (1%)	65 33
6	F	78/81 (96%)	76 (97%)	2 (3%)	40 7
6	S	78/81 (96%)	77 (99%)	1 (1%)	61 26
7	G	63/69 (91%)	61 (97%)	2 (3%)	34 4
7	T	63/69 (91%)	61 (97%)	2 (3%)	34 4
8	H	67/75 (89%)	65 (97%)	2 (3%)	36 5
8	U	67/75 (89%)	64 (96%)	3 (4%)	24 2
9	I	55/58 (95%)	54 (98%)	1 (2%)	51 16
9	V	55/58 (95%)	48 (87%)	7 (13%)	4 0
10	J	47/50 (94%)	46 (98%)	1 (2%)	47 11
10	W	47/50 (94%)	46 (98%)	1 (2%)	47 11
11	K	39/46 (85%)	38 (97%)	1 (3%)	40 7
11	X	39/46 (85%)	38 (97%)	1 (3%)	40 7
12	L	37/40 (92%)	37 (100%)	0	100 100
12	Y	37/40 (92%)	37 (100%)	0	100 100
13	M	34/38 (90%)	34 (100%)	0	100 100
13	Z	34/38 (90%)	34 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3042/3086 (99%)	2985 (98%)	57 (2%)	50 14

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	128	VAL
1	A	138	HIS
1	A	369	ASP
2	B	33	LEU
2	B	59	GLN
2	B	60	GLU
2	B	65	TRP
2	B	75	LEU
2	B	78	LEU
2	B	91	ASN
2	B	115	ASP
3	C	159	MET
3	C	230	ASN
6	F	37	LYS
6	F	80	GLN
7	G	33	LEU
7	G	37	LEU
8	H	60	TYR
8	H	61	LYS
9	I	36	LYS
10	J	7	GLU
11	K	54	ARG
1	N	363	LEU
1	N	369	ASP
2	O	33	LEU
2	O	60	GLU
2	O	68	LEU
2	O	78	LEU
2	O	87[A]	MET
2	O	87[B]	MET
2	O	91	ASN
2	O	92	ASN
2	O	115	ASP
2	O	217	LYS
2	O	226	MET
3	P	159	MET
3	P	230	ASN

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Mol	Chain	Res	Type
4	Q	10	ASP
4	Q	19	ARG
4	Q	31	LYS
4	Q	51	LEU
5	R	79	LYS
6	S	54	ASN
7	T	33	LEU
7	T	37	LEU
8	U	46	LYS
8	U	60	TYR
8	U	61	LYS
9	V	8	GLN
9	V	29	LEU
9	V	36	LYS
9	V	43	ARG
9	V	61	GLU
9	V	65	LYS
9	V	68	ILE
10	W	50	LEU
11	X	52	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	170	ASN
1	A	422	ASN
2	B	10	GLN
3	C	50	ASN
3	C	56	GLN
3	C	76	GLN
4	D	76	ASN
4	D	109	HIS
4	D	119	GLN
5	E	94	ASN
6	F	54	ASN
8	H	32	ASN
8	H	37	HIS
11	K	35	GLN
1	N	55	ASN
1	N	170	ASN
1	N	422	ASN

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Mol	Chain	Res	Type
3	P	50	ASN
3	P	56	GLN
4	Q	101	HIS
4	Q	109	HIS
5	R	94	ASN
6	S	54	ASN
8	U	37	HIS
9	V	8	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\| > 2$
1	FME	A	1	1	8,9,10	0.53	0	8,9,11	0.81	0
1	FME	N	1	1	8,9,10	0.62	0	8,9,11	0.86	0
2	FME	B	1	2	8,9,10	3.20	3 (37%)	8,9,11	3.53	3 (37%)
2	FME	O	1	2	8,9,10	0.87	0	8,9,11	0.83	0

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
1	FME	A	1	1	-	2/7/9/11	-
1	FME	N	1	1	-	2/7/9/11	-
2	FME	B	1	2	-	2/7/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FME	O	1	2	-	0/7/9/11	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	FME	CA-N	8.21	1.58	1.46
2	B	1	FME	CG-SD	-2.59	1.68	1.81
2	B	1	FME	CB-CG	2.34	1.60	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1	FME	CA-N-CN	-7.41	111.43	122.82
2	B	1	FME	C-CA-N	6.05	121.17	109.50
2	B	1	FME	O1-CN-N	-2.05	120.02	125.32

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	N-CA-CB-CG
2	B	1	FME	O1-CN-N-CA
2	B	1	FME	CB-CA-N-CN
1	N	1	FME	N-CA-CB-CG
1	N	1	FME	C-CA-CB-CG
1	A	1	FME	C-CA-CB-CG

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1	FME	1	0
2	B	1	FME	4	0
2	O	1	FME	2	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 135 ligands modelled in this entry, 8 are monoatomic and 2 are unknown - leaving 125 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
23	EDO	C	827	-	3,3,3	0.50	0	2,2,2	0.74	0
20	DMU	O	731	-	10,10,34	0.20	0	9,9,45	0.46	0
20	DMU	G	712	-	10,10,34	0.22	0	9,9,45	0.59	0
22	LFA	G	621	-	16,16,19	0.35	0	15,15,18	0.61	0
22	LFA	N	628	-	13,13,19	0.56	0	12,12,18	0.53	0
20	DMU	B	742	-	22,22,34	0.70	0	27,27,45	1.18	2 (7%)
22	LFA	P	615	-	10,10,19	0.20	0	9,9,18	0.18	0
23	EDO	B	805	-	3,3,3	1.03	0	2,2,2	0.91	0
22	LFA	C	614	-	14,14,19	0.25	0	13,13,18	0.22	0
23	EDO	N	825	-	3,3,3	0.51	0	2,2,2	0.16	0
20	DMU	G	711	-	22,22,34	0.74	1 (4%)	27,27,45	1.38	3 (11%)
23	EDO	N	829	-	3,3,3	0.16	0	2,2,2	0.21	0
20	DMU	N	745	-	34,34,34	1.43	4 (11%)	45,45,45	1.34	6 (13%)
23	EDO	E	811	-	3,3,3	0.19	0	2,2,2	0.37	0
20	DMU	J	732	-	10,10,34	0.14	0	9,9,45	0.64	0
22	LFA	C	623	-	13,13,19	0.28	0	12,12,18	0.19	0
20	DMU	L	747	-	22,22,34	0.72	0	27,27,45	1.29	3 (11%)
20	DMU	T	712	-	10,10,34	0.47	0	9,9,45	0.59	0
27	PGV	P	266	-	50,50,50	0.93	3 (6%)	53,56,56	1.22	2 (3%)
23	EDO	A	825	-	3,3,3	0.37	0	2,2,2	0.49	0
18	CDL	A	522	-	63,63,99	0.55	0	69,75,111	1.19	6 (8%)
23	EDO	C	809	-	3,3,3	0.20	0	2,2,2	0.51	0
22	LFA	G	622	-	10,10,19	0.17	0	9,9,18	0.17	0
20	DMU	O	742	-	22,22,34	1.03	2 (9%)	27,27,45	1.09	3 (11%)
23	EDO	G	821	-	3,3,3	0.22	0	2,2,2	0.22	0
18	CDL	A	521	-	93,93,99	0.50	0	99,105,111	0.60	2 (2%)
22	LFA	A	627	-	13,13,19	0.83	0	12,12,18	0.31	0
22	LFA	C	612	-	5,5,19	0.20	0	4,4,18	0.17	0
23	EDO	A	801	-	3,3,3	0.65	0	2,2,2	0.86	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	DMU	C	715[A]	-	34,34,34	1.28	6 (17%)	45,45,45	1.38	3 (6%)
23	EDO	N	823	-	3,3,3	0.62	0	2,2,2	0.33	0
22	LFA	C	624	-	10,10,19	0.30	0	9,9,18	0.22	0
22	LFA	C	611	-	10,10,19	0.31	0	9,9,18	0.32	0
22	LFA	T	621	-	16,16,19	0.45	0	15,15,18	0.31	0
20	DMU	W	61	-	34,34,34	0.73	0	45,45,45	1.51	5 (11%)
20	DMU	B	731	-	10,10,34	0.30	0	9,9,45	0.54	0
14	HEA	A	515[B]	-	67,67,67	1.69	14 (20%)	81,103,103	2.32	25 (30%)
22	LFA	C	716[B]	-	17,17,19	0.17	0	16,16,18	0.17	0
22	LFA	N	627	-	13,13,19	0.36	0	12,12,18	0.54	0
20	DMU	N	526	-	34,34,34	0.98	2 (5%)	45,45,45	1.16	3 (6%)
23	EDO	F	819	-	3,3,3	0.44	0	2,2,2	0.39	0
23	EDO	N	803	-	3,3,3	0.19	0	2,2,2	0.41	0
20	DMU	C	722	-	22,22,34	0.52	0	27,27,45	0.95	2 (7%)
14	HEA	A	515[A]	-	67,67,67	1.70	15 (22%)	81,103,103	2.33	25 (30%)
20	DMU	P	733	-	34,34,34	0.80	2 (5%)	45,45,45	1.47	4 (8%)
19	CHD	P	271	-	32,32,32	0.60	0	51,51,51	1.60	8 (15%)
19	CHD	C	271	-	32,32,32	0.71	0	51,51,51	1.57	9 (17%)
20	DMU	A	743	-	6,6,34	0.31	0	5,5,45	0.39	0
20	DMU	N	744	-	34,34,34	1.40	7 (20%)	45,45,45	1.56	5 (11%)
22	LFA	P	611	-	10,10,19	0.29	0	9,9,18	0.20	0
22	LFA	P	614	-	14,14,19	0.18	0	13,13,18	0.17	0
14	HEA	A	516	1,21	67,67,67	2.01	18 (26%)	81,103,103	2.62	30 (37%)
20	DMU	A	745	-	34,34,34	1.17	3 (8%)	45,45,45	1.03	2 (4%)
22	LFA	C	625	-	14,14,19	0.29	0	13,13,18	0.44	0
20	DMU	P	734	-	34,34,34	0.92	1 (2%)	45,45,45	1.19	2 (4%)
23	EDO	A	823	-	3,3,3	0.53	0	2,2,2	0.48	0
23	EDO	N	801	-	3,3,3	0.54	0	2,2,2	0.17	0
19	CHD	N	525	-	32,32,32	1.03	2 (6%)	51,51,51	0.94	1 (1%)
22	LFA	P	623	-	13,13,19	0.25	0	12,12,18	0.28	0
21	PER	N	520	14,15	1,1,1	1.75	0	-		
18	CDL	N	521	-	93,93,99	0.38	0	99,105,111	0.46	0
20	DMU	B	741	-	10,10,34	0.35	0	9,9,45	0.56	0
22	LFA	A	628	-	13,13,19	0.51	0	12,12,18	0.70	0
24	CUA	B	228	2	0,1,1	-	-	-		
19	CHD	G	86	-	32,32,32	0.78	0	51,51,51	1.10	3 (5%)
23	EDO	P	809	-	3,3,3	0.38	0	2,2,2	0.33	0
20	DMU	C	734	-	34,34,34	0.96	1 (2%)	45,45,45	1.06	3 (6%)
23	EDO	R	815	-	3,3,3	0.14	0	2,2,2	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	PEK	C	264	-	52,52,52	0.60	2 (3%)	55,57,57	0.81	2 (3%)
20	DMU	P	721	-	6,6,34	0.20	0	5,5,45	0.65	0
19	CHD	T	86	-	32,32,32	0.88	1 (3%)	51,51,51	1.09	2 (3%)
27	PGV	C	266	-	50,50,50	1.10	4 (8%)	53,56,56	1.08	3 (5%)
26	PEK	P	264	-	52,52,52	0.74	2 (3%)	55,57,57	1.01	4 (7%)
20	DMU	P	272	-	10,10,34	0.25	0	9,9,45	0.70	0
20	DMU	P	715[A]	-	34,34,34	1.19	4 (11%)	45,45,45	1.27	3 (6%)
20	DMU	O	741	-	10,10,34	0.57	0	9,9,45	0.55	0
22	LFA	P	624	-	10,10,19	0.20	0	9,9,18	0.15	0
22	LFA	T	622	-	10,10,19	0.25	0	9,9,18	0.12	0
23	EDO	P	827	-	3,3,3	0.55	0	2,2,2	1.12	0
23	EDO	F	817	-	3,3,3	0.64	0	2,2,2	0.31	0
23	EDO	O	805	-	3,3,3	0.55	0	2,2,2	0.12	0
20	DMU	M	746	-	7,7,34	0.25	0	6,6,45	0.83	0
20	DMU	G	713	-	22,22,34	0.53	0	27,27,45	1.19	3 (11%)
14	HEA	N	515[B]	-	67,67,67	1.61	13 (19%)	81,103,103	2.00	23 (28%)
20	DMU	C	714	-	34,34,34	0.84	1 (2%)	45,45,45	1.27	6 (13%)
23	EDO	A	803	-	3,3,3	0.08	0	2,2,2	0.10	0
23	EDO	P	807	-	3,3,3	0.07	0	2,2,2	0.07	0
23	EDO	T	821	-	3,3,3	0.44	0	2,2,2	0.28	0
20	DMU	T	711	-	22,22,34	0.79	0	27,27,45	1.46	4 (14%)
18	CDL	C	270	-	86,86,99	0.58	1 (1%)	92,98,111	1.07	9 (9%)
23	EDO	S	819	-	3,3,3	0.31	0	2,2,2	0.26	0
14	HEA	N	515[A]	-	67,67,67	1.59	13 (19%)	81,103,103	2.04	21 (25%)
23	EDO	S	817	-	3,3,3	0.94	0	2,2,2	0.12	0
22	LFA	P	612	-	5,5,19	0.09	0	4,4,18	0.21	0
20	DMU	C	733	-	34,34,34	1.17	5 (14%)	45,45,45	1.21	5 (11%)
22	LFA	C	615	-	10,10,19	0.16	0	9,9,18	0.16	0
20	DMU	W	732	-	10,10,34	0.15	0	9,9,45	0.57	0
23	EDO	R	811	-	3,3,3	0.12	0	2,2,2	0.09	0
20	DMU	A	526	-	34,34,34	1.08	2 (5%)	45,45,45	1.13	2 (4%)
23	EDO	C	807	-	3,3,3	0.17	0	2,2,2	0.20	0
18	CDL	N	522	-	63,63,99	0.51	1 (1%)	69,75,111	1.05	5 (7%)
20	DMU	Y	747	-	22,22,34	0.56	0	27,27,45	1.20	2 (7%)
23	EDO	E	813	-	3,3,3	0.36	0	2,2,2	0.13	0
20	DMU	P	722	-	22,22,34	0.45	0	27,27,45	1.07	2 (7%)
27	PGV	C	267	-	50,50,50	0.91	3 (6%)	53,56,56	1.10	3 (5%)
27	PGV	P	267	-	50,50,50	0.77	1 (2%)	53,56,56	0.93	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	DMU	A	744	-	34,34,34	1.44	6 (17%)	45,45,45	1.21	4 (8%)
22	LFA	C	626	-	12,12,19	0.21	0	11,11,18	0.26	0
22	LFA	P	626	-	12,12,19	0.34	0	11,11,18	0.31	0
20	DMU	P	714	-	34,34,34	0.71	0	45,45,45	1.07	3 (6%)
23	EDO	R	813	-	3,3,3	0.19	0	2,2,2	0.07	0
22	LFA	P	716[B]	-	17,17,19	0.14	0	16,16,18	0.12	0
20	DMU	N	743	-	6,6,34	0.36	0	5,5,45	0.37	0
19	CHD	A	525	-	32,32,32	1.01	2 (6%)	51,51,51	1.12	4 (7%)
14	HEA	N	516	1,21	67,67,67	1.93	16 (23%)	81,103,103	2.96	26 (32%)
20	DMU	C	721	-	6,6,34	0.23	0	5,5,45	0.61	0
21	PER	A	520	14,15	1,1,1	1.97	0	-		
23	EDO	E	815	-	3,3,3	0.39	0	2,2,2	0.51	0
20	DMU	T	713	-	22,22,34	0.68	0	27,27,45	1.39	5 (18%)
22	LFA	P	625	-	14,14,19	0.34	0	13,13,18	0.54	0
20	DMU	C	272	-	10,10,34	0.34	0	9,9,45	0.60	0
20	DMU	J	61	-	34,34,34	0.84	1 (2%)	45,45,45	1.07	2 (4%)
18	CDL	P	270	-	86,86,99	0.49	0	92,98,111	0.96	7 (7%)
24	CUA	O	228	2	0,1,1	-	-	-		
20	DMU	Z	746	-	7,7,34	0.16	0	6,6,45	0.49	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	EDO	C	827	-	-	1/1/1/1	-
20	DMU	O	731	-	-	4/8/8/59	-
20	DMU	G	712	-	-	4/8/8/59	-
22	LFA	G	621	-	-	9/14/14/17	-
22	LFA	N	628	-	-	6/11/11/17	-
20	DMU	B	742	-	-	8/13/33/59	0/1/1/2
22	LFA	P	615	-	-	5/8/8/17	-
23	EDO	B	805	-	-	0/1/1/1	-
22	LFA	C	614	-	-	7/12/12/17	-
23	EDO	N	825	-	-	0/1/1/1	-
20	DMU	G	711	-	-	3/13/33/59	0/1/1/2
23	EDO	N	829	-	-	0/1/1/1	-
20	DMU	N	745	-	-	7/19/59/59	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	EDO	E	811	-	-	0/1/1/1	-
20	DMU	J	732	-	-	5/8/8/59	-
22	LFA	C	623	-	-	5/11/11/17	-
20	DMU	L	747	-	-	10/13/33/59	0/1/1/2
20	DMU	T	712	-	-	4/8/8/59	-
27	PGV	P	266	-	-	8/55/55/55	-
23	EDO	A	825	-	-	1/1/1/1	-
18	CDL	A	522	-	-	31/74/74/110	-
23	EDO	C	809	-	-	0/1/1/1	-
22	LFA	G	622	-	-	3/8/8/17	-
20	DMU	O	742	-	-	7/13/33/59	0/1/1/2
23	EDO	G	821	-	-	0/1/1/1	-
18	CDL	A	521	-	-	49/104/104/110	-
22	LFA	A	627	-	-	5/11/11/17	-
22	LFA	C	612	-	-	1/3/3/17	-
23	EDO	A	801	-	-	0/1/1/1	-
20	DMU	C	715[A]	-	-	3/19/59/59	0/2/2/2
23	EDO	N	823	-	-	0/1/1/1	-
22	LFA	C	624	-	-	4/8/8/17	-
22	LFA	C	611	-	-	5/8/8/17	-
22	LFA	T	621	-	-	9/14/14/17	-
20	DMU	W	61	-	-	3/19/59/59	0/2/2/2
20	DMU	B	731	-	-	6/8/8/59	-
14	HEA	A	515[B]	-	-	3/36/76/76	-
22	LFA	C	716[B]	-	-	5/15/15/17	-
22	LFA	N	627	-	-	5/11/11/17	-
20	DMU	N	526	-	-	6/19/59/59	0/2/2/2
23	EDO	F	819	-	-	0/1/1/1	-
23	EDO	N	803	-	-	1/1/1/1	-
20	DMU	C	722	-	-	10/13/33/59	0/1/1/2
14	HEA	A	515[A]	-	-	6/36/76/76	-
20	DMU	P	733	-	-	6/19/59/59	0/2/2/2
19	CHD	P	271	-	-	8/9/74/74	0/4/4/4
19	CHD	C	271	-	-	8/9/74/74	0/4/4/4
20	DMU	A	743	-	-	2/4/4/59	-
20	DMU	N	744	-	-	6/19/59/59	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	LFA	P	611	-	-	5/8/8/17	-
22	LFA	P	614	-	-	6/12/12/17	-
14	HEA	A	516	1,21	-	5/36/76/76	-
20	DMU	A	745	-	-	5/19/59/59	0/2/2/2
22	LFA	C	625	-	-	3/12/12/17	-
20	DMU	P	734	-	-	9/19/59/59	0/2/2/2
23	EDO	A	823	-	-	0/1/1/1	-
23	EDO	N	801	-	-	0/1/1/1	-
19	CHD	N	525	-	-	2/9/74/74	0/4/4/4
22	LFA	P	623	-	-	5/11/11/17	-
18	CDL	N	521	-	-	52/104/104/110	-
20	DMU	B	741	-	-	4/8/8/59	-
22	LFA	A	628	-	-	5/11/11/17	-
19	CHD	G	86	-	-	2/9/74/74	0/4/4/4
23	EDO	P	809	-	-	0/1/1/1	-
20	DMU	C	734	-	-	8/19/59/59	0/2/2/2
23	EDO	R	815	-	-	1/1/1/1	-
26	PEK	C	264	-	-	14/56/56/56	-
20	DMU	P	721	-	-	3/4/4/59	-
19	CHD	T	86	-	-	2/9/74/74	0/4/4/4
27	PGV	C	266	-	-	7/55/55/55	-
26	PEK	P	264	-	-	18/56/56/56	-
20	DMU	P	272	-	-	0/8/8/59	-
20	DMU	P	715[A]	-	-	5/19/59/59	0/2/2/2
20	DMU	O	741	-	-	4/8/8/59	-
22	LFA	P	624	-	-	6/8/8/17	-
22	LFA	T	622	-	-	4/8/8/17	-
23	EDO	P	827	-	-	0/1/1/1	-
23	EDO	F	817	-	-	0/1/1/1	-
23	EDO	O	805	-	-	0/1/1/1	-
20	DMU	M	746	-	-	5/5/5/59	-
20	DMU	G	713	-	-	7/13/33/59	0/1/1/2
14	HEA	N	515[B]	-	-	2/36/76/76	-
20	DMU	C	714	-	-	9/19/59/59	0/2/2/2
23	EDO	A	803	-	-	0/1/1/1	-
23	EDO	P	807	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	EDO	T	821	-	-	0/1/1/1	-
20	DMU	T	711	-	-	7/13/33/59	0/1/1/2
18	CDL	C	270	-	-	49/97/97/110	-
23	EDO	S	819	-	-	0/1/1/1	-
14	HEA	N	515[A]	-	-	5/36/76/76	-
23	EDO	S	817	-	-	0/1/1/1	-
22	LFA	P	612	-	-	1/3/3/17	-
20	DMU	C	733	-	-	9/19/59/59	0/2/2/2
22	LFA	C	615	-	-	2/8/8/17	-
20	DMU	W	732	-	-	7/8/8/59	-
23	EDO	R	811	-	-	1/1/1/1	-
20	DMU	A	526	-	-	4/19/59/59	0/2/2/2
23	EDO	C	807	-	-	0/1/1/1	-
18	CDL	N	522	-	-	34/74/74/110	-
20	DMU	Y	747	-	-	9/13/33/59	0/1/1/2
23	EDO	E	813	-	-	0/1/1/1	-
20	DMU	P	722	-	-	7/13/33/59	0/1/1/2
27	PGV	C	267	-	-	12/55/55/55	-
27	PGV	P	267	-	-	12/55/55/55	-
20	DMU	A	744	-	-	7/19/59/59	0/2/2/2
22	LFA	C	626	-	-	4/10/10/17	-
22	LFA	P	626	-	-	5/10/10/17	-
20	DMU	P	714	-	-	5/19/59/59	0/2/2/2
23	EDO	R	813	-	-	0/1/1/1	-
22	LFA	P	716[B]	-	-	6/15/15/17	-
20	DMU	N	743	-	-	3/4/4/59	-
19	CHD	A	525	-	-	2/9/74/74	0/4/4/4
14	HEA	N	516	1,21	-	5/36/76/76	-
20	DMU	C	721	-	-	2/4/4/59	-
23	EDO	E	815	-	-	1/1/1/1	-
20	DMU	T	713	-	-	4/13/33/59	0/1/1/2
22	LFA	P	625	-	-	4/12/12/17	-
20	DMU	C	272	-	-	3/8/8/59	-
20	DMU	J	61	-	-	4/19/59/59	0/2/2/2
18	CDL	P	270	-	-	48/97/97/110	-
20	DMU	Z	746	-	-	2/5/5/59	-

All (159) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	516	HEA	CHD-C1D	6.74	1.52	1.38
14	N	516	HEA	C1D-ND	-6.70	1.28	1.40
14	A	516	HEA	C3B-C2B	5.40	1.47	1.34
14	N	515[A]	HEA	CHB-C4A	4.80	1.47	1.38
14	N	515[B]	HEA	CHB-C4A	4.80	1.47	1.38
20	N	745	DMU	O16-C6	-4.65	1.32	1.40
14	N	516	HEA	C3C-C4C	4.52	1.55	1.42
14	N	516	HEA	C3B-C2B	4.44	1.44	1.34
14	A	515[A]	HEA	C16-C17	-4.38	1.39	1.53
14	A	515[B]	HEA	C16-C17	-4.38	1.39	1.53
20	A	744	DMU	O49-C1	-4.15	1.32	1.43
14	A	515[A]	HEA	CBD-CGD	4.15	1.60	1.50
14	A	515[B]	HEA	CBD-CGD	4.15	1.60	1.50
14	N	516	HEA	CHD-C1D	4.13	1.46	1.38
20	P	715[A]	DMU	O3-C5	-4.12	1.32	1.43
14	A	516	HEA	CMB-C2B	-4.07	1.42	1.50
14	A	516	HEA	O1A-CGA	3.85	1.34	1.22
14	N	516	HEA	CMD-C2D	-3.83	1.42	1.50
20	C	733	DMU	O16-C6	-3.80	1.33	1.40
14	A	516	HEA	CHC-C4B	3.80	1.46	1.38
14	A	515[A]	HEA	CHB-C4A	3.70	1.45	1.38
14	A	515[B]	HEA	CHB-C4A	3.70	1.45	1.38
14	N	515[A]	HEA	C16-C17	-3.69	1.41	1.53
14	N	515[B]	HEA	C16-C17	-3.69	1.41	1.53
14	A	516	HEA	C3D-C2D	3.69	1.44	1.36
14	A	516	HEA	C4C-NC	-3.68	1.32	1.39
27	C	266	PGV	C21-C20	3.64	1.65	1.52
14	N	516	HEA	C3D-C2D	3.63	1.44	1.36
14	N	516	HEA	CHB-C1B	3.54	1.47	1.39
20	P	734	DMU	O3-C5	-3.46	1.34	1.43
26	P	264	PEK	C2-C1	3.35	1.60	1.50
14	A	516	HEA	CHB-C1B	3.31	1.46	1.39
14	N	515[A]	HEA	CHD-C1D	3.28	1.45	1.38
14	N	515[B]	HEA	CHD-C1D	3.28	1.45	1.38
20	N	744	DMU	O49-C1	-3.24	1.34	1.43
14	A	515[A]	HEA	C4D-C3D	-3.24	1.39	1.45
14	A	515[B]	HEA	C4D-C3D	-3.24	1.39	1.45
20	N	745	DMU	C10-C5	-3.19	1.43	1.52
20	C	715[A]	DMU	O5-C6	-3.17	1.33	1.41
20	N	744	DMU	O5-C6	-3.13	1.33	1.41
14	A	515[A]	HEA	C4B-C3B	-3.11	1.39	1.44
14	A	515[B]	HEA	C4B-C3B	-3.11	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	C	734	DMU	O3-C5	-3.11	1.35	1.43
14	N	515[A]	HEA	CHC-C4B	3.11	1.44	1.38
14	N	515[B]	HEA	CHC-C4B	3.11	1.44	1.38
14	N	516	HEA	C1B-NB	-3.10	1.32	1.38
19	A	525	CHD	O25-C24	3.06	1.32	1.22
20	N	526	DMU	O16-C6	-3.00	1.35	1.40
14	A	515[A]	HEA	C14-C15	-2.98	1.26	1.33
14	A	515[B]	HEA	C14-C15	-2.98	1.26	1.33
14	A	515[A]	HEA	CHD-C1D	2.91	1.44	1.38
14	A	515[B]	HEA	CHD-C1D	2.91	1.44	1.38
14	A	516	HEA	FE-NB	2.90	2.03	1.94
14	N	515[A]	HEA	C1A-NA	2.90	1.45	1.39
14	N	515[B]	HEA	C1A-NA	2.90	1.45	1.39
20	A	745	DMU	C10-C5	-2.89	1.44	1.52
14	A	516	HEA	CMD-C2D	-2.88	1.44	1.50
14	N	515[A]	HEA	CBD-CGD	2.85	1.57	1.50
14	N	515[B]	HEA	CBD-CGD	2.85	1.57	1.50
14	N	516	HEA	O1A-CGA	2.84	1.31	1.22
20	C	715[A]	DMU	O3-C5	-2.81	1.36	1.43
14	N	515[A]	HEA	C3B-C2B	2.81	1.41	1.34
14	N	515[B]	HEA	C3B-C2B	2.81	1.41	1.34
20	O	742	DMU	O16-C6	-2.76	1.35	1.40
27	C	267	PGV	O01-C02	-2.75	1.40	1.46
14	A	516	HEA	C4B-C3B	-2.75	1.39	1.44
14	A	516	HEA	C1B-NB	-2.69	1.33	1.38
26	P	264	PEK	C23-C22	-2.68	1.42	1.52
20	O	742	DMU	O16-C18	2.67	1.50	1.43
20	A	744	DMU	O55-C2	2.65	1.49	1.43
14	A	515[A]	HEA	C3D-C2D	2.62	1.42	1.36
14	A	515[B]	HEA	C3D-C2D	2.62	1.42	1.36
20	N	744	DMU	O1-C10	2.61	1.48	1.41
14	N	516	HEA	C4D-C3D	-2.60	1.40	1.45
14	N	516	HEA	CMB-C2B	-2.59	1.45	1.50
14	A	516	HEA	C3A-C4A	2.59	1.50	1.46
20	N	744	DMU	C10-C5	-2.57	1.45	1.52
20	C	733	DMU	O3-C5	-2.57	1.36	1.43
18	C	270	CDL	C11-CA5	2.56	1.58	1.50
27	P	267	PGV	P-O14	-2.52	1.43	1.55
14	N	515[A]	HEA	C4C-NC	-2.51	1.34	1.39
14	N	515[B]	HEA	C4C-NC	-2.51	1.34	1.39
20	N	745	DMU	C7-C5	-2.51	1.45	1.52
20	C	715[A]	DMU	C10-C5	-2.50	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	515[A]	HEA	CHC-C4B	2.46	1.43	1.38
14	A	515[B]	HEA	CHC-C4B	2.46	1.43	1.38
14	N	515[A]	HEA	CBA-CGA	2.44	1.56	1.50
14	N	515[B]	HEA	CBA-CGA	2.44	1.56	1.50
19	N	525	CHD	O26-C24	-2.41	1.22	1.30
14	A	515[A]	HEA	C4B-NB	-2.41	1.36	1.40
14	A	515[B]	HEA	C4B-NB	-2.41	1.36	1.40
27	C	266	PGV	P-O13	-2.40	1.42	1.50
14	N	516	HEA	CHC-C4B	2.40	1.43	1.38
27	C	266	PGV	P-O14	-2.39	1.44	1.55
26	C	264	PEK	C22-C21	2.39	1.57	1.50
14	A	516	HEA	C3C-C4C	2.39	1.49	1.42
19	A	525	CHD	O26-C24	-2.39	1.22	1.30
14	N	515[A]	HEA	CHA-C4D	2.38	1.44	1.39
14	N	515[B]	HEA	CHA-C4D	2.38	1.44	1.39
20	C	733	DMU	O5-C6	-2.38	1.35	1.41
14	A	516	HEA	CHC-C1C	-2.37	1.34	1.39
20	C	715[A]	DMU	O2-C8	2.36	1.48	1.43
14	N	516	HEA	C4C-NC	-2.35	1.35	1.39
20	N	744	DMU	O16-C6	-2.35	1.36	1.40
20	A	744	DMU	O16-C6	-2.35	1.36	1.40
20	A	744	DMU	O3-C5	-2.34	1.37	1.43
20	N	744	DMU	O3-C5	-2.34	1.37	1.43
14	A	516	HEA	C1D-ND	-2.33	1.36	1.40
20	C	714	DMU	C7-C5	-2.32	1.46	1.52
19	N	525	CHD	O25-C24	2.32	1.29	1.22
20	C	715[A]	DMU	O16-C6	-2.31	1.36	1.40
20	G	711	DMU	C3-C4	-2.30	1.48	1.53
20	P	715[A]	DMU	C7-C5	-2.30	1.46	1.52
14	A	515[A]	HEA	C12-C11	-2.28	1.49	1.53
14	A	515[B]	HEA	C12-C11	-2.28	1.49	1.53
20	P	715[A]	DMU	C10-C5	-2.28	1.45	1.52
27	C	267	PGV	C22-C21	2.28	1.63	1.51
27	C	267	PGV	O04-C19	-2.27	1.15	1.22
20	C	715[A]	DMU	C7-C5	-2.26	1.46	1.52
18	N	522	CDL	OA7-CA5	-2.25	1.15	1.22
19	T	86	CHD	O26-C24	-2.24	1.23	1.30
14	N	516	HEA	C1C-NC	-2.24	1.35	1.39
14	N	516	HEA	C3A-C4A	2.23	1.49	1.46
20	N	526	DMU	O1-C10	2.23	1.47	1.41
20	A	526	DMU	C10-C5	-2.21	1.46	1.52
14	A	515[A]	HEA	C27-C19	-2.20	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	N	745	DMU	O1-C10	2.18	1.47	1.41
20	P	733	DMU	O5-C6	-2.18	1.36	1.41
14	A	515[A]	HEA	C4C-NC	-2.18	1.35	1.39
14	A	515[B]	HEA	C4C-NC	-2.18	1.35	1.39
27	P	266	PGV	O03-C01	2.17	1.50	1.45
20	N	744	DMU	C7-C5	-2.16	1.46	1.52
20	C	733	DMU	C7-C5	-2.15	1.46	1.52
20	A	744	DMU	O5-C6	-2.14	1.36	1.41
20	A	526	DMU	C7-C5	-2.14	1.46	1.52
26	C	264	PEK	C23-C22	-2.13	1.44	1.52
20	J	61	DMU	C7-C5	-2.11	1.46	1.52
20	A	745	DMU	C3-C4	2.09	1.58	1.52
14	A	516	HEA	C18-C19	2.09	1.37	1.33
27	P	266	PGV	P-O14	-2.09	1.45	1.55
14	A	515[A]	HEA	C12-C13	2.08	1.60	1.53
14	A	515[B]	HEA	C12-C13	2.08	1.60	1.53
20	C	733	DMU	C10-C5	-2.08	1.46	1.52
20	P	715[A]	DMU	O5-C6	-2.07	1.36	1.41
20	A	745	DMU	O7-C10	2.07	1.47	1.41
27	C	266	PGV	C03-C02	2.06	1.57	1.50
20	A	744	DMU	O1-C10	2.06	1.47	1.41
20	P	733	DMU	C6-C1	-2.05	1.46	1.52
14	N	515[A]	HEA	O11-C11	2.05	1.47	1.42
14	N	515[B]	HEA	O11-C11	2.05	1.47	1.42
14	A	516	HEA	C11-C3B	2.05	1.53	1.51
27	P	266	PGV	O01-C02	-2.04	1.41	1.46
14	N	515[A]	HEA	C4B-C3B	-2.03	1.41	1.44
14	N	515[B]	HEA	C4B-C3B	-2.03	1.41	1.44
14	A	515[A]	HEA	CBA-CGA	2.02	1.55	1.50
14	A	515[B]	HEA	CBA-CGA	2.02	1.55	1.50
14	N	516	HEA	FE-NB	2.01	2.01	1.94
14	N	515[A]	HEA	C1C-C2C	2.01	1.47	1.43
14	N	515[B]	HEA	C1C-C2C	2.01	1.47	1.43

All (308) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	N	516	HEA	C2D-C1D-ND	10.39	121.78	109.84
14	N	516	HEA	C1D-C2D-C3D	-8.10	98.46	106.98
14	A	515[A]	HEA	C3C-C4C-NC	7.88	116.44	109.80
14	A	515[B]	HEA	C3C-C4C-NC	7.88	116.44	109.80
14	N	516	HEA	CMD-C2D-C1D	7.73	137.11	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	N	516	HEA	C2B-C1B-NB	7.70	118.80	109.90
14	A	516	HEA	C1B-C2B-C3B	-7.61	97.99	106.80
14	N	516	HEA	CHB-C1B-C2B	-7.06	113.89	125.03
14	N	516	HEA	CMB-C2B-C1B	7.04	136.03	125.03
14	A	516	HEA	C2B-C1B-NB	6.99	117.99	109.90
14	A	516	HEA	CMB-C2B-C1B	6.95	135.90	125.03
14	A	516	HEA	C2D-C1D-ND	6.92	117.80	109.84
20	N	744	DMU	O16-C6-C1	6.56	118.23	108.27
14	A	515[A]	HEA	C3D-C4D-ND	6.45	116.58	110.35
14	A	515[B]	HEA	C3D-C4D-ND	6.45	116.58	110.35
14	N	516	HEA	C1B-C2B-C3B	-6.40	99.39	106.80
19	P	271	CHD	C17-C13-C14	-6.36	93.73	100.11
14	A	516	HEA	CMD-C2D-C1D	5.96	134.35	125.03
14	N	516	HEA	C4C-C3C-C2C	-5.93	99.93	107.30
18	A	522	CDL	OA6-CA4-CA3	5.86	129.36	108.34
20	P	715[A]	DMU	O16-C6-C1	5.61	116.80	108.27
20	C	715[A]	DMU	O16-C6-C1	5.45	116.55	108.27
20	W	61	DMU	C10-C5-C7	5.36	121.29	110.01
14	N	515[A]	HEA	C27-C19-C20	5.36	124.54	115.23
14	A	516	HEA	CHB-C1B-C2B	-5.30	116.66	125.03
19	C	271	CHD	C17-C13-C14	-5.21	94.88	100.11
27	P	266	PGV	O03-C19-O04	-5.10	110.86	123.63
14	N	515[A]	HEA	C2D-C1D-ND	5.06	115.66	109.84
14	N	515[B]	HEA	C2D-C1D-ND	5.06	115.66	109.84
20	P	734	DMU	C10-C5-C7	5.02	120.58	110.01
20	W	61	DMU	O16-C6-C1	4.94	115.78	108.27
20	P	733	DMU	C10-C5-C7	4.90	120.31	110.01
14	A	516	HEA	C1D-C2D-C3D	-4.89	101.83	106.98
14	N	515[A]	HEA	C3C-C4C-NC	4.88	113.91	109.80
14	N	515[B]	HEA	C3C-C4C-NC	4.88	113.91	109.80
20	T	711	DMU	O5-C6-C1	4.87	120.38	110.37
20	G	711	DMU	O5-C6-C1	4.85	120.34	110.37
20	T	713	DMU	O16-C6-C1	4.84	115.63	108.27
14	N	516	HEA	C1D-ND-C4D	-4.75	99.58	105.21
19	C	271	CHD	C16-C17-C20	4.74	119.35	112.18
18	N	522	CDL	OA6-CA5-C11	4.68	121.60	111.48
27	C	267	PGV	C23-C22-C21	4.67	137.97	114.37
20	Y	747	DMU	O16-C6-C1	4.64	115.32	108.27
14	A	515[A]	HEA	C26-C15-C16	-4.62	107.21	115.23
14	A	515[B]	HEA	C26-C15-C16	-4.62	107.21	115.23
14	A	515[A]	HEA	C2D-C1D-ND	4.62	115.15	109.84
14	A	515[B]	HEA	C2D-C1D-ND	4.62	115.15	109.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	515[A]	HEA	CHA-C4D-ND	-4.62	119.45	124.42
14	A	515[B]	HEA	CHA-C4D-ND	-4.62	119.45	124.42
14	N	516	HEA	C3B-C4B-NB	4.60	115.13	109.84
14	N	515[A]	HEA	C1D-ND-C4D	-4.59	99.77	105.21
14	N	515[B]	HEA	C1D-ND-C4D	-4.59	99.77	105.21
14	N	515[A]	HEA	C3B-C4B-NB	4.59	115.11	109.84
14	N	515[B]	HEA	C3B-C4B-NB	4.59	115.11	109.84
19	C	271	CHD	C14-C13-C12	4.56	111.58	107.42
14	A	515[A]	HEA	C1D-ND-C4D	-4.47	99.92	105.21
14	A	515[B]	HEA	C1D-ND-C4D	-4.47	99.92	105.21
20	J	61	DMU	O16-C6-C1	4.45	115.04	108.27
14	N	515[A]	HEA	C3D-C4D-ND	4.45	114.65	110.35
14	N	515[B]	HEA	C3D-C4D-ND	4.45	114.65	110.35
14	A	515[A]	HEA	C3B-C4B-NB	4.42	114.92	109.84
14	A	515[B]	HEA	C3B-C4B-NB	4.42	114.92	109.84
26	P	264	PEK	O01-C1-O02	-4.42	113.37	123.70
20	L	747	DMU	O16-C6-C1	4.39	114.94	108.27
14	A	516	HEA	CHB-C4A-NA	4.34	129.18	124.45
14	N	515[A]	HEA	C2B-C1B-NB	4.31	114.88	109.90
14	N	515[B]	HEA	C2B-C1B-NB	4.31	114.88	109.90
14	N	515[A]	HEA	CHC-C4B-NB	-4.25	119.11	124.37
14	N	515[B]	HEA	CHC-C4B-NB	-4.25	119.11	124.37
14	A	515[A]	HEA	C4C-C3C-C2C	-4.24	102.03	107.30
14	A	515[B]	HEA	C4C-C3C-C2C	-4.24	102.03	107.30
19	P	271	CHD	C14-C13-C12	4.23	111.28	107.42
20	B	742	DMU	O16-C6-C1	4.22	114.69	108.27
14	N	515[A]	HEA	C4B-NB-C1B	-4.21	100.22	105.21
14	N	515[B]	HEA	C4B-NB-C1B	-4.21	100.22	105.21
20	A	744	DMU	O16-C6-C1	4.21	114.67	108.27
14	A	515[A]	HEA	C2B-C1B-NB	4.19	114.74	109.90
14	A	515[B]	HEA	C2B-C1B-NB	4.19	114.74	109.90
18	A	522	CDL	CA4-OA6-CA5	4.17	127.78	117.80
14	A	515[A]	HEA	C27-C19-C20	4.13	122.40	115.23
20	N	526	DMU	O16-C6-C1	4.13	114.54	108.27
14	A	515[A]	HEA	C1B-C2B-C3B	-4.12	102.03	106.80
14	A	515[B]	HEA	C1B-C2B-C3B	-4.12	102.03	106.80
20	A	526	DMU	O16-C6-C1	4.08	114.47	108.27
14	N	516	HEA	C4B-NB-C1B	-4.07	100.38	105.21
20	A	745	DMU	C10-O1-C9	4.06	121.65	113.72
20	P	714	DMU	O16-C6-C1	4.03	114.39	108.27
19	P	271	CHD	C16-C17-C20	4.01	118.25	112.18
14	A	516	HEA	C3D-C4D-ND	4.00	114.22	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	P	733	DMU	C6-O5-C4	3.99	121.50	113.72
14	N	516	HEA	CHD-C1D-C2D	-3.98	115.63	126.95
20	G	713	DMU	O16-C6-C1	3.92	114.22	108.27
20	C	714	DMU	O16-C6-C1	3.88	114.17	108.27
18	C	270	CDL	OB6-CB5-C51	3.87	119.84	111.48
14	A	515[A]	HEA	CHC-C4B-NB	-3.83	119.63	124.37
14	A	515[B]	HEA	CHC-C4B-NB	-3.83	119.63	124.37
18	P	270	CDL	OB6-CB5-C51	3.80	119.70	111.48
14	A	515[A]	HEA	C1D-C2D-C3D	-3.78	103.00	106.98
14	A	515[B]	HEA	C1D-C2D-C3D	-3.78	103.00	106.98
14	N	515[A]	HEA	CHB-C4A-NA	-3.77	120.35	124.45
14	N	515[B]	HEA	CHB-C4A-NA	-3.77	120.35	124.45
14	A	516	HEA	CHC-C1C-C2C	-3.74	116.56	127.43
20	P	733	DMU	O5-C6-C1	3.72	118.02	110.37
14	N	515[A]	HEA	C13-C12-C11	-3.70	108.48	114.39
14	N	515[B]	HEA	C13-C12-C11	-3.70	108.48	114.39
18	C	270	CDL	OA6-CA5-OA7	-3.68	115.09	123.70
14	A	516	HEA	C1D-ND-C4D	-3.67	100.86	105.21
14	A	515[A]	HEA	C4B-NB-C1B	-3.64	100.89	105.21
14	A	515[B]	HEA	C4B-NB-C1B	-3.64	100.89	105.21
20	C	734	DMU	C10-C5-C7	3.63	117.66	110.01
20	N	745	DMU	C10-O1-C9	3.56	120.67	113.72
20	P	733	DMU	O5-C4-C3	3.55	117.07	109.72
20	C	715[A]	DMU	C10-O1-C9	3.55	120.66	113.72
27	P	266	PGV	O03-C19-C20	3.52	122.57	111.83
14	N	515[A]	HEA	CHA-C4D-ND	-3.49	120.66	124.42
14	N	515[B]	HEA	CHA-C4D-ND	-3.49	120.66	124.42
14	A	516	HEA	O1A-CGA-CBA	-3.48	112.06	123.09
14	A	516	HEA	C4A-C3A-C2A	-3.45	103.82	106.81
14	A	516	HEA	O2A-CGA-CBA	3.44	124.88	114.00
14	N	516	HEA	CHC-C4B-NB	-3.39	120.17	124.37
18	C	270	CDL	OA7-CA5-C11	3.39	137.02	123.78
14	N	515[B]	HEA	C27-C19-C20	3.37	121.08	115.23
14	A	516	HEA	CHC-C1C-NC	3.35	129.94	123.86
19	G	86	CHD	C18-C13-C12	3.32	112.38	109.06
14	N	516	HEA	C3D-C4D-ND	3.30	113.54	110.35
18	P	270	CDL	OB5-PB2-OB3	3.28	121.93	108.94
18	C	270	CDL	OB5-PB2-OB3	3.26	121.86	108.94
14	A	515[A]	HEA	C13-C12-C11	-3.26	109.19	114.39
14	A	515[B]	HEA	C13-C12-C11	-3.26	109.19	114.39
20	A	744	DMU	C10-C5-C7	3.17	116.68	110.01
14	A	516	HEA	O1D-CGD-CBD	-3.13	113.15	123.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	T	711	DMU	O16-C6-C1	3.13	113.02	108.27
20	N	526	DMU	O3-C5-C10	3.12	117.51	110.08
18	N	522	CDL	OA6-CA4-CA3	3.11	119.50	108.34
14	N	516	HEA	CAD-CBD-CGD	-3.09	105.48	113.67
14	A	516	HEA	CHD-C1D-C2D	-3.07	118.21	126.95
14	N	516	HEA	CHB-C4A-NA	3.07	127.79	124.45
14	A	516	HEA	CHD-C4C-NC	3.06	129.41	123.86
14	N	516	HEA	CMB-C2B-C3B	-3.04	124.39	130.28
19	T	86	CHD	C18-C13-C12	3.03	112.09	109.06
27	C	267	PGV	C24-C23-C22	3.02	129.61	114.37
20	C	714	DMU	C6-O5-C4	3.01	119.61	113.72
14	A	516	HEA	CMC-C2C-C1C	2.99	129.97	125.42
14	A	516	HEA	CHA-C4D-ND	-2.95	121.24	124.42
14	N	515[A]	HEA	C4A-NA-C1A	-2.95	101.01	105.82
14	N	515[B]	HEA	C4A-NA-C1A	-2.95	101.01	105.82
14	A	515[A]	HEA	CHB-C1B-C2B	-2.94	120.39	125.03
14	A	515[B]	HEA	CHB-C1B-C2B	-2.94	120.39	125.03
14	N	515[A]	HEA	C1D-C2D-C3D	-2.92	103.91	106.98
14	N	515[B]	HEA	C1D-C2D-C3D	-2.92	103.91	106.98
20	C	733	DMU	C10-C5-C7	2.91	116.13	110.01
14	A	515[A]	HEA	C20-C19-C18	-2.89	114.68	121.17
20	G	711	DMU	C6-C1-C2	2.88	116.07	110.01
18	N	522	CDL	OA8-CA6-CA4	2.86	116.64	108.40
20	O	742	DMU	O16-C6-C1	2.85	112.60	108.27
14	N	516	HEA	C3C-C4C-NC	2.84	112.19	109.80
26	P	264	PEK	O02-C1-C2	2.84	134.89	123.78
14	A	515[B]	HEA	C27-C19-C20	2.78	120.05	115.23
14	A	516	HEA	O2D-CGD-CBD	2.76	122.72	114.00
19	C	271	CHD	C16-C17-C13	-2.75	100.87	103.54
18	A	522	CDL	OA8-CA6-CA4	2.74	116.31	108.40
20	N	744	DMU	C6-O5-C4	-2.73	108.40	113.72
20	C	714	DMU	O5-C6-C1	2.72	115.96	110.37
20	N	745	DMU	C57-C4-C3	-2.72	105.74	113.38
27	C	266	PGV	O03-C19-O04	-2.71	116.85	123.63
20	P	722	DMU	O5-C6-C1	2.69	115.90	110.37
14	N	515[A]	HEA	C1B-C2B-C3B	-2.69	103.68	106.80
14	N	515[B]	HEA	C1B-C2B-C3B	-2.69	103.68	106.80
18	A	521	CDL	OB5-PB2-OB3	-2.67	98.34	108.94
19	A	525	CHD	C22-C20-C17	-2.66	104.81	110.33
19	C	271	CHD	C22-C23-C24	-2.65	105.42	112.49
20	C	733	DMU	O5-C6-C1	2.65	115.82	110.37
14	N	516	HEA	CHB-C1B-NB	2.65	127.27	124.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	516	HEA	C4C-CHD-C1D	-2.65	120.03	126.25
20	C	714	DMU	O3-C5-C10	2.64	116.37	110.08
14	A	515[A]	HEA	O1D-CGD-CBD	-2.64	114.73	123.09
14	A	515[B]	HEA	O1D-CGD-CBD	-2.64	114.73	123.09
20	O	742	DMU	C57-C4-C3	-2.63	106.56	113.02
20	N	744	DMU	C11-C9-C8	-2.62	106.58	113.02
20	N	745	DMU	C10-O7-C3	-2.62	111.77	117.98
18	N	522	CDL	OA6-CA4-CA6	-2.61	98.97	108.34
26	P	264	PEK	O13-P-O14	2.61	124.60	112.44
14	A	516	HEA	C4A-CHB-C1B	-2.61	120.48	126.02
18	P	270	CDL	OA4-PA1-OA3	2.61	124.57	112.44
18	N	522	CDL	OA6-CA5-OA7	-2.60	117.63	123.70
14	N	516	HEA	C4A-CHB-C1B	-2.60	120.50	126.02
19	T	86	CHD	C17-C13-C12	-2.59	115.34	117.67
18	P	270	CDL	OA5-PA1-OA3	2.58	119.18	108.94
18	A	522	CDL	OA6-CA5-C11	2.58	117.06	111.48
20	T	711	DMU	C6-C1-C2	2.57	115.43	110.01
14	A	516	HEA	CHB-C4A-C3A	-2.54	120.92	125.21
14	N	516	HEA	O1A-CGA-CBA	-2.54	115.04	123.09
14	A	515[A]	HEA	C4C-NC-C1C	-2.54	101.69	105.82
14	A	515[B]	HEA	C4C-NC-C1C	-2.54	101.69	105.82
18	C	270	CDL	OA5-PA1-OA3	2.53	118.97	108.94
19	A	525	CHD	C5-C6-C7	2.48	117.35	114.40
26	P	264	PEK	C2-C3-C4	2.48	118.77	113.35
14	A	516	HEA	C3A-C2A-C1A	2.48	109.39	107.05
14	N	515[A]	HEA	CHB-C1B-C2B	-2.47	121.12	125.03
14	N	515[B]	HEA	CHB-C1B-C2B	-2.47	121.12	125.03
19	P	271	CHD	C16-C17-C13	-2.47	101.14	103.54
18	A	522	CDL	OA7-CA5-C11	-2.46	114.17	123.78
20	C	734	DMU	O5-C6-O16	2.45	115.84	110.04
20	L	747	DMU	C6-O5-C4	2.45	118.51	113.72
19	P	271	CHD	C18-C13-C17	2.45	115.04	111.20
20	T	713	DMU	O5-C4-C3	2.45	114.11	109.70
20	C	722	DMU	O5-C6-C1	2.45	115.39	110.37
19	A	525	CHD	O12-C12-C13	-2.44	106.90	111.02
20	A	744	DMU	C2-C3-C4	-2.44	105.52	110.93
20	L	747	DMU	O5-C6-C1	2.44	115.38	110.37
20	N	745	DMU	C7-C8-C9	2.43	114.64	110.23
14	A	515[A]	HEA	O1A-CGA-CBA	-2.42	115.42	123.09
14	A	515[B]	HEA	O1A-CGA-CBA	-2.42	115.42	123.09
20	T	713	DMU	C2-C3-C4	2.39	114.56	110.23
14	A	515[A]	HEA	C17-C16-C15	2.38	121.08	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	515[B]	HEA	C17-C16-C15	2.38	121.08	113.19
20	C	715[A]	DMU	O5-C6-C1	2.38	115.26	110.37
20	A	526	DMU	C10-C5-C7	2.38	115.02	110.01
20	G	711	DMU	O16-C6-C1	2.38	111.89	108.27
20	W	61	DMU	O1-C10-C5	2.36	115.23	110.37
20	P	715[A]	DMU	C10-O7-C3	-2.36	112.38	117.98
14	A	515[A]	HEA	O2D-CGD-O1D	2.36	129.40	123.33
14	A	515[B]	HEA	O2D-CGD-O1D	2.36	129.40	123.33
20	B	742	DMU	O5-C6-C1	2.35	115.21	110.37
20	P	734	DMU	O5-C6-O16	2.35	115.60	110.04
14	A	516	HEA	CAD-CBD-CGD	-2.34	107.46	113.67
20	Y	747	DMU	O5-C6-C1	2.34	115.17	110.37
27	C	266	PGV	C15-C14-C13	-2.34	102.63	113.86
18	C	270	CDL	OB2-PB2-OB3	-2.33	99.69	108.94
14	N	516	HEA	C13-C12-C11	-2.33	110.67	114.39
20	N	744	DMU	C2-C3-C4	-2.33	105.77	110.93
20	P	714	DMU	O3-C5-C10	2.32	115.61	110.08
14	A	515[A]	HEA	C16-C15-C14	2.32	126.37	121.17
14	A	515[B]	HEA	C16-C15-C14	2.32	126.37	121.17
20	J	61	DMU	C10-C5-C7	2.32	114.88	110.01
20	C	733	DMU	C8-C7-C5	2.31	114.88	110.83
20	O	742	DMU	O5-C4-C57	2.30	112.13	106.44
19	G	86	CHD	C14-C13-C12	-2.29	105.32	107.42
20	C	733	DMU	C6-C1-C2	2.29	114.83	110.01
14	N	515[A]	HEA	O1D-CGD-CBD	-2.29	115.84	123.09
14	N	515[B]	HEA	O1D-CGD-CBD	-2.29	115.84	123.09
20	C	733	DMU	C10-O7-C3	-2.28	112.58	117.98
14	A	515[A]	HEA	O11-C11-C12	2.28	115.17	109.14
14	A	515[B]	HEA	O11-C11-C12	2.28	115.17	109.14
20	G	713	DMU	O5-C6-O16	2.26	115.40	110.04
14	A	515[B]	HEA	C21-C20-C19	-2.26	105.70	113.19
18	P	270	CDL	OA4-PA1-OA5	-2.25	97.38	107.57
20	P	714	DMU	C10-C5-C7	2.25	114.74	110.01
14	N	516	HEA	O2A-CGA-CBA	2.25	121.10	114.00
19	N	525	CHD	C22-C20-C17	-2.24	105.69	110.33
18	A	522	CDL	OA5-PA1-OA3	-2.23	100.08	108.94
14	A	516	HEA	CMB-C2B-C3B	-2.23	125.95	130.28
20	T	713	DMU	O5-C6-O16	2.23	115.31	110.04
18	P	270	CDL	OA6-CA5-C11	-2.23	106.66	111.48
20	N	745	DMU	O5-C6-C1	2.23	114.94	110.37
14	A	516	HEA	C27-C19-C20	2.22	119.09	115.23
19	A	525	CHD	C13-C17-C20	2.22	122.17	119.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	C	264	PEK	O13-P-O14	2.21	122.74	112.44
18	A	521	CDL	OB4-PB2-OB2	2.21	117.56	107.57
27	C	266	PGV	O14-P-O12	-2.20	97.60	107.57
18	C	270	CDL	O1-C1-CB2	2.19	117.27	109.70
14	N	516	HEA	C25-C23-C22	-2.17	116.13	122.66
19	P	271	CHD	C17-C13-C12	-2.17	115.71	117.67
20	W	61	DMU	O1-C9-C8	-2.17	105.79	109.70
14	N	515[B]	HEA	C17-C18-C19	2.16	132.56	127.62
20	P	722	DMU	O16-C6-C1	2.15	111.54	108.27
26	C	264	PEK	C03-C02-C01	2.15	116.80	111.78
20	N	744	DMU	C10-O1-C9	2.14	117.91	113.72
20	C	714	DMU	C10-C5-C7	2.14	114.51	110.01
14	N	516	HEA	C27-C19-C20	2.12	118.90	115.23
27	P	267	PGV	O04-C19-C20	2.12	132.06	123.78
14	A	515[A]	HEA	CAD-C3D-C4D	2.11	128.37	124.70
14	A	515[B]	HEA	CAD-C3D-C4D	2.11	128.37	124.70
19	G	86	CHD	O25-C24-C23	-2.11	116.40	123.09
19	C	271	CHD	C6-C7-C8	2.11	113.80	111.50
19	P	271	CHD	O25-C24-C23	-2.10	116.42	123.09
27	C	267	PGV	C25-C24-C23	2.10	124.98	114.37
20	C	734	DMU	O3-C5-C7	2.10	115.31	110.38
20	W	61	DMU	O7-C10-O1	-2.09	105.19	110.69
14	N	515[A]	HEA	C20-C19-C18	-2.09	116.48	121.17
14	N	515[A]	HEA	CHC-C1C-NC	2.09	127.64	123.86
14	N	515[B]	HEA	CHC-C1C-NC	2.09	127.64	123.86
20	C	722	DMU	O16-C6-C1	2.09	111.44	108.27
19	C	271	CHD	C4-C5-C10	2.08	114.88	112.66
14	N	515[B]	HEA	C21-C20-C19	-2.08	106.30	113.19
14	N	516	HEA	CAD-C3D-C4D	2.08	128.32	124.70
19	C	271	CHD	C17-C13-C12	-2.07	115.81	117.67
14	N	515[A]	HEA	C4A-C3A-C2A	-2.07	105.02	106.81
14	N	515[B]	HEA	C4A-C3A-C2A	-2.07	105.02	106.81
20	T	711	DMU	C57-C4-C3	-2.06	107.96	113.02
20	P	715[A]	DMU	O5-C4-C57	2.06	111.54	106.44
20	N	526	DMU	C10-O7-C3	-2.06	113.10	117.98
18	C	270	CDL	CA6-CA4-CA3	2.06	116.58	111.78
19	C	271	CHD	C18-C13-C17	2.05	114.42	111.20
20	A	744	DMU	O7-C3-C2	2.05	112.44	107.23
14	N	515[B]	HEA	C25-C23-C22	-2.04	116.53	122.66
19	P	271	CHD	C15-C14-C8	2.04	121.15	118.36
18	C	270	CDL	OA6-CA4-CA6	-2.03	101.05	108.34
14	A	516	HEA	C2C-C1C-NC	2.03	113.40	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	745	DMU	C10-C5-C7	2.03	114.27	110.01
14	A	516	HEA	C1C-CHC-C4B	-2.03	121.48	126.25
18	P	270	CDL	CA6-CA4-CA3	2.02	116.50	111.78
20	C	714	DMU	C18-O16-C6	-2.02	110.23	113.68
20	T	713	DMU	C57-C4-C3	-2.02	108.07	113.02
20	G	713	DMU	O5-C6-C1	2.00	114.48	110.37
20	N	745	DMU	O1-C9-C8	2.00	113.31	109.70
14	N	515[A]	HEA	O1A-CGA-CBA	-2.00	116.75	123.09
14	N	515[B]	HEA	O1A-CGA-CBA	-2.00	116.75	123.09

There are no chirality outliers.

All (742) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	515[A]	HEA	C18-C19-C20-C21
14	A	515[A]	HEA	C27-C19-C20-C21
18	A	521	CDL	CA2-OA2-PA1-OA3
18	A	521	CDL	C11-CA5-OA6-CA4
18	A	521	CDL	CB2-OB2-PB2-OB3
18	A	521	CDL	CB3-OB5-PB2-OB2
18	A	521	CDL	CB3-OB5-PB2-OB4
18	A	521	CDL	C51-CB5-OB6-CB4
18	A	522	CDL	C1-CA2-OA2-PA1
18	A	522	CDL	C51-CB5-OB6-CB4
18	C	270	CDL	C1-CA2-OA2-PA1
18	C	270	CDL	CA2-OA2-PA1-OA3
18	C	270	CDL	CA2-OA2-PA1-OA5
18	C	270	CDL	CA3-OA5-PA1-OA2
18	C	270	CDL	C11-CA5-OA6-CA4
18	C	270	CDL	CB3-OB5-PB2-OB4
18	C	270	CDL	OB7-CB5-OB6-CB4
18	C	270	CDL	C51-CB5-OB6-CB4
18	N	521	CDL	CA2-OA2-PA1-OA3
18	N	521	CDL	CA3-OA5-PA1-OA3
18	N	521	CDL	C11-CA5-OA6-CA4
18	N	521	CDL	CB2-OB2-PB2-OB5
18	N	521	CDL	C51-CB5-OB6-CB4
18	N	522	CDL	CA2-C1-CB2-OB2
18	N	522	CDL	C1-CA2-OA2-PA1
18	N	522	CDL	C11-CA5-OA6-CA4
18	N	522	CDL	CB3-OB5-PB2-OB2
18	N	522	CDL	CB3-OB5-PB2-OB3

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Mol	Chain	Res	Type	Atoms
18	N	522	CDL	CB3-OB5-PB2-OB4
18	N	522	CDL	C51-CB5-OB6-CB4
18	P	270	CDL	C1-CA2-OA2-PA1
18	P	270	CDL	CA2-OA2-PA1-OA3
18	P	270	CDL	CA2-OA2-PA1-OA5
18	P	270	CDL	CA3-OA5-PA1-OA2
18	P	270	CDL	CB3-OB5-PB2-OB4
18	P	270	CDL	OB7-CB5-OB6-CB4
18	P	270	CDL	C51-CB5-OB6-CB4
19	P	271	CHD	C13-C17-C20-C21
20	C	722	DMU	C1-C6-O16-C18
20	G	711	DMU	C19-C18-O16-C6
20	L	747	DMU	C1-C6-O16-C18
20	L	747	DMU	O5-C6-O16-C18
20	N	744	DMU	O5-C6-O16-C18
20	T	711	DMU	C19-C18-O16-C6
20	Y	747	DMU	O5-C6-O16-C18
26	C	264	PEK	C12-C13-C14-C15
26	P	264	PEK	C9-C10-C11-C12
26	P	264	PEK	C11-C12-C13-C14
26	P	264	PEK	C12-C13-C14-C15
18	C	270	CDL	OB9-CB7-OB8-CB6
19	P	271	CHD	C16-C17-C20-C21
19	C	271	CHD	C13-C17-C20-C21
19	P	271	CHD	C13-C17-C20-C22
18	A	521	CDL	OA7-CA5-OA6-CA4
18	A	521	CDL	OB7-CB5-OB6-CB4
18	A	522	CDL	OB7-CB5-OB6-CB4
18	C	270	CDL	OA7-CA5-OA6-CA4
18	N	521	CDL	OA7-CA5-OA6-CA4
18	N	521	CDL	OB7-CB5-OB6-CB4
18	N	522	CDL	OA7-CA5-OA6-CA4
18	N	522	CDL	OB7-CB5-OB6-CB4
20	L	747	DMU	C3-C4-C57-O61
19	C	271	CHD	C16-C17-C20-C21
19	P	271	CHD	C16-C17-C20-C22
19	C	271	CHD	C13-C17-C20-C22
20	C	734	DMU	O5-C4-C57-O61
18	A	521	CDL	C31-CA7-OA8-CA6
18	C	270	CDL	C71-CB7-OB8-CB6
18	N	521	CDL	C31-CA7-OA8-CA6
18	A	521	CDL	OA9-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
18	N	521	CDL	OA9-CA7-OA8-CA6
19	C	271	CHD	C16-C17-C20-C22
18	C	270	CDL	O1-C1-CB2-OB2
18	N	522	CDL	O1-C1-CB2-OB2
18	P	270	CDL	O1-C1-CB2-OB2
18	N	522	CDL	C31-CA7-OA8-CA6
20	A	745	DMU	O5-C4-C57-O61
20	P	734	DMU	O5-C4-C57-O61
20	G	711	DMU	O5-C4-C57-O61
18	P	270	CDL	C11-CA5-OA6-CA4
20	C	714	DMU	C3-C4-C57-O61
20	P	733	DMU	O6-C11-C9-C8
20	C	714	DMU	O5-C4-C57-O61
20	T	711	DMU	O5-C4-C57-O61
14	N	515[A]	HEA	C15-C16-C17-C18
20	L	747	DMU	O5-C4-C57-O61
20	P	734	DMU	O6-C11-C9-O1
20	W	61	DMU	O6-C11-C9-O1
20	P	734	DMU	C3-C4-C57-O61
20	C	722	DMU	O5-C6-O16-C18
20	P	733	DMU	O6-C11-C9-O1
20	C	734	DMU	C3-C4-C57-O61
20	A	745	DMU	O6-C11-C9-C8
20	C	733	DMU	O6-C11-C9-C8
20	W	61	DMU	O6-C11-C9-C8
18	C	270	CDL	C51-C52-C53-C54
22	P	614	LFA	C9-C10-C11-C12
22	P	716[B]	LFA	C12-C13-C14-C15
18	N	522	CDL	OA9-CA7-OA8-CA6
18	A	522	CDL	OA7-CA5-OA6-CA4
18	P	270	CDL	C31-CA7-OA8-CA6
18	P	270	CDL	C71-CB7-OB8-CB6
20	A	745	DMU	O6-C11-C9-O1
20	T	711	DMU	C3-C4-C57-O61
18	A	521	CDL	C72-C73-C74-C75
22	C	614	LFA	C10-C11-C12-C13
20	G	711	DMU	C3-C4-C57-O61
20	A	745	DMU	C3-C4-C57-O61
20	N	745	DMU	O6-C11-C9-C8
20	P	734	DMU	O6-C11-C9-C8
20	C	733	DMU	C1-C6-O16-C18
22	N	628	LFA	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
19	P	271	CHD	C21-C20-C22-C23
27	P	267	PGV	C28-C29-C30-C31
18	N	521	CDL	CA5-C11-C12-C13
20	G	713	DMU	O5-C4-C57-O61
19	P	271	CHD	C17-C20-C22-C23
20	C	733	DMU	O6-C11-C9-O1
18	N	521	CDL	OB6-CB4-CB6-OB8
27	C	266	PGV	C26-C27-C28-C29
27	P	266	PGV	C23-C24-C25-C26
14	N	515[A]	HEA	C27-C19-C20-C21
18	P	270	CDL	OA7-CA5-OA6-CA4
20	G	713	DMU	C3-C4-C57-O61
18	A	521	CDL	CA7-C31-C32-C33
18	A	522	CDL	CA5-C11-C12-C13
18	N	522	CDL	CA7-C31-C32-C33
18	P	270	CDL	CA7-C31-C32-C33
18	P	270	CDL	OB9-CB7-OB8-CB6
20	N	745	DMU	O5-C4-C57-O61
20	G	713	DMU	O16-C18-C19-C22
18	A	522	CDL	CA7-C31-C32-C33
18	C	270	CDL	CB5-C51-C52-C53
18	P	270	CDL	CB5-C51-C52-C53
20	C	733	DMU	O5-C6-O16-C18
18	P	270	CDL	C51-C52-C53-C54
18	A	521	CDL	O1-C1-CB2-OB2
18	N	521	CDL	O1-C1-CB2-OB2
14	N	515[A]	HEA	C18-C19-C20-C21
20	C	722	DMU	O16-C18-C19-C22
18	A	521	CDL	CA5-C11-C12-C13
27	P	266	PGV	C26-C27-C28-C29
18	N	522	CDL	CA5-C11-C12-C13
18	A	521	CDL	CA2-C1-CB2-OB2
18	N	521	CDL	CA2-C1-CB2-OB2
18	C	270	CDL	C31-CA7-OA8-CA6
22	P	716[B]	LFA	C11-C10-C9-C8
22	C	716[B]	LFA	C12-C13-C14-C15
20	P	733	DMU	O16-C18-C19-C22
20	P	715[A]	DMU	O5-C4-C57-O61
20	B	742	DMU	C1-C6-O16-C18
20	G	713	DMU	C1-C6-O16-C18
20	P	715[A]	DMU	C1-C6-O16-C18
26	P	264	PEK	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
20	N	745	DMU	O6-C11-C9-O1
20	N	526	DMU	O6-C11-C9-C8
20	Y	747	DMU	O16-C18-C19-C22
18	P	270	CDL	OA9-CA7-OA8-CA6
18	A	522	CDL	C11-CA5-OA6-CA4
20	N	526	DMU	O16-C18-C19-C22
20	N	526	DMU	O6-C11-C9-O1
18	C	270	CDL	C73-C74-C75-C76
18	P	270	CDL	C54-C55-C56-C57
18	A	521	CDL	C22-C23-C24-C25
20	C	721	DMU	C31-C34-C37-C40
20	C	722	DMU	C31-C34-C37-C40
20	W	732	DMU	C31-C34-C37-C40
22	G	621	LFA	C11-C12-C13-C14
18	C	270	CDL	C35-C36-C37-C38
20	B	741	DMU	C19-C22-C25-C28
20	C	722	DMU	C22-C25-C28-C31
22	C	614	LFA	C7-C8-C9-C10
22	P	614	LFA	C2-C3-C4-C5
27	C	266	PGV	C29-C30-C31-C32
20	A	744	DMU	C19-C18-O16-C6
20	O	742	DMU	C19-C18-O16-C6
20	P	722	DMU	C19-C18-O16-C6
18	A	521	CDL	C77-C78-C79-C80
18	N	521	CDL	C14-C15-C16-C17
20	B	742	DMU	C19-C22-C25-C28
26	C	264	PEK	C26-C27-C28-C29
26	P	264	PEK	C1-C2-C3-C4
27	C	267	PGV	C7-C8-C9-C10
22	C	614	LFA	C6-C7-C8-C9
22	P	623	LFA	C4-C5-C6-C7
26	C	264	PEK	C28-C29-C30-C31
18	A	522	CDL	C31-C32-C33-C34
27	C	266	PGV	C30-C31-C32-C33
27	C	267	PGV	C28-C29-C30-C31
18	C	270	CDL	OA9-CA7-OA8-CA6
18	A	521	CDL	C76-C77-C78-C79
22	T	621	LFA	C4-C5-C6-C7
18	A	522	CDL	C73-C74-C75-C76
20	C	733	DMU	C25-C28-C31-C34
20	C	714	DMU	C19-C22-C25-C28
20	B	742	DMU	O16-C18-C19-C22

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Mol	Chain	Res	Type	Atoms
18	N	521	CDL	C80-C81-C82-C83
20	B	731	DMU	C19-C22-C25-C28
20	L	747	DMU	C31-C34-C37-C40
20	Z	746	DMU	C25-C28-C31-C34
22	N	627	LFA	C6-C7-C8-C9
18	P	270	CDL	C71-C72-C73-C74
20	L	747	DMU	C22-C25-C28-C31
22	C	624	LFA	C5-C6-C7-C8
26	C	264	PEK	C34-C35-C36-C37
20	C	733	DMU	C19-C22-C25-C28
20	G	712	DMU	C19-C22-C25-C28
20	N	745	DMU	C31-C34-C37-C40
22	C	615	LFA	C5-C6-C7-C8
22	P	611	LFA	C5-C6-C7-C8
27	C	267	PGV	C22-C23-C24-C25
27	P	267	PGV	C7-C8-C9-C10
27	P	267	PGV	C30-C31-C32-C33
20	C	734	DMU	O6-C11-C9-C8
22	C	611	LFA	C4-C5-C6-C7
23	P	807	EDO	O1-C1-C2-O2
20	O	741	DMU	C19-C22-C25-C28
20	P	733	DMU	C28-C31-C34-C37
22	P	615	LFA	C3-C4-C5-C6
20	W	61	DMU	O16-C18-C19-C22
20	C	714	DMU	C28-C31-C34-C37
22	P	623	LFA	C3-C4-C5-C6
20	P	733	DMU	C18-C19-C22-C25
18	C	270	CDL	CA7-C31-C32-C33
22	C	624	LFA	C1-C2-C3-C4
18	C	270	CDL	C56-C57-C58-C59
20	C	733	DMU	C28-C31-C34-C37
20	N	526	DMU	C22-C25-C28-C31
27	C	267	PGV	C27-C28-C29-C30
18	N	521	CDL	C13-C14-C15-C16
18	P	270	CDL	C73-C74-C75-C76
20	Y	747	DMU	C22-C25-C28-C31
22	P	611	LFA	C4-C5-C6-C7
18	N	521	CDL	C63-C64-C65-C66
18	N	521	CDL	C76-C77-C78-C79
27	C	267	PGV	C13-C14-C15-C16
18	A	521	CDL	C17-C18-C19-C20
18	C	270	CDL	C71-C72-C73-C74

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Mol	Chain	Res	Type	Atoms
18	P	270	CDL	C11-C12-C13-C14
20	B	731	DMU	C31-C34-C37-C40
20	M	746	DMU	C25-C28-C31-C34
22	C	611	LFA	C5-C6-C7-C8
22	N	628	LFA	C6-C7-C8-C9
20	L	747	DMU	O16-C18-C19-C22
20	J	732	DMU	C31-C34-C37-C40
22	P	614	LFA	C11-C12-C13-C14
22	P	615	LFA	C7-C8-C9-C10
20	B	731	DMU	C18-C19-C22-C25
20	Y	747	DMU	C18-C19-C22-C25
20	C	722	DMU	O5-C4-C57-O61
22	C	625	LFA	C4-C5-C6-C7
27	P	266	PGV	C29-C30-C31-C32
18	A	521	CDL	C14-C15-C16-C17
18	P	270	CDL	C75-C76-C77-C78
22	P	614	LFA	C7-C8-C9-C10
22	P	623	LFA	C6-C7-C8-C9
26	P	264	PEK	C17-C18-C19-C20
18	N	522	CDL	C73-C74-C75-C76
20	B	742	DMU	C18-C19-C22-C25
20	A	526	DMU	C19-C22-C25-C28
22	P	615	LFA	C6-C7-C8-C9
26	C	264	PEK	C15-C16-C17-C18
27	P	266	PGV	C12-C13-C14-C15
18	P	270	CDL	C56-C57-C58-C59
22	A	628	LFA	C6-C7-C8-C9
18	A	522	CDL	C78-C79-C80-C81
18	N	521	CDL	C77-C78-C79-C80
22	T	621	LFA	C11-C12-C13-C14
22	C	615	LFA	C3-C4-C5-C6
26	C	264	PEK	C25-C26-C27-C28
27	C	267	PGV	C14-C15-C16-C17
27	P	267	PGV	C24-C25-C26-C27
22	C	625	LFA	C9-C10-C11-C12
20	P	721	DMU	C28-C31-C34-C37
22	C	611	LFA	C3-C4-C5-C6
20	A	745	DMU	C31-C34-C37-C40
18	C	270	CDL	C54-C55-C56-C57
22	C	626	LFA	C2-C3-C4-C5
22	P	716[B]	LFA	C2-C3-C4-C5
22	T	622	LFA	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
22	C	716[B]	LFA	C2-C3-C4-C5
18	C	270	CDL	C78-C79-C80-C81
18	N	522	CDL	OA6-CA4-CA6-OA8
18	A	521	CDL	C74-C75-C76-C77
18	N	522	CDL	C15-C16-C17-C18
20	A	526	DMU	C22-C25-C28-C31
20	P	734	DMU	O16-C18-C19-C22
18	C	270	CDL	C22-C23-C24-C25
18	N	522	CDL	C71-C72-C73-C74
18	N	522	CDL	C74-C75-C76-C77
22	P	615	LFA	C4-C5-C6-C7
27	C	267	PGV	C21-C22-C23-C24
20	A	744	DMU	C4-C3-O7-C10
18	A	521	CDL	C13-C14-C15-C16
18	A	521	CDL	C51-C52-C53-C54
18	A	521	CDL	C71-C72-C73-C74
27	P	266	PGV	C30-C31-C32-C33
18	C	270	CDL	C33-C34-C35-C36
20	O	731	DMU	O16-C18-C19-C22
18	A	522	CDL	C71-C72-C73-C74
18	N	521	CDL	O1-C1-CA2-OA2
20	P	715[A]	DMU	C25-C28-C31-C34
22	C	626	LFA	C5-C6-C7-C8
18	A	522	CDL	C77-C78-C79-C80
18	P	270	CDL	C22-C23-C24-C25
20	G	712	DMU	C31-C34-C37-C40
19	C	271	CHD	C21-C20-C22-C23
22	C	623	LFA	C4-C5-C6-C7
18	N	521	CDL	C71-C72-C73-C74
22	P	716[B]	LFA	C6-C7-C8-C9
20	B	742	DMU	C31-C34-C37-C40
18	C	270	CDL	C79-C80-C81-C82
18	N	521	CDL	C19-C20-C21-C22
22	G	621	LFA	C6-C7-C8-C9
20	P	722	DMU	O16-C18-C19-C22
22	T	621	LFA	C13-C14-C15-C16
18	A	521	CDL	C80-C81-C82-C83
20	P	722	DMU	C28-C31-C34-C37
20	O	742	DMU	O16-C18-C19-C22
18	A	522	CDL	C74-C75-C76-C77
20	P	714	DMU	C18-C19-C22-C25
20	T	712	DMU	O16-C18-C19-C22

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Mol	Chain	Res	Type	Atoms
18	N	521	CDL	C22-C23-C24-C25
20	B	741	DMU	C25-C28-C31-C34
20	N	526	DMU	C25-C28-C31-C34
22	C	626	LFA	C4-C5-C6-C7
20	G	712	DMU	C18-C19-C22-C25
26	P	264	PEK	C4-C5-C6-C7
18	A	522	CDL	CB3-CB4-CB6-OB8
18	N	521	CDL	CB3-CB4-CB6-OB8
22	P	624	LFA	C11-C10-C9-C8
22	C	624	LFA	C4-C5-C6-C7
20	C	734	DMU	O6-C11-C9-O1
26	P	264	PEK	C2-C3-C4-C5
18	P	270	CDL	C82-C83-C84-C85
18	A	522	CDL	C16-C17-C18-C19
20	G	713	DMU	C19-C22-C25-C28
20	G	712	DMU	O16-C18-C19-C22
20	O	741	DMU	O16-C18-C19-C22
22	C	614	LFA	C11-C10-C9-C8
22	P	624	LFA	C7-C8-C9-C10
22	C	623	LFA	C11-C10-C9-C8
18	N	521	CDL	C57-C58-C59-C60
22	G	621	LFA	C4-C5-C6-C7
20	T	713	DMU	C18-C19-C22-C25
26	C	264	PEK	C33-C34-C35-C36
20	Y	747	DMU	O5-C4-C57-O61
20	P	714	DMU	C19-C22-C25-C28
18	A	522	CDL	C17-C18-C19-C20
20	J	732	DMU	O16-C18-C19-C22
27	P	267	PGV	C12-C13-C14-C15
18	A	521	CDL	C36-C37-C38-C39
18	A	521	CDL	C58-C59-C60-C61
18	A	522	CDL	C12-C13-C14-C15
18	N	522	CDL	C16-C17-C18-C19
18	P	270	CDL	C13-C14-C15-C16
20	C	721	DMU	C28-C31-C34-C37
18	P	270	CDL	C33-C34-C35-C36
20	P	733	DMU	C19-C22-C25-C28
22	N	627	LFA	C2-C3-C4-C5
20	B	741	DMU	C18-C19-C22-C25
20	C	722	DMU	C28-C31-C34-C37
22	G	621	LFA	C5-C6-C7-C8
22	G	621	LFA	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
18	A	521	CDL	C84-C85-C86-C87
20	A	743	DMU	C34-C37-C40-C43
22	T	621	LFA	C14-C15-C16-C17
22	N	628	LFA	C2-C3-C4-C5
26	P	264	PEK	C26-C27-C28-C29
18	A	521	CDL	C59-C60-C61-C62
20	T	713	DMU	C22-C25-C28-C31
22	T	622	LFA	C3-C4-C5-C6
20	C	714	DMU	C34-C37-C40-C43
20	J	61	DMU	C34-C37-C40-C43
20	P	734	DMU	C25-C28-C31-C34
20	W	732	DMU	C25-C28-C31-C34
20	C	272	DMU	C28-C31-C34-C37
22	C	611	LFA	C11-C10-C9-C8
22	P	626	LFA	C1-C2-C3-C4
18	A	521	CDL	C12-C13-C14-C15
22	N	628	LFA	C1-C2-C3-C4
20	B	731	DMU	O16-C18-C19-C22
18	P	270	CDL	C57-C58-C59-C60
20	W	732	DMU	C19-C22-C25-C28
26	C	264	PEK	C17-C18-C19-C20
20	C	272	DMU	C22-C25-C28-C31
18	N	522	CDL	C17-C18-C19-C20
18	N	522	CDL	C78-C79-C80-C81
18	P	270	CDL	C35-C36-C37-C38
22	A	627	LFA	C9-C10-C11-C12
18	N	521	CDL	C52-C53-C54-C55
22	C	624	LFA	C11-C10-C9-C8
26	P	264	PEK	C13-C14-C15-C16
20	B	742	DMU	C25-C28-C31-C34
20	J	61	DMU	O16-C18-C19-C22
20	T	711	DMU	C34-C37-C40-C43
20	W	732	DMU	C18-C19-C22-C25
22	N	628	LFA	C5-C6-C7-C8
20	C	722	DMU	C19-C18-O16-C6
20	C	733	DMU	C19-C18-O16-C6
20	G	713	DMU	C19-C18-O16-C6
20	N	744	DMU	C19-C18-O16-C6
20	B	741	DMU	O16-C18-C19-C22
22	P	626	LFA	C6-C7-C8-C9
18	A	522	CDL	C15-C16-C17-C18
18	N	521	CDL	C78-C79-C80-C81

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Mol	Chain	Res	Type	Atoms
20	O	742	DMU	C19-C22-C25-C28
20	N	526	DMU	C34-C37-C40-C43
20	Y	747	DMU	C1-C6-O16-C18
18	A	521	CDL	C34-C35-C36-C37
22	T	621	LFA	C6-C7-C8-C9
18	C	270	CDL	C13-C14-C15-C16
18	P	270	CDL	C21-C22-C23-C24
26	C	264	PEK	C35-C36-C37-C38
18	A	522	CDL	C79-C80-C81-C82
22	P	626	LFA	C9-C10-C11-C12
27	C	267	PGV	C23-C24-C25-C26
22	P	611	LFA	C11-C10-C9-C8
26	C	264	PEK	C29-C30-C31-C32
20	L	747	DMU	C34-C37-C40-C43
18	N	521	CDL	C79-C80-C81-C82
18	A	522	CDL	C31-CA7-OA8-CA6
20	P	722	DMU	C31-C34-C37-C40
22	N	627	LFA	C7-C8-C9-C10
27	P	267	PGV	C22-C23-C24-C25
20	B	742	DMU	C34-C37-C40-C43
20	A	744	DMU	C2-C3-O7-C10
22	C	612	LFA	C2-C3-C4-C5
18	A	521	CDL	C57-C58-C59-C60
18	N	521	CDL	C53-C54-C55-C56
18	A	522	CDL	CA3-CA4-CA6-OA8
18	C	270	CDL	CB3-CB4-CB6-OB8
20	P	734	DMU	C34-C37-C40-C43
20	A	743	DMU	C25-C28-C31-C34
18	P	270	CDL	C59-C60-C61-C62
20	L	747	DMU	C25-C28-C31-C34
22	C	611	LFA	C7-C8-C9-C10
22	P	625	LFA	C5-C6-C7-C8
18	N	521	CDL	OB5-CB3-CB4-OB6
20	O	742	DMU	C18-C19-C22-C25
20	P	714	DMU	C28-C31-C34-C37
20	O	731	DMU	C18-C19-C22-C25
26	C	264	PEK	C9-C10-C11-C12
26	P	264	PEK	C11-C10-C9-C8
22	A	627	LFA	C2-C3-C4-C5
18	N	521	CDL	C37-C38-C39-C40
27	P	267	PGV	C11-C12-C13-C14
20	T	713	DMU	C19-C22-C25-C28

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Mol	Chain	Res	Type	Atoms
22	P	716[B]	LFA	C7-C8-C9-C10
27	P	266	PGV	C14-C15-C16-C17
22	G	621	LFA	C14-C15-C16-C17
22	P	624	LFA	C4-C5-C6-C7
18	P	270	CDL	C24-C25-C26-C27
20	N	743	DMU	C34-C37-C40-C43
14	A	515[A]	HEA	C15-C16-C17-C18
18	N	522	CDL	C77-C78-C79-C80
22	C	614	LFA	C9-C10-C11-C12
18	A	522	CDL	CA2-C1-CB2-OB2
20	T	712	DMU	C28-C31-C34-C37
22	P	624	LFA	C1-C2-C3-C4
18	P	270	CDL	C79-C80-C81-C82
22	C	614	LFA	C2-C3-C4-C5
18	C	270	CDL	CA4-CA3-OA5-PA1
20	T	712	DMU	C19-C22-C25-C28
22	G	622	LFA	C5-C6-C7-C8
18	N	521	CDL	CA7-C31-C32-C33
20	C	734	DMU	C25-C28-C31-C34
20	W	732	DMU	C28-C31-C34-C37
20	N	744	DMU	C4-C3-O7-C10
20	C	715[A]	DMU	C19-C22-C25-C28
20	O	742	DMU	O5-C4-C57-O61
20	P	721	DMU	C31-C34-C37-C40
20	Y	747	DMU	C31-C34-C37-C40
22	C	625	LFA	C5-C6-C7-C8
18	A	521	CDL	C20-C21-C22-C23
22	P	625	LFA	C4-C5-C6-C7
18	C	270	CDL	C74-C75-C76-C77
18	C	270	CDL	C75-C76-C77-C78
20	T	711	DMU	C18-C19-C22-C25
27	C	266	PGV	C11-C10-C9-C8
26	P	264	PEK	C22-C23-C24-C25
18	N	521	CDL	C60-C61-C62-C63
18	P	270	CDL	C72-C73-C74-C75
18	C	270	CDL	O1-C1-CA2-OA2
22	T	622	LFA	C6-C7-C8-C9
22	T	621	LFA	C10-C11-C12-C13
18	N	521	CDL	C51-C52-C53-C54
18	N	522	CDL	CA3-CA4-CA6-OA8
22	A	628	LFA	C11-C10-C9-C8
18	P	270	CDL	C78-C79-C80-C81

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Mol	Chain	Res	Type	Atoms
18	N	521	CDL	C54-C55-C56-C57
20	P	722	DMU	C18-C19-C22-C25
20	N	745	DMU	C3-C4-C57-O61
20	P	721	DMU	C25-C28-C31-C34
22	A	628	LFA	C11-C12-C13-C14
18	P	270	CDL	C19-C20-C21-C22
22	P	623	LFA	C10-C11-C12-C13
20	O	742	DMU	C31-C34-C37-C40
22	C	623	LFA	C5-C6-C7-C8
26	C	264	PEK	C27-C28-C29-C30
18	A	521	CDL	OB9-CB7-OB8-CB6
18	A	521	CDL	C53-C54-C55-C56
20	P	734	DMU	C19-C22-C25-C28
22	G	622	LFA	C2-C3-C4-C5
27	P	267	PGV	C02-C03-O11-P
20	O	731	DMU	C19-C22-C25-C28
18	C	270	CDL	C18-C19-C20-C21
27	P	266	PGV	C11-C10-C9-C8
20	O	741	DMU	C28-C31-C34-C37
22	P	626	LFA	C5-C6-C7-C8
22	P	626	LFA	C2-C3-C4-C5
18	N	522	CDL	C75-C76-C77-C78
20	O	741	DMU	C25-C28-C31-C34
20	W	732	DMU	C34-C37-C40-C43
22	P	625	LFA	C9-C10-C11-C12
18	A	521	CDL	C71-CB7-OB8-CB6
18	A	521	CDL	C78-C79-C80-C81
20	M	746	DMU	C34-C37-C40-C43
20	C	714	DMU	C18-C19-C22-C25
20	C	722	DMU	C18-C19-C22-C25
20	C	715[A]	DMU	C3-C4-C57-O61
18	A	521	CDL	OA5-CA3-CA4-CA6
18	N	521	CDL	OB5-CB3-CB4-CB6
18	N	521	CDL	C32-C33-C34-C35
18	N	521	CDL	C35-C36-C37-C38
22	T	621	LFA	C1-C2-C3-C4
22	P	611	LFA	C1-C2-C3-C4
18	P	270	CDL	C80-C81-C82-C83
18	N	521	CDL	C64-C65-C66-C67
20	C	733	DMU	C3-C4-C57-O61
27	C	267	PGV	C02-C03-O11-P
18	C	270	CDL	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
18	A	521	CDL	OA5-CA3-CA4-OA6
18	A	522	CDL	OA5-CA3-CA4-OA6
18	N	522	CDL	C79-C80-C81-C82
26	P	264	PEK	C30-C31-C32-C33
20	T	711	DMU	C31-C34-C37-C40
18	N	522	CDL	C72-C73-C74-C75
20	Z	746	DMU	C34-C37-C40-C43
18	C	270	CDL	OB6-CB4-CB6-OB8
18	N	521	CDL	CB2-C1-CA2-OA2
22	A	627	LFA	C11-C12-C13-C14
18	P	270	CDL	CB3-CB4-CB6-OB8
18	C	270	CDL	C14-C15-C16-C17
20	B	731	DMU	C25-C28-C31-C34
20	P	722	DMU	C19-C22-C25-C28
22	G	622	LFA	C1-C2-C3-C4
22	A	628	LFA	C10-C11-C12-C13
18	A	521	CDL	CB3-OB5-PB2-OB3
18	C	270	CDL	CA2-OA2-PA1-OA4
18	C	270	CDL	CA3-OA5-PA1-OA3
18	C	270	CDL	CB3-OB5-PB2-OB2
18	N	521	CDL	CA3-OA5-PA1-OA4
18	P	270	CDL	CA3-OA5-PA1-OA3
18	P	270	CDL	CB3-OB5-PB2-OB2
20	A	526	DMU	C34-C37-C40-C43
22	G	621	LFA	C2-C3-C4-C5
18	N	522	CDL	C52-C51-CB5-OB6
20	A	526	DMU	C25-C28-C31-C34
22	A	628	LFA	C5-C6-C7-C8
18	C	270	CDL	CB7-C71-C72-C73
18	P	270	CDL	CA4-CA3-OA5-PA1
20	B	731	DMU	C34-C37-C40-C43
18	P	270	CDL	C14-C15-C16-C17
18	A	521	CDL	C38-C39-C40-C41
18	P	270	CDL	CB7-C71-C72-C73
22	P	614	LFA	C1-C2-C3-C4
18	C	270	CDL	C12-C11-CA5-OA6
20	N	745	DMU	C19-C22-C25-C28
20	J	732	DMU	C25-C28-C31-C34
20	A	744	DMU	C28-C31-C34-C37
20	T	712	DMU	C34-C37-C40-C43
22	P	612	LFA	C1-C2-C3-C4
20	N	744	DMU	C2-C3-O7-C10

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Mol	Chain	Res	Type	Atoms
22	C	626	LFA	C10-C11-C12-C13
20	C	734	DMU	C34-C37-C40-C43
27	P	267	PGV	C15-C16-C17-C18
20	W	732	DMU	O16-C18-C19-C22
22	C	614	LFA	C11-C12-C13-C14
20	M	746	DMU	C22-C25-C28-C31
20	C	734	DMU	C31-C34-C37-C40
18	N	521	CDL	C72-C73-C74-C75
20	C	715[A]	DMU	C25-C28-C31-C34
22	N	628	LFA	C3-C4-C5-C6
18	A	522	CDL	OB6-CB4-CB6-OB8
18	P	270	CDL	C12-C11-CA5-OA6
27	C	267	PGV	C31-C32-C33-C34
20	N	743	DMU	C28-C31-C34-C37
18	A	522	CDL	C72-C73-C74-C75
18	A	522	CDL	OA9-CA7-OA8-CA6
18	N	522	CDL	C31-C32-C33-C34
18	C	270	CDL	C82-C83-C84-C85
22	A	627	LFA	C4-C5-C6-C7
27	C	266	PGV	C11-C12-C13-C14
18	N	522	CDL	C52-C51-CB5-OB7
18	C	270	CDL	C11-C12-C13-C14
22	T	622	LFA	C5-C6-C7-C8
22	P	615	LFA	C5-C6-C7-C8
18	N	522	CDL	CB2-C1-CA2-OA2
20	P	734	DMU	C18-C19-C22-C25
22	N	627	LFA	C11-C12-C13-C14
22	N	627	LFA	C3-C4-C5-C6
20	P	714	DMU	C4-C3-O7-C10
22	A	627	LFA	C6-C7-C8-C9
18	C	270	CDL	C20-C21-C22-C23
18	N	521	CDL	C17-C18-C19-C20
20	P	722	DMU	C3-C4-C57-O61
26	P	264	PEK	C10-C11-C12-C13
22	C	623	LFA	C6-C7-C8-C9
20	P	714	DMU	C2-C3-O7-C10
20	A	744	DMU	O16-C18-C19-C22
20	O	742	DMU	C25-C28-C31-C34
22	C	716[B]	LFA	C5-C6-C7-C8
22	P	624	LFA	C2-C3-C4-C5
22	C	716[B]	LFA	C14-C15-C16-C17
18	P	270	CDL	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
20	M	746	DMU	C28-C31-C34-C37
22	P	624	LFA	C3-C4-C5-C6
19	T	86	CHD	C22-C23-C24-O25
19	T	86	CHD	C22-C23-C24-O26
18	A	522	CDL	CA3-CA4-OA6-CA5
23	N	803	EDO	O1-C1-C2-O2
23	R	811	EDO	O1-C1-C2-O2
20	P	715[A]	DMU	C19-C22-C25-C28
27	P	267	PGV	C29-C30-C31-C32
19	G	86	CHD	C22-C23-C24-O25
20	Y	747	DMU	C34-C37-C40-C43
18	N	521	CDL	C20-C21-C22-C23
18	P	270	CDL	C74-C75-C76-C77
18	C	270	CDL	C84-C85-C86-C87
18	A	521	CDL	C19-C20-C21-C22
27	C	267	PGV	C05-C04-O12-P
19	G	86	CHD	C22-C23-C24-O26
18	A	521	CDL	C52-C53-C54-C55
18	C	270	CDL	C21-C22-C23-C24
19	C	271	CHD	C22-C23-C24-O25
14	N	516	HEA	CAD-CBD-CGD-O2D
20	A	744	DMU	C31-C34-C37-C40
18	A	522	CDL	CB4-CB3-OB5-PB2
26	P	264	PEK	C16-C17-C18-C19
26	P	264	PEK	C32-C33-C34-C35
27	C	266	PGV	O03-C19-C20-C21
20	Y	747	DMU	C19-C18-O16-C6
19	C	271	CHD	C22-C23-C24-O26
19	N	525	CHD	C22-C23-C24-O26
27	P	266	PGV	O03-C19-C20-C21
14	A	516	HEA	CAA-CBA-CGA-O1A
14	N	516	HEA	CAA-CBA-CGA-O1A
20	B	742	DMU	C22-C25-C28-C31
20	C	272	DMU	C31-C34-C37-C40
20	G	713	DMU	C28-C31-C34-C37
18	A	522	CDL	OA5-CA3-CA4-CA6
18	A	521	CDL	OB6-CB4-CB6-OB8
14	N	516	HEA	CAD-CBD-CGD-O1D
22	C	623	LFA	C10-C11-C12-C13
22	G	621	LFA	C3-C4-C5-C6
22	P	625	LFA	C11-C10-C9-C8
27	P	267	PGV	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
19	N	525	CHD	C22-C23-C24-O25
18	P	270	CDL	C17-C18-C19-C20
14	A	516	HEA	CAD-CBD-CGD-O1D
18	N	522	CDL	C20-C21-C22-C23
20	N	743	DMU	C25-C28-C31-C34
14	N	515[A]	HEA	CAD-CBD-CGD-O1D
14	N	515[B]	HEA	CAD-CBD-CGD-O1D
20	T	713	DMU	C28-C31-C34-C37
20	C	714	DMU	C4-C3-O7-C10
19	A	525	CHD	C22-C23-C24-O25
19	A	525	CHD	C22-C23-C24-O26
20	J	61	DMU	C28-C31-C34-C37
19	P	271	CHD	C22-C23-C24-O26
18	C	270	CDL	C57-C58-C59-C60
22	C	716[B]	LFA	C1-C2-C3-C4
20	N	744	DMU	C28-C31-C34-C37
22	P	716[B]	LFA	C3-C4-C5-C6
14	A	516	HEA	CAD-CBD-CGD-O2D
19	P	271	CHD	C22-C23-C24-O25
18	N	521	CDL	C59-C60-C61-C62
20	P	715[A]	DMU	C3-C4-C57-O61
18	A	521	CDL	C54-C55-C56-C57
18	A	521	CDL	C73-C74-C75-C76
22	P	611	LFA	C3-C4-C5-C6
23	A	825	EDO	O1-C1-C2-O2
23	C	827	EDO	O1-C1-C2-O2
23	E	815	EDO	O1-C1-C2-O2
23	R	815	EDO	O1-C1-C2-O2
26	C	264	PEK	C23-C24-C25-C26
20	T	711	DMU	C25-C28-C31-C34
20	N	745	DMU	O16-C18-C19-C22
18	A	521	CDL	C60-C61-C62-C63
20	C	722	DMU	C3-C4-C57-O61
19	C	271	CHD	C17-C20-C22-C23
20	A	744	DMU	C19-C22-C25-C28
27	C	266	PGV	C31-C32-C33-C34
20	M	746	DMU	C31-C34-C37-C40
14	N	516	HEA	CAA-CBA-CGA-O2A
20	O	731	DMU	C22-C25-C28-C31
14	A	515[A]	HEA	CAD-CBD-CGD-O1D
14	A	515[B]	HEA	CAD-CBD-CGD-O1D
18	N	522	CDL	C32-C31-CA7-OA8

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Mol	Chain	Res	Type	Atoms
22	T	621	LFA	C12-C13-C14-C15
18	N	521	CDL	C58-C59-C60-C61
14	N	515[A]	HEA	CAD-CBD-CGD-O2D
14	N	515[B]	HEA	CAD-CBD-CGD-O2D
18	A	521	CDL	C72-C71-CB7-OB8
20	C	714	DMU	C31-C34-C37-C40
18	A	522	CDL	O1-C1-CB2-OB2
18	N	521	CDL	C12-C11-CA5-OA6
20	C	714	DMU	C2-C3-O7-C10
18	A	522	CDL	C19-C20-C21-C22
22	T	621	LFA	C9-C10-C11-C12
26	P	264	PEK	C2-C1-O01-C02
14	A	515[A]	HEA	CAD-CBD-CGD-O2D
14	A	515[B]	HEA	CAD-CBD-CGD-O2D
26	P	264	PEK	O01-C1-C2-C3
20	C	734	DMU	O16-C18-C19-C22
18	P	270	CDL	C1-CB2-OB2-PB2
27	P	267	PGV	C05-C04-O12-P
14	A	516	HEA	CAA-CBA-CGA-O2A
14	A	516	HEA	C26-C15-C16-C17
14	N	516	HEA	C26-C15-C16-C17
18	N	522	CDL	C32-C31-CA7-OA9
20	L	747	DMU	C18-C19-C22-C25
26	C	264	PEK	C31-C32-C33-C34
18	C	270	CDL	C80-C81-C82-C83
20	J	61	DMU	C5-C10-O7-C3
20	J	732	DMU	C18-C19-C22-C25
22	P	614	LFA	C4-C5-C6-C7
18	N	521	CDL	CB7-C71-C72-C73
18	N	521	CDL	C32-C31-CA7-OA8
22	P	623	LFA	C1-C2-C3-C4
27	C	267	PGV	C15-C16-C17-C18
18	C	270	CDL	C12-C11-CA5-OA7
18	N	521	CDL	C12-C11-CA5-OA7
18	N	521	CDL	C32-C31-CA7-OA9
22	G	621	LFA	C11-C10-C9-C8
20	N	744	DMU	O1-C10-O7-C3
20	J	732	DMU	C28-C31-C34-C37
18	N	521	CDL	C72-C71-CB7-OB8
14	A	515[A]	HEA	CAA-CBA-CGA-O1A
14	A	515[B]	HEA	CAA-CBA-CGA-O1A
18	A	521	CDL	C72-C71-CB7-OB9

There are no ring outliers.

50 monomers are involved in 150 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	O	731	DMU	1	0
20	G	712	DMU	1	0
22	N	628	LFA	6	0
22	P	615	LFA	1	0
27	P	266	PGV	1	0
18	A	522	CDL	1	0
22	G	622	LFA	1	0
20	O	742	DMU	1	0
18	A	521	CDL	9	0
22	A	627	LFA	7	0
22	C	624	LFA	2	0
22	T	621	LFA	3	0
20	W	61	DMU	7	0
22	C	716[B]	LFA	3	0
22	N	627	LFA	3	0
14	A	515[A]	HEA	7	0
20	P	733	DMU	1	0
19	P	271	CHD	1	0
20	A	743	DMU	1	0
20	N	744	DMU	2	0
22	P	611	LFA	1	0
14	A	516	HEA	1	0
22	C	625	LFA	1	0
21	N	520	PER	1	0
18	N	521	CDL	7	0
22	A	628	LFA	11	0
19	G	86	CHD	1	0
26	C	264	PEK	5	0
19	T	86	CHD	1	0
27	C	266	PGV	2	0
26	P	264	PEK	3	0
20	P	715[A]	DMU	1	0
22	P	624	LFA	1	0
22	T	622	LFA	1	0
14	N	515[B]	HEA	1	0
20	T	711	DMU	1	0
18	C	270	CDL	15	0
14	N	515[A]	HEA	6	0
20	C	733	DMU	2	0
20	A	526	DMU	1	0

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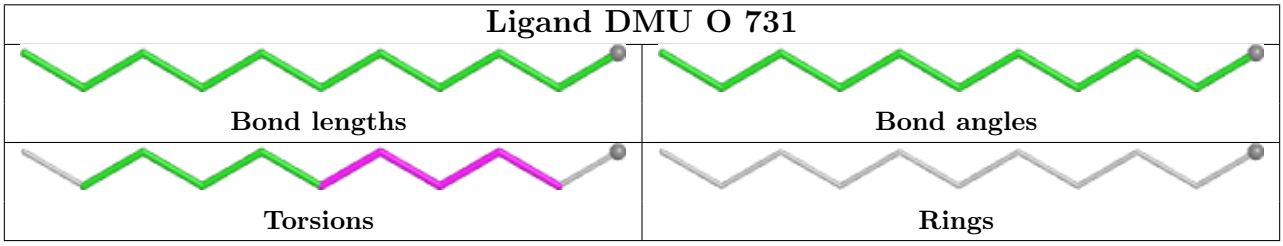
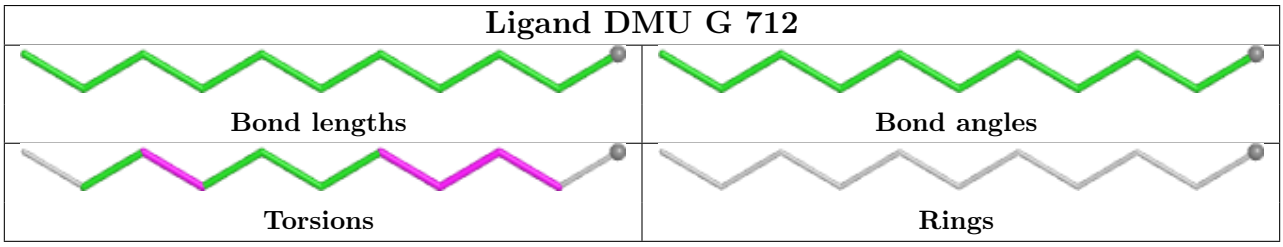
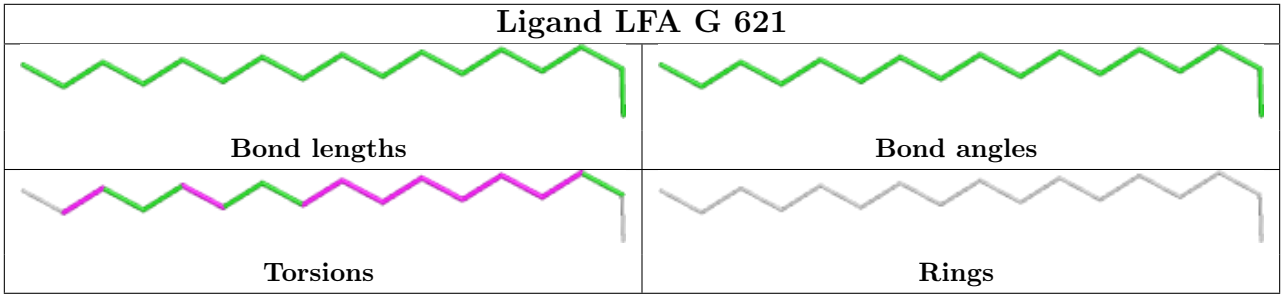
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	N	522	CDL	1	0
27	C	267	PGV	1	0
20	A	744	DMU	4	0
22	C	626	LFA	2	0
20	P	714	DMU	1	0
22	P	716[B]	LFA	1	0
14	N	516	HEA	2	0
21	A	520	PER	1	0
20	J	61	DMU	6	0
18	P	270	CDL	13	0

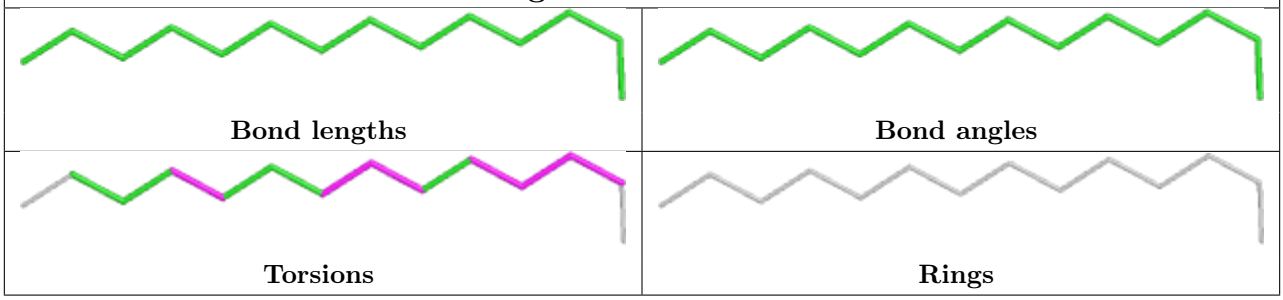
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



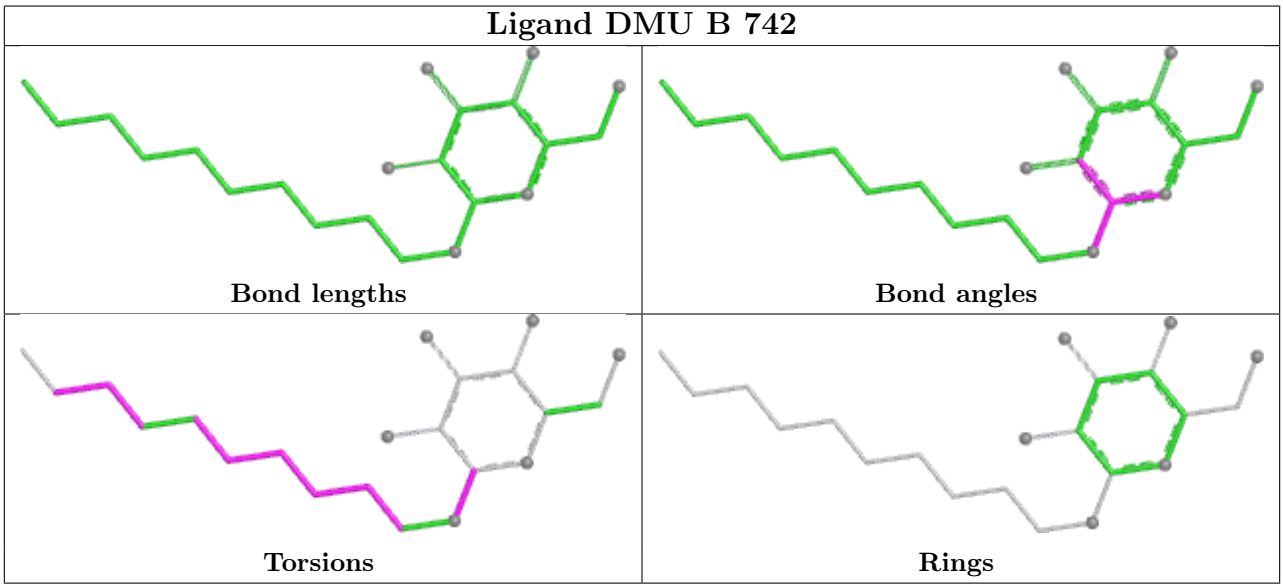




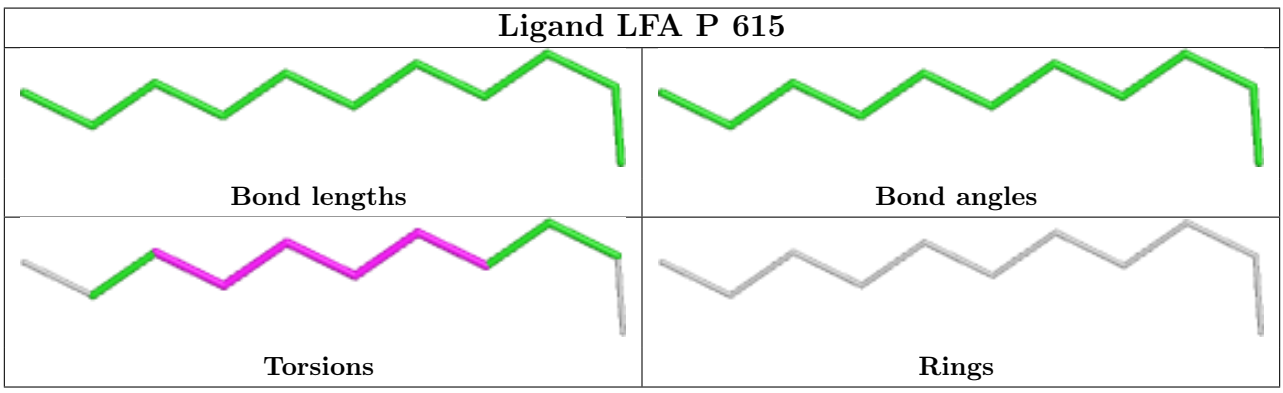
Ligand LFA N 628



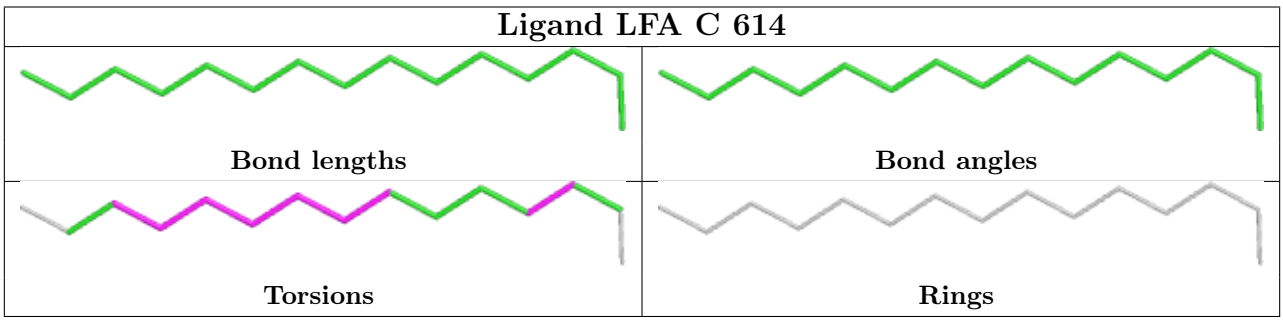
Ligand DMU B 742



Ligand LFA P 615



Ligand LFA C 614



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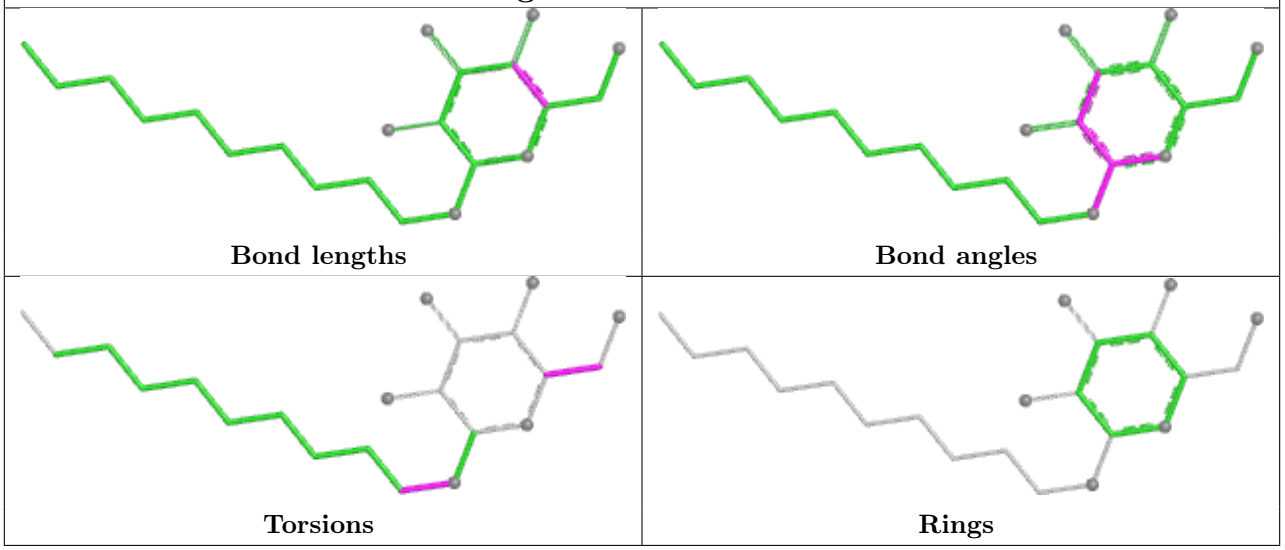

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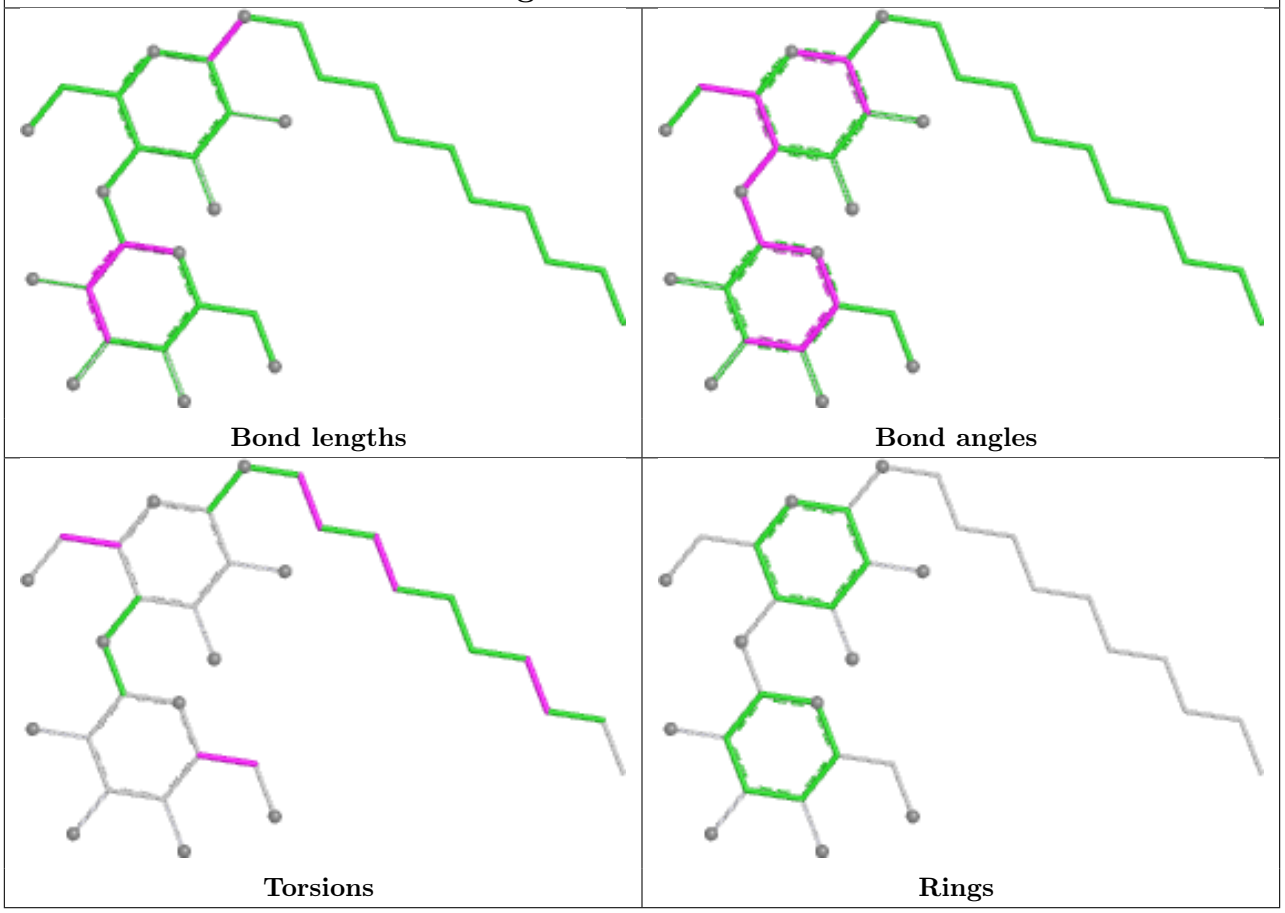

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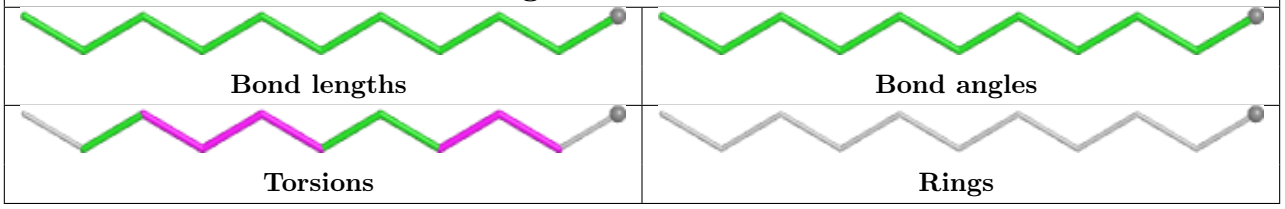

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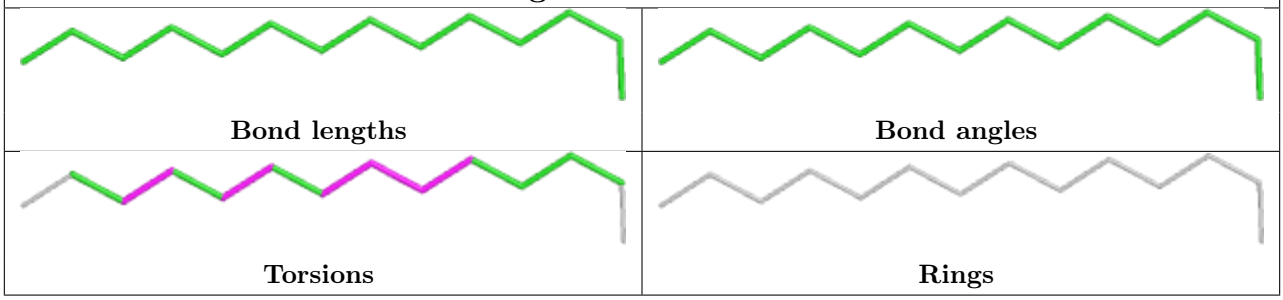
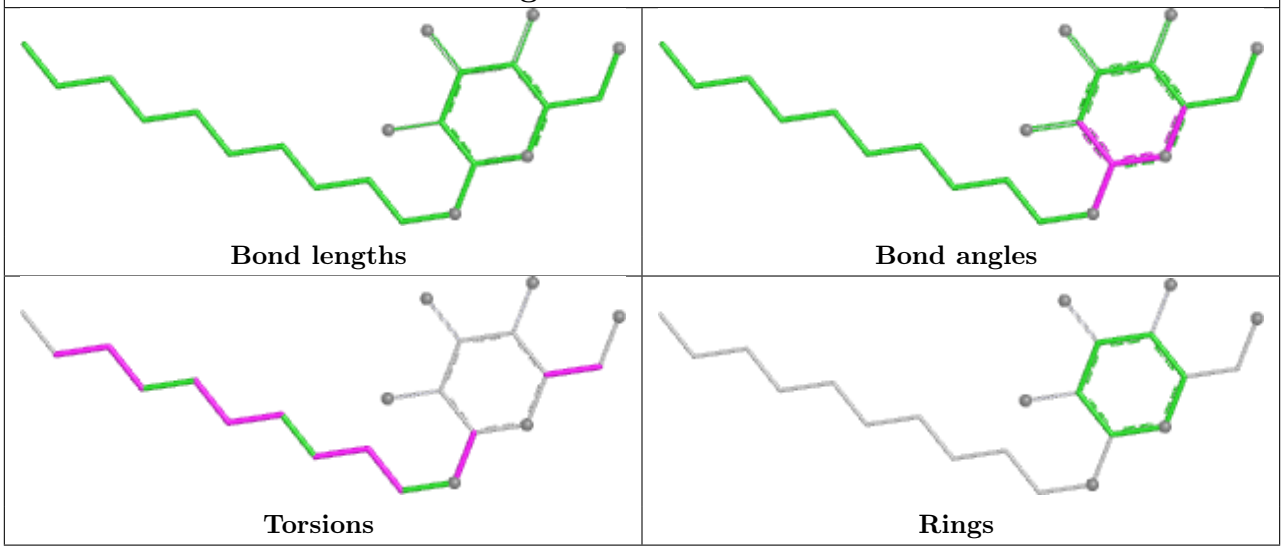
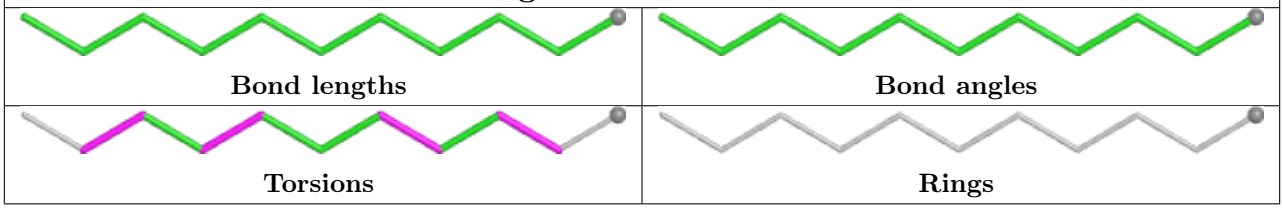


Ligand DMU L 747

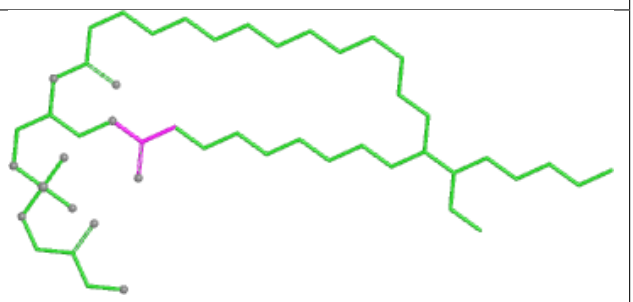


Ligand DMU T 712



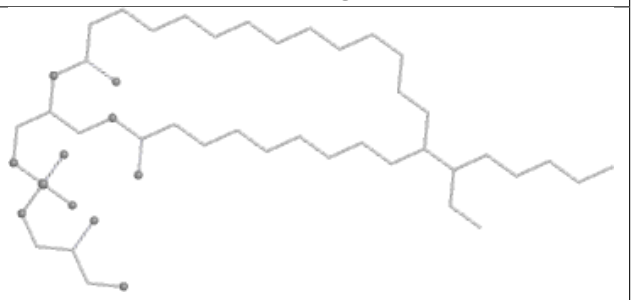
Ligand PGV P 266

Bond lengths



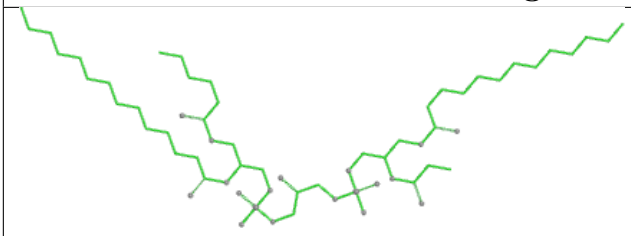
Bond angles

Torsions

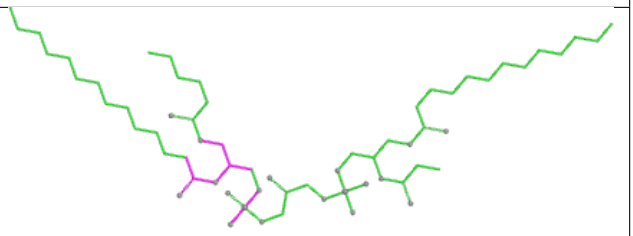


Rings

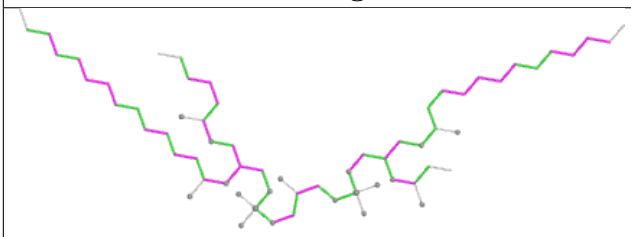
Ligand CDL A 522



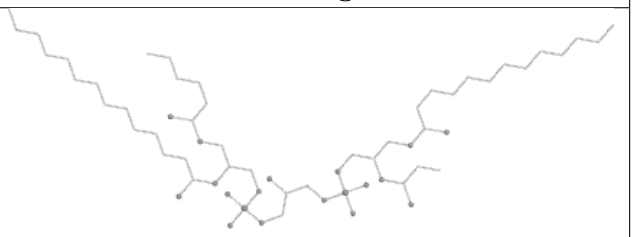
Bond lengths



Bond angles

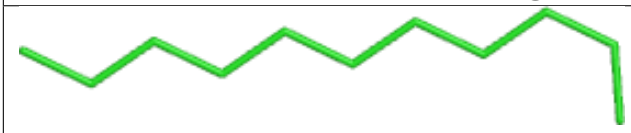


Torsions

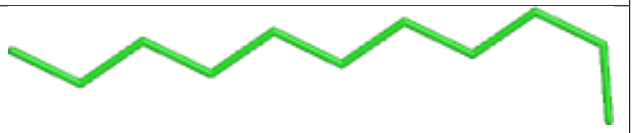


Rings

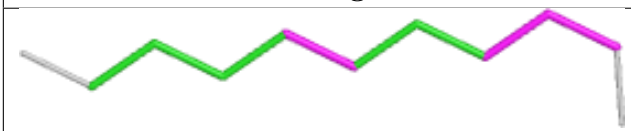
Ligand LFA G 622



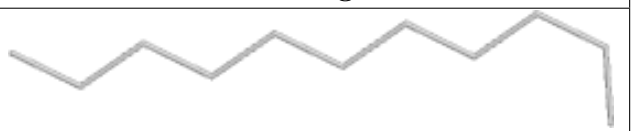
Bond lengths



Bond angles

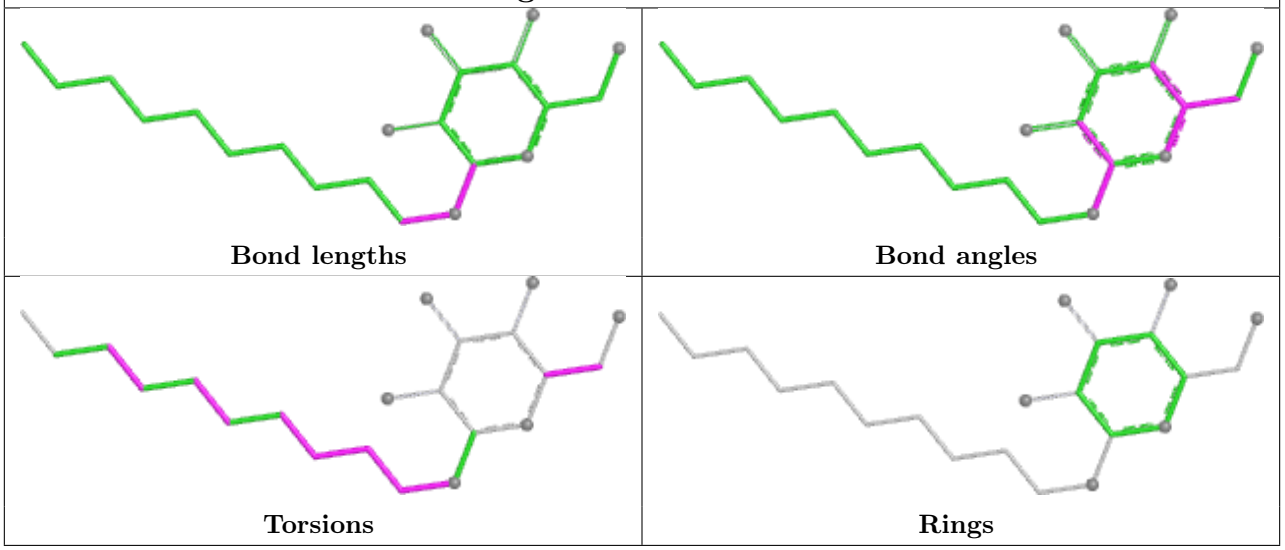


Torsions

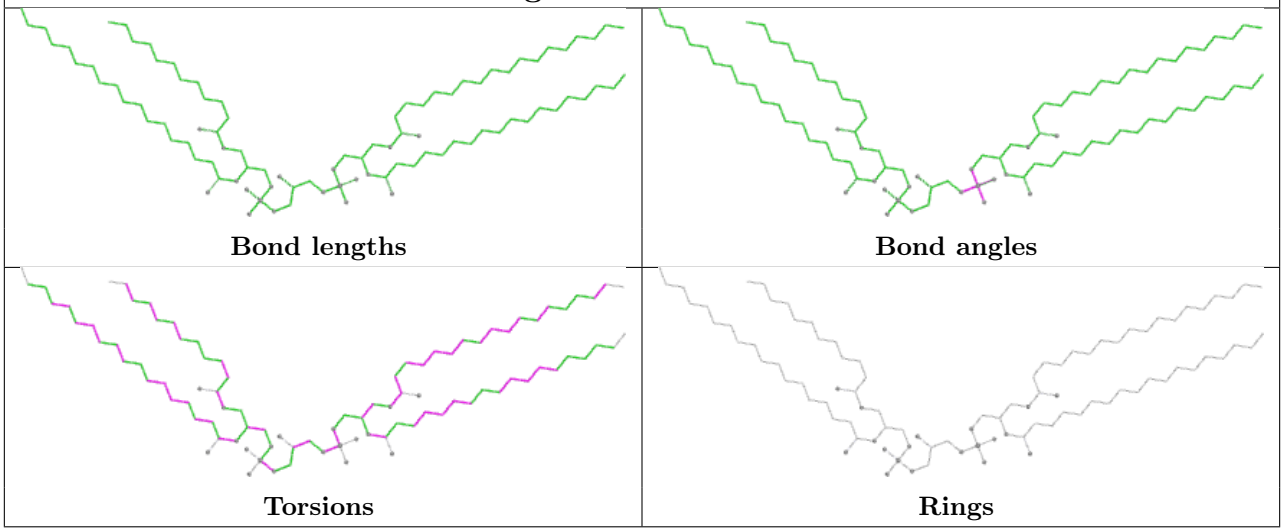


Rings

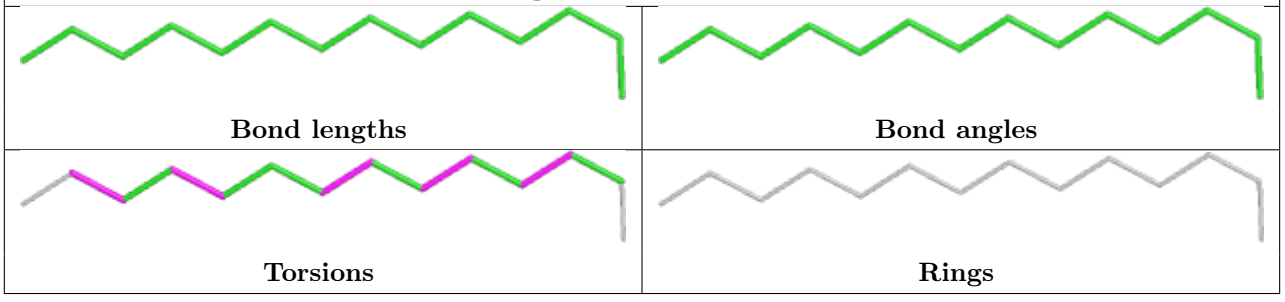
Ligand DMU O 742



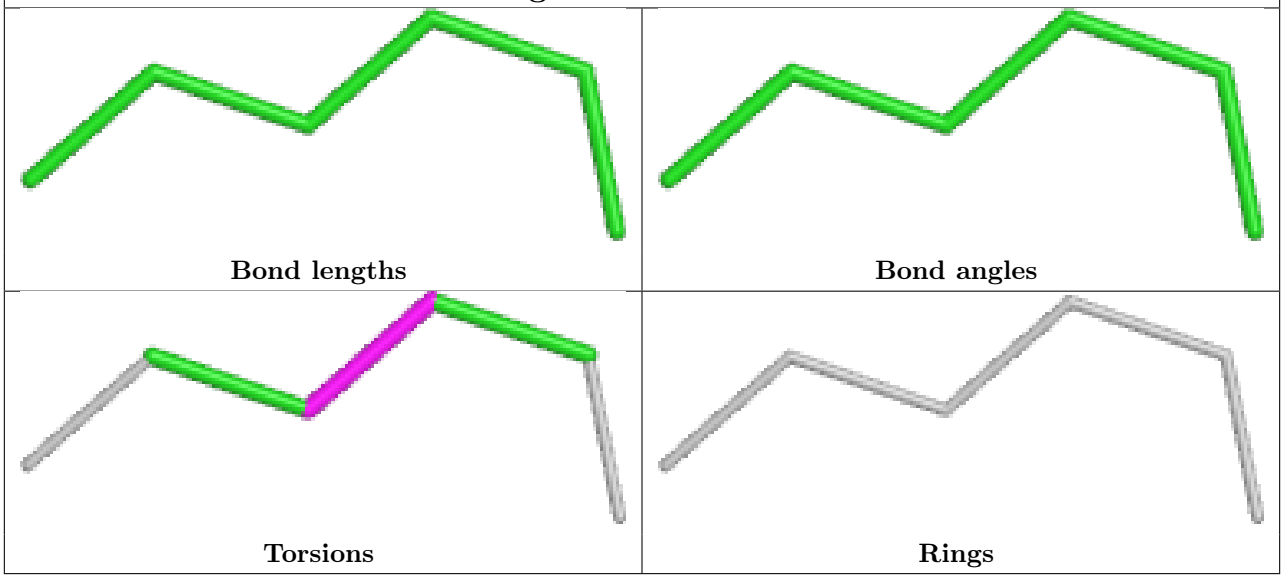
Ligand CDL A 521



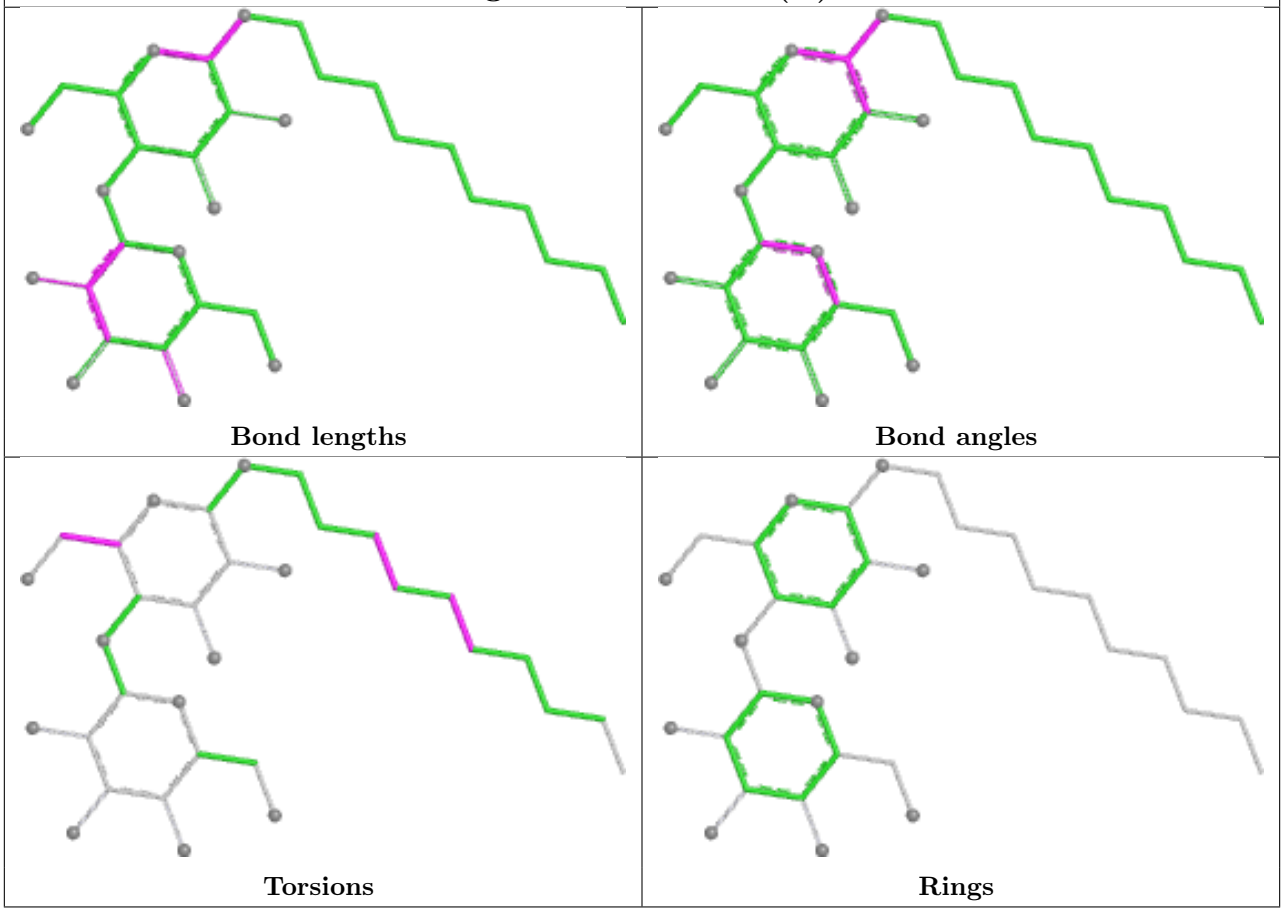
Ligand LFA A 627



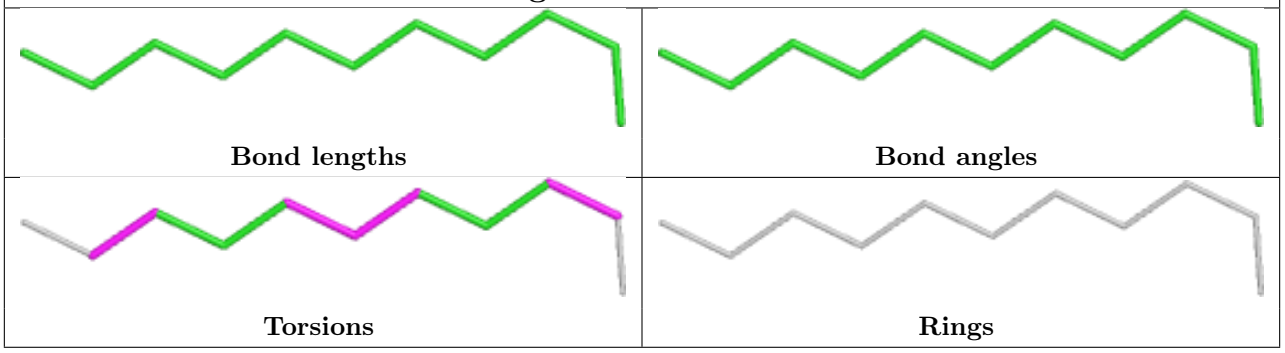
Ligand LFA C 612



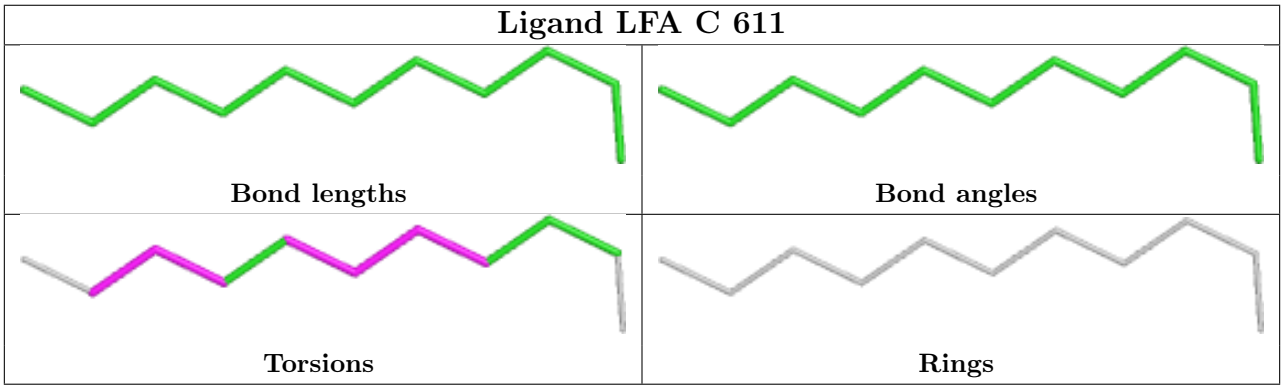
Ligand DMU C 715 (A)



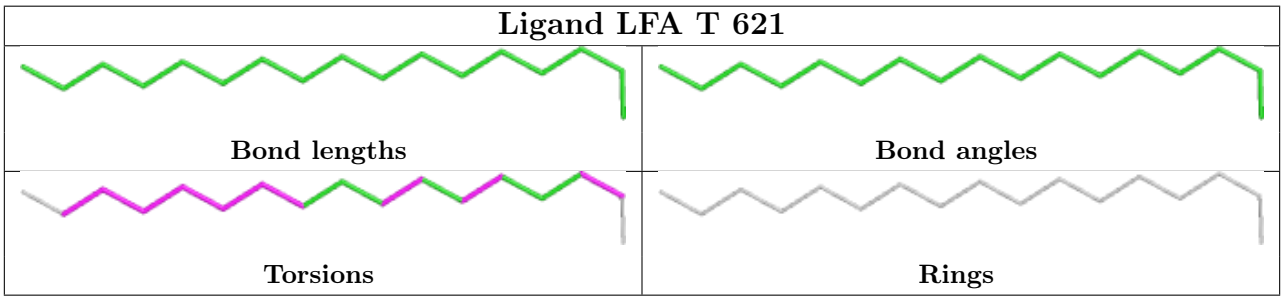
Ligand LFA C 624



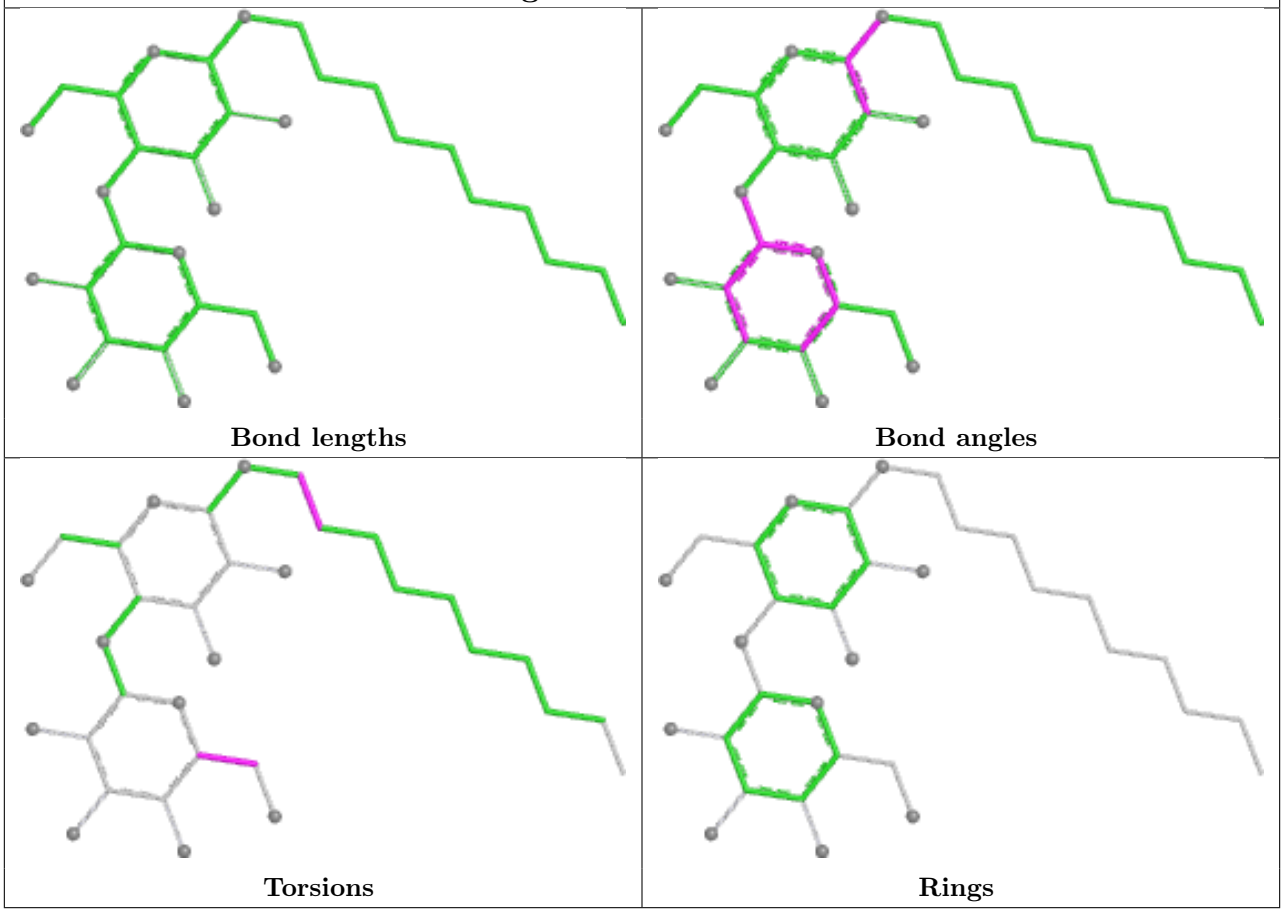
Ligand LFA C 611



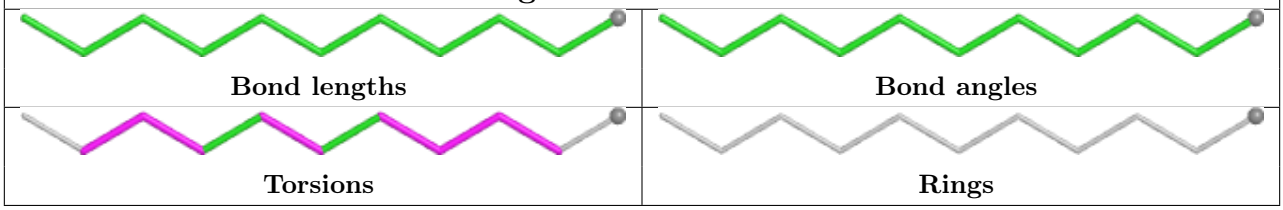
Ligand LFA T 621



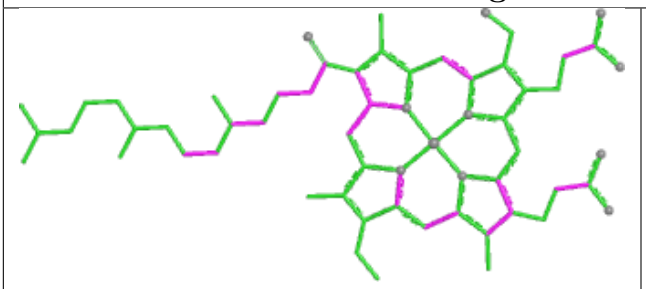
Ligand DMU W 61



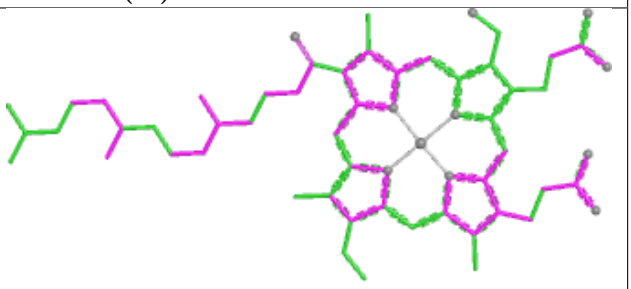
Ligand DMU B 731



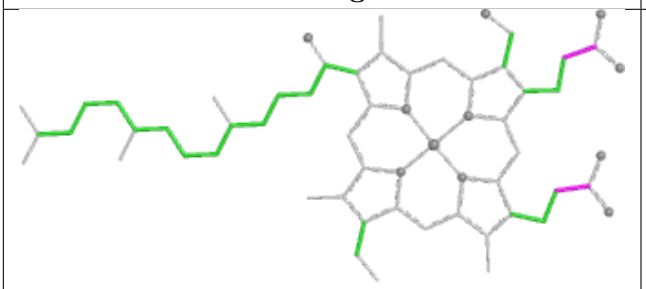
Ligand HEA A 515 (B)



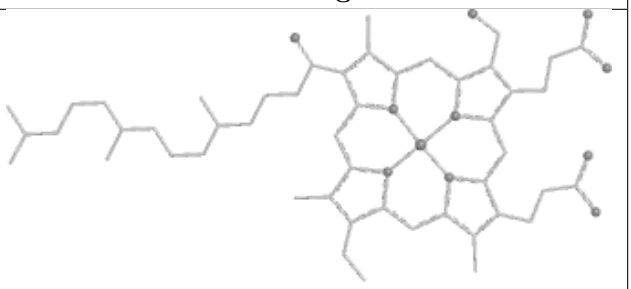
Bond lengths



Bond angles



Torsions

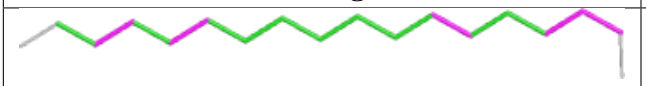


Rings

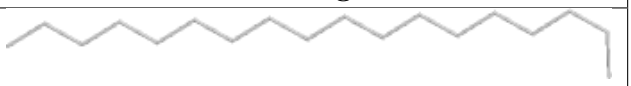
Ligand LFA C 716 (B)

Bond lengths

Bond angles

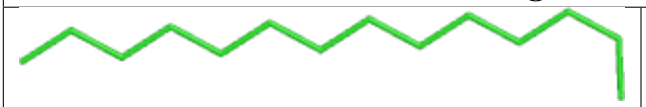


Torsions

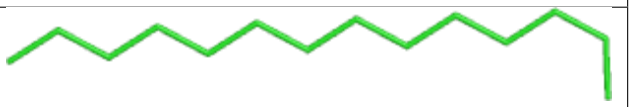


Rings

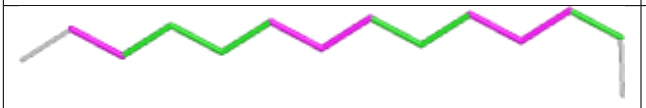
Ligand LFA N 627



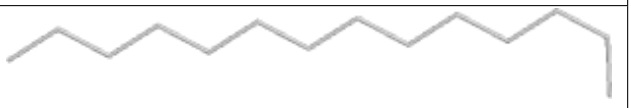
Bond lengths



Bond angles

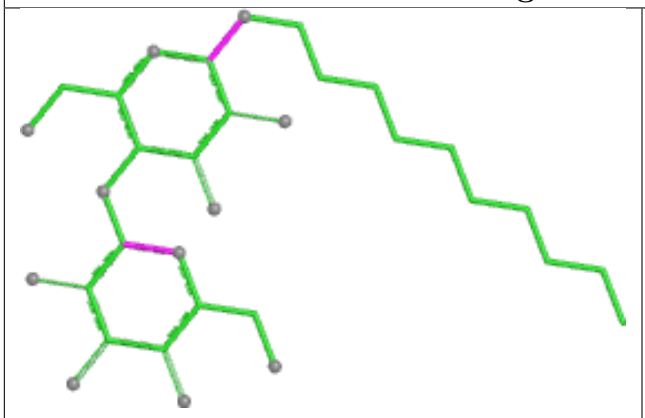


Torsions

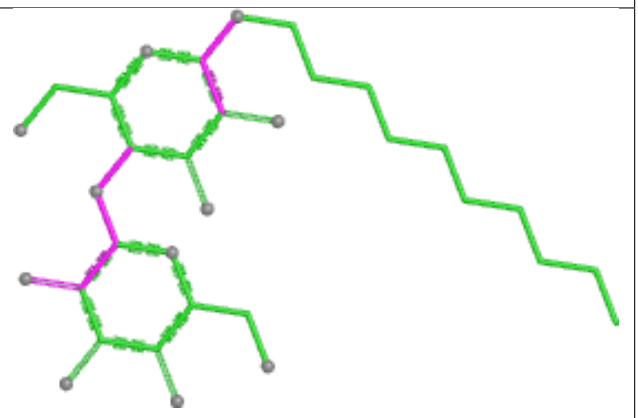


Rings

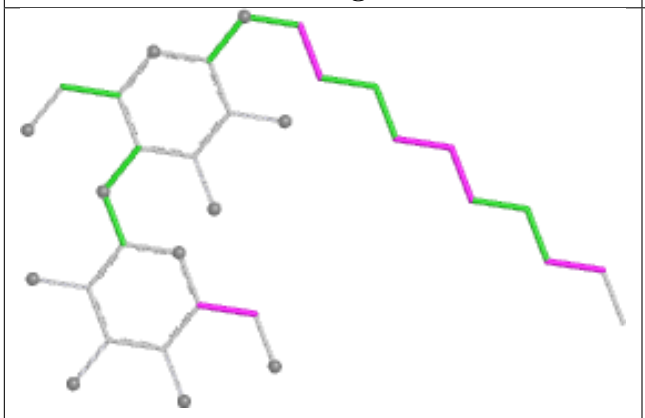
Ligand DMU N 526



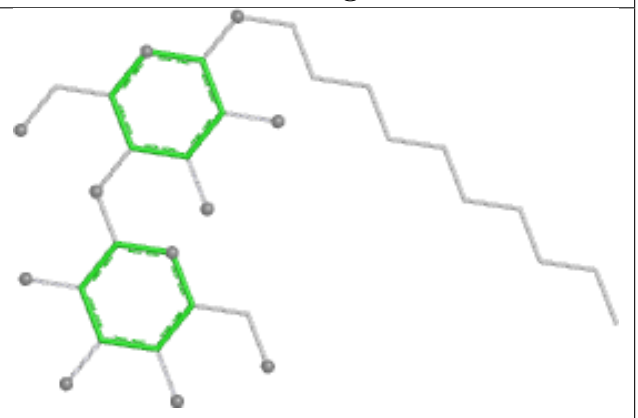
Bond lengths



Bond angles

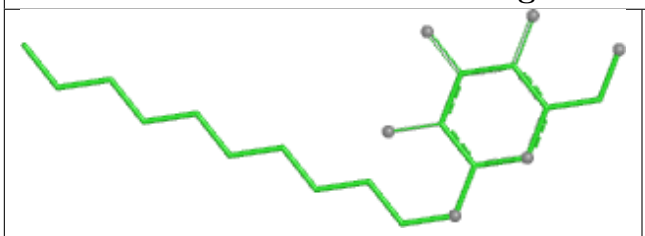


Torsions

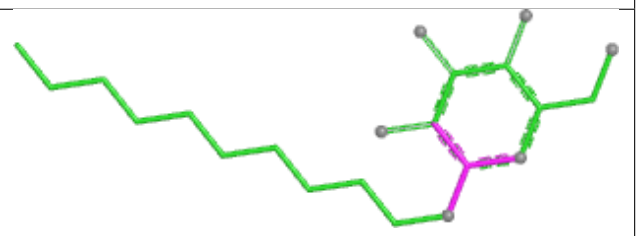


Rings

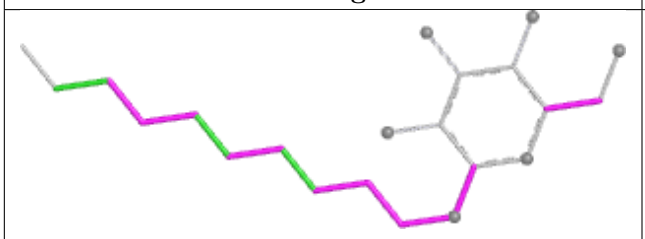
Ligand DMU C 722



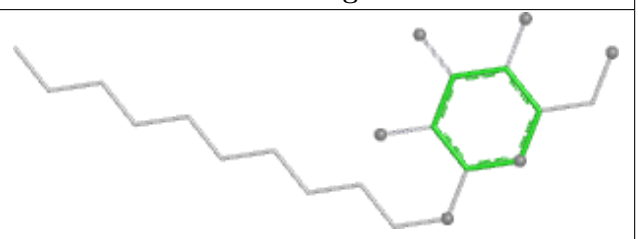
Bond lengths



Bond angles

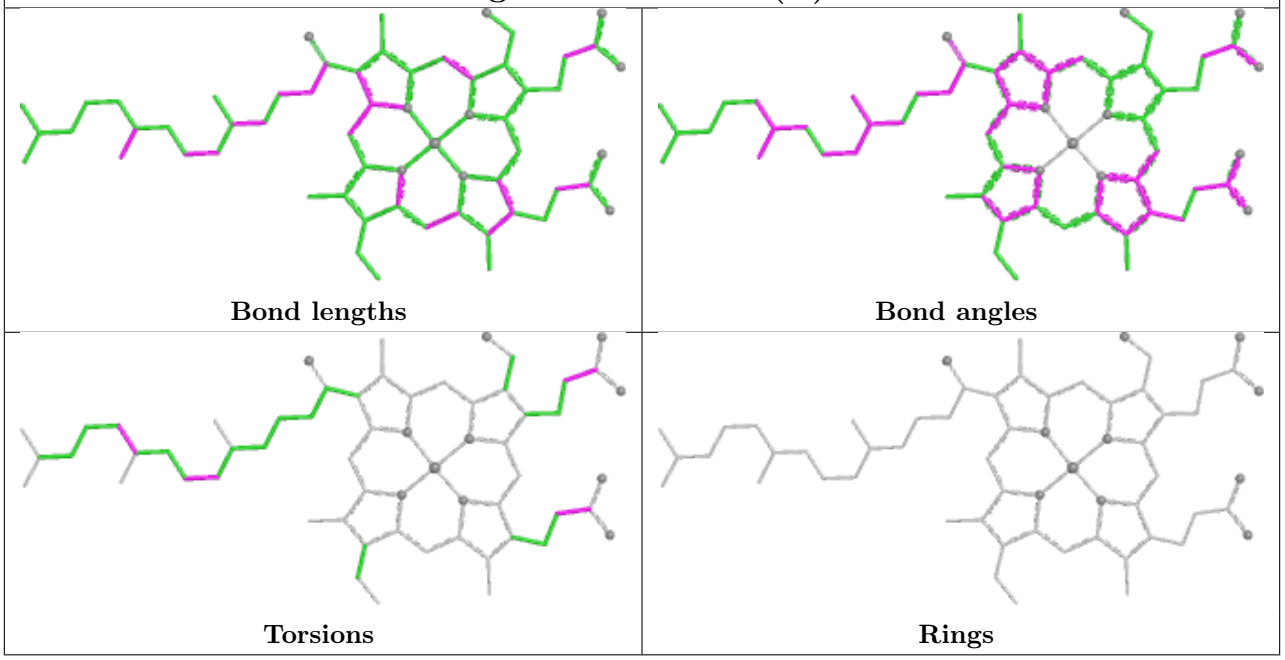


Torsions

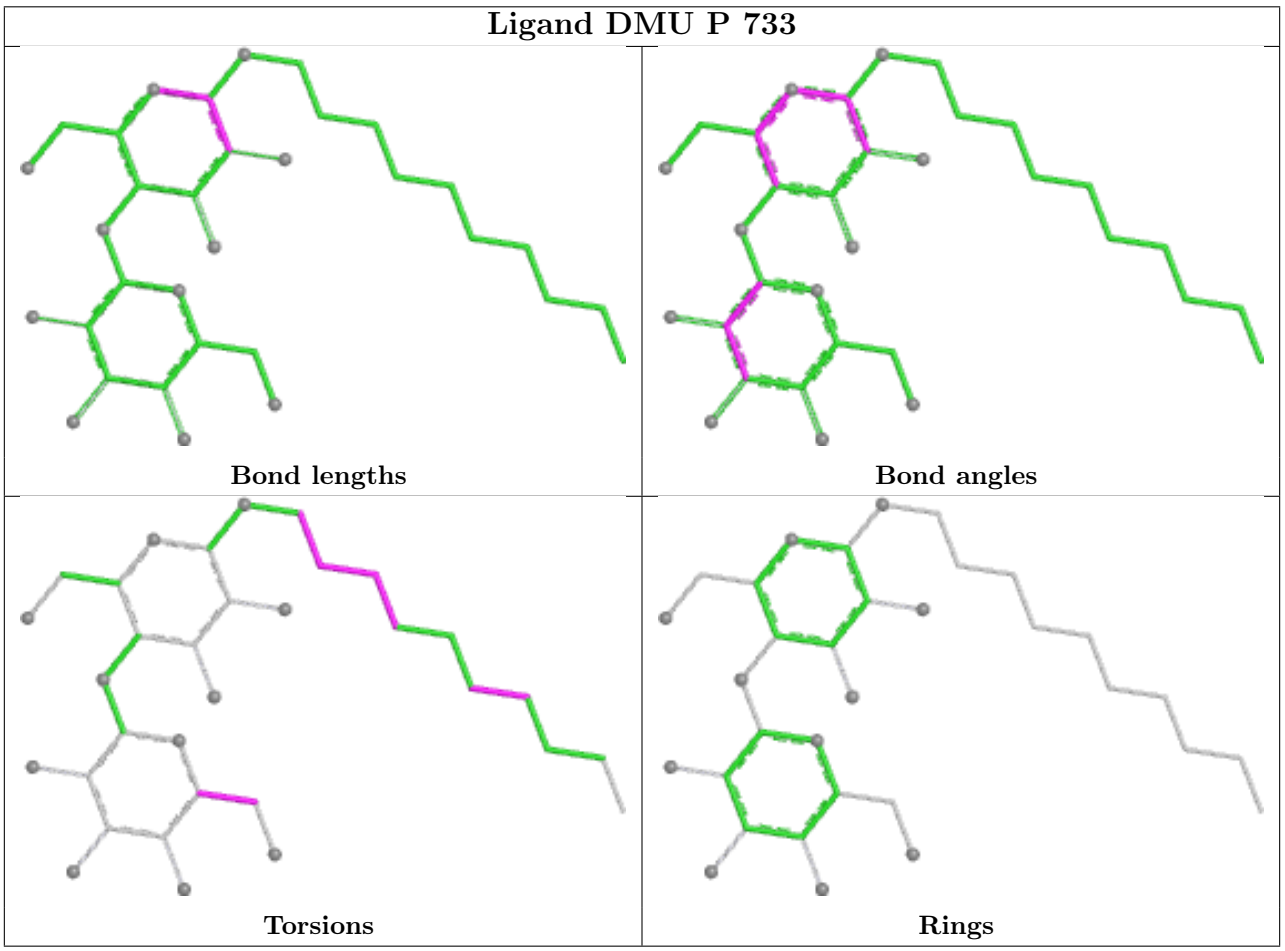


Rings

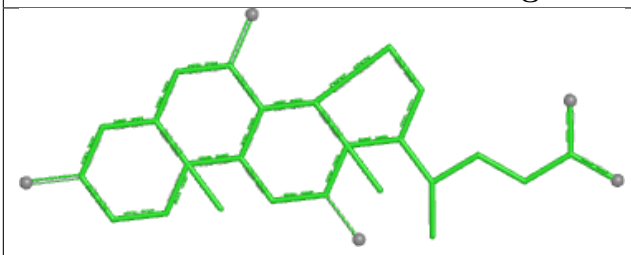
Ligand HEA A 515 (A)



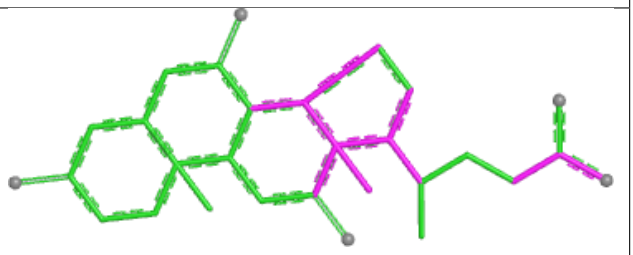
Ligand DMU P 733



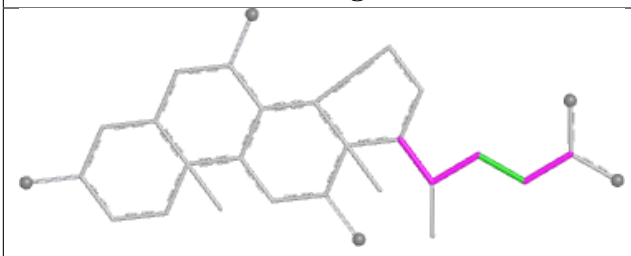
Ligand CHD P 271



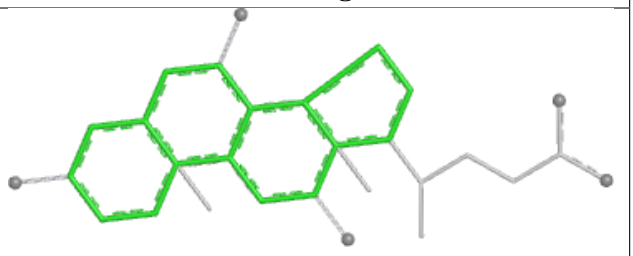
Bond lengths



Bond angles

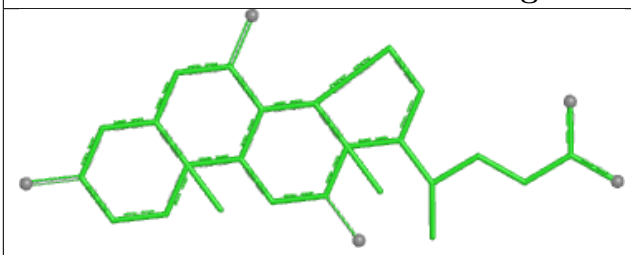


Torsions

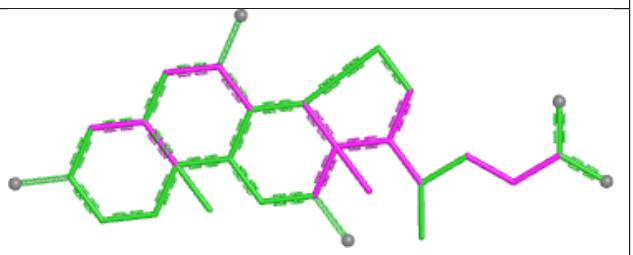


Rings

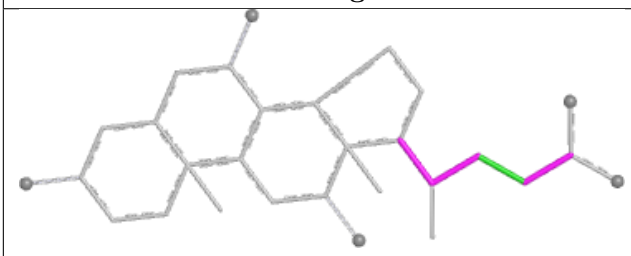
Ligand CHD C 271



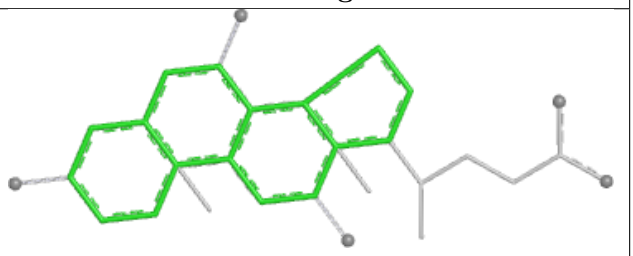
Bond lengths



Bond angles



Torsions



Rings

Ligand DMU A 743

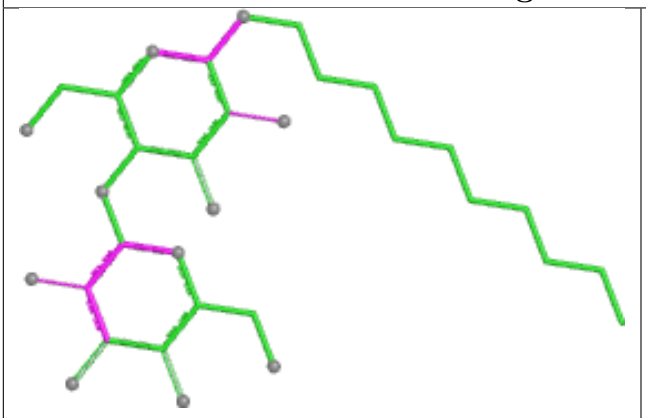
Bond lengths

Bond angles

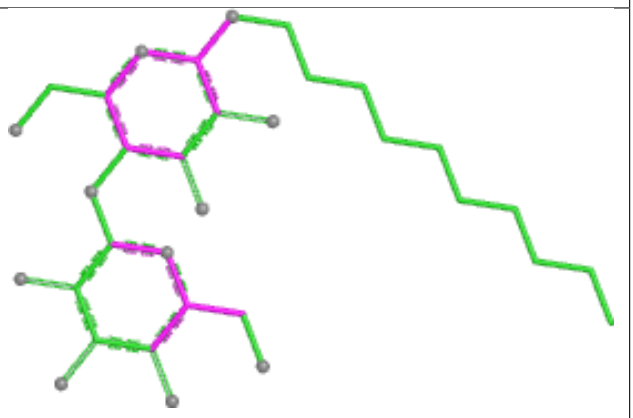
Torsions

Rings

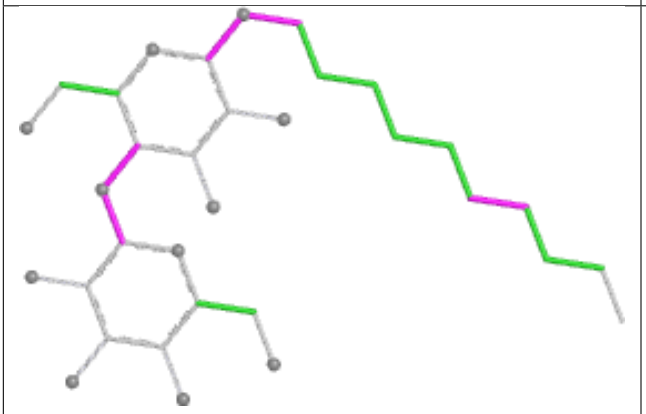
Ligand DMU N 744



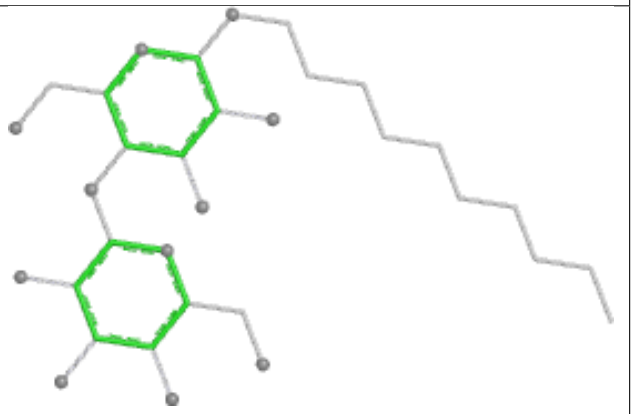
Bond lengths



Bond angles

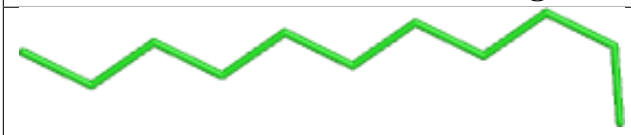


Torsions



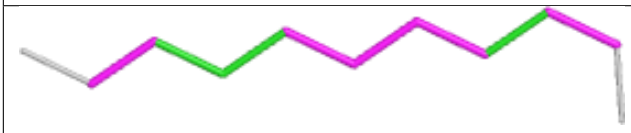
Rings

Ligand LFA P 611

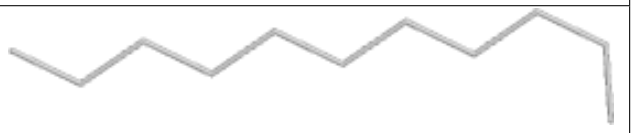


Bond lengths

Bond angles

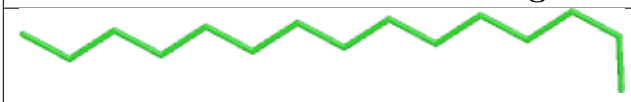


Torsions



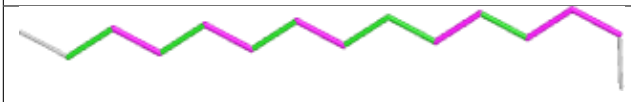
Rings

Ligand LFA P 614

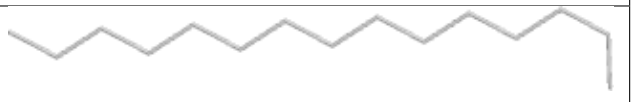


Bond lengths

Bond angles

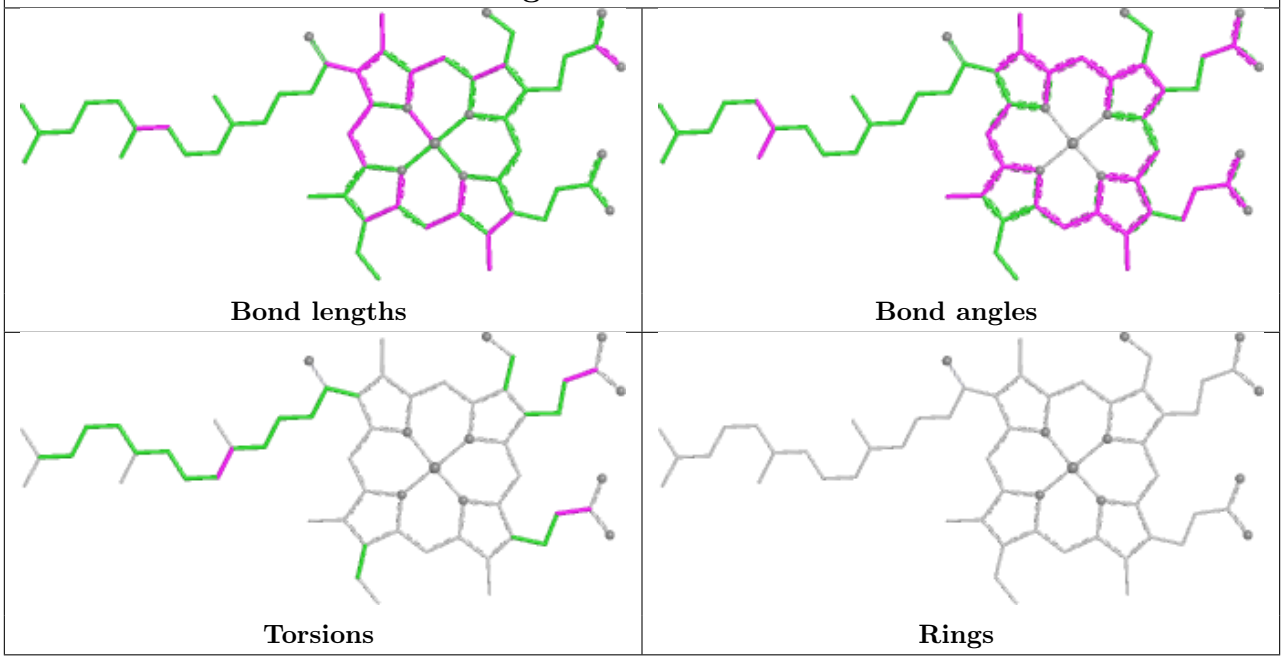


Torsions

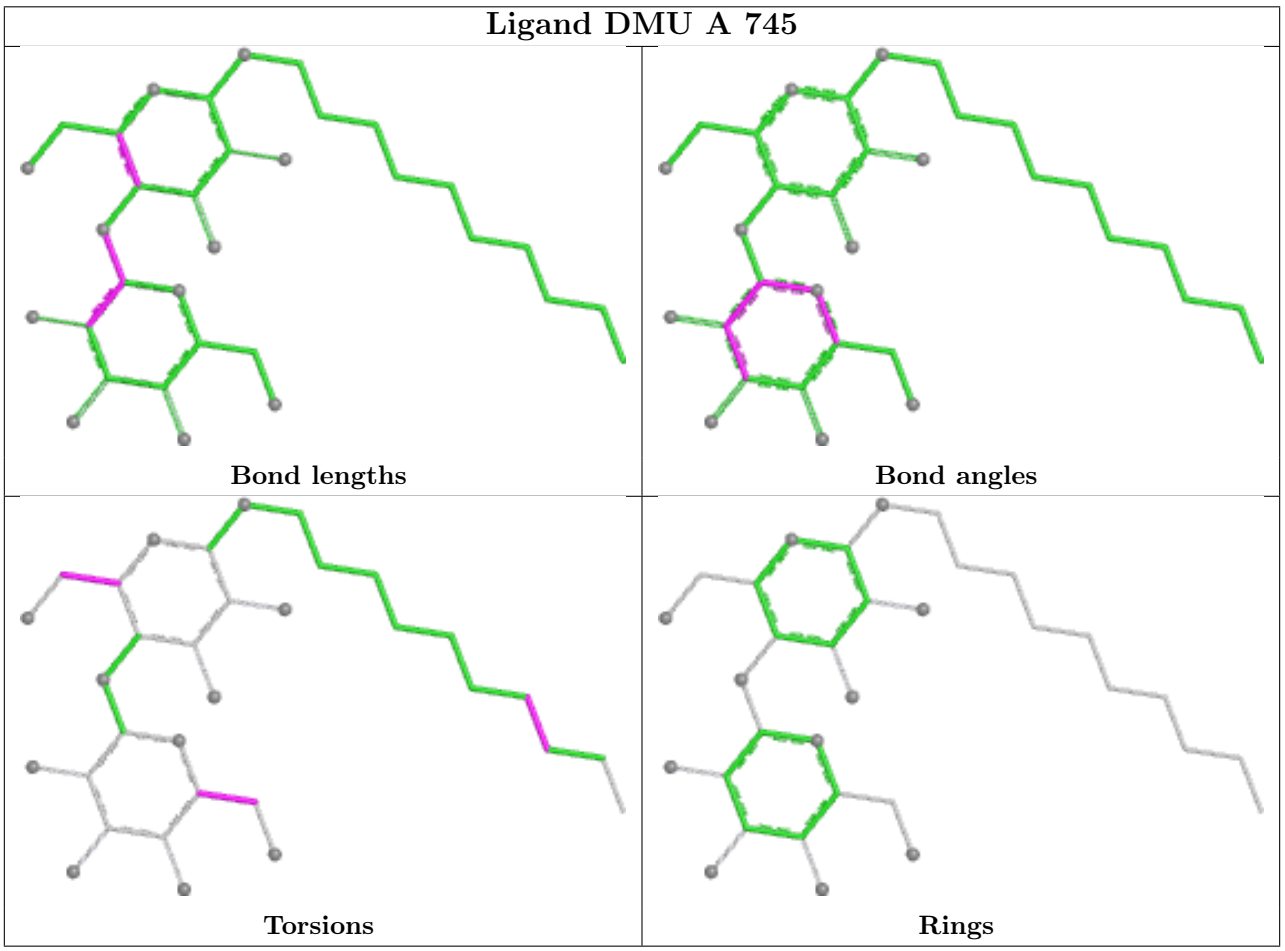


Rings

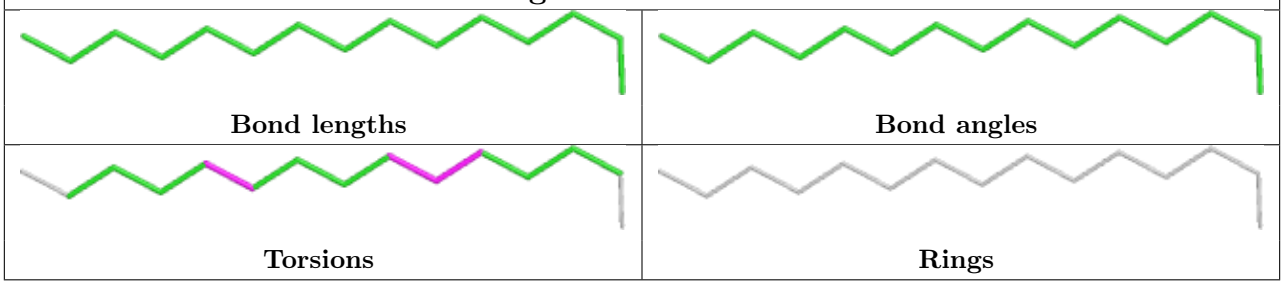
Ligand HEA A 516



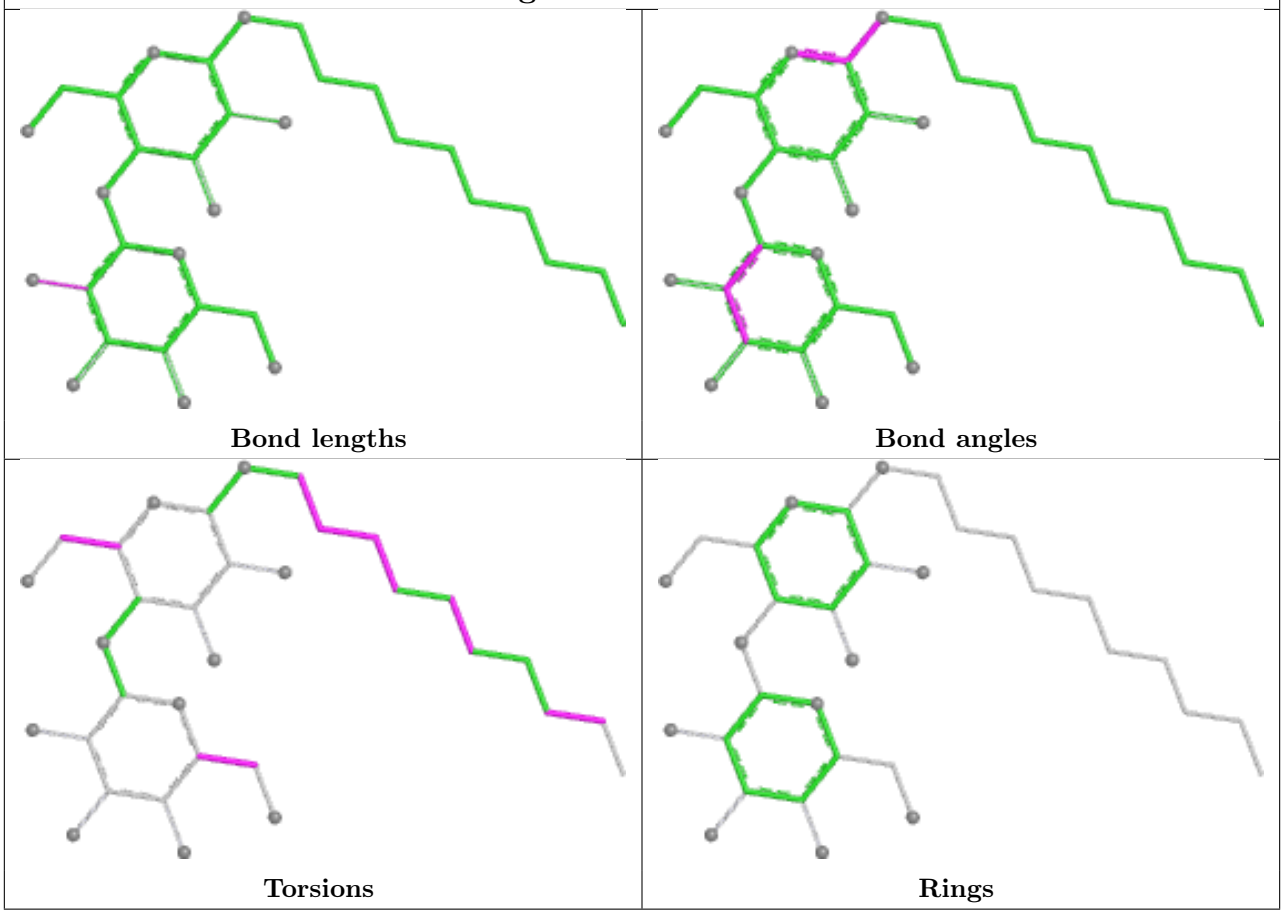
Ligand DMU A 745



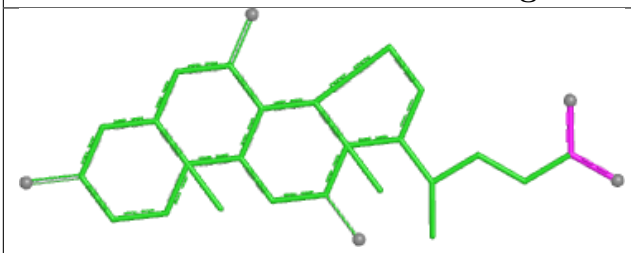
Ligand LFA C 625

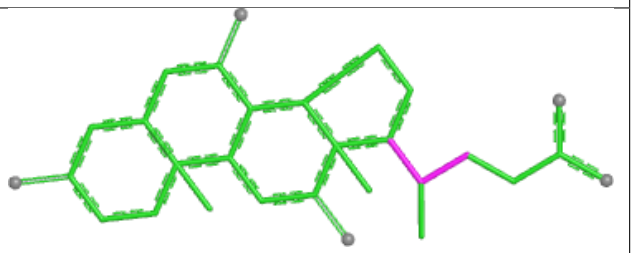


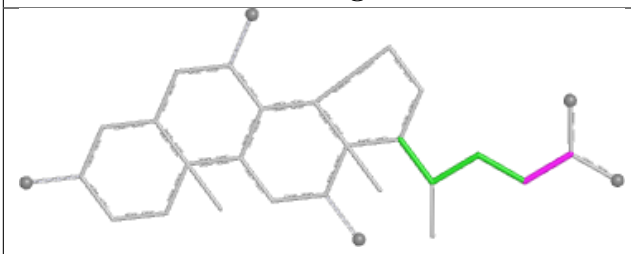
Ligand DMU P 734

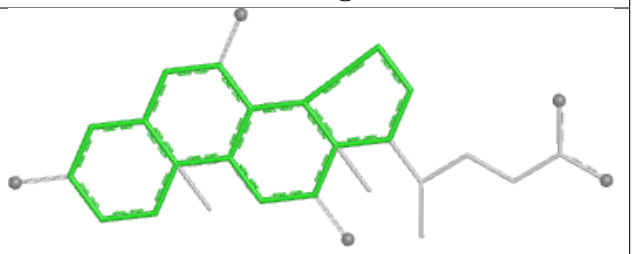


Ligand CHD N 525

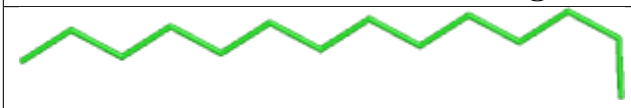

Bond lengths

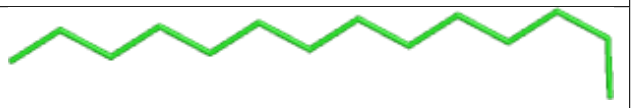

Bond angles

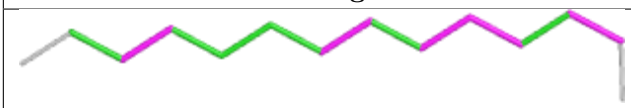

Torsions

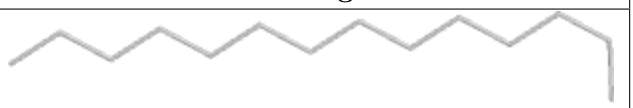

Rings

Ligand LFA P 623

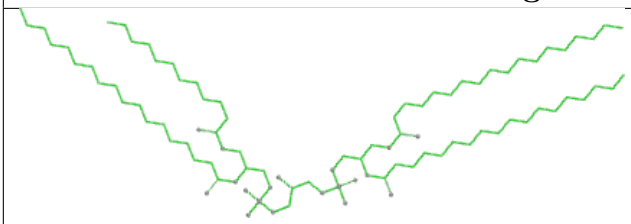

Bond lengths

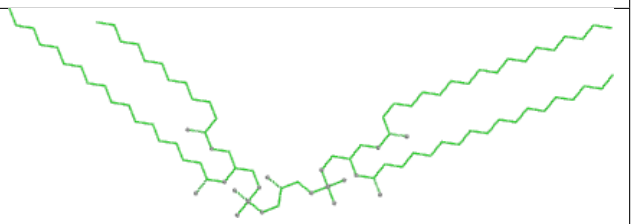

Bond angles

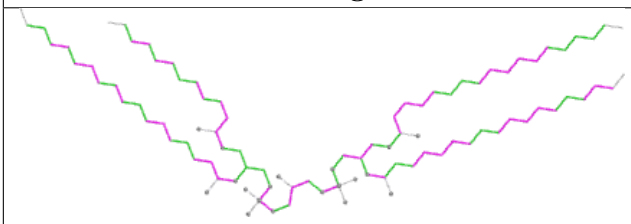

Torsions

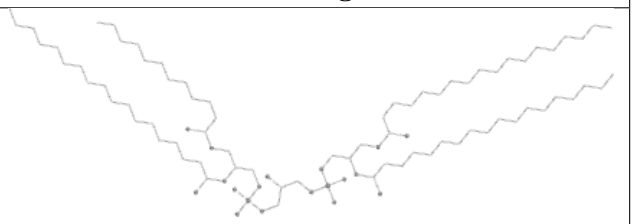

Rings

Ligand CDL N 521

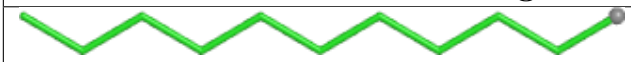

Bond lengths


Bond angles


Torsions


Rings

Ligand DMU B 741

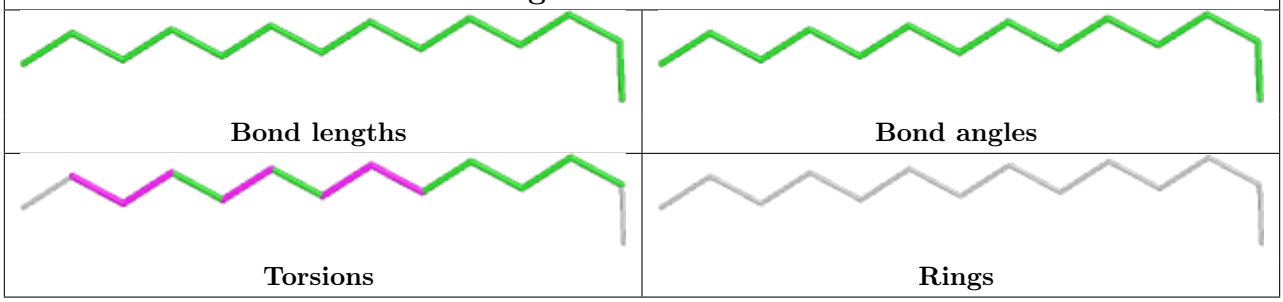

Bond lengths

Bond angles

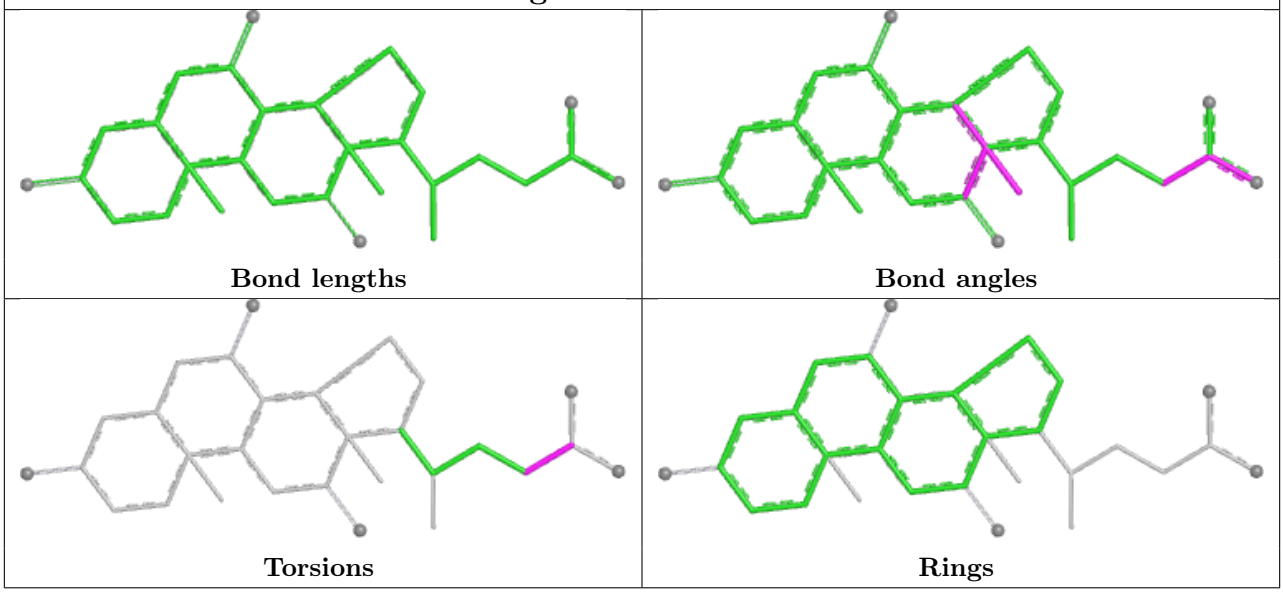
Torsions

Rings

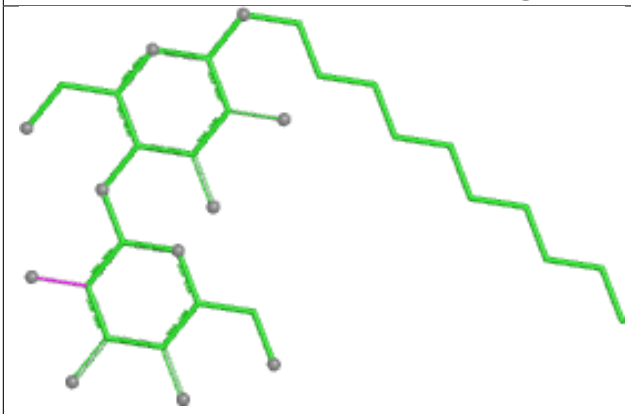
Ligand LFA A 628



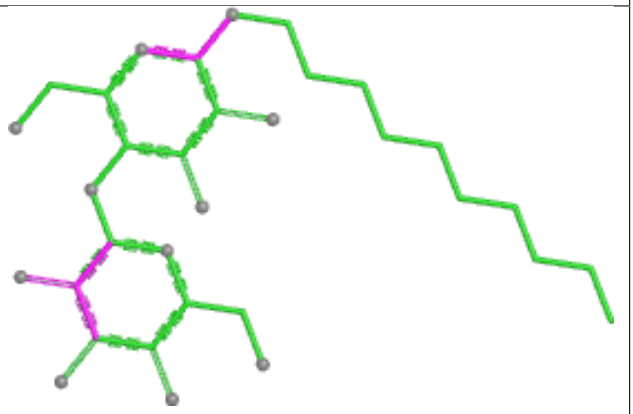
Ligand CHD G 86



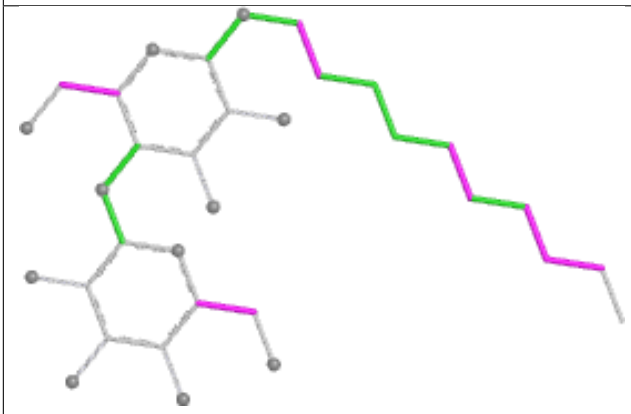
Ligand DMU C 734



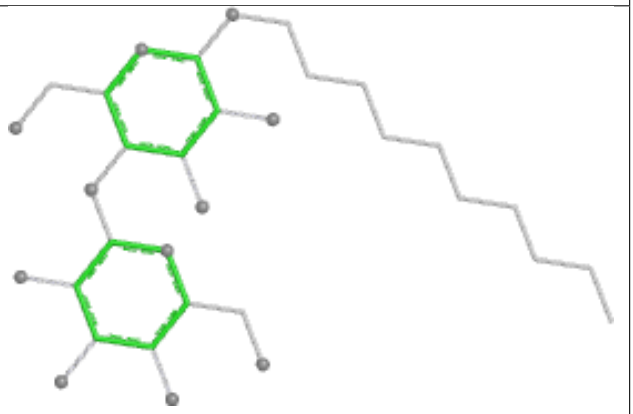
Bond lengths



Bond angles

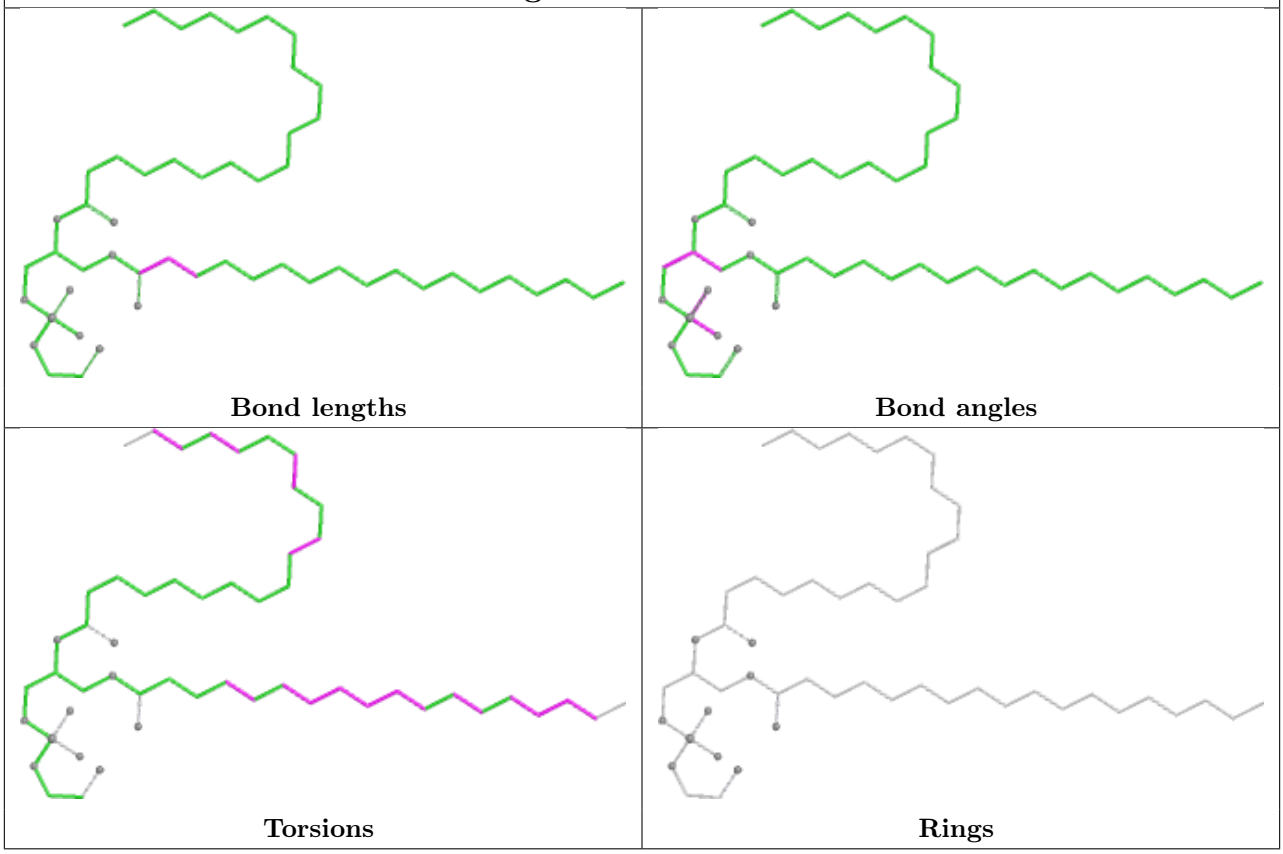


Torsions

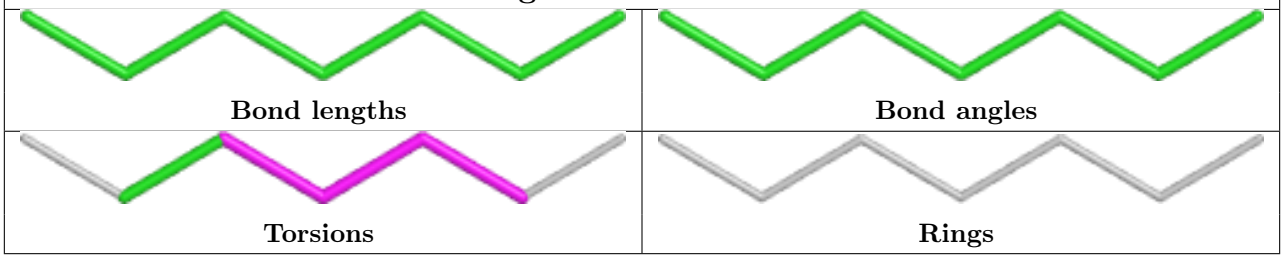


Rings

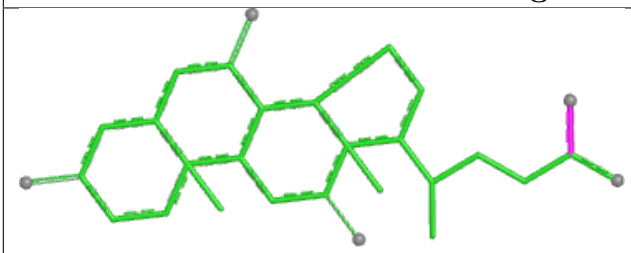
Ligand PEK C 264



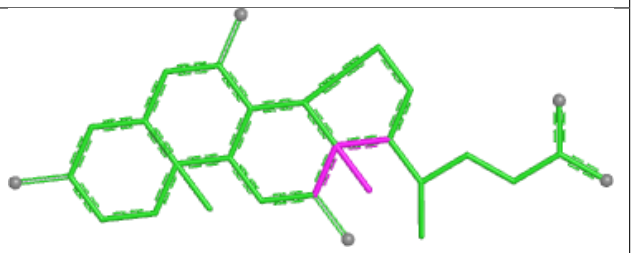
Ligand DMU P 721



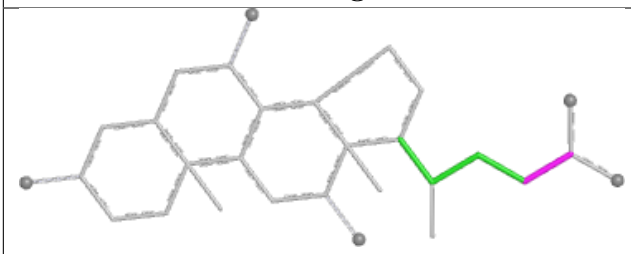
Ligand CHD T 86



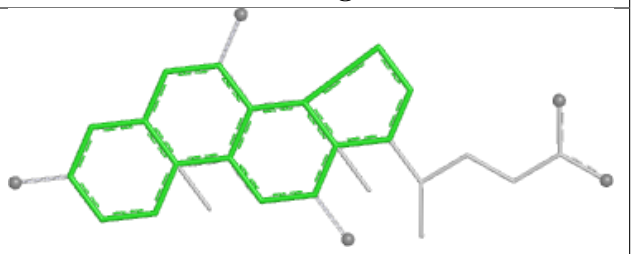
Bond lengths



Bond angles

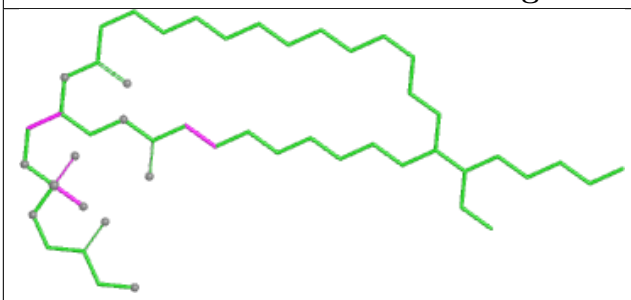


Torsions

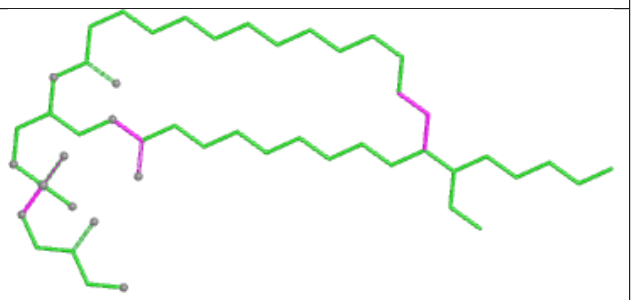


Rings

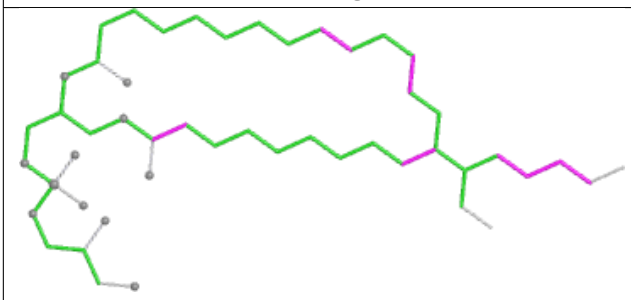
Ligand PGV C 266



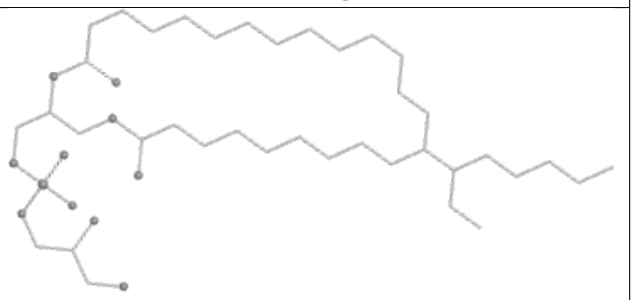
Bond lengths



Bond angles

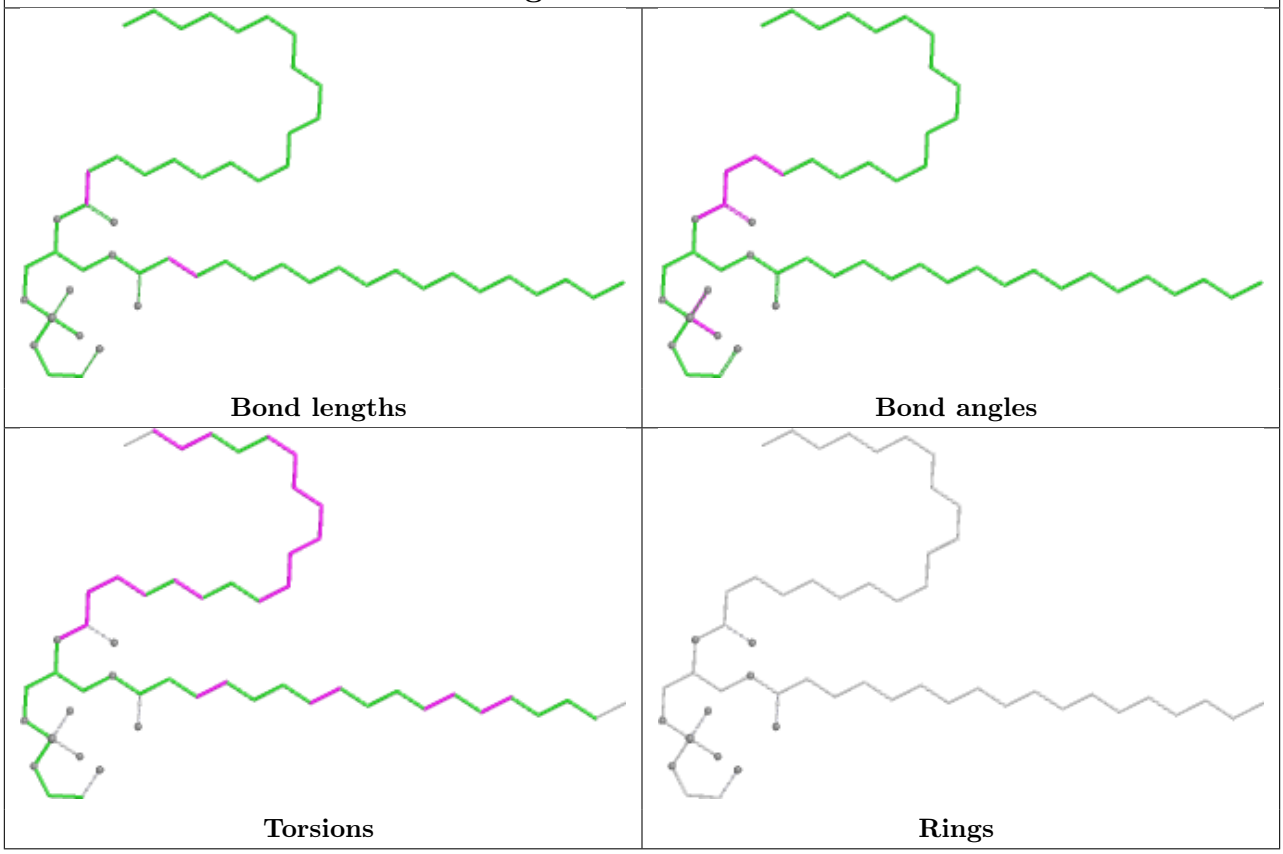


Torsions

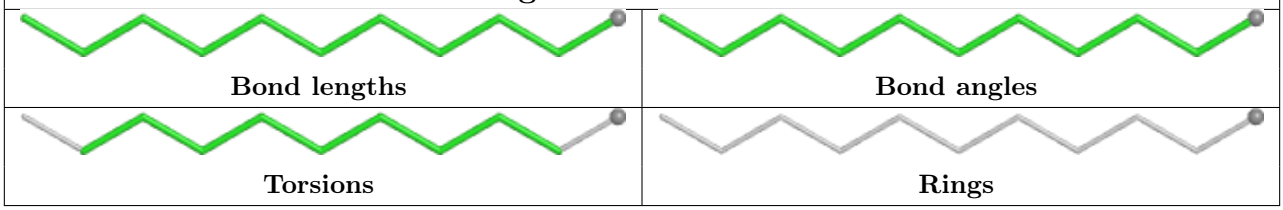


Rings

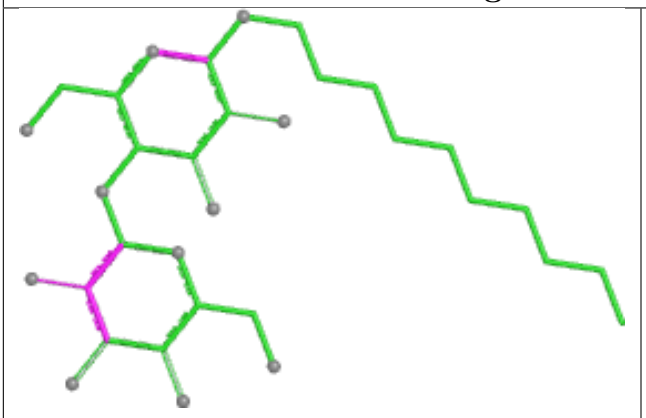
Ligand PEK P 264



Ligand DMU P 272

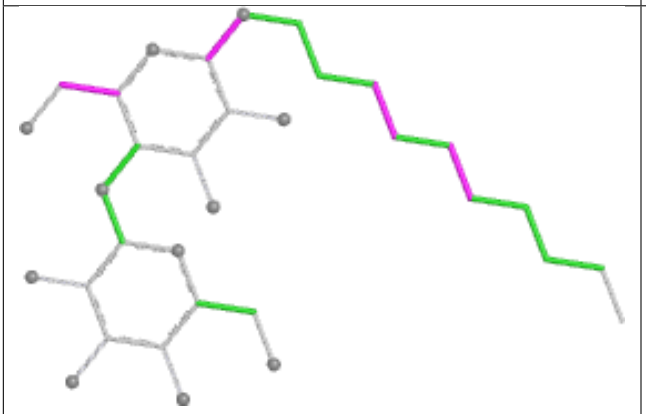


Ligand DMU P 715 (A)

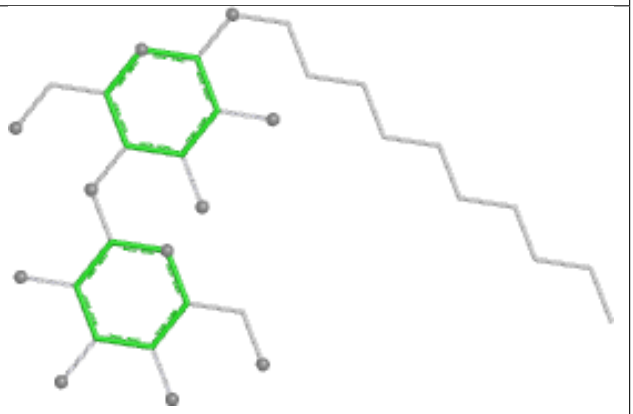


Bond lengths

Bond angles



Torsions



Rings

Ligand DMU O 741

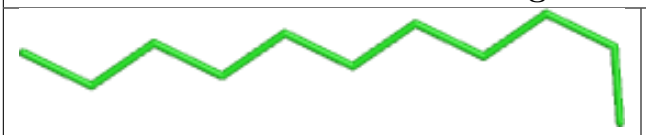
Bond lengths

Bond angles

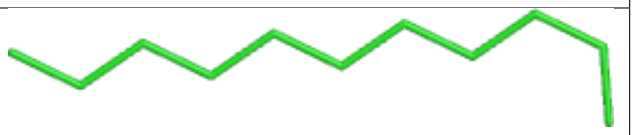
Torsions

Rings

Ligand LFA P 624

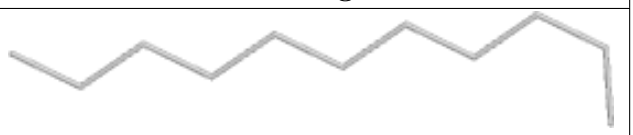


Bond lengths



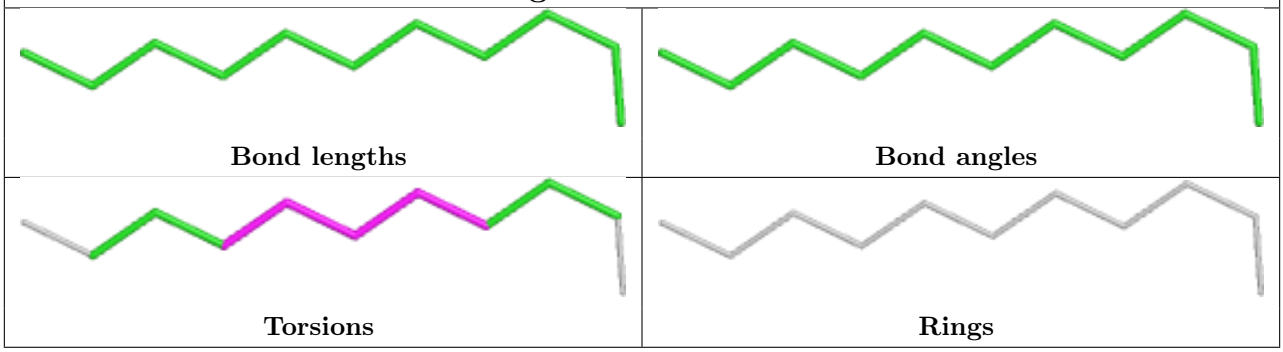
Bond angles

Torsions

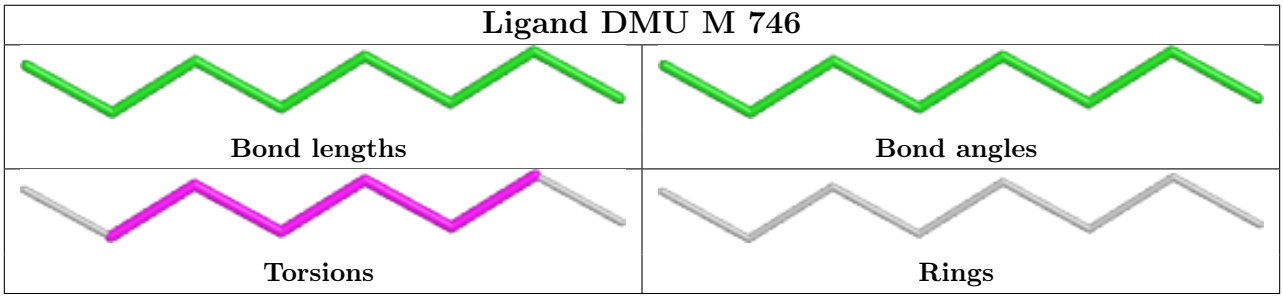


Rings

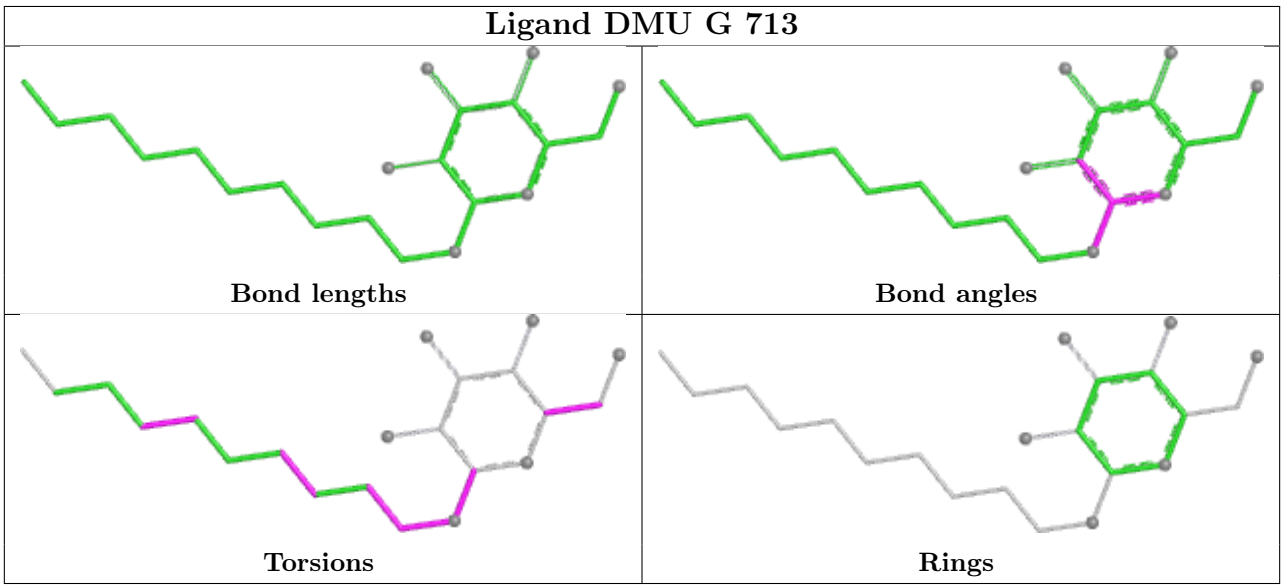
Ligand LFA T 622



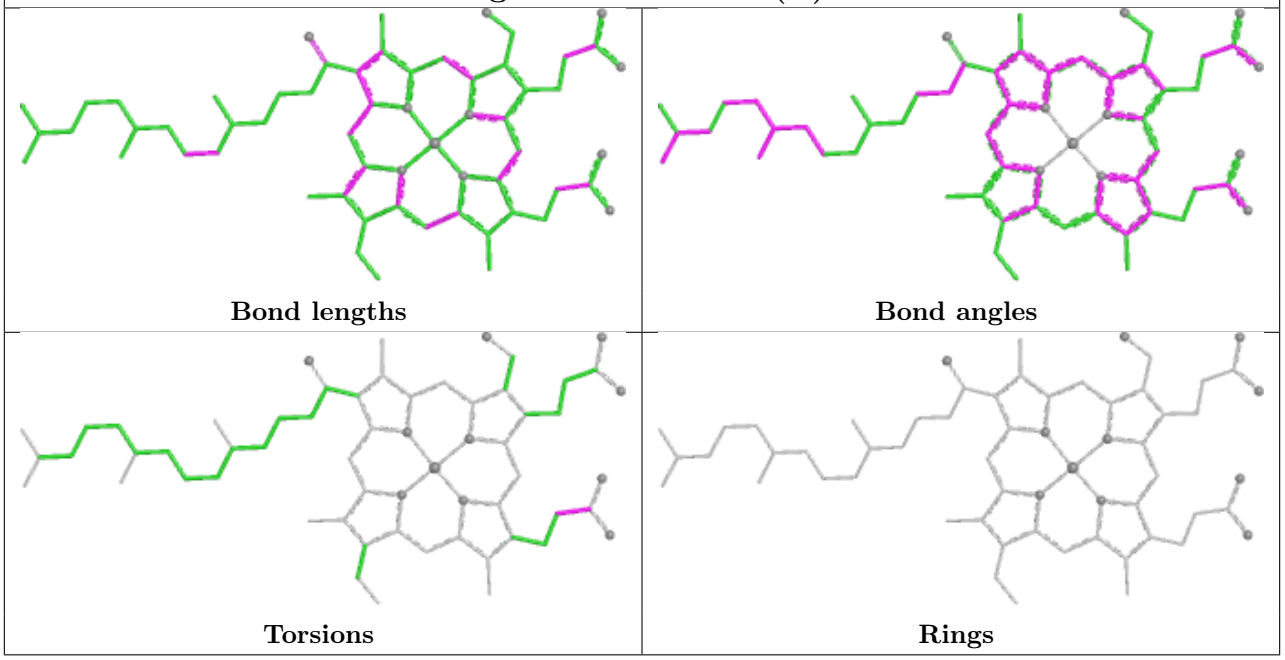
Ligand DMU M 746



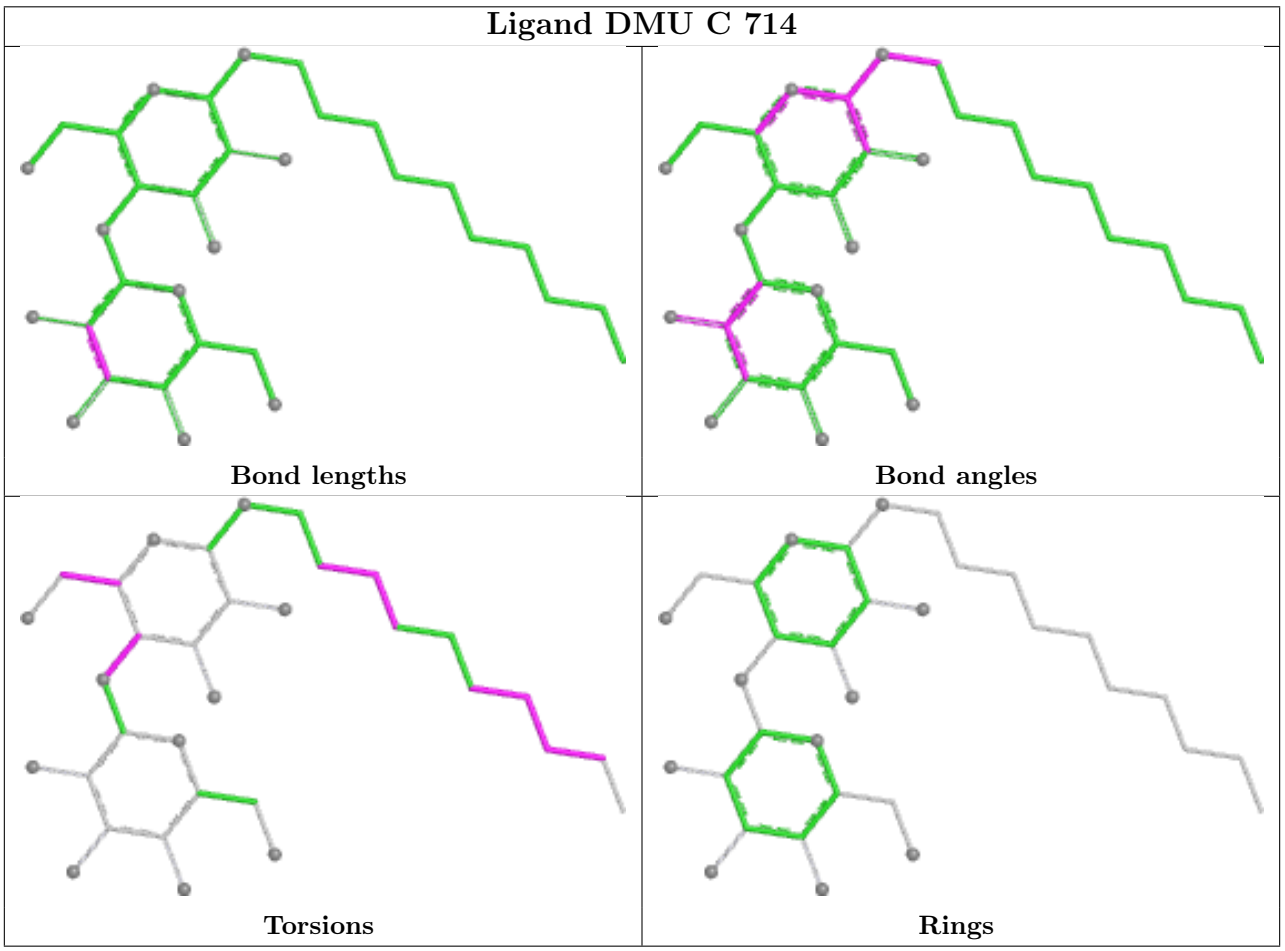
Ligand DMU G 713



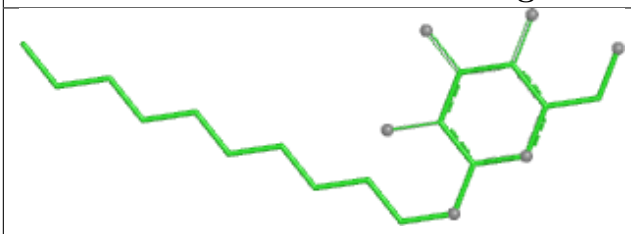
Ligand HEA N 515 (B)



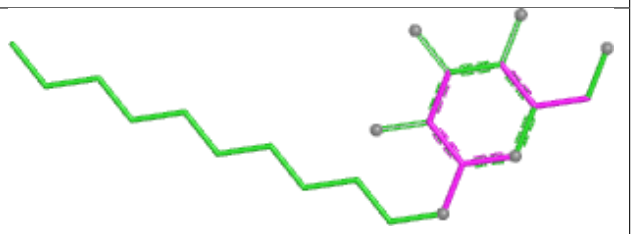
Ligand DMU C 714



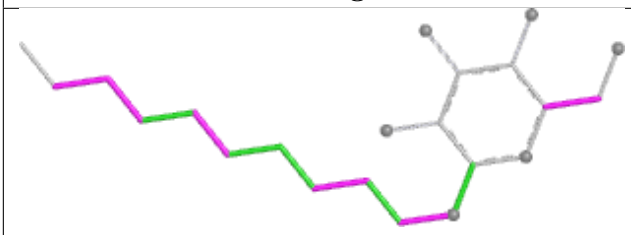
Ligand DMU T 711



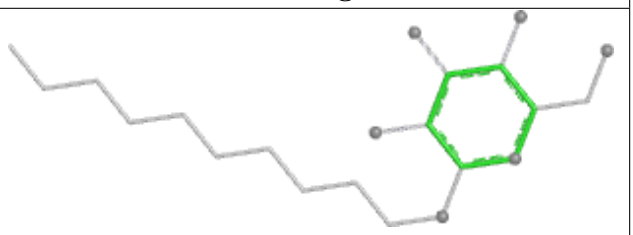
Bond lengths



Bond angles

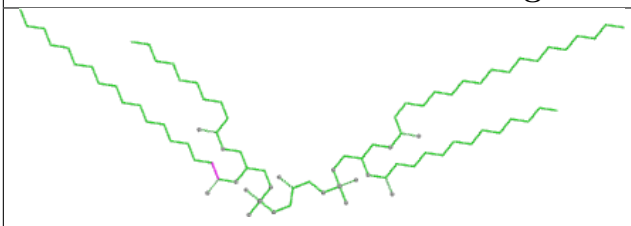


Torsions

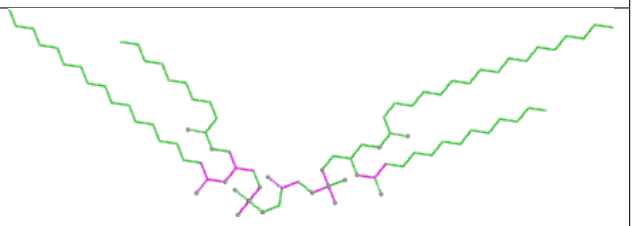


Rings

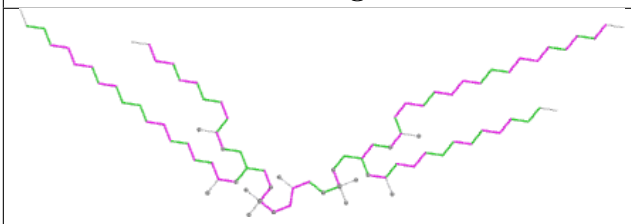
Ligand CDL C 270



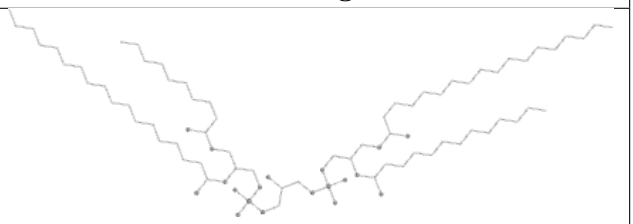
Bond lengths



Bond angles

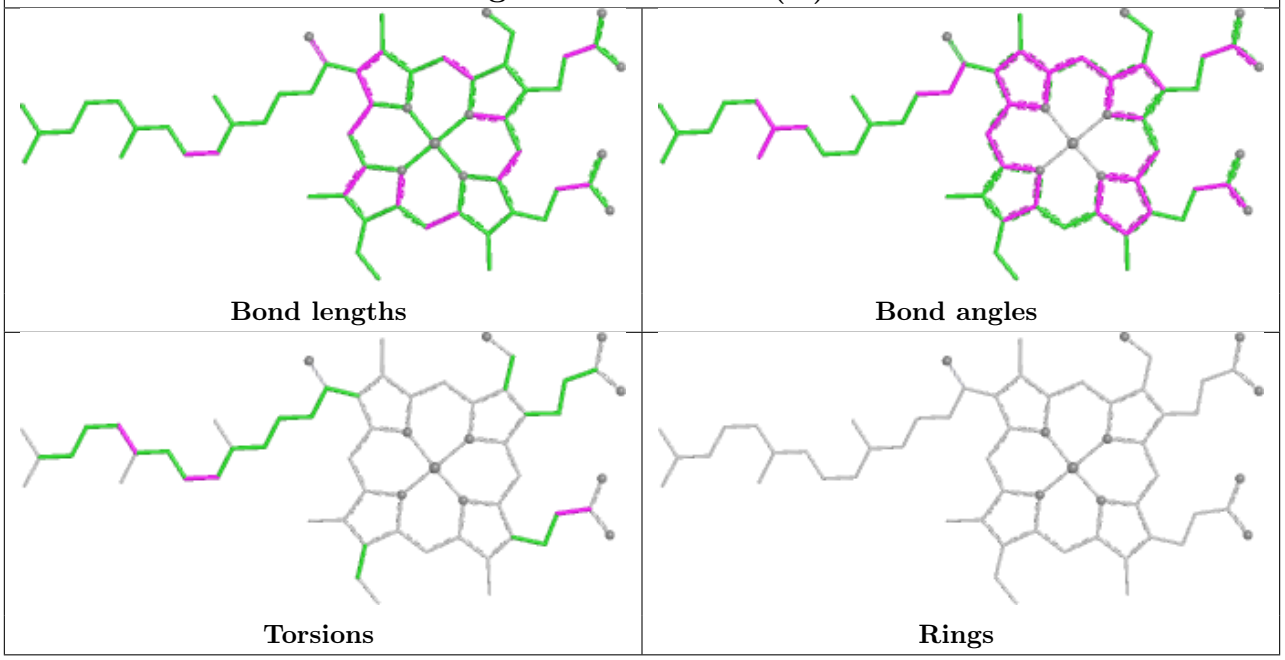


Torsions

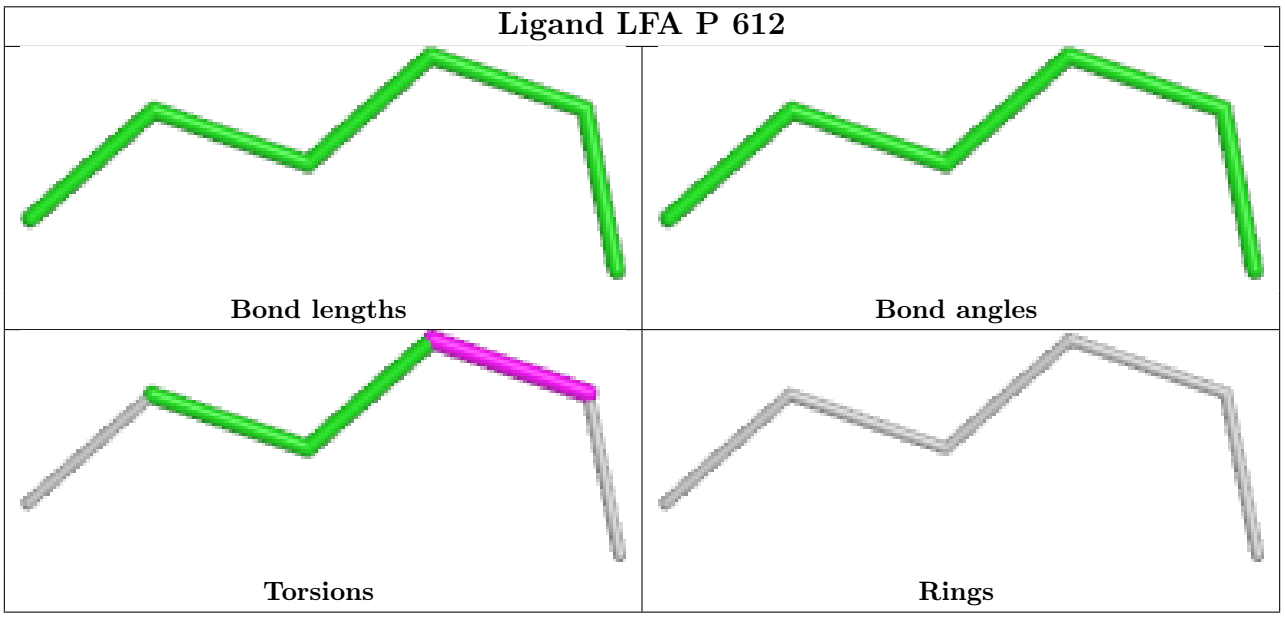


Rings

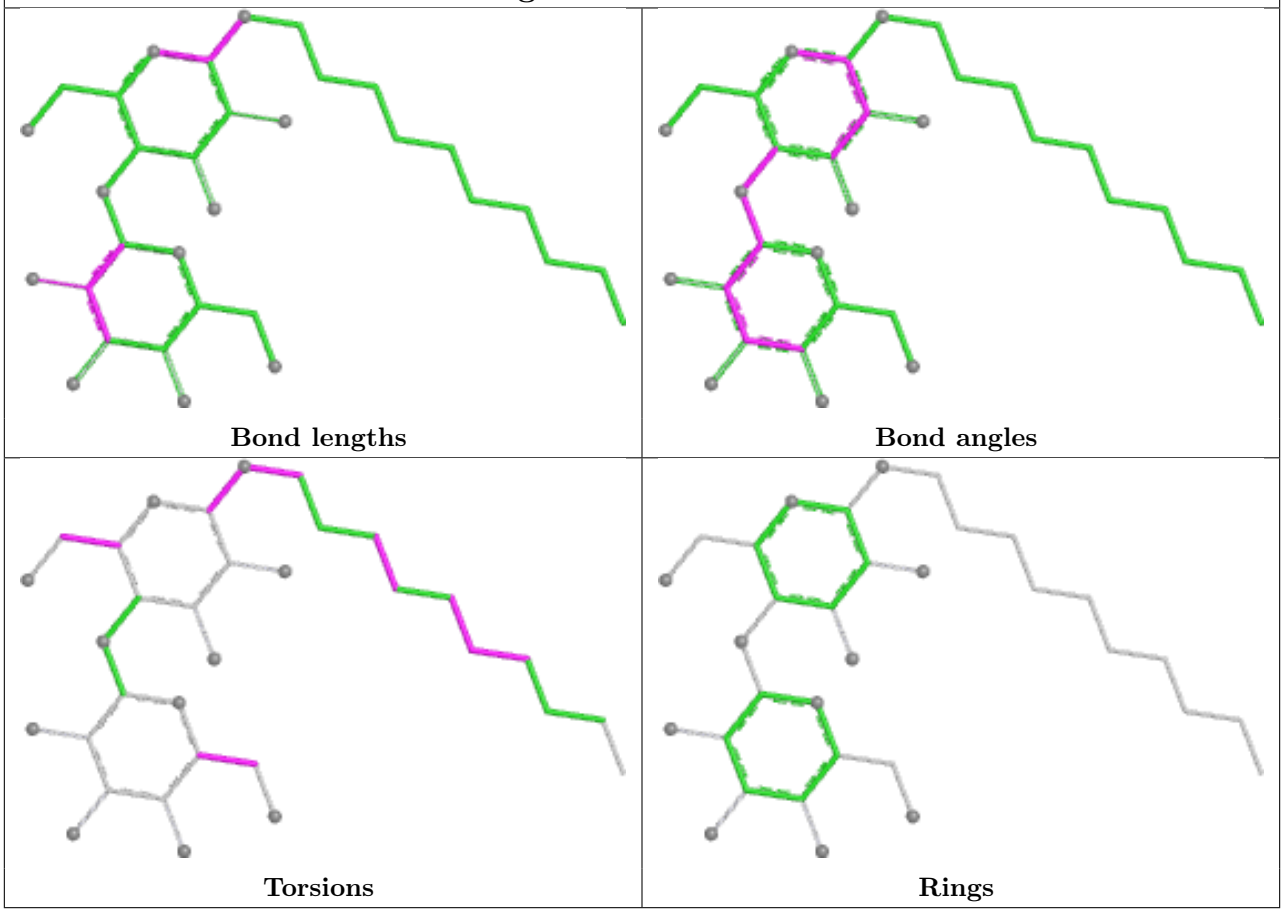
Ligand HEA N 515 (A)



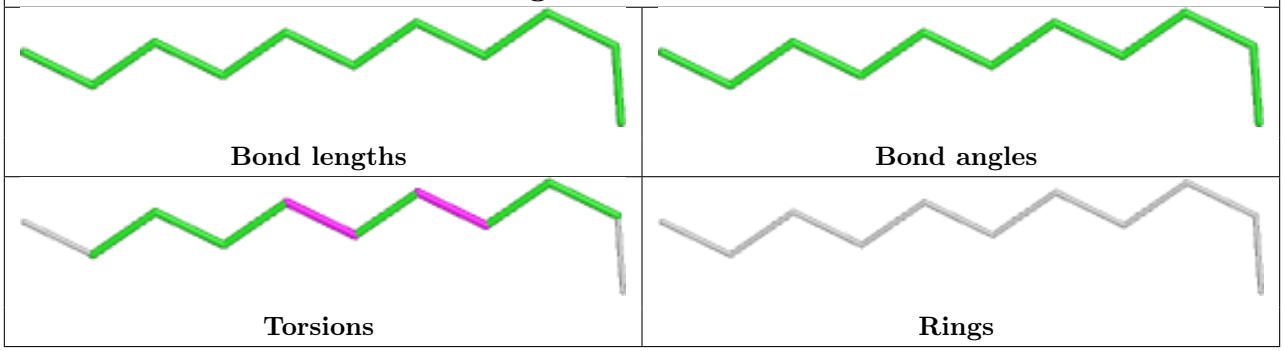
Ligand LFA P 612



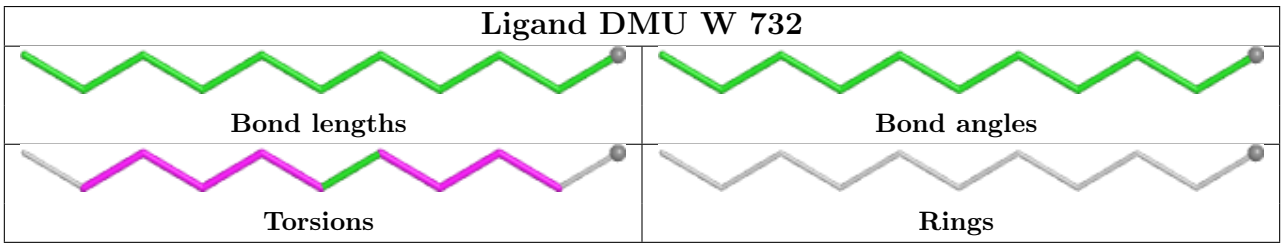
Ligand DMU C 733



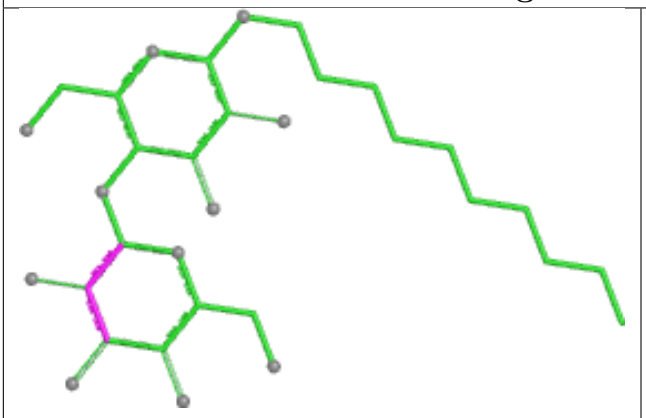
Ligand LFA C 615



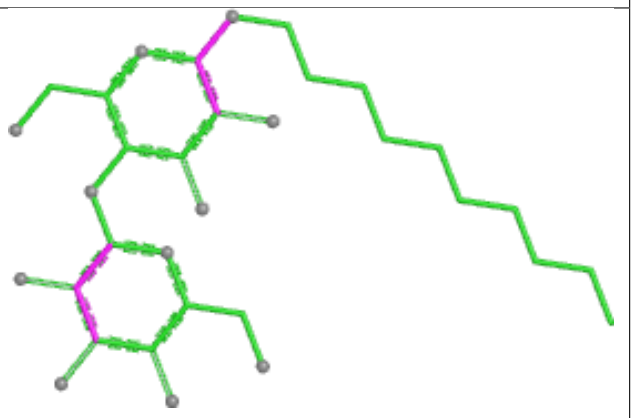
Ligand DMU W 732



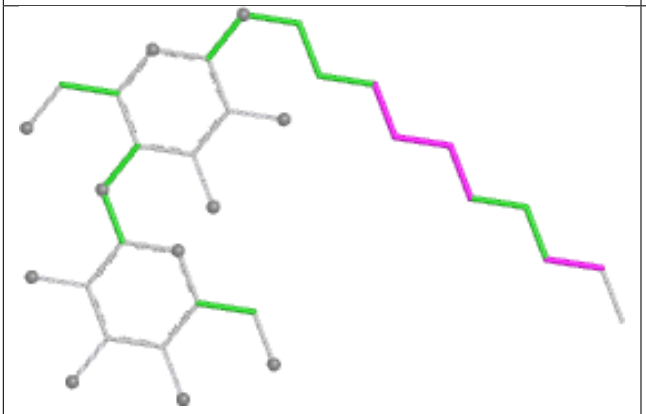
Ligand DMU A 526



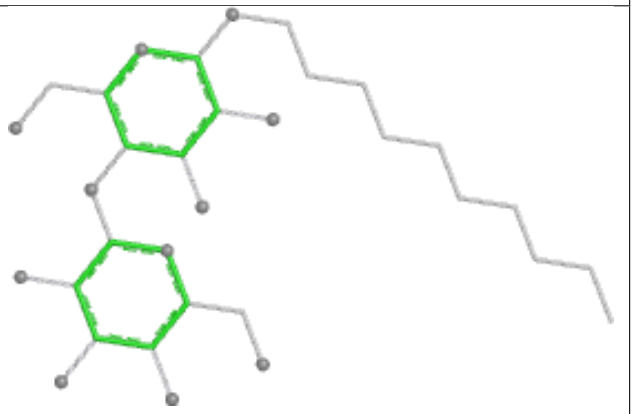
Bond lengths



Bond angles

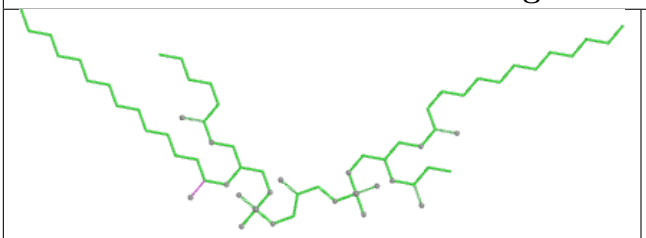


Torsions

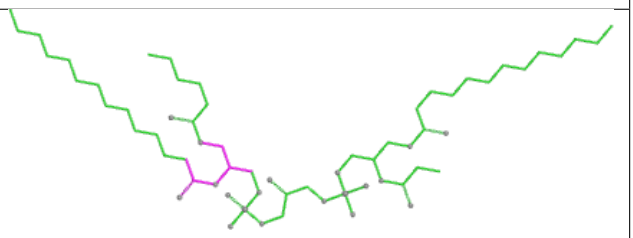


Rings

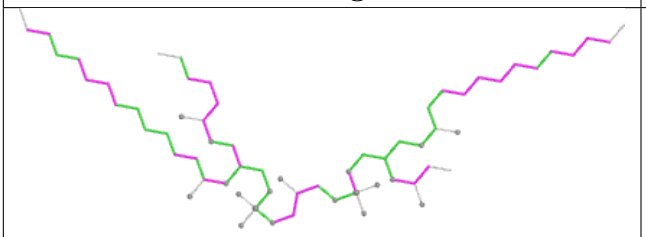
Ligand CDL N 522



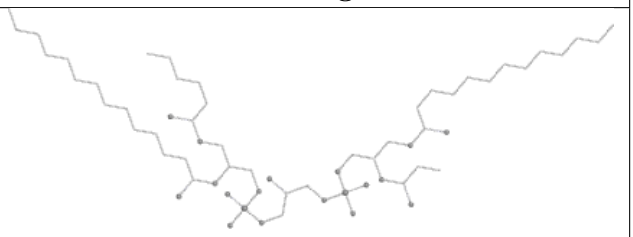
Bond lengths



Bond angles

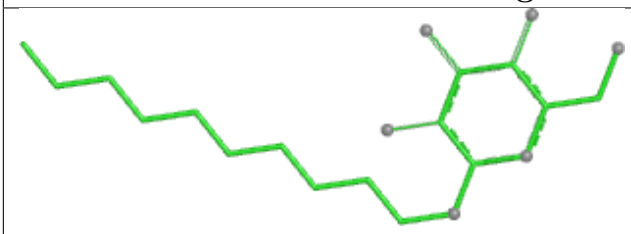


Torsions

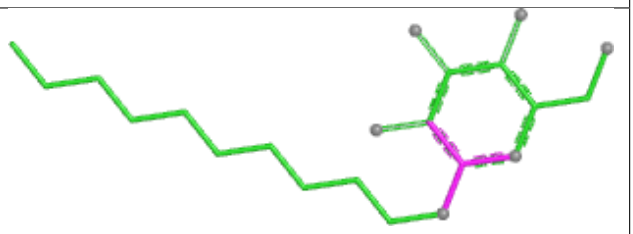


Rings

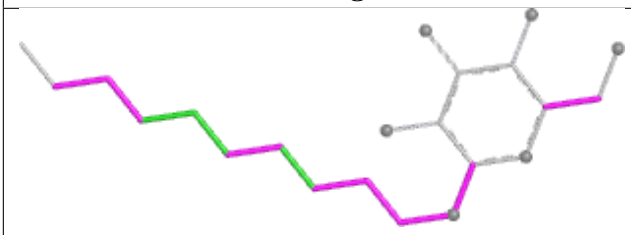
Ligand DMU Y 747



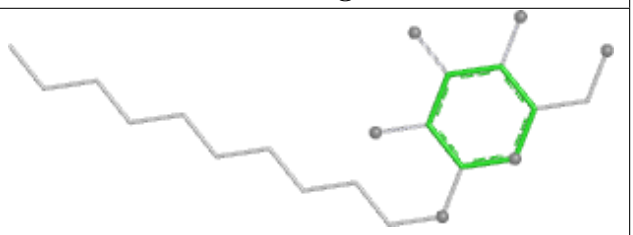
Bond lengths



Bond angles

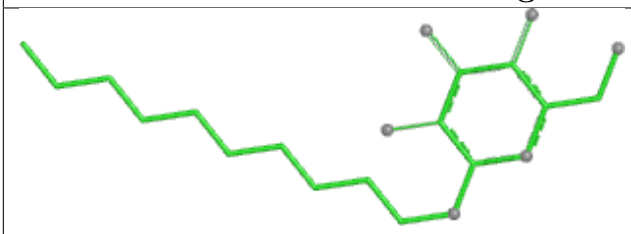


Torsions

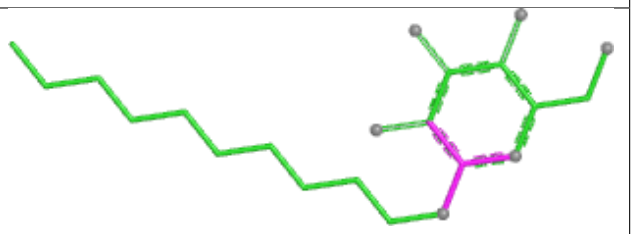


Rings

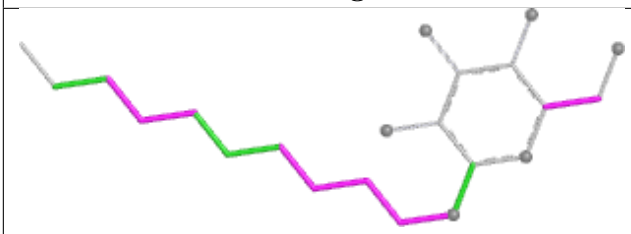
Ligand DMU P 722



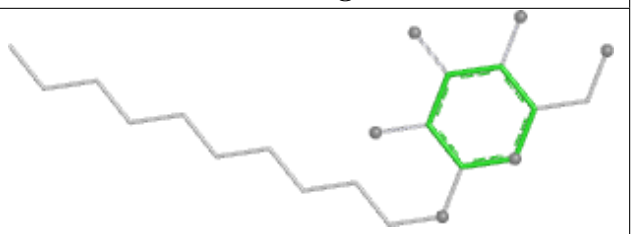
Bond lengths



Bond angles

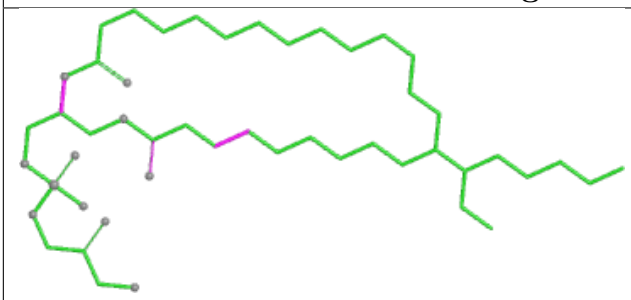


Torsions

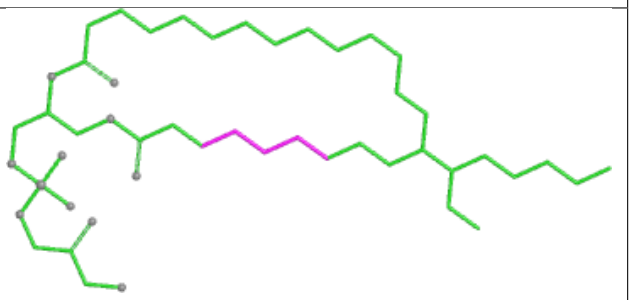


Rings

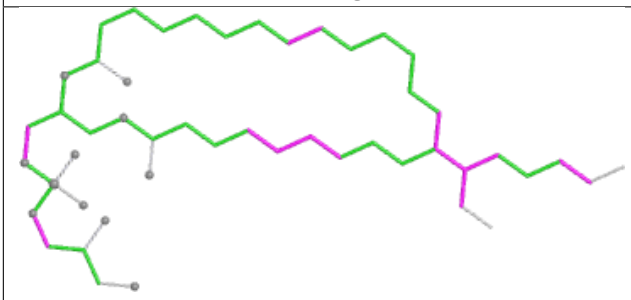
Ligand PGV C 267



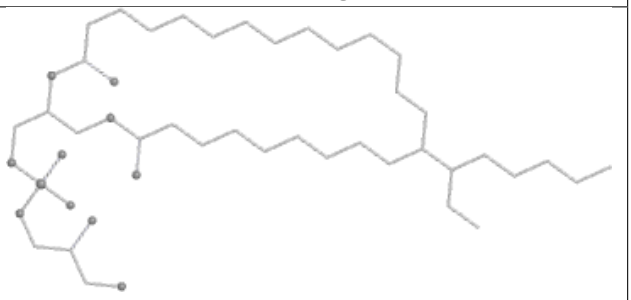
Bond lengths



Bond angles

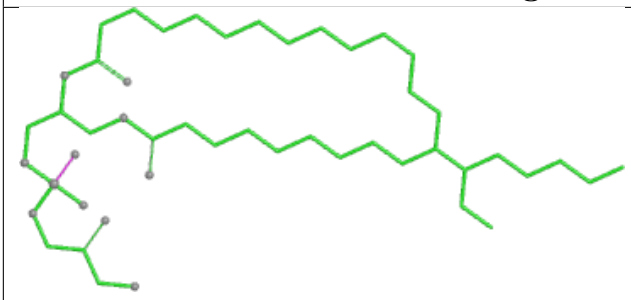


Torsions



Rings

Ligand PGV P 267



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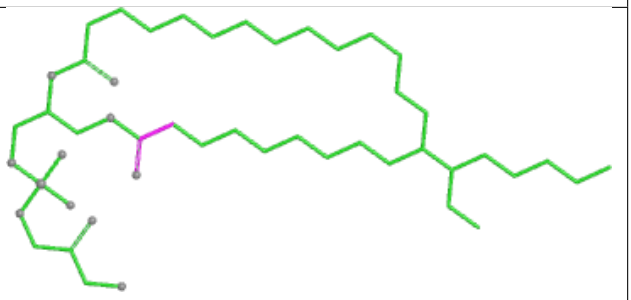
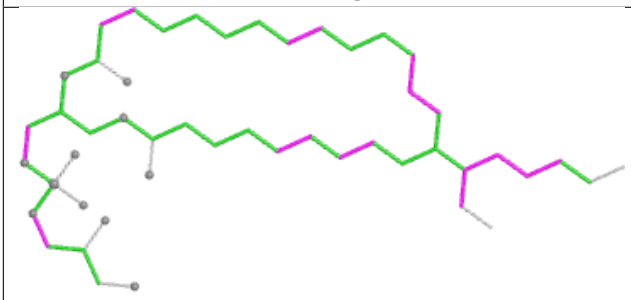
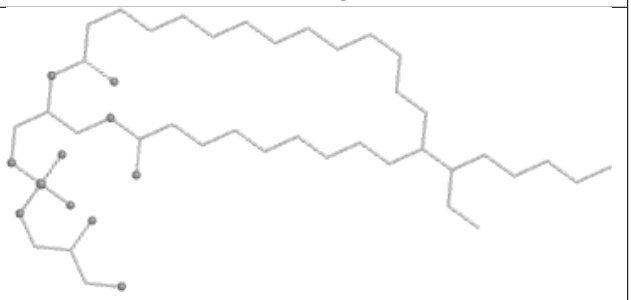


Bond angles

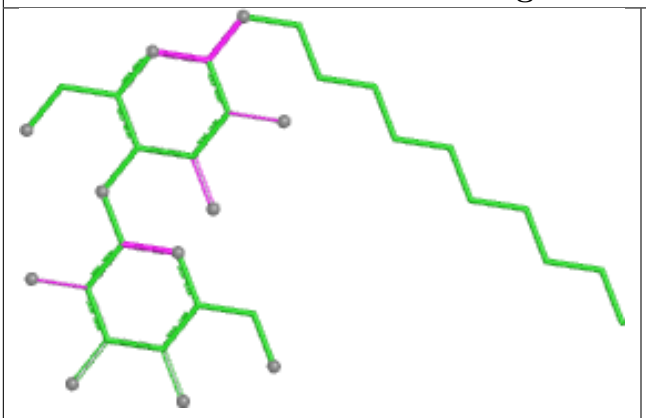


Torsions

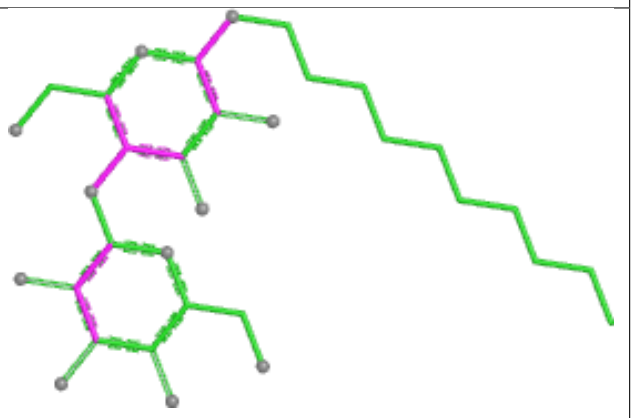


Rings

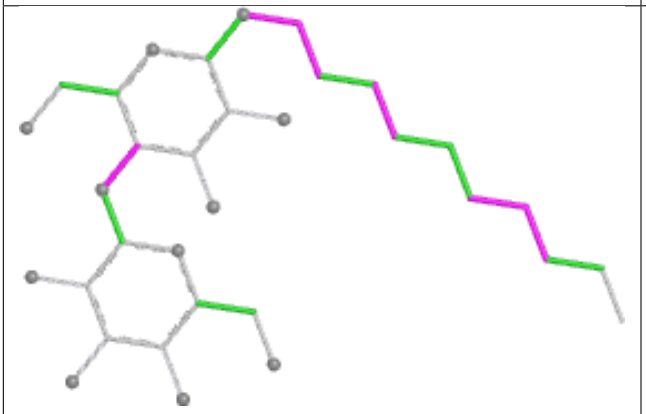
Ligand DMU A 744



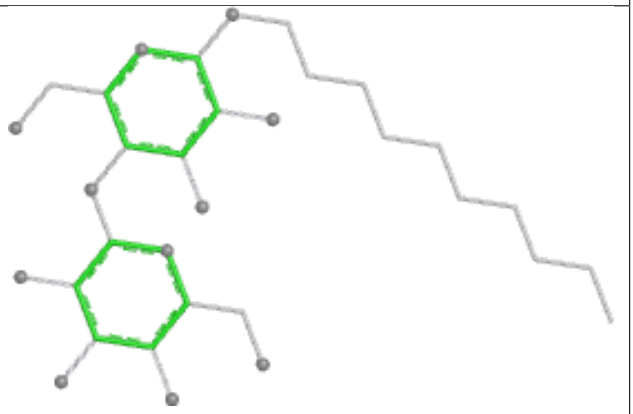
Bond lengths



Bond angles

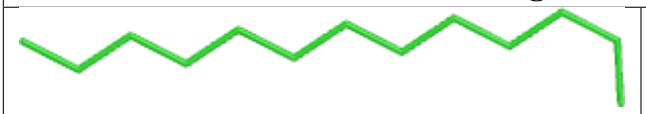


Torsions

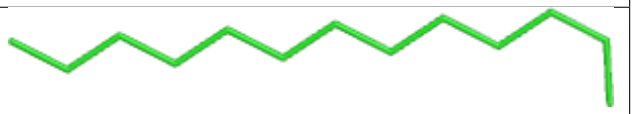


Rings

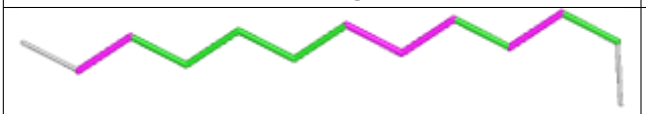
Ligand LFA C 626



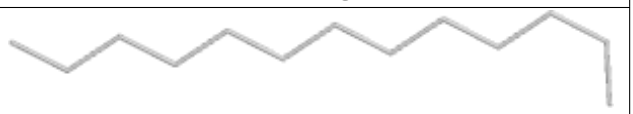
Bond lengths



Bond angles

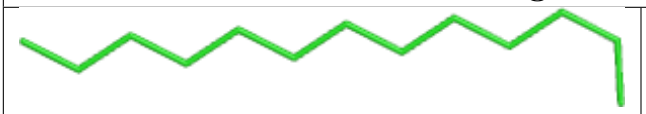


Torsions

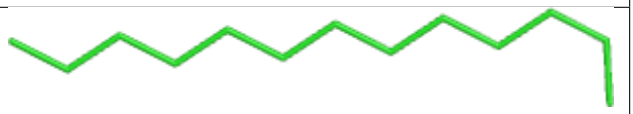


Rings

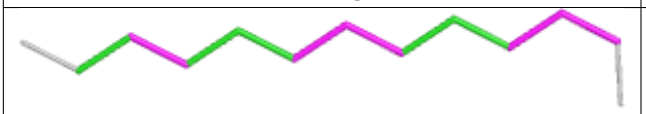
Ligand LFA P 626



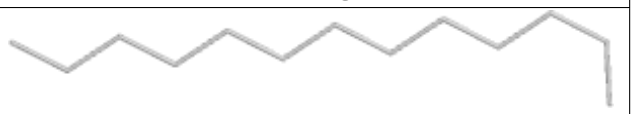
Bond lengths



Bond angles

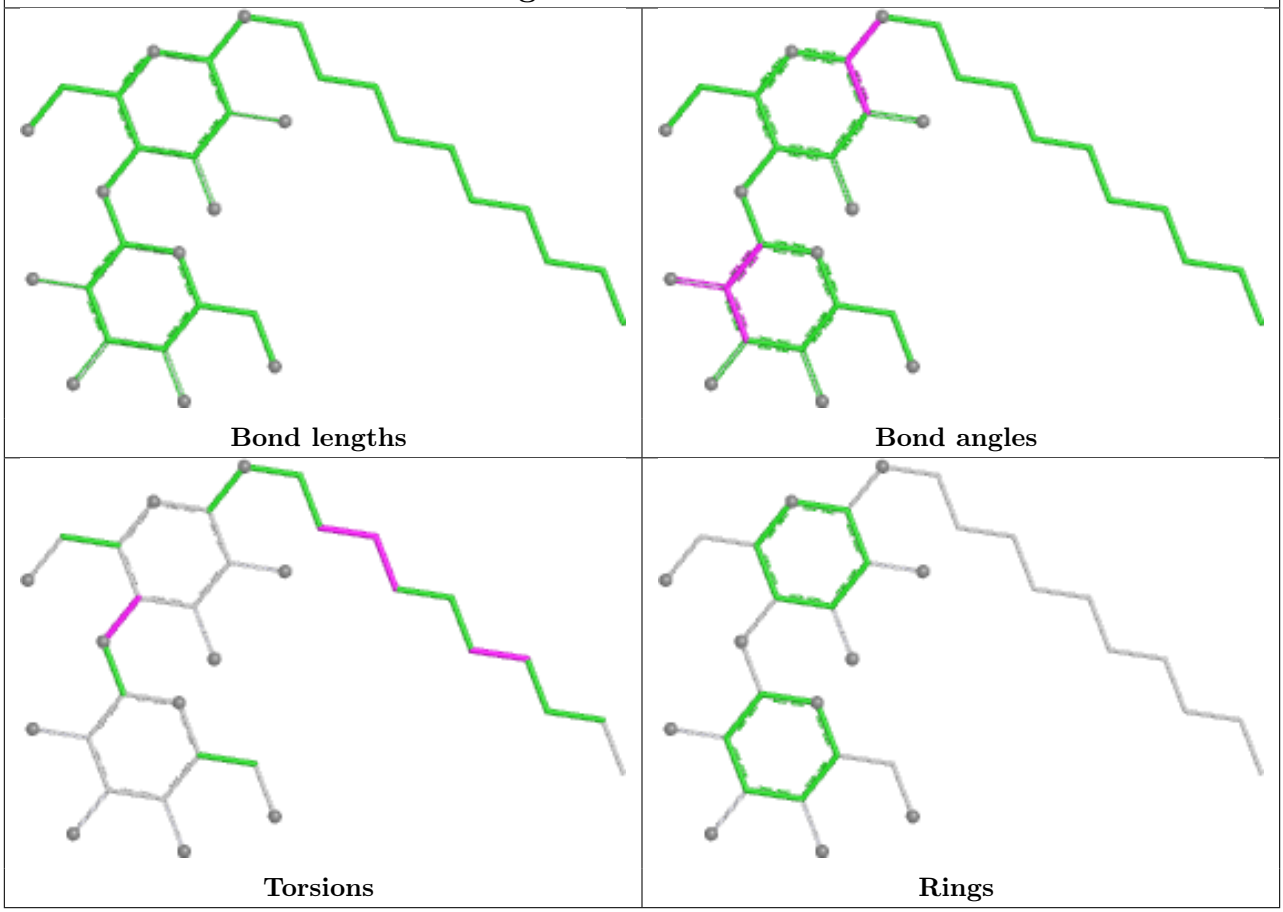


Torsions

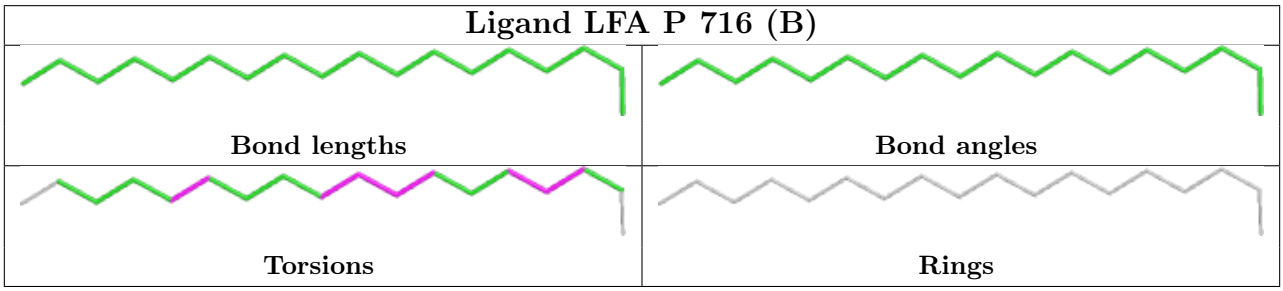


Rings

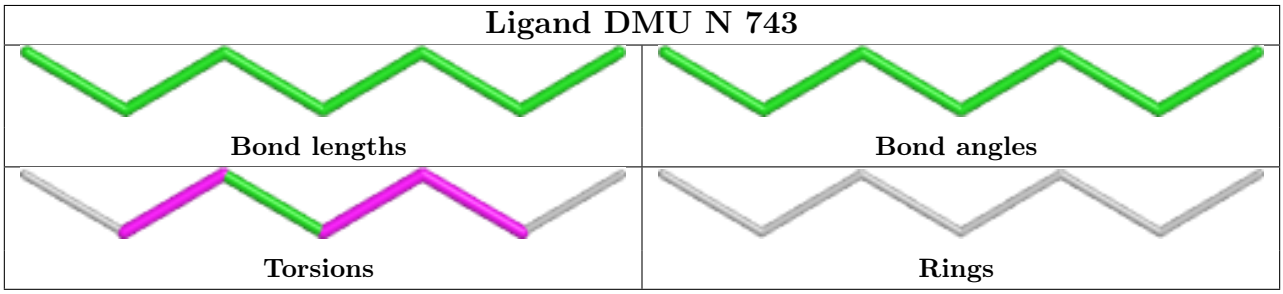
Ligand DMU P 714



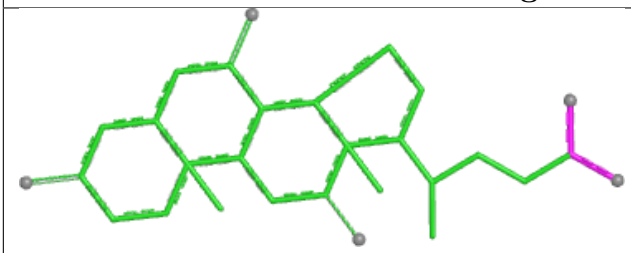
Ligand LFA P 716 (B)



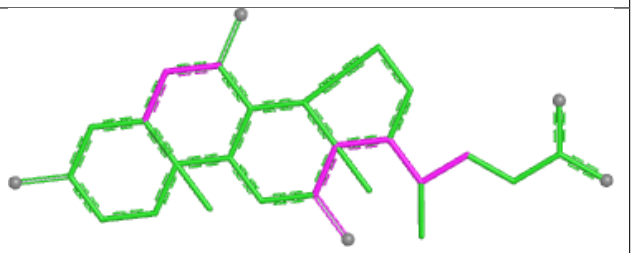
Ligand DMU N 743



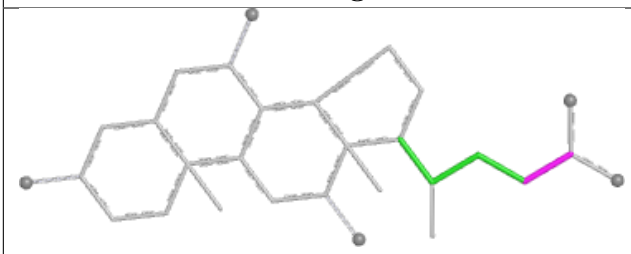
Ligand CHD A 525



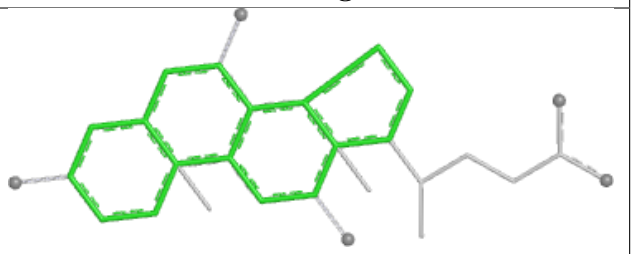
Bond lengths



Bond angles

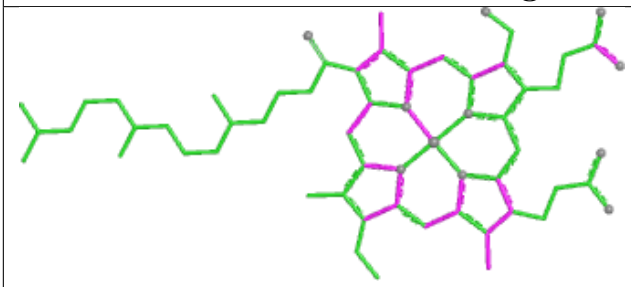


Torsions

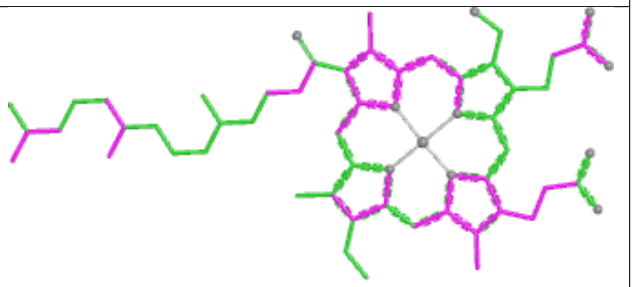


Rings

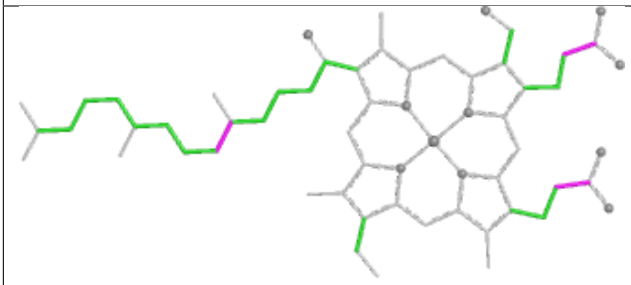
Ligand HEA N 516



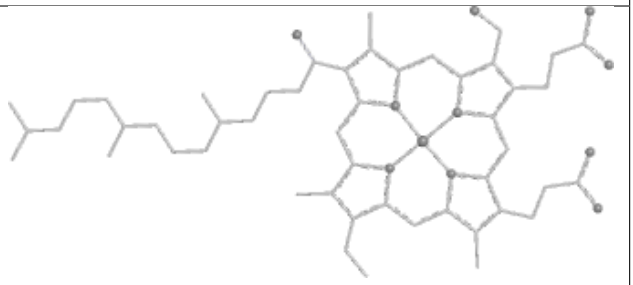
Bond lengths



Bond angles



Torsions



Rings

Ligand DMU C 721

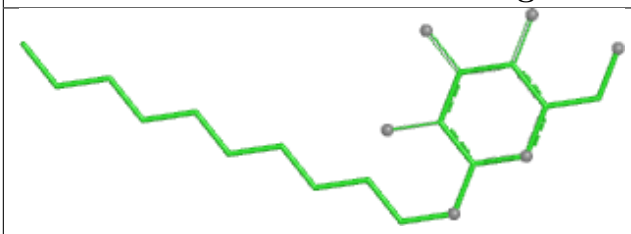
Bond lengths

Bond angles

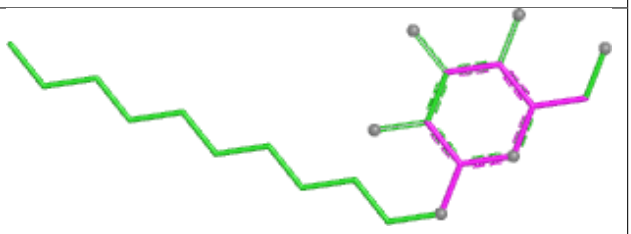
Torsions

Rings

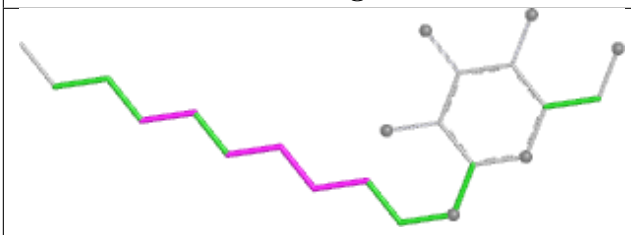
Ligand DMU T 713



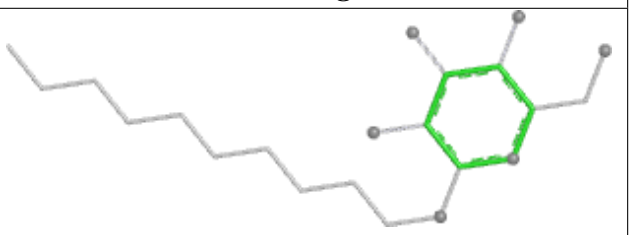
Bond lengths



Bond angles

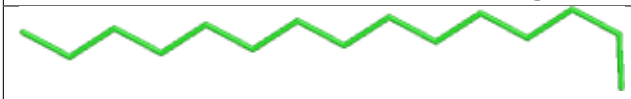


Torsions

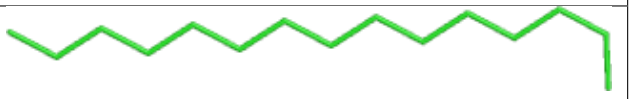


Rings

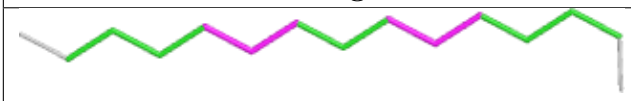
Ligand LFA P 625



Bond lengths



Bond angles



Torsions

Rings

Ligand DMU C 272

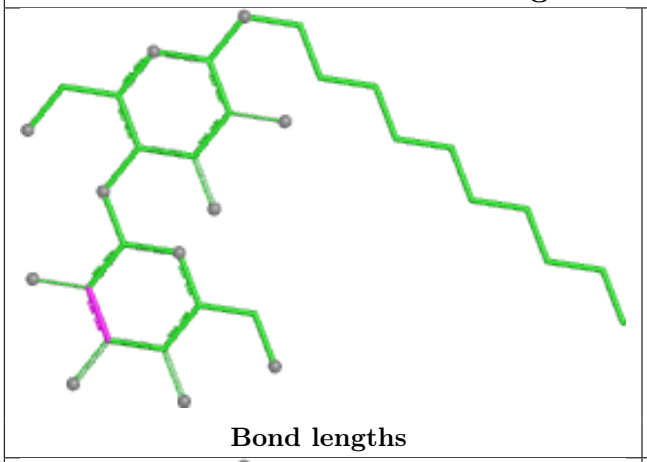
Bond lengths

Bond angles

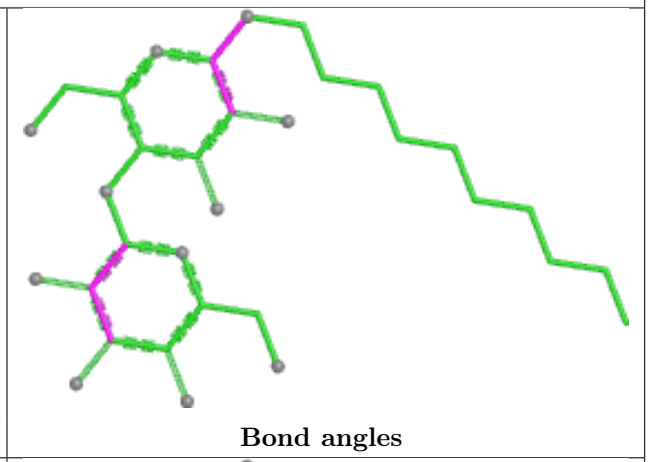
Torsions

Rings

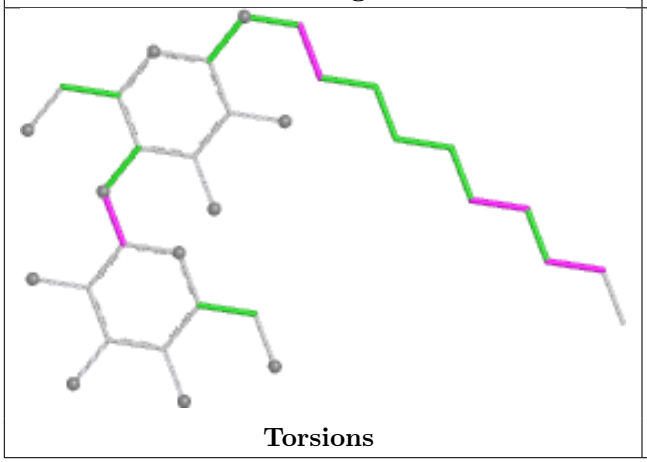
Ligand DMU J 61



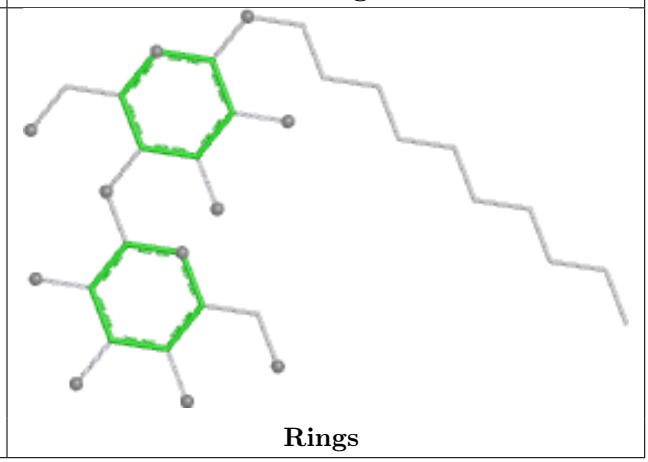
Bond lengths



Bond angles

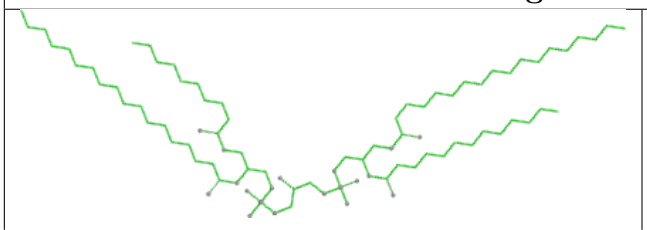


Torsions

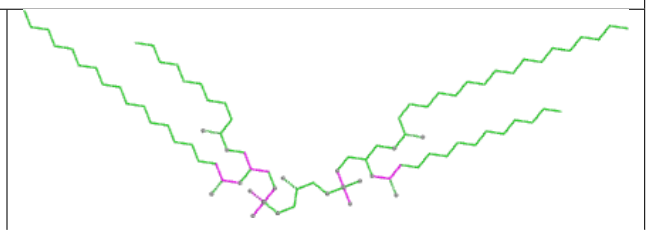


Rings

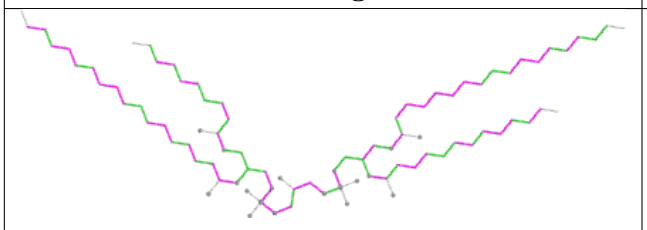
Ligand CDL P 270



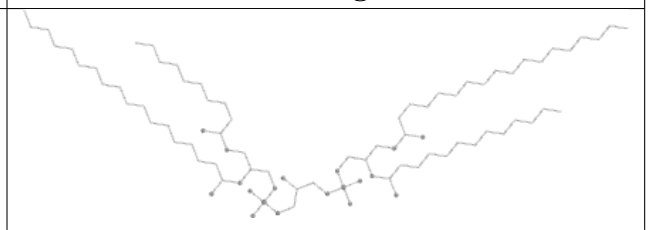
Bond lengths



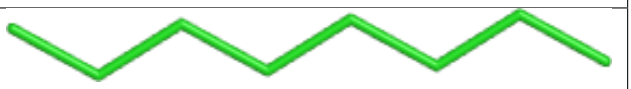
Bond angles



Torsions



Rings

Ligand DMU Z 746	
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	A	512/514 (99%)	-0.11	4 (0%) 82 86	9, 20, 27, 45	15 (2%)
1	N	512/514 (99%)	0.12	8 (1%) 70 74	10, 23, 32, 48	15 (2%)
2	B	226/227 (99%)	0.37	20 (8%) 15 17	14, 25, 47, 74	5 (2%)
2	O	226/227 (99%)	0.49	12 (5%) 32 37	16, 31, 57, 113	5 (2%)
3	C	258/261 (98%)	0.17	5 (1%) 66 70	10, 23, 34, 49	9 (3%)
3	P	258/261 (98%)	0.23	3 (1%) 76 80	10, 25, 37, 58	9 (3%)
4	D	143/147 (97%)	0.27	2 (1%) 73 77	13, 28, 42, 61	1 (0%)
4	Q	137/147 (93%)	0.90	17 (12%) 8 9	19, 41, 72, 88	1 (0%)
5	E	102/109 (93%)	0.15	2 (1%) 65 69	22, 28, 44, 60	0
5	R	102/109 (93%)	0.41	2 (1%) 65 69	26, 38, 54, 68	0
6	F	91/98 (92%)	0.29	3 (3%) 49 55	14, 29, 50, 59	2 (2%)
6	S	91/98 (92%)	0.49	3 (3%) 49 55	14, 28, 51, 57	2 (2%)
7	G	72/85 (84%)	0.71	8 (11%) 10 11	15, 30, 76, 94	1 (1%)
7	T	72/85 (84%)	0.81	8 (11%) 10 11	16, 34, 77, 99	1 (1%)
8	H	75/85 (88%)	0.71	9 (12%) 9 10	23, 32, 79, 107	0
8	U	75/85 (88%)	0.77	10 (13%) 7 8	28, 36, 79, 101	0
9	I	70/73 (95%)	0.88	10 (14%) 6 6	26, 38, 63, 85	0
9	V	70/73 (95%)	1.00	8 (11%) 10 11	25, 46, 64, 94	0
10	J	56/59 (94%)	0.66	6 (10%) 11 12	25, 34, 61, 67	0
10	W	56/59 (94%)	0.99	6 (10%) 11 12	27, 38, 58, 81	0
11	K	49/56 (87%)	0.66	2 (4%) 41 47	26, 33, 49, 59	0
11	X	49/56 (87%)	1.15	6 (12%) 8 9	33, 43, 69, 81	0
12	L	44/47 (93%)	0.27	3 (6%) 23 27	21, 25, 38, 57	0
12	Y	44/47 (93%)	0.63	1 (2%) 61 66	27, 33, 50, 58	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	M	40/46 (86%)	0.42	2 (5%) 34 39	21, 25, 46, 63	0
13	Z	40/46 (86%)	0.86	5 (12%) 8 9	30, 37, 69, 71	0
All	All	3470/3614 (96%)	0.35	165 (4%) 35 41	9, 27, 54, 113	66 (1%)

All (165) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	T	36	TRP	9.1
7	G	36	TRP	6.8
2	O	227	LEU	6.6
6	S	93	PRO	6.6
10	W	1	PHE	6.2
6	S	3	GLY	5.9
2	B	65	TRP	5.8
2	O	113	TYR	5.6
4	Q	35	ALA	5.4
8	H	45	ALA	5.4
1	N	113[A]	LEU	5.3
9	V	37	PHE	5.2
11	X	6	ALA	5.1
9	I	37	PHE	5.0
9	V	3	ALA	4.9
8	U	52	VAL	4.8
2	O	90	ILE	4.8
2	B	110	TYR	4.6
8	H	46	LYS	4.5
1	A	113[A]	LEU	4.5
1	N	136[A]	LEU	4.5
10	J	1	PHE	4.5
2	B	59	GLN	4.5
3	P	37	PHE	4.5
6	F	3	GLY	4.3
9	I	3	ALA	4.2
2	B	61	VAL	4.2
4	D	5	VAL	4.2
8	U	47	GLY	4.2
4	D	4	SER	4.2
3	C	258	TRP	4.2
7	T	38	HIS	4.1
2	O	32[A]	PHE	4.1
10	W	52	TRP	4.1

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Mol	Chain	Res	Type	RSRZ
11	X	13	TYR	4.0
8	U	45	ALA	4.0
4	Q	51	LEU	3.9
2	B	32[A]	PHE	3.9
2	O	91	ASN	3.9
10	W	48	TYR	3.9
9	I	25	PHE	3.8
5	R	7	THR	3.7
11	K	6	ALA	3.7
8	U	48	GLY	3.7
7	G	37	LEU	3.6
2	B	90	ILE	3.6
9	V	72	ALA	3.5
13	M	40	TYR	3.5
7	G	30	LEU	3.5
8	H	11	TYR	3.5
7	T	30	LEU	3.4
5	E	39	TYR	3.4
7	G	33	LEU	3.4
8	H	48	GLY	3.4
4	Q	10	ASP	3.3
3	C	38	ASN	3.3
3	P	258	TRP	3.3
2	B	55	THR	3.3
10	W	55	PHE	3.3
5	R	108	LYS	3.3
8	H	51	SER	3.2
4	Q	39	ALA	3.2
9	V	36	LYS	3.2
11	K	47	ARG	3.1
7	T	37	LEU	3.1
2	B	113	TYR	3.1
11	X	54	ARG	3.1
4	Q	131	ILE	3.1
12	L	45	LEU	3.1
5	E	7	THR	3.1
3	C	260	GLY	3.0
12	L	46	LYS	3.0
2	B	58	ALA	3.0
4	Q	17[A]	VAL	3.0
1	A	189	MET	3.0
7	G	40	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	16[A]	ILE	3.0
8	U	46	LYS	3.0
9	I	29	LEU	3.0
11	X	7	PRO	2.9
1	N	483	LEU	2.9
13	Z	1	ILE	2.9
12	Y	24	MET	2.9
13	Z	40	TYR	2.8
10	J	52	TRP	2.8
10	J	56	PRO	2.8
8	H	47	GLY	2.8
8	H	50	VAL	2.8
9	I	19	PHE	2.8
7	G	45	PRO	2.8
2	B	91	ASN	2.7
10	W	27	THR	2.7
2	B	60	GLU	2.7
7	T	39	SER	2.7
2	O	16[A]	ILE	2.7
2	B	115	ASP	2.7
4	Q	52	SER	2.7
1	A	311[A]	ILE	2.6
7	T	40	GLY	2.6
9	V	8	GLN	2.6
1	N	513	LEU	2.6
7	G	42	ARG	2.6
7	G	41	HIS	2.6
7	T	33	LEU	2.6
8	U	49	ASP	2.6
10	J	55	PHE	2.6
13	Z	39	ASN	2.6
13	M	32	TRP	2.5
9	V	25	PHE	2.5
8	U	85	ILE	2.5
13	Z	13	LYS	2.5
7	T	42	ARG	2.5
3	C	102	TYR	2.5
8	U	50	VAL	2.5
2	B	86	MET	2.5
1	A	513	LEU	2.4
4	Q	57	VAL	2.4
9	V	34	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
2	O	22[A]	HIS	2.4
2	O	115	ASP	2.4
1	N	311[A]	ILE	2.3
13	Z	32	TRP	2.3
8	H	43	MET	2.3
1	N	334	TRP	2.3
2	B	57	ASP	2.3
4	Q	74	SER	2.3
4	Q	19	ARG	2.3
11	X	47	ARG	2.3
8	H	44	THR	2.3
4	Q	87	PHE	2.3
9	I	34	PHE	2.3
1	N	35	LEU	2.3
4	Q	27	VAL	2.3
4	Q	73	ARG	2.2
8	U	44	THR	2.2
10	J	27	THR	2.2
3	C	259	TRP	2.2
10	J	48	TYR	2.2
4	Q	117	ALA	2.2
2	B	56	MET	2.2
4	Q	33	LEU	2.2
9	I	72	ALA	2.2
2	O	217	LYS	2.2
4	Q	72	ASN	2.2
4	Q	11	TYR	2.1
6	F	87[A]	THR	2.1
8	U	42	ALA	2.1
10	W	56	PRO	2.1
6	S	19	GLU	2.1
2	O	87[A]	MET	2.1
9	I	26	MET	2.1
2	B	131	GLY	2.1
3	P	259	TRP	2.1
6	F	53	THR	2.1
9	I	31	PHE	2.1
9	V	33	THR	2.1
1	N	49	GLY	2.1
12	L	24	MET	2.1
2	B	40	TYR	2.1
2	O	60	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	22[A]	HIS	2.0
9	I	32	ALA	2.0
2	B	67	ILE	2.0
2	O	86	MET	2.0
11	X	34	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
2	FME	B	1	10/11	0.94	0.15	21,34,59,119	0
1	FME	A	1	10/11	0.95	0.12	32,41,68,95	0
1	FME	N	1	10/11	0.95	0.12	35,41,72,79	0
2	FME	O	1	10/11	0.96	0.09	28,32,40,54	0

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
20	DMU	C	722	22/33	0.66	0.40	32,56,76,90	22
20	DMU	P	722	22/33	0.68	0.38	31,63,73,87	22
22	LFA	P	615	11/20	0.68	0.49	52,57,67,74	11
22	LFA	C	626	13/20	0.73	0.31	41,45,51,54	13
23	EDO	C	807	4/4	0.74	0.41	42,45,46,60	4
19	CHD	P	271	29/29	0.76	0.20	48,66,110,128	0
22	LFA	P	716[B]	18/20	0.77	0.28	37,49,60,62	18
22	LFA	P	624	11/20	0.77	0.41	42,47,54,60	11
22	LFA	P	623	14/20	0.78	0.41	32,53,60,63	14

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	LFA	C	615	11/20	0.78	0.45	45,55,74,75	11
20	DMU	G	711	22/33	0.78	0.33	42,56,77,88	22
20	DMU	P	733	33/33	0.78	0.38	40,50,59,68	33
22	LFA	P	614	15/20	0.79	0.41	40,46,58,59	15
20	DMU	T	711	22/33	0.79	0.33	43,53,69,80	22
22	LFA	C	612	6/20	0.79	0.44	39,43,45,49	6
20	DMU	B	741	11/33	0.79	0.33	49,56,63,66	11
22	LFA	C	623	14/20	0.79	0.38	34,48,54,55	14
20	DMU	P	714	33/33	0.79	0.33	34,42,59,78	33
22	LFA	C	614	15/20	0.80	0.38	38,46,57,58	15
20	DMU	C	733	33/33	0.80	0.38	38,48,60,65	33
20	DMU	W	732	11/33	0.80	0.40	49,54,59,70	11
22	LFA	C	625	15/20	0.80	0.28	33,41,54,57	15
20	DMU	P	734	33/33	0.80	0.31	48,60,72,80	33
22	LFA	T	622	11/20	0.80	0.36	41,54,62,65	11
22	LFA	G	622	11/20	0.80	0.34	39,51,56,60	11
23	EDO	E	811	4/4	0.80	0.31	29,31,33,35	4
20	DMU	C	714	33/33	0.81	0.33	33,39,57,61	33
20	DMU	N	744	33/33	0.81	0.24	28,43,59,67	33
22	LFA	C	624	11/20	0.81	0.37	37,48,53,54	11
23	EDO	C	827	4/4	0.81	0.28	23,26,27,29	4
22	LFA	P	611	11/20	0.81	0.33	28,39,44,46	11
22	LFA	C	716[B]	18/20	0.82	0.29	34,49,89,90	18
22	LFA	P	626	13/20	0.82	0.32	38,50,62,64	13
20	DMU	C	734	33/33	0.82	0.27	38,54,63,66	33
20	DMU	W	61	33/33	0.82	0.22	36,48,77,81	33
22	LFA	A	628	14/20	0.82	0.29	33,41,48,51	14
19	CHD	C	271	29/29	0.82	0.17	44,58,76,95	0
20	DMU	J	732	11/33	0.82	0.41	47,50,57,68	11
20	DMU	T	712	11/33	0.83	0.36	45,52,60,60	11
20	DMU	J	61	33/33	0.83	0.20	33,43,65,71	33
20	DMU	N	743	7/33	0.83	0.34	45,49,56,57	7
20	DMU	A	743	7/33	0.83	0.34	42,46,50,53	7
20	DMU	N	745	33/33	0.83	0.28	33,46,72,87	33
20	DMU	O	742	22/33	0.83	0.26	33,38,44,48	22
22	LFA	A	627	14/20	0.84	0.28	28,38,66,70	14
22	LFA	G	621	17/20	0.84	0.29	29,53,64,64	17
23	EDO	N	801	4/4	0.84	0.17	17,17,19,23	4
23	EDO	P	827	4/4	0.84	0.25	23,24,30,32	4
23	EDO	A	801	4/4	0.85	0.14	17,18,20,22	4
22	LFA	P	625	15/20	0.85	0.22	35,41,61,63	15
23	EDO	C	809	4/4	0.85	0.17	22,23,29,32	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
20	DMU	Y	747	22/33	0.85	0.38	35,55,76,79	22
20	DMU	O	731	11/33	0.85	0.38	46,48,52,67	11
22	LFA	T	621	17/20	0.85	0.31	34,49,66,69	17
18	CDL	P	270	87/100	0.85	0.21	34,78,126,150	0
20	DMU	C	715[A]	33/33	0.86	0.23	26,35,43,61	33
20	DMU	G	713	22/33	0.86	0.30	41,52,58,61	22
18	CDL	C	270	87/100	0.86	0.20	34,82,121,135	0
20	DMU	B	742	22/33	0.86	0.25	34,48,57,69	22
18	CDL	N	522	64/100	0.86	0.18	46,82,132,158	0
20	DMU	P	715[A]	33/33	0.86	0.23	27,37,49,61	33
20	DMU	P	721	7/33	0.86	0.37	43,53,63,70	7
22	LFA	P	612	6/20	0.86	0.33	39,40,41,44	6
20	DMU	T	713	22/33	0.87	0.27	37,48,54,59	22
20	DMU	G	712	11/33	0.87	0.33	35,46,52,65	11
20	DMU	A	745	33/33	0.87	0.21	24,32,44,57	33
23	EDO	A	803	4/4	0.87	0.23	23,29,37,39	4
20	DMU	C	721	7/33	0.87	0.32	45,49,53,64	7
18	CDL	N	521	94/100	0.87	0.19	37,83,124,140	0
20	DMU	O	741	11/33	0.87	0.30	40,45,52,66	11
20	DMU	L	747	22/33	0.87	0.33	37,47,57,64	22
23	EDO	F	817	4/4	0.87	0.15	13,13,16,20	4
20	DMU	M	746	8/33	0.87	0.26	35,44,48,49	8
23	EDO	N	803	4/4	0.87	0.21	26,26,37,42	4
22	LFA	N	628	14/20	0.87	0.28	35,42,66,68	14
22	LFA	C	611	11/20	0.88	0.32	36,43,48,49	11
22	LFA	N	627	14/20	0.88	0.26	28,38,54,55	14
18	CDL	A	522	64/100	0.88	0.17	38,71,110,133	0
23	EDO	A	825	4/4	0.89	0.19	33,33,34,42	4
20	DMU	B	731	11/33	0.89	0.31	36,51,59,63	11
20	DMU	P	272	11/33	0.89	0.27	42,47,55,60	11
20	DMU	A	744	33/33	0.90	0.17	21,32,44,65	33
20	DMU	Z	746	8/33	0.90	0.26	44,47,52,56	8
23	EDO	P	807	4/4	0.90	0.23	47,48,50,59	4
18	CDL	A	521	94/100	0.90	0.17	28,71,121,139	0
20	DMU	C	272	11/33	0.91	0.23	45,51,57,68	11
23	EDO	F	819	4/4	0.91	0.14	22,22,27,29	4
23	EDO	S	817	4/4	0.91	0.11	13,14,16,19	4
23	EDO	N	829	4/4	0.92	0.14	27,30,31,33	4
20	DMU	N	526	33/33	0.92	0.11	41,49,61,72	0
23	EDO	R	815	4/4	0.93	0.17	38,39,42,43	4
23	EDO	P	809	4/4	0.93	0.15	27,28,28,36	4
23	EDO	G	821	4/4	0.94	0.12	23,24,29,30	4

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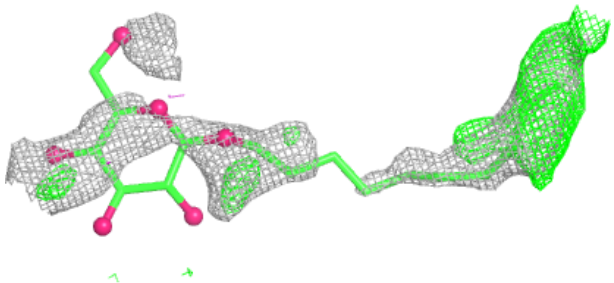
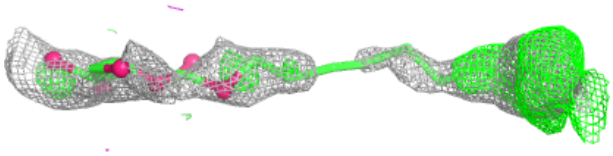
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	EDO	A	823	4/4	0.94	0.15	17,17,19,24	4
23	EDO	B	805	4/4	0.94	0.13	17,21,21,25	4
23	EDO	S	819	4/4	0.94	0.12	20,21,21,30	4
23	EDO	N	825	4/4	0.95	0.13	27,28,29,30	4
23	EDO	E	815	4/4	0.95	0.13	25,28,29,32	4
19	CHD	A	525	29/29	0.95	0.08	22,26,29,33	0
20	DMU	A	526	33/33	0.95	0.09	32,39,54,58	0
23	EDO	R	811	4/4	0.96	0.26	45,46,50,53	4
23	EDO	N	823	4/4	0.96	0.15	19,21,22,22	4
19	CHD	N	525	29/29	0.96	0.07	23,26,29,34	0
23	EDO	E	813	4/4	0.96	0.12	22,24,25,25	4
26	PEK	P	264	53/53	0.96	0.13	26,46,102,108	0
19	CHD	G	86	29/29	0.97	0.06	20,23,28,36	0
23	EDO	R	813	4/4	0.97	0.11	27,28,29,29	4
23	EDO	T	821	4/4	0.97	0.07	25,27,29,32	4
26	PEK	C	264	53/53	0.97	0.12	24,42,96,129	0
19	CHD	T	86	29/29	0.97	0.07	21,24,28,35	0
27	PGV	P	266	51/51	0.97	0.10	22,31,61,65	0
23	EDO	O	805	4/4	0.98	0.10	23,24,27,29	4
25	UNX	C	262	1/1	0.98	0.25	36,36,36,36	0
27	PGV	C	266	51/51	0.98	0.10	19,28,65,76	0
27	PGV	C	267	51/51	0.98	0.10	20,28,75,94	0
25	UNX	P	262	1/1	0.98	0.21	34,34,34,34	0
27	PGV	P	267	51/51	0.98	0.10	20,30,91,105	0
21	PER	N	520	2/2	0.99	0.12	19,19,19,26	0
14	HEA	A	515[A]	60/60	0.99	0.05	15,18,29,35	9
14	HEA	A	515[B]	60/60	0.99	0.05	15,18,29,34	9
14	HEA	A	516	60/60	0.99	0.05	15,17,23,26	0
14	HEA	N	515[A]	60/60	0.99	0.05	19,21,32,39	9
14	HEA	N	515[B]	60/60	0.99	0.05	19,21,29,33	9
14	HEA	N	516	60/60	0.99	0.05	18,19,25,28	0
21	PER	A	520	2/2	0.99	0.10	20,20,20,26	0
16	MG	N	518	1/1	1.00	0.02	23,23,23,23	0
17	NA	A	519	1/1	1.00	0.03	21,21,21,21	0
17	NA	N	519	1/1	1.00	0.02	28,28,28,28	0
15	CU	A	517	1/1	1.00	0.02	17,17,17,17	0
15	CU	N	517	1/1	1.00	0.02	20,20,20,20	0
16	MG	A	518	1/1	1.00	0.03	19,19,19,19	0
24	CUA	B	228	2/2	1.00	0.01	19,19,19,19	0
24	CUA	O	228	2/2	1.00	0.01	24,24,24,25	0
28	ZN	F	99	1/1	1.00	0.02	24,24,24,24	0
28	ZN	S	99	1/1	1.00	0.02	25,25,25,25	0

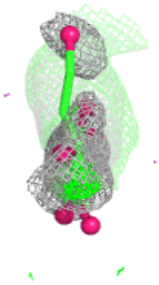
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DMU C 722:

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

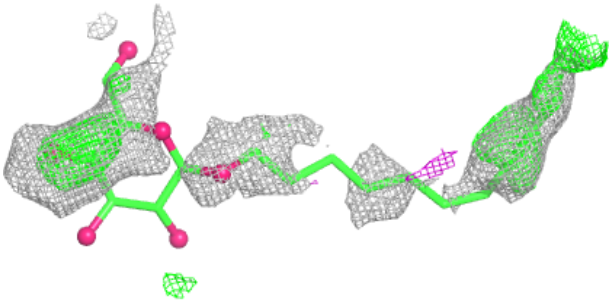


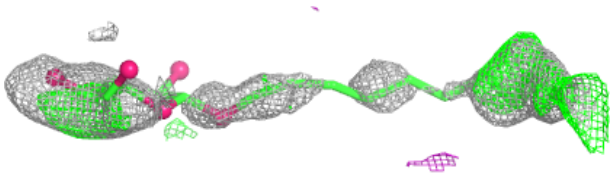


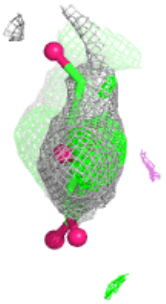


Electron density around DMU P 722:

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

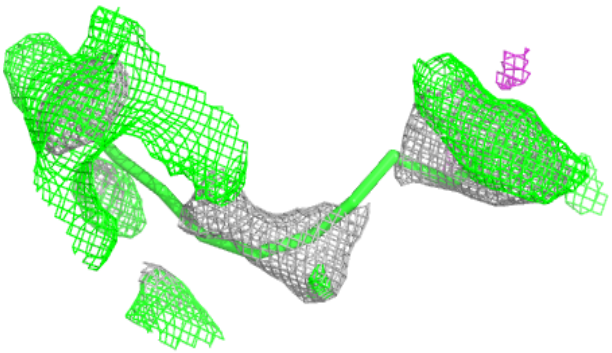


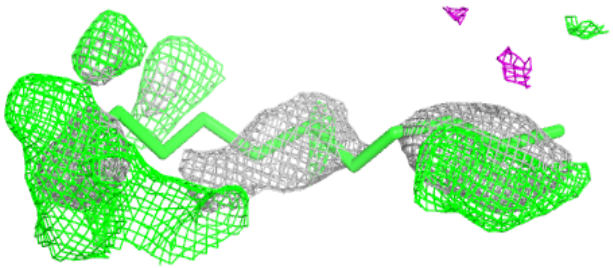


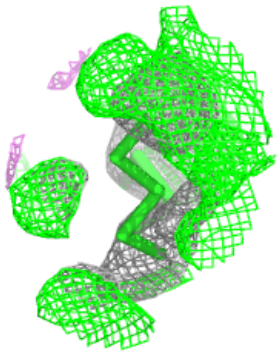


Electron density around LFA P 615:

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

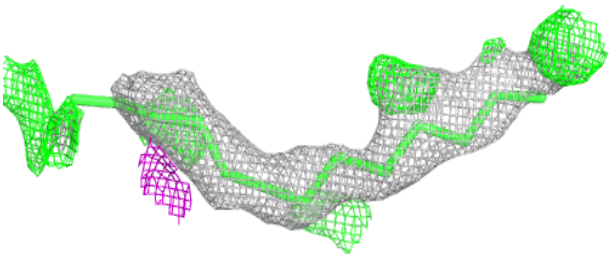


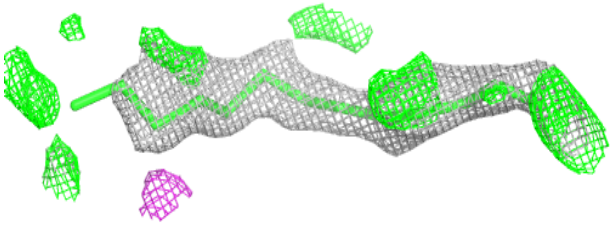


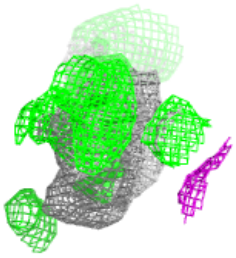


Electron density around LFA C 626:

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

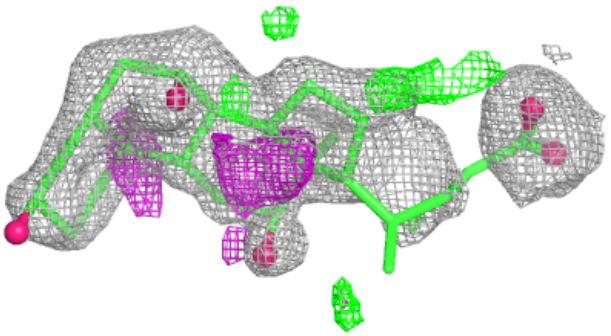


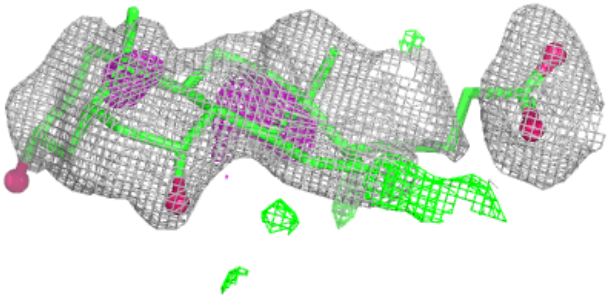


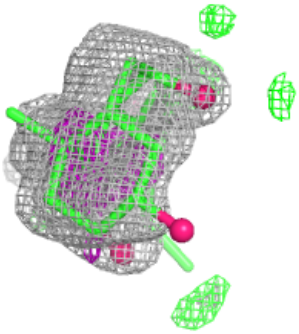


Electron density around CHD P 271:

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

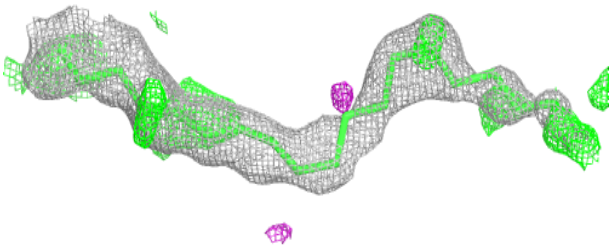


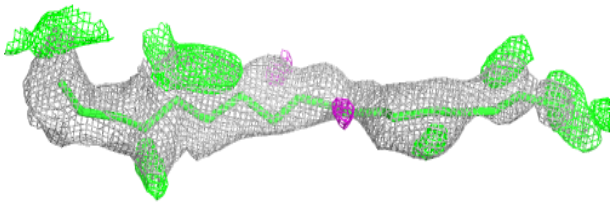


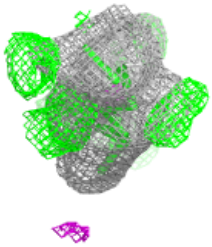


Electron density around LFA P 716 (B):

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

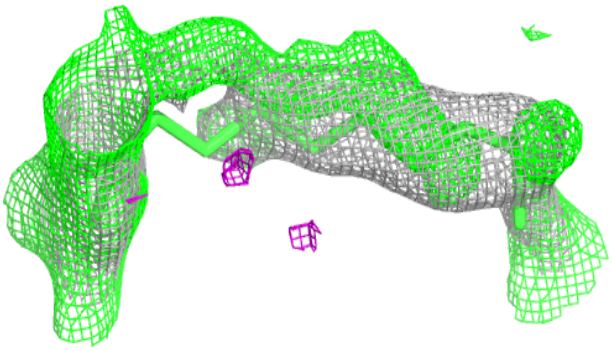


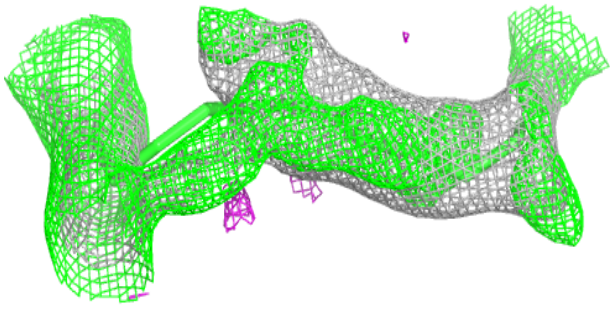


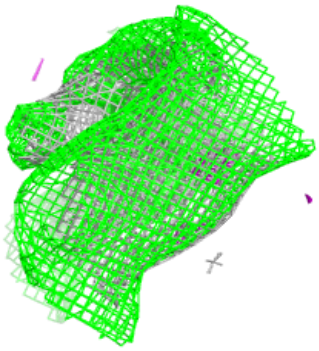


Electron density around LFA P 624:

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

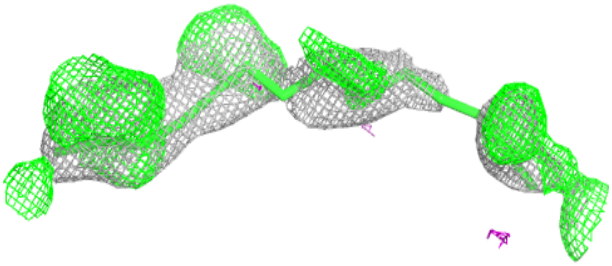


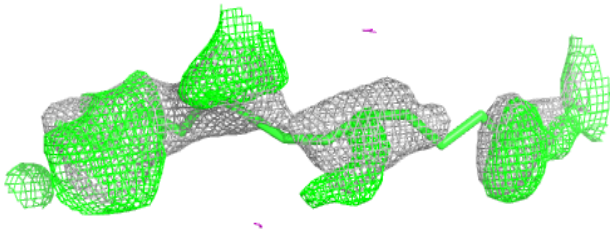


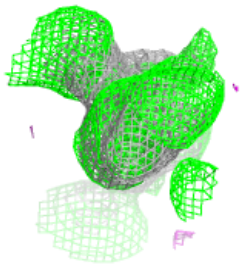


Electron density around LFA P 623:

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

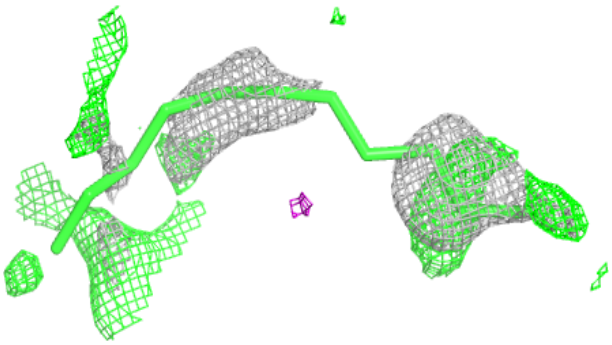


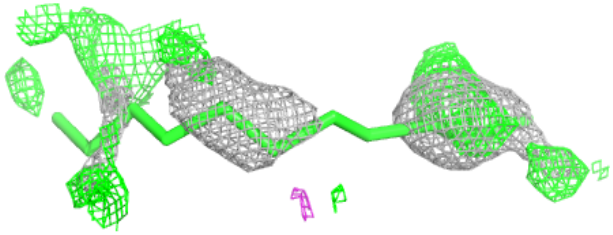


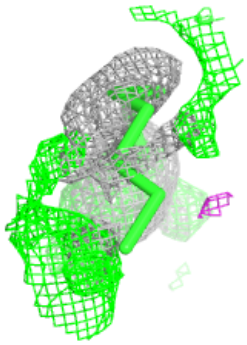


Electron density around LFA C 615:

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

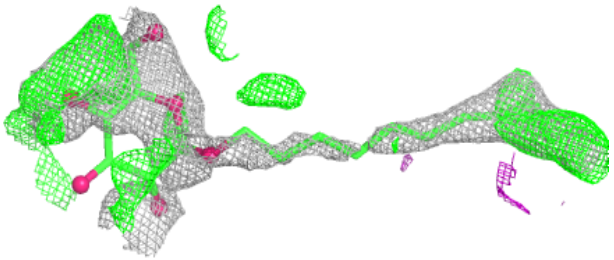


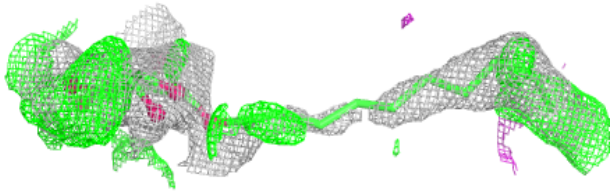


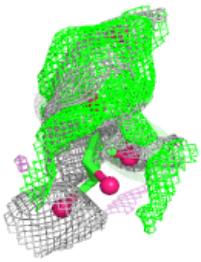


Electron density around DMU G 711:

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

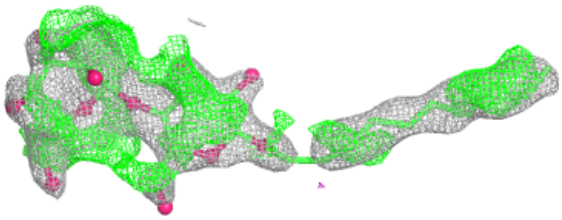


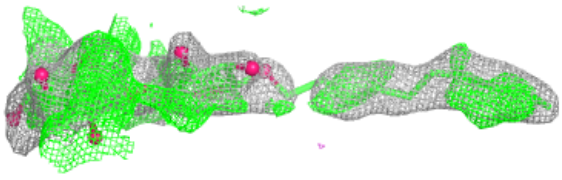


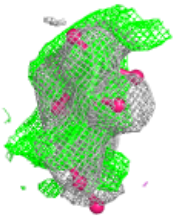


Electron density around DMU P 733:

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

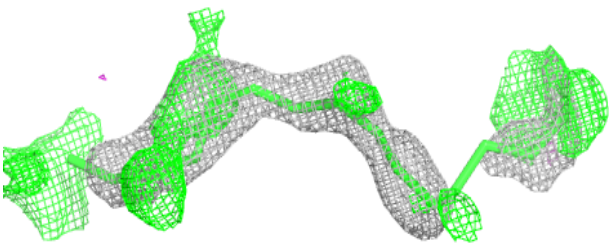


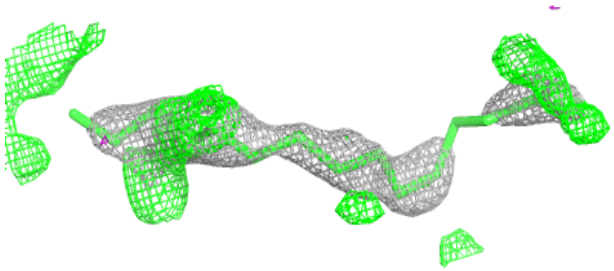


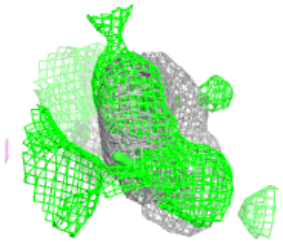


Electron density around LFA P 614:

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

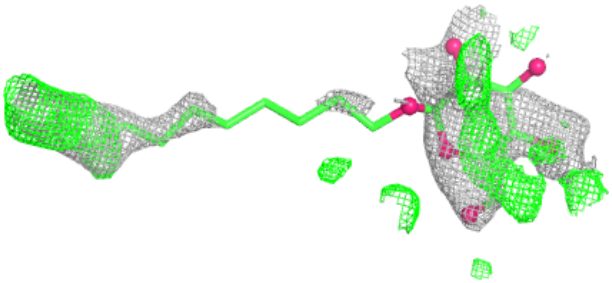


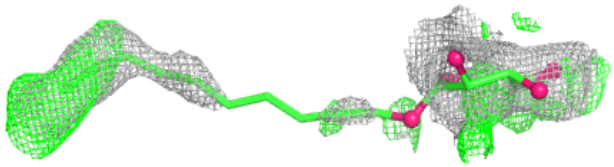


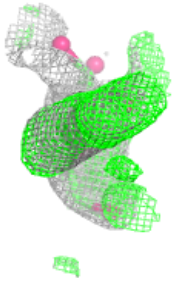


Electron density around DMU T 711:

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

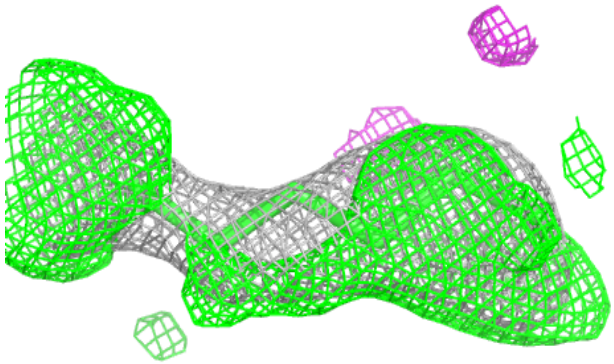


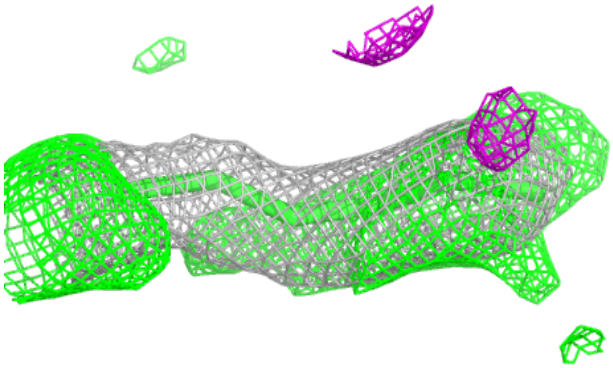


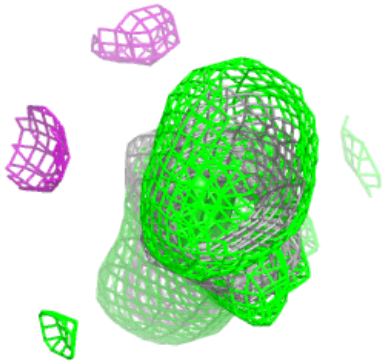


Electron density around LFA C 612:

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

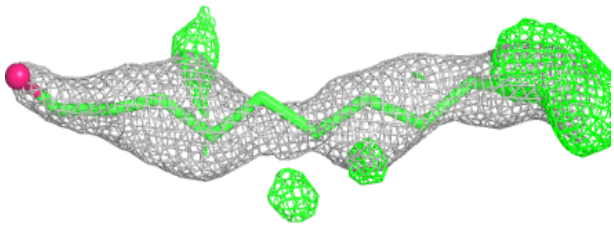


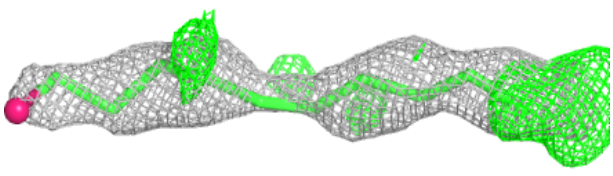


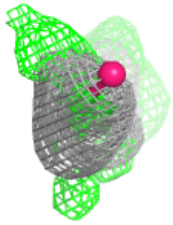


Electron density around DMU B 741:

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

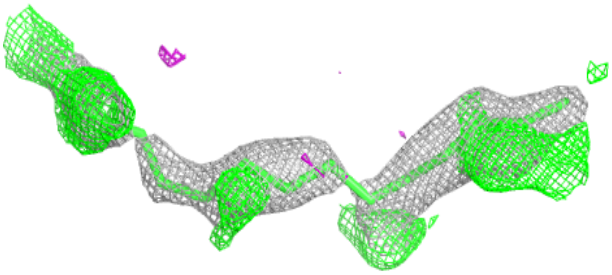


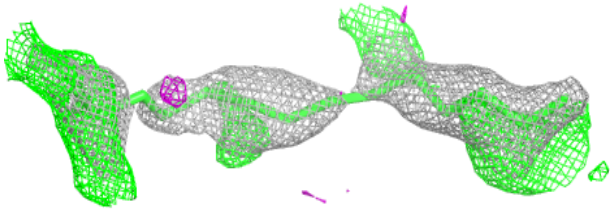


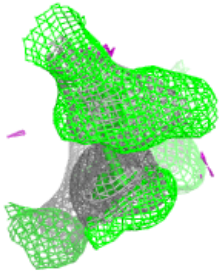


Electron density around LFA C 623:

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

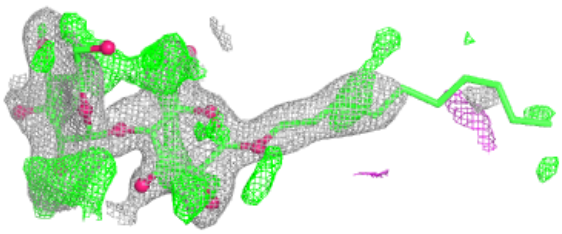


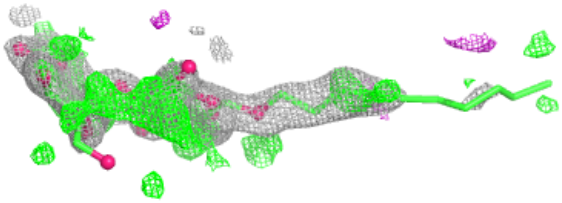


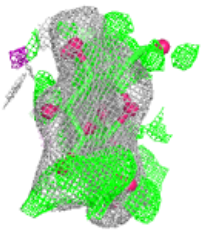


Electron density around DMU P 714:

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

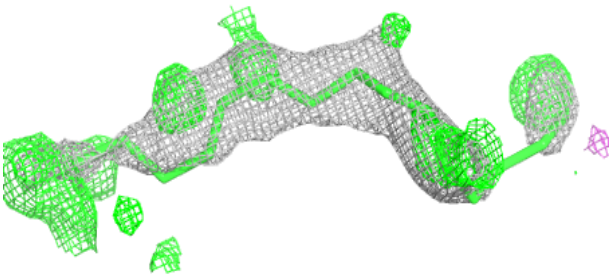


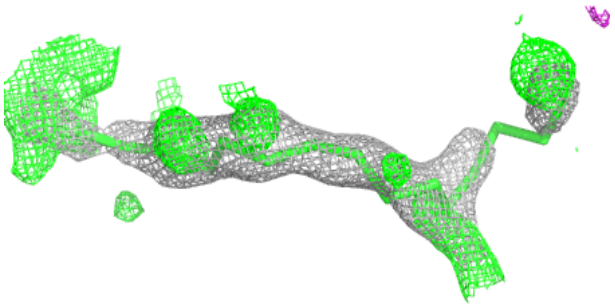


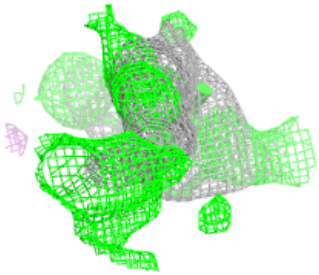


Electron density around LFA C 614:

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

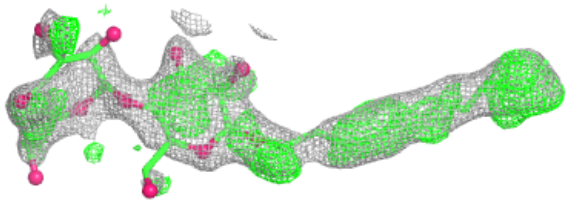


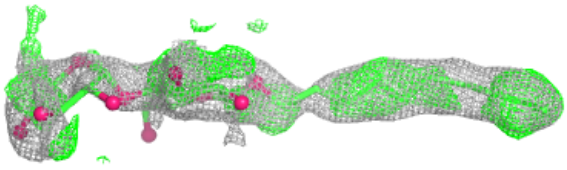


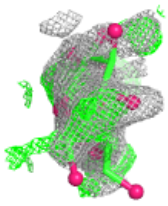


Electron density around DMU C 733:

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

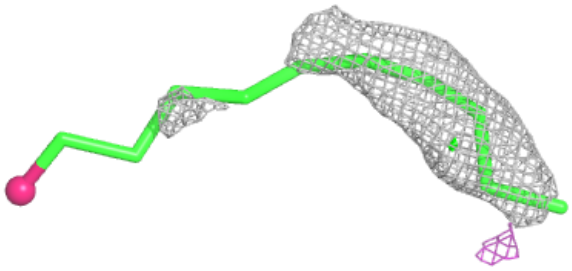


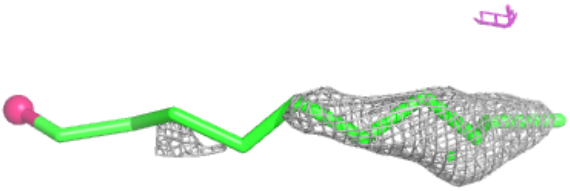


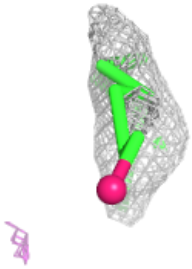


Electron density around DMU W 732:

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

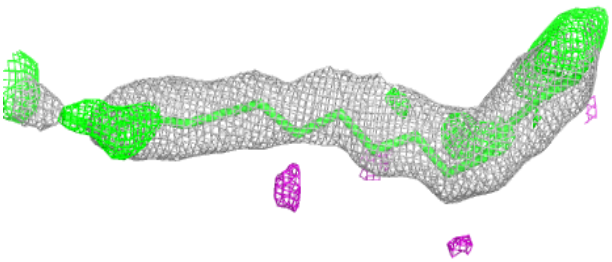


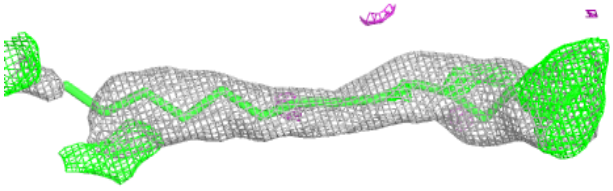


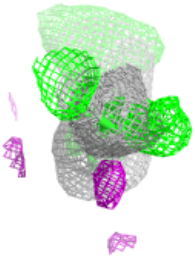


Electron density around LFA C 625:

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

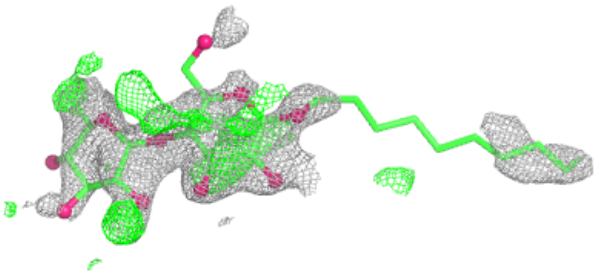


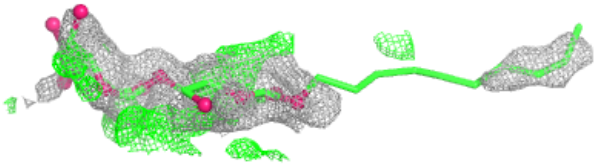


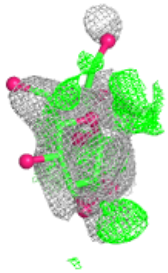


Electron density around DMU P 734:

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

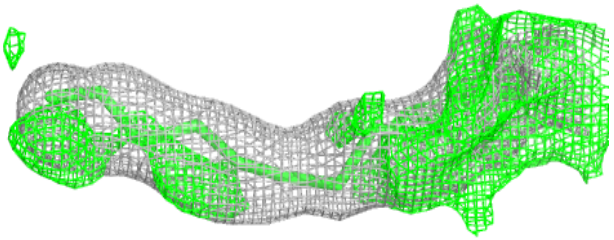


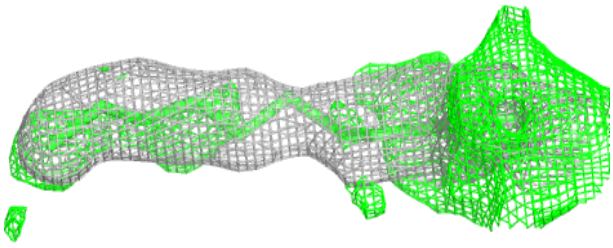


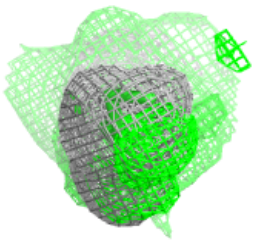


Electron density around LFA T 622:

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

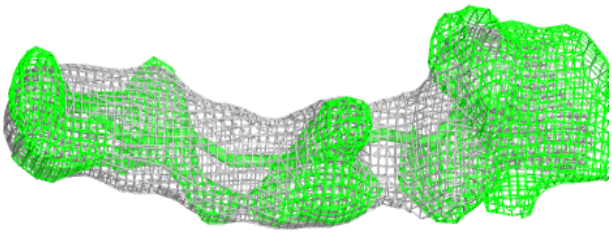


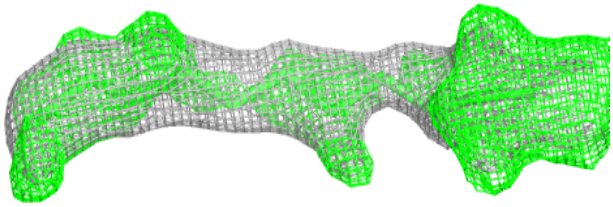


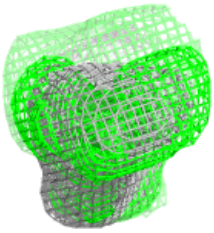


Electron density around LFA G 622:

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

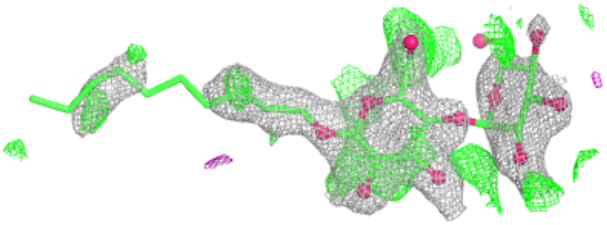


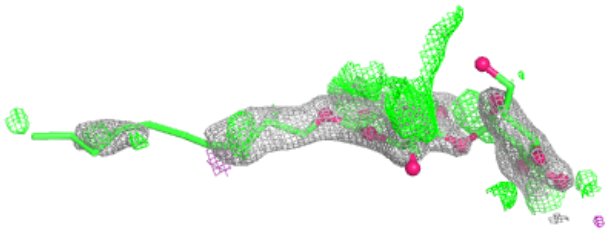


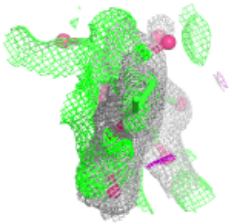


Electron density around DMU C 714:

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

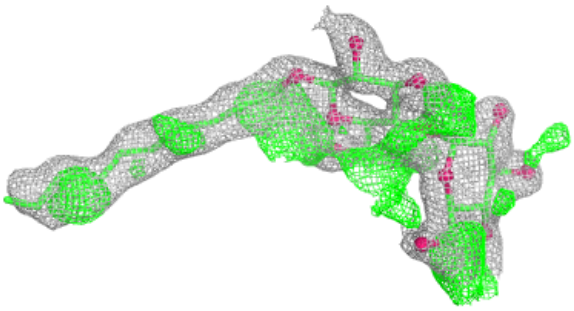


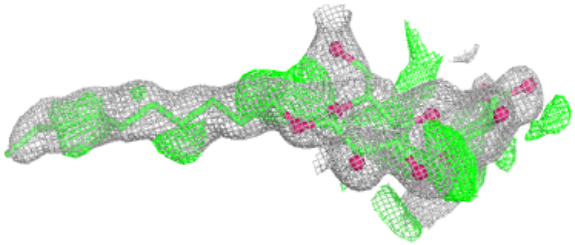


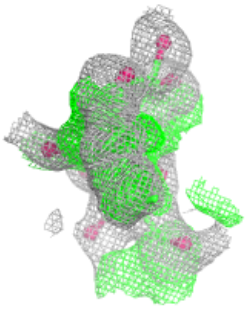


Electron density around DMU N 744:

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

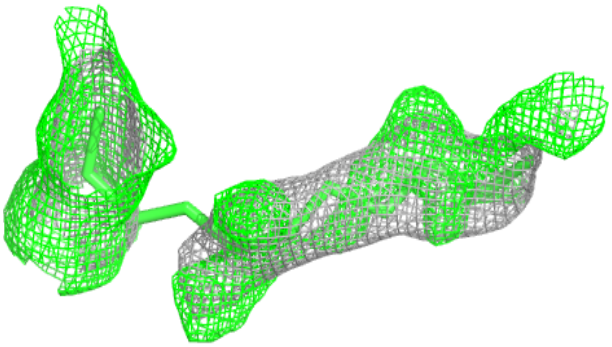


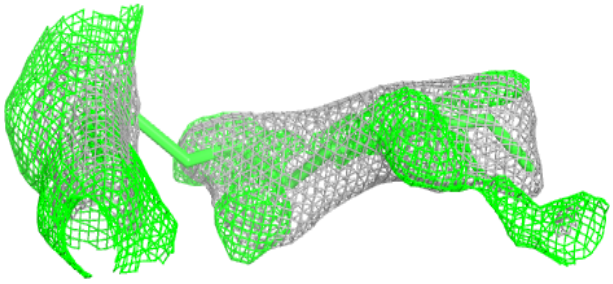


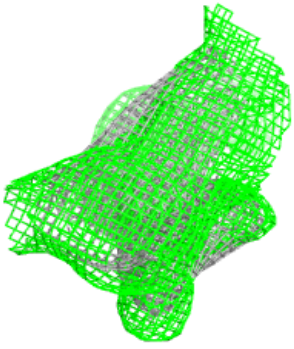


Electron density around LFA C 624:

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

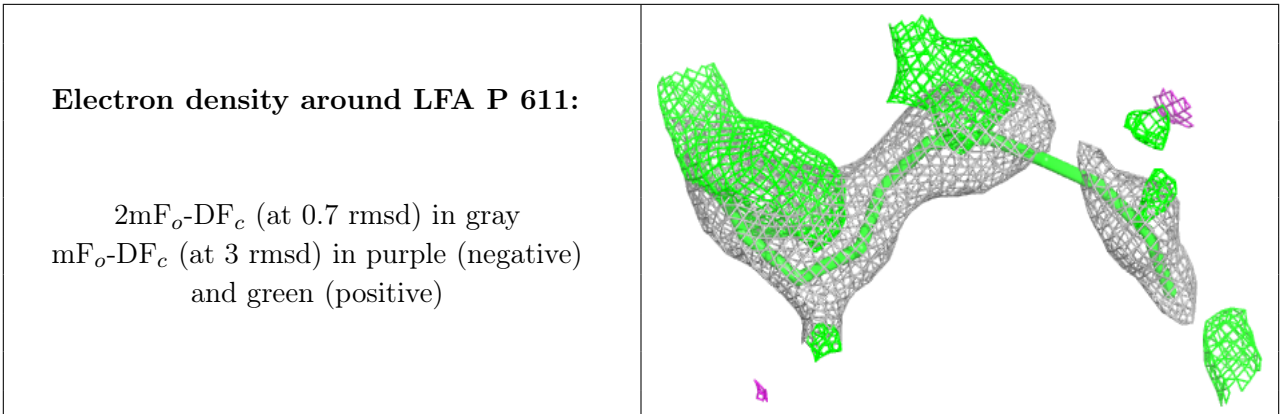


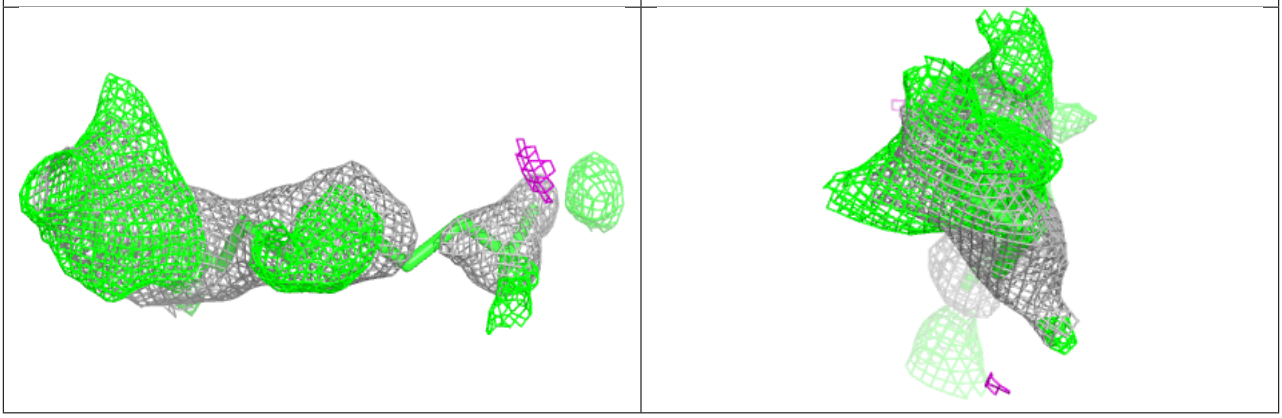




Electron density around LFA P 611:

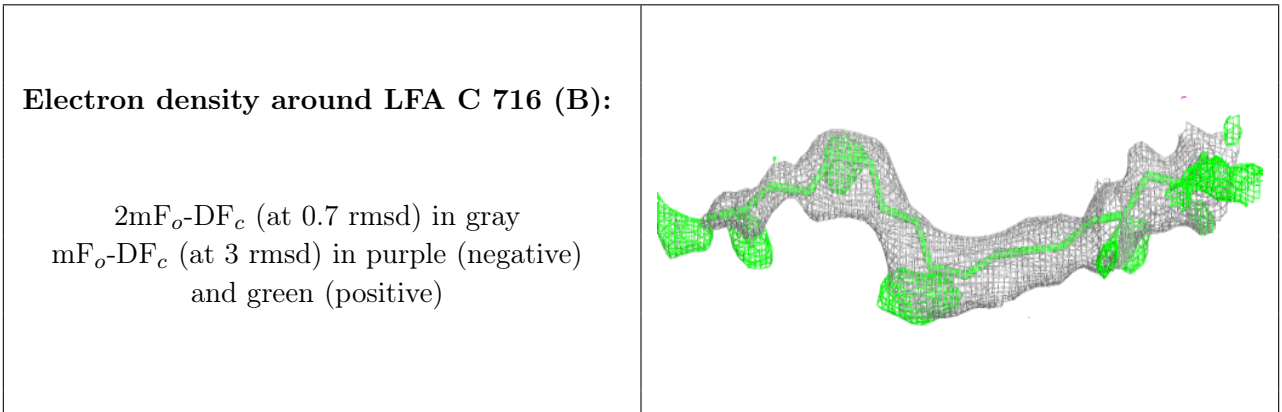
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

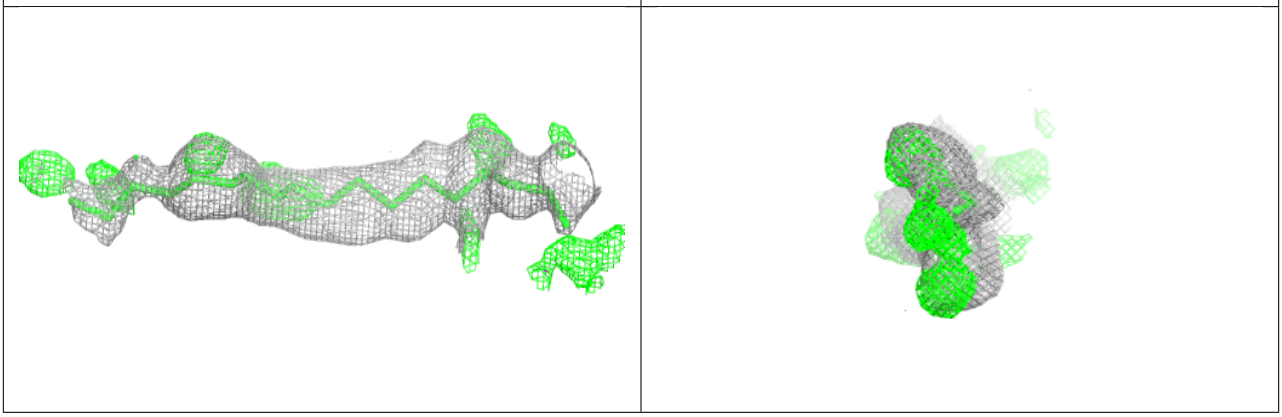




Electron density around LFA C 716 (B):

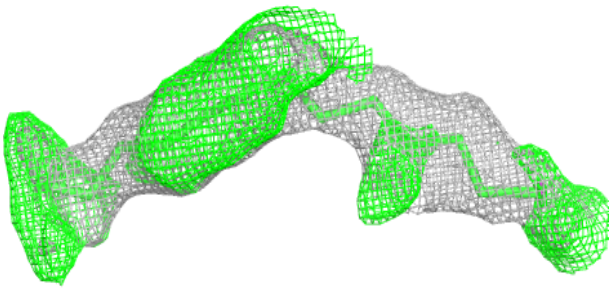
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

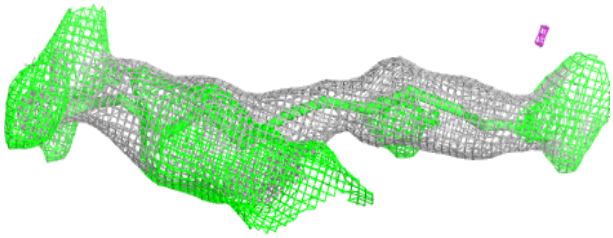


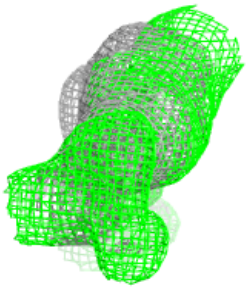


Electron density around LFA P 626:

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

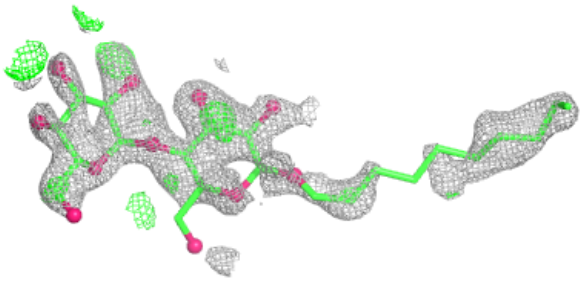


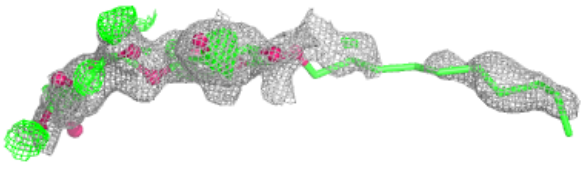


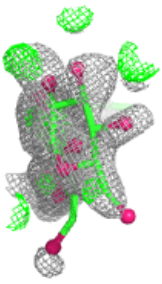


Electron density around DMU C 734:

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

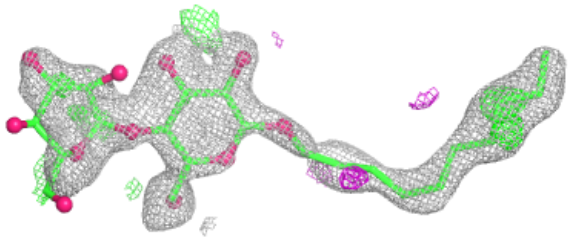


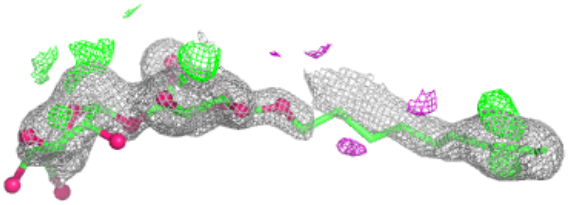


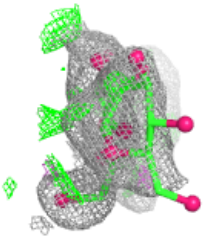


Electron density around DMU W 61:

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

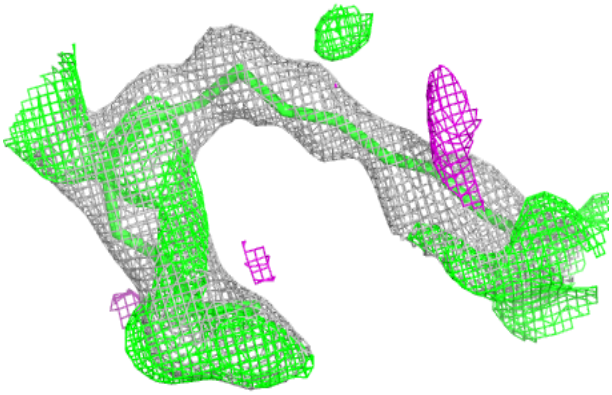


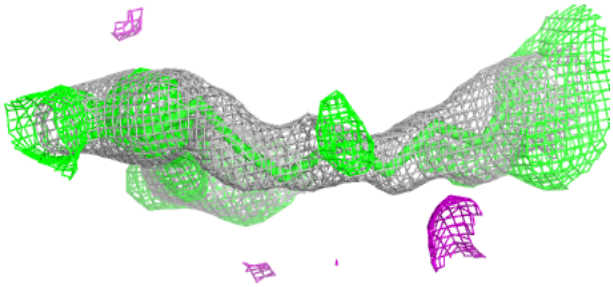


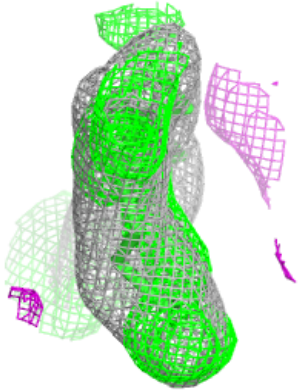


Electron density around LFA A 628:

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

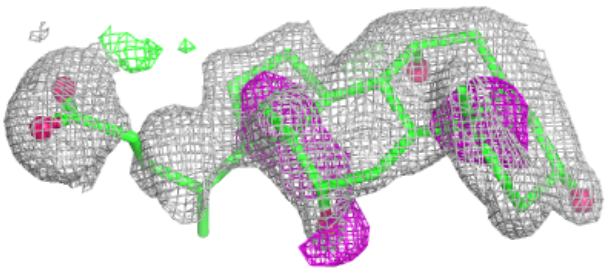


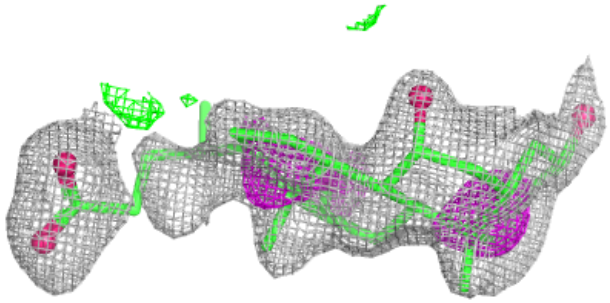


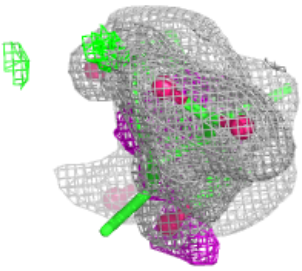


Electron density around CHD C 271:

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

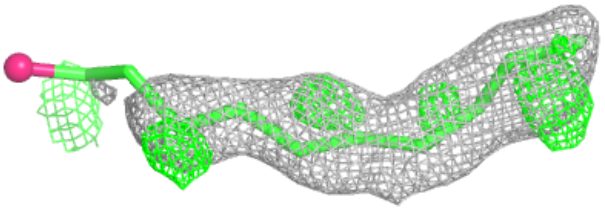


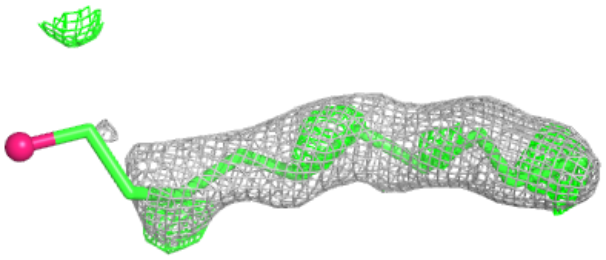


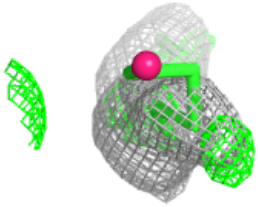


Electron density around DMU J 732:

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

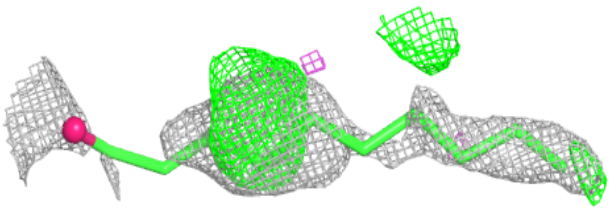


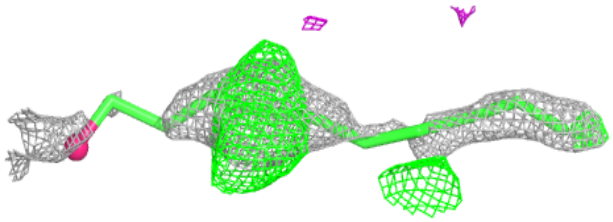


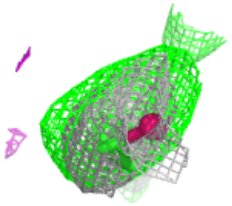


Electron density around DMU T 712:

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

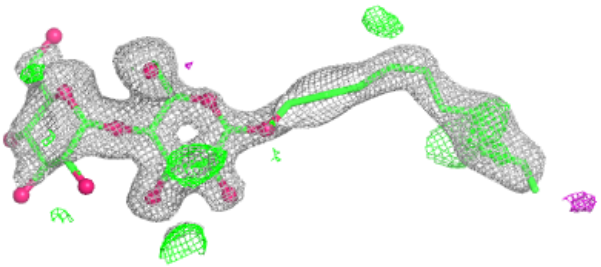


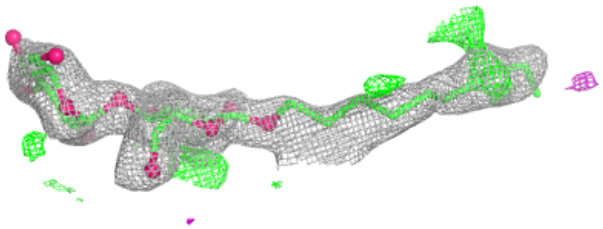


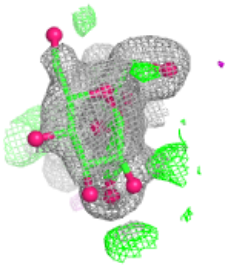


Electron density around DMU J 61:

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

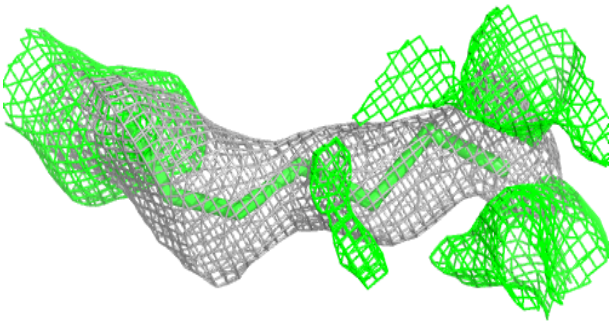


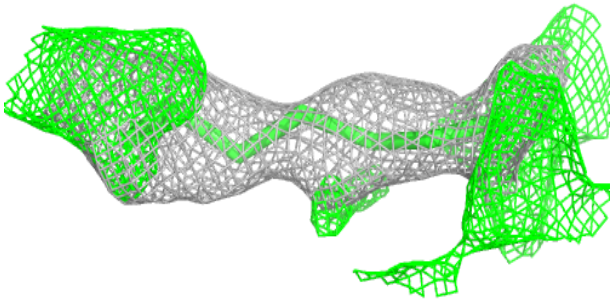


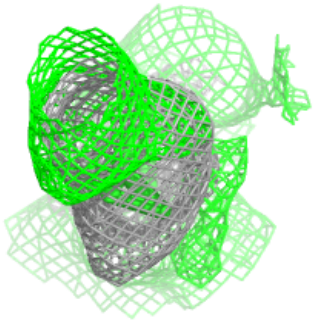


Electron density around DMU N 743:

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

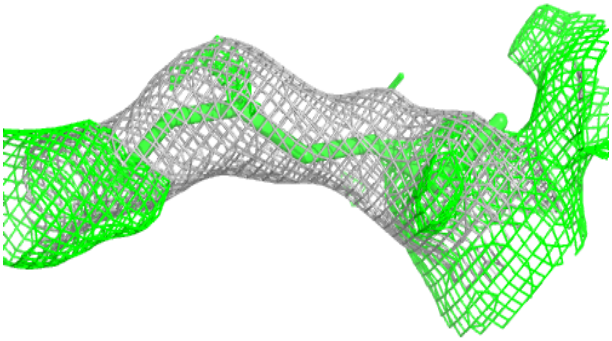


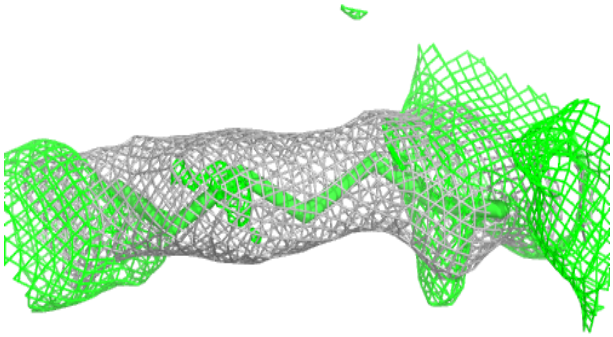


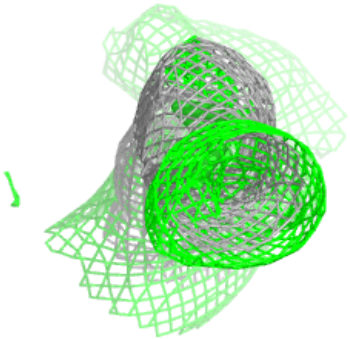


Electron density around DMU A 743:

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

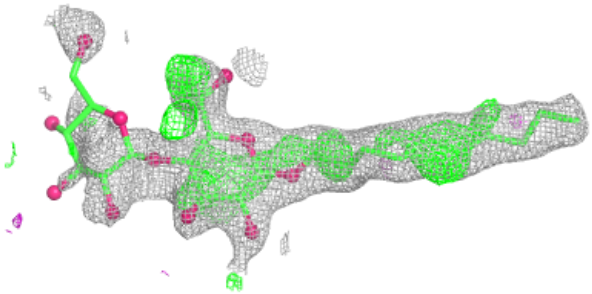


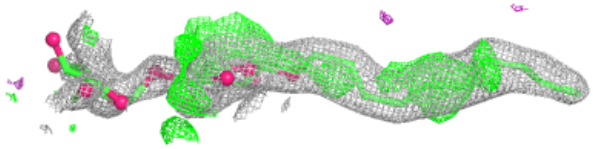


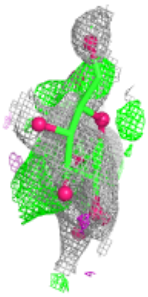


Electron density around DMU N 745:

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

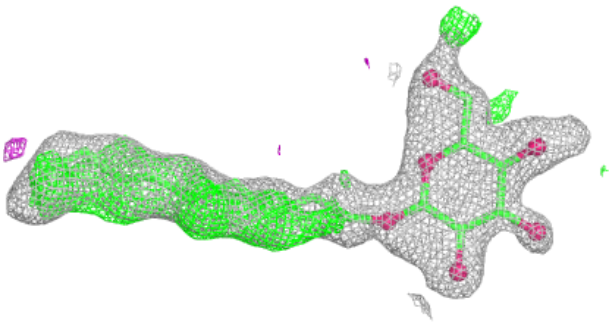


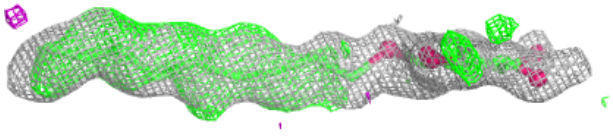


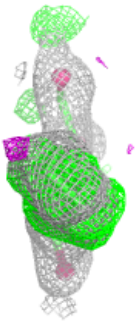


Electron density around DMU O 742:

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

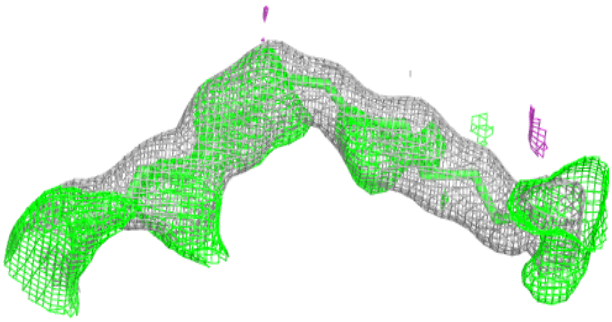


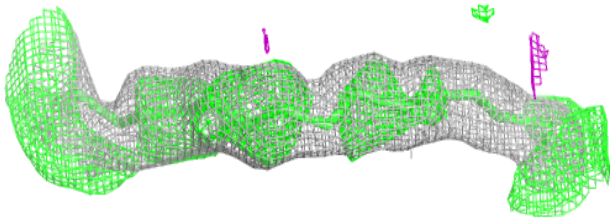


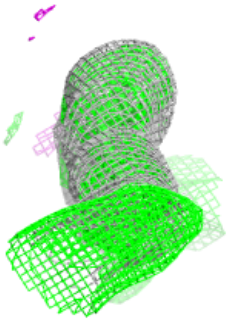


Electron density around LFA A 627:

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

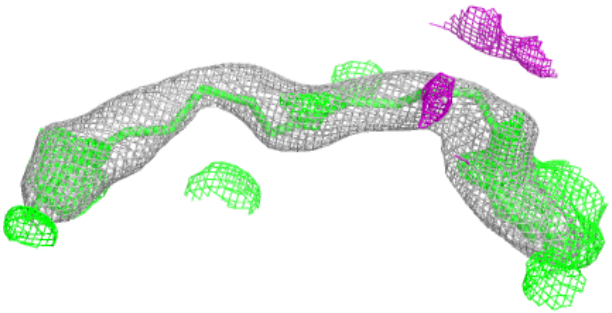


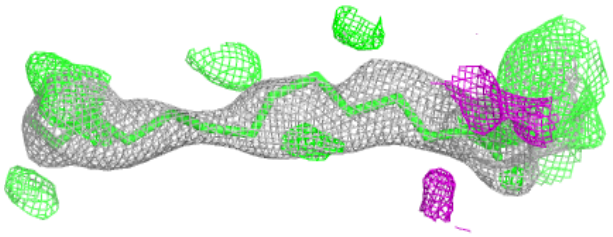


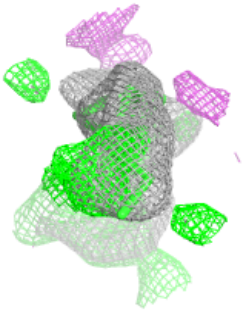


Electron density around LFA G 621:

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

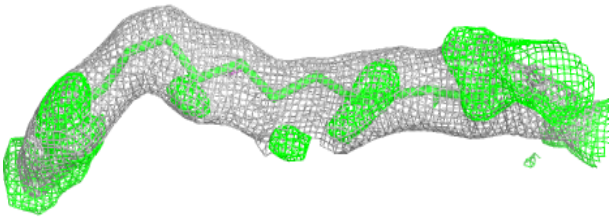


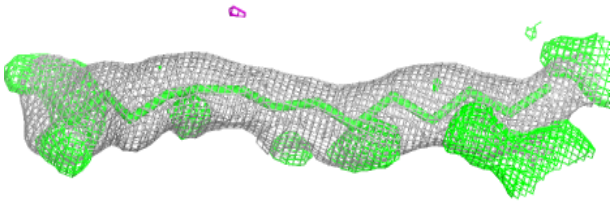


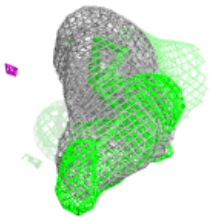


Electron density around LFA P 625:

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

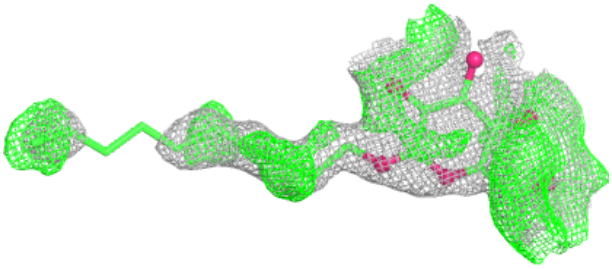


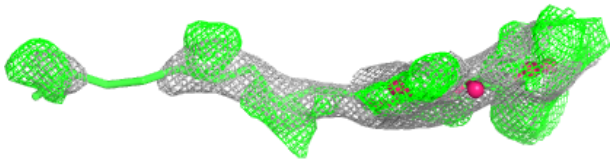


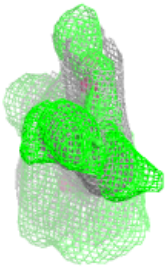


Electron density around DMU Y 747:

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

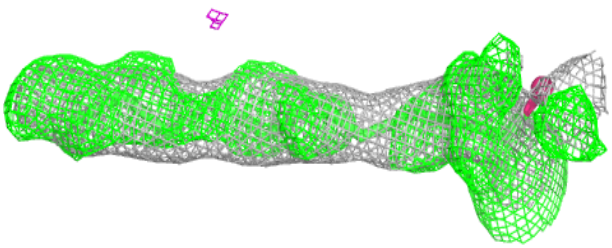


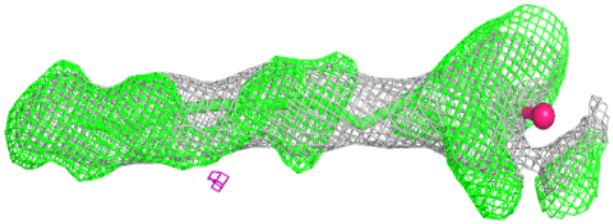


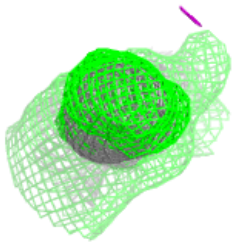


Electron density around DMU O 731:

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

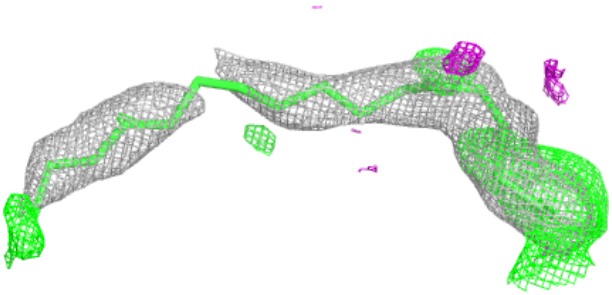


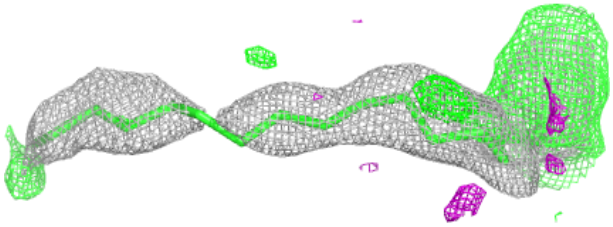


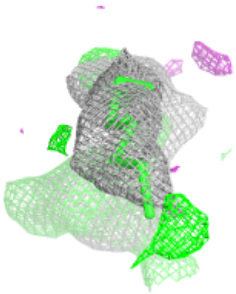


Electron density around LFA T 621:

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

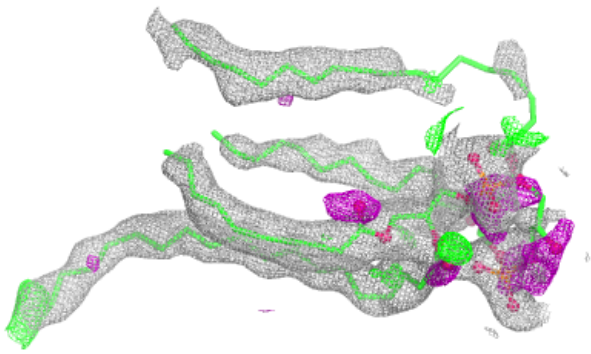


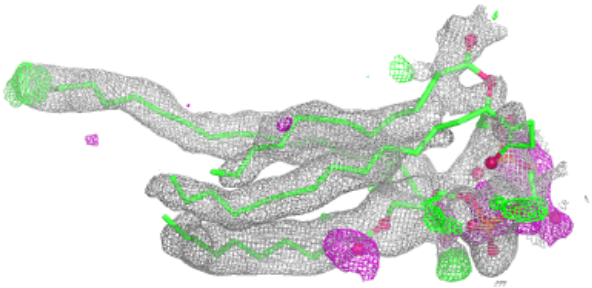


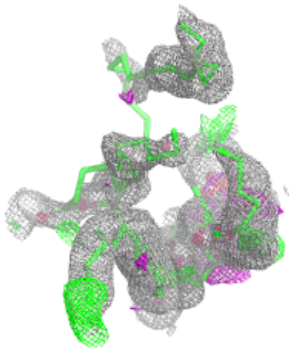


Electron density around CDL P 270:

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

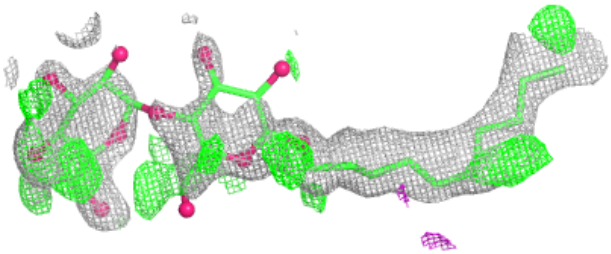


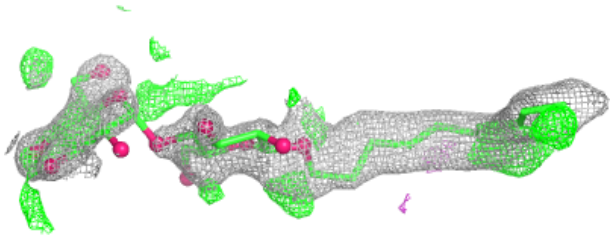


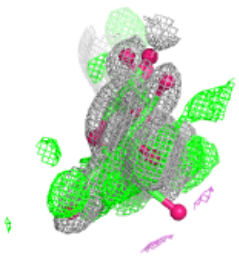


Electron density around DMU C 715 (A):

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

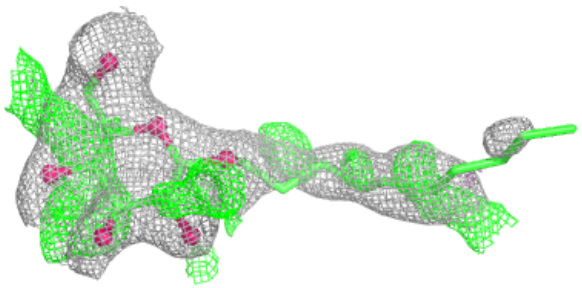


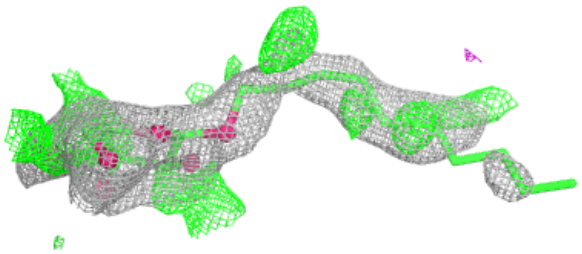


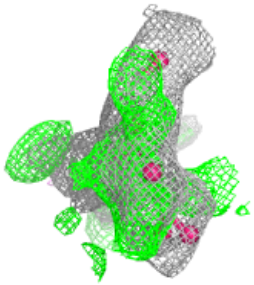


Electron density around DMU G 713:

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

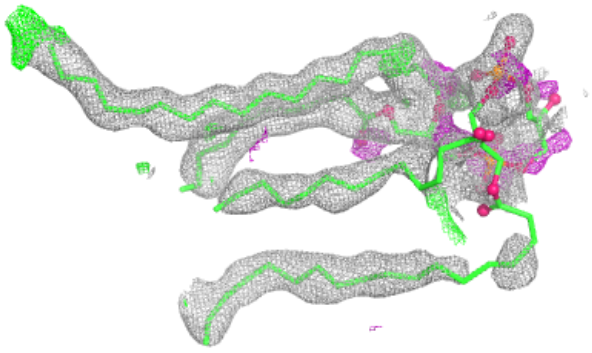


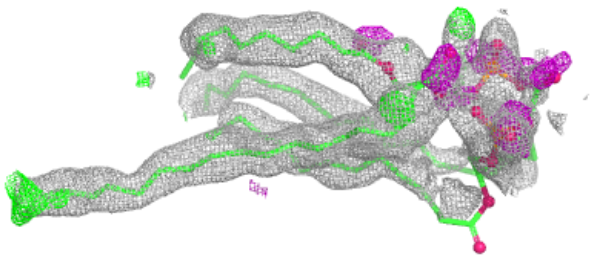


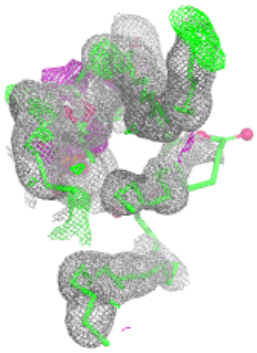


Electron density around CDL C 270:

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

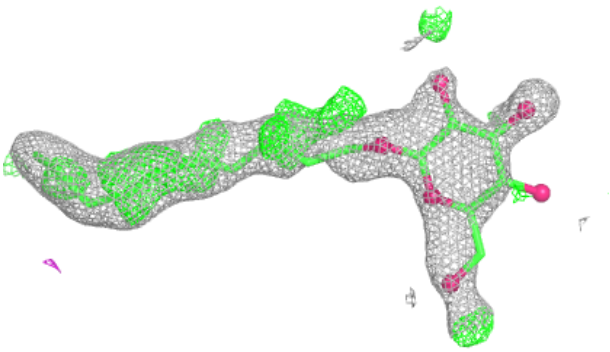


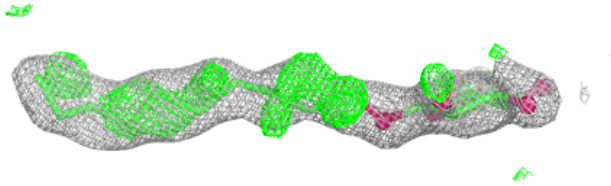


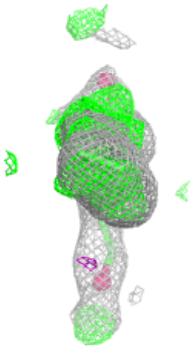


Electron density around DMU B 742:

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

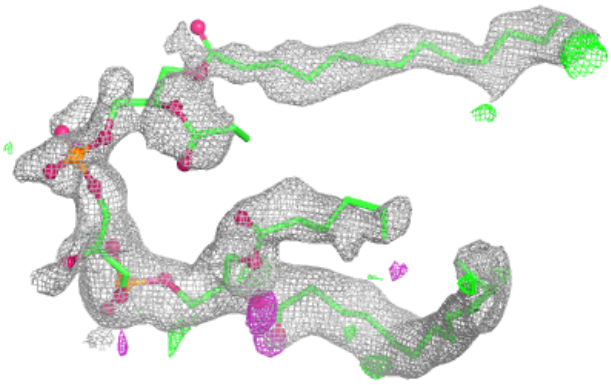


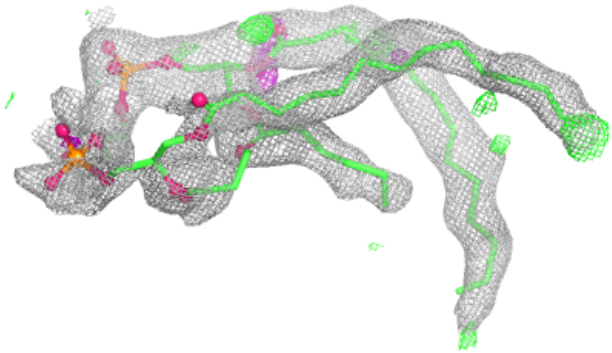


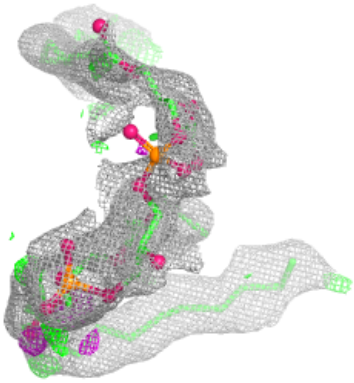


Electron density around CDL N 522:

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

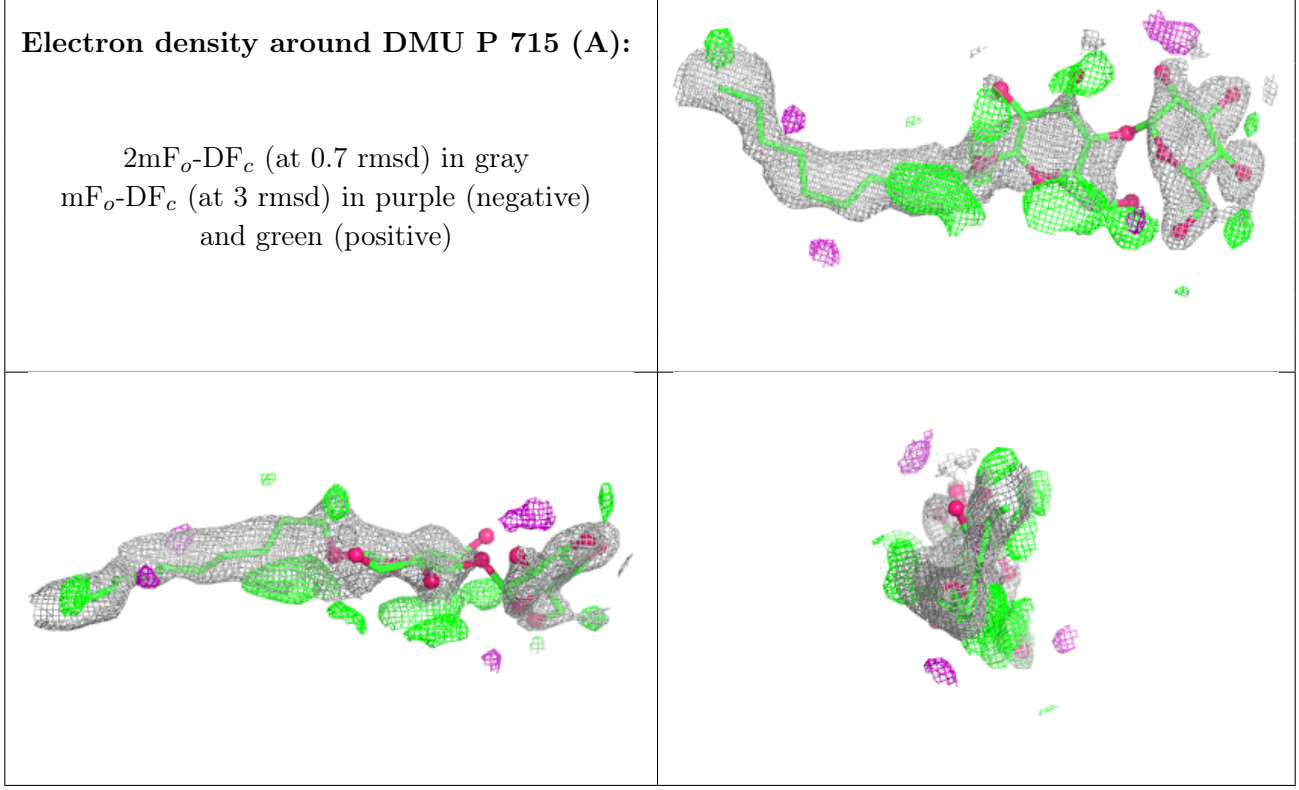






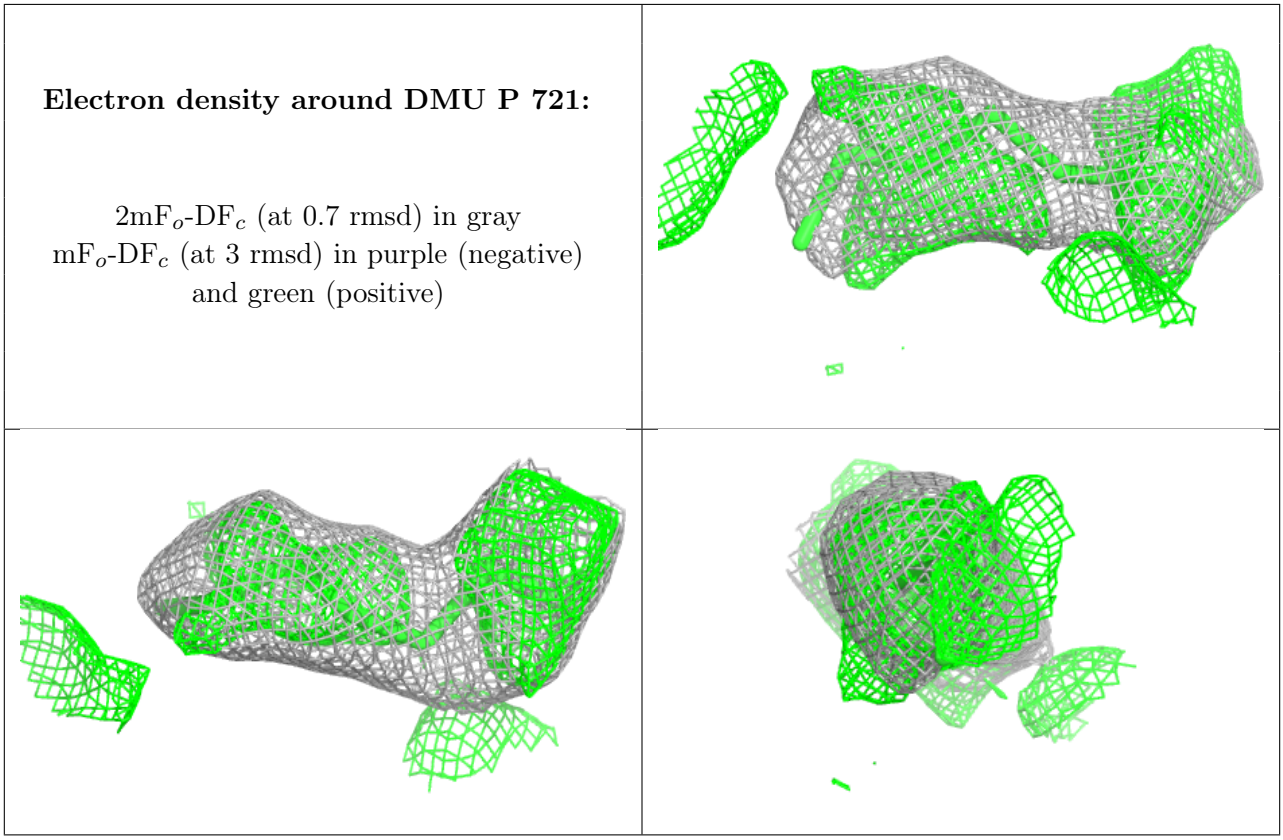
Electron density around DMU P 715 (A):

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



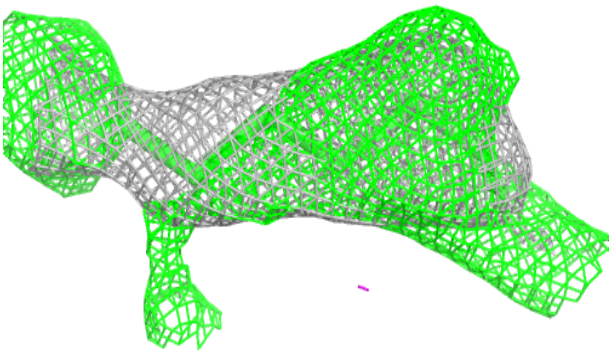
Electron density around DMU P 721:

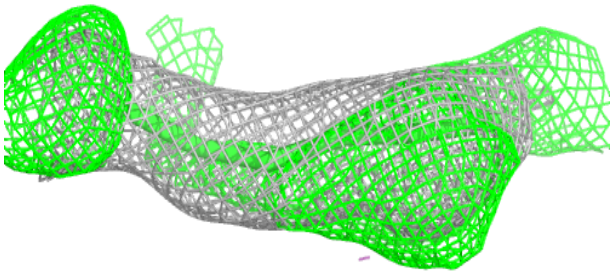
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

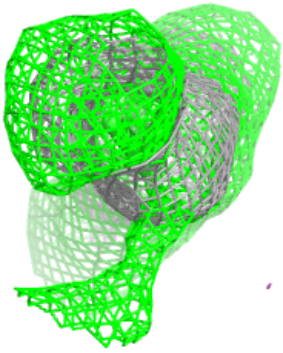


Electron density around LFA P 612:

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

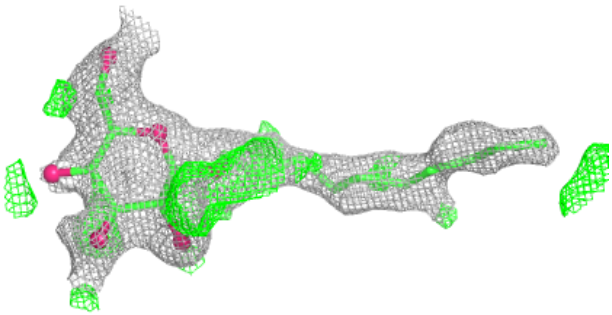


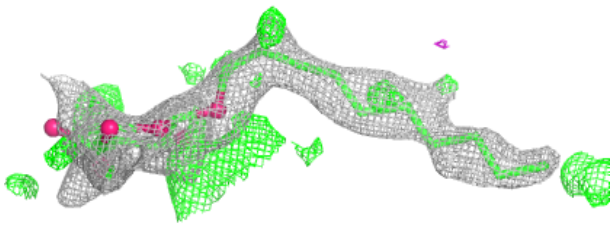


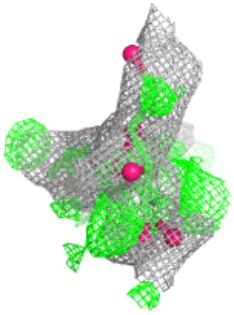


Electron density around DMU T 713:

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

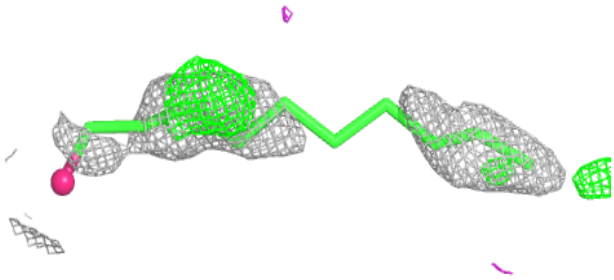


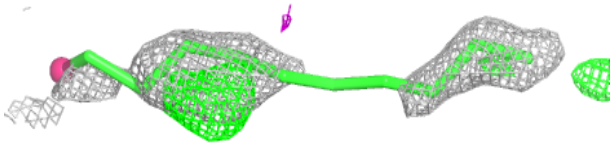


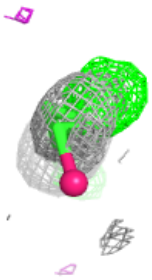


Electron density around DMU G 712:

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

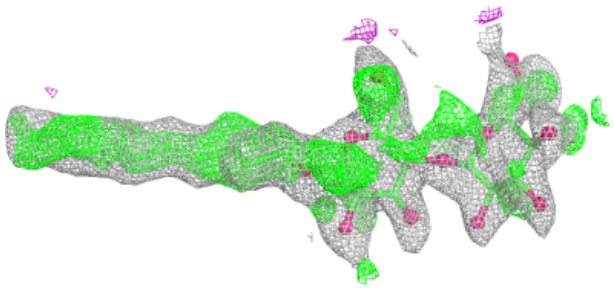


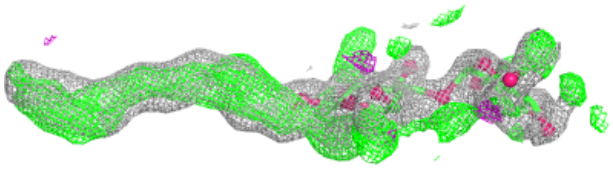


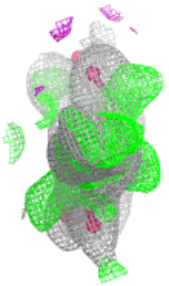


Electron density around DMU A 745:

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

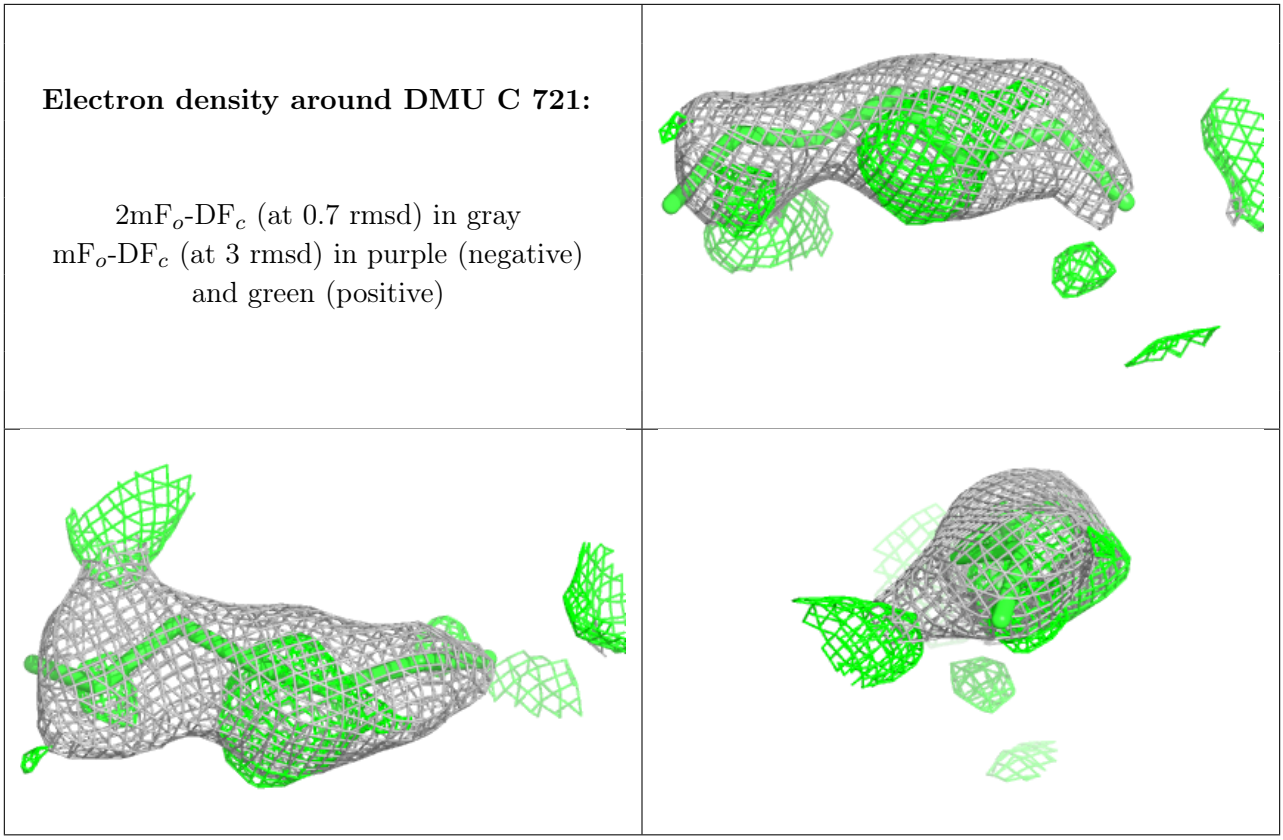






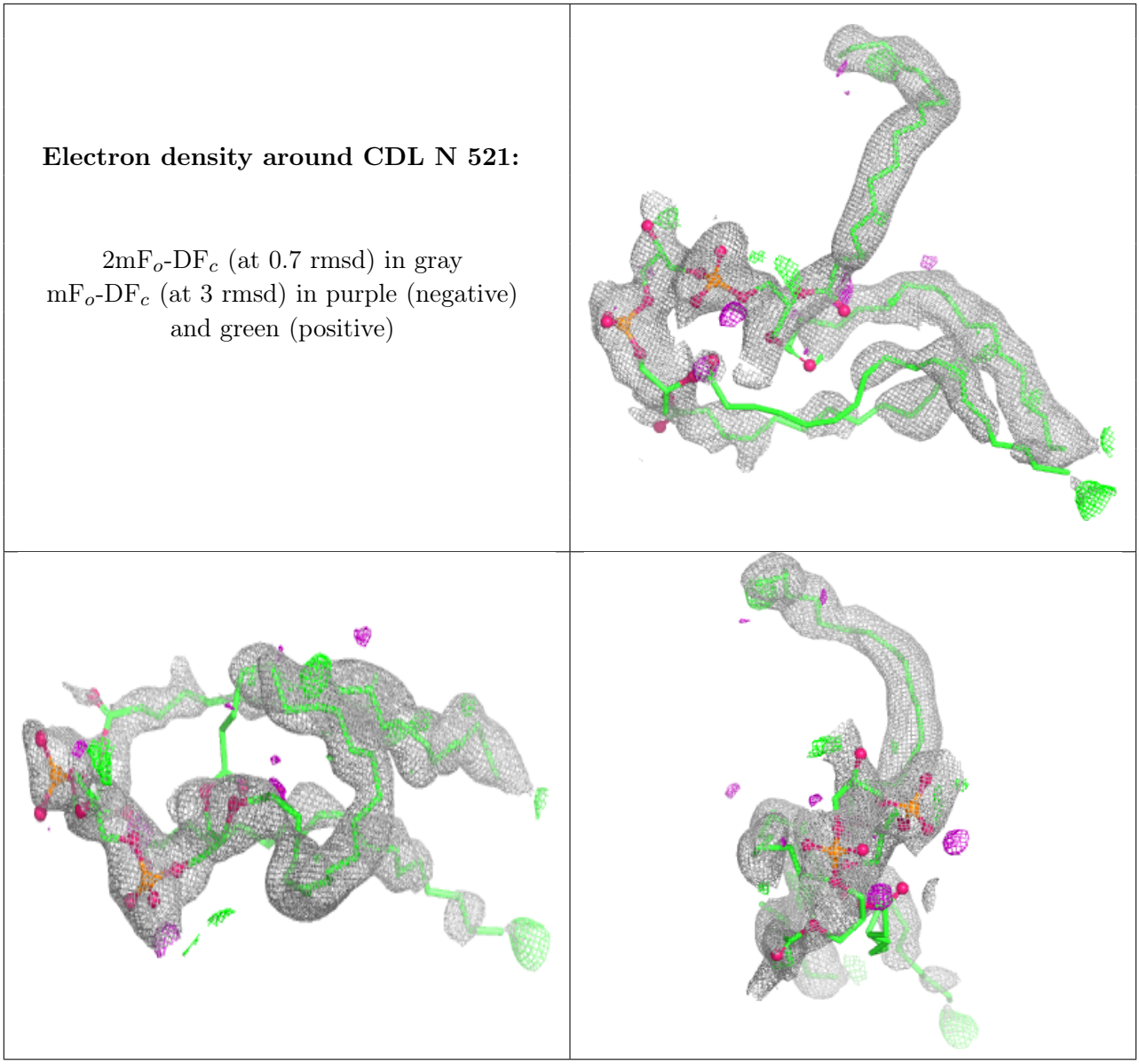
Electron density around DMU C 721:

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



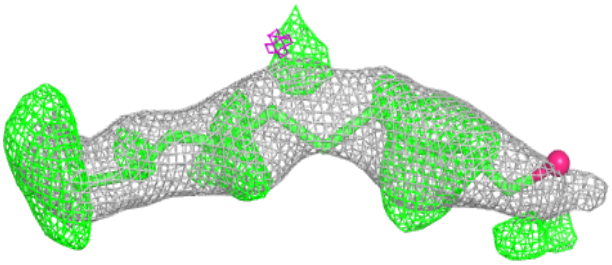
Electron density around CDL N 521:

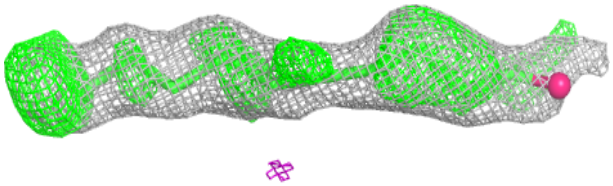
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

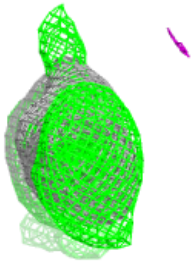


Electron density around DMU O 741:

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

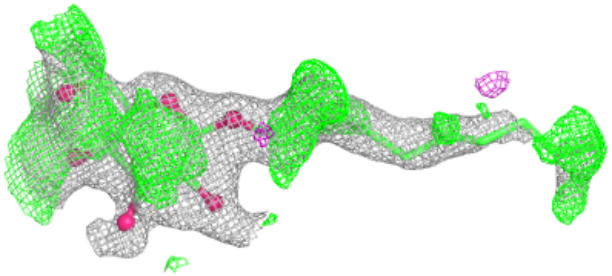


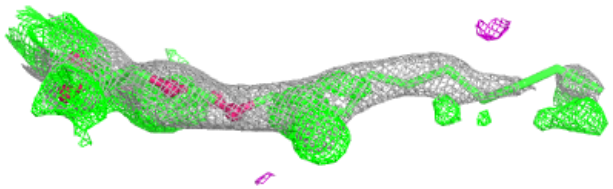


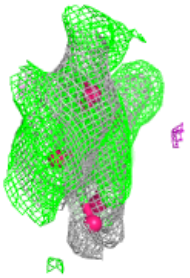


Electron density around DMU L 747:

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

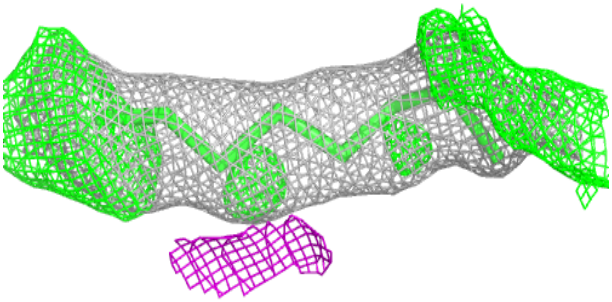


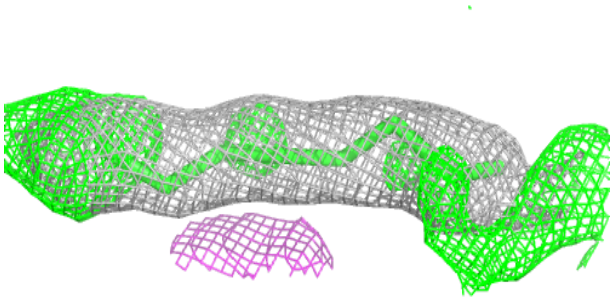


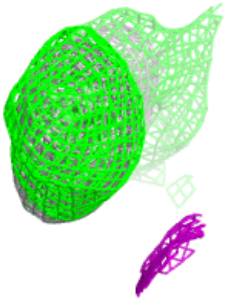


Electron density around DMU M 746:

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

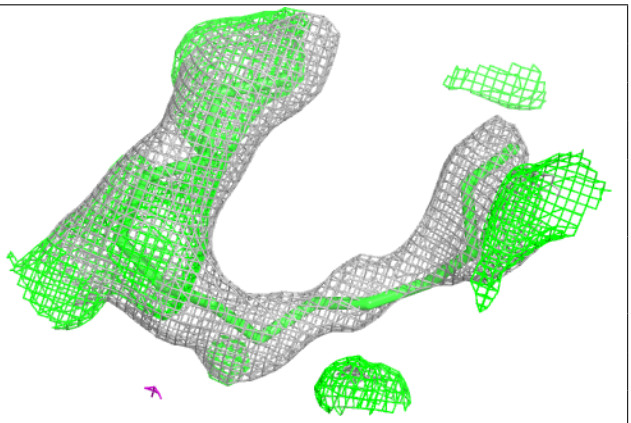


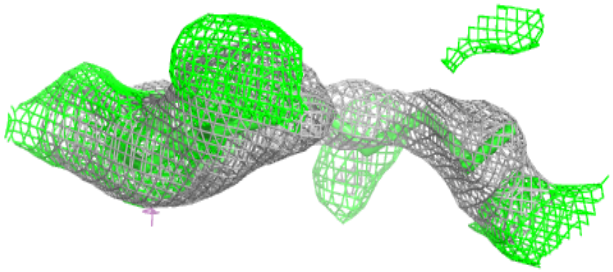


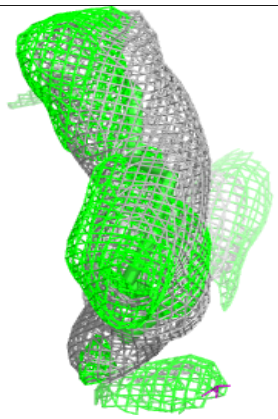


Electron density around LFA N 628:

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

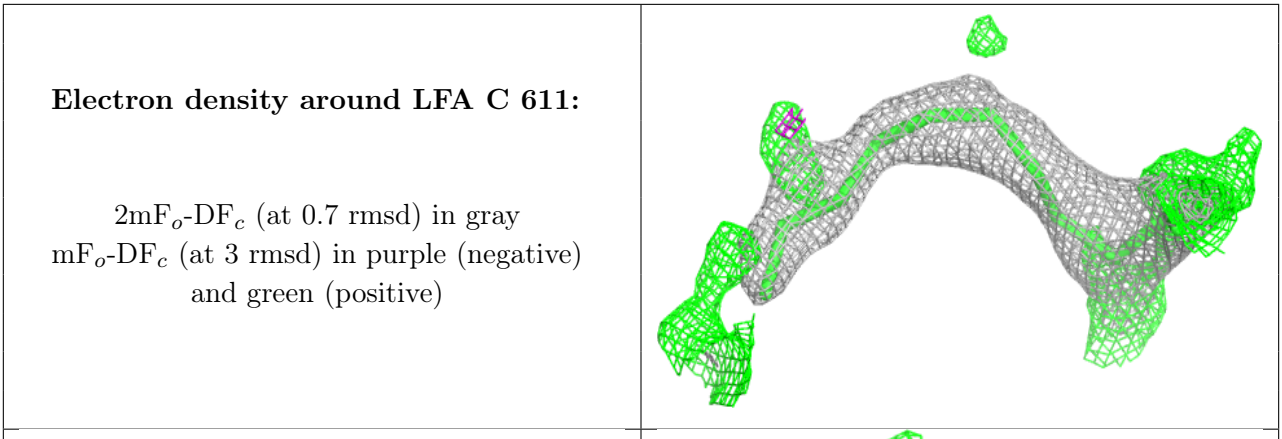






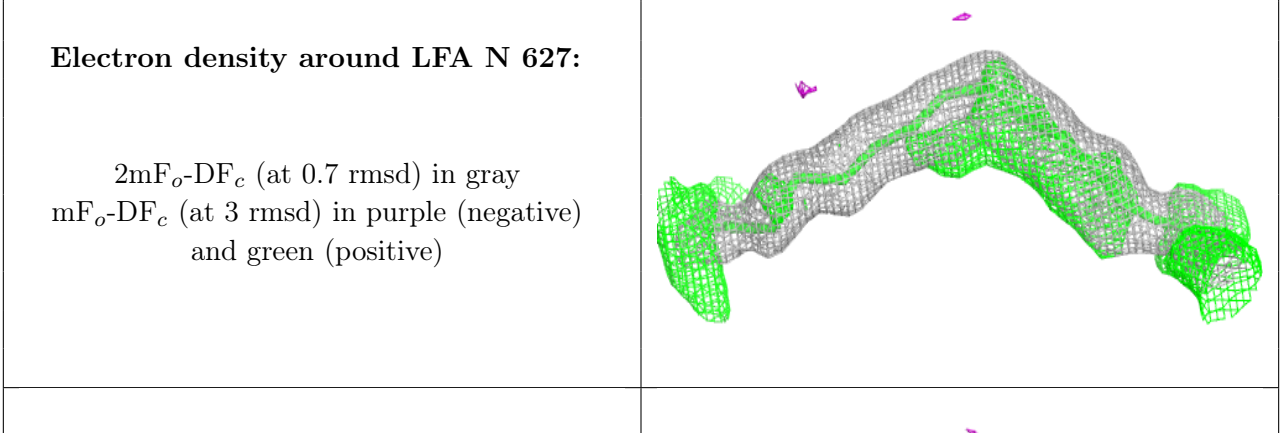
Electron density around LFA C 611:

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



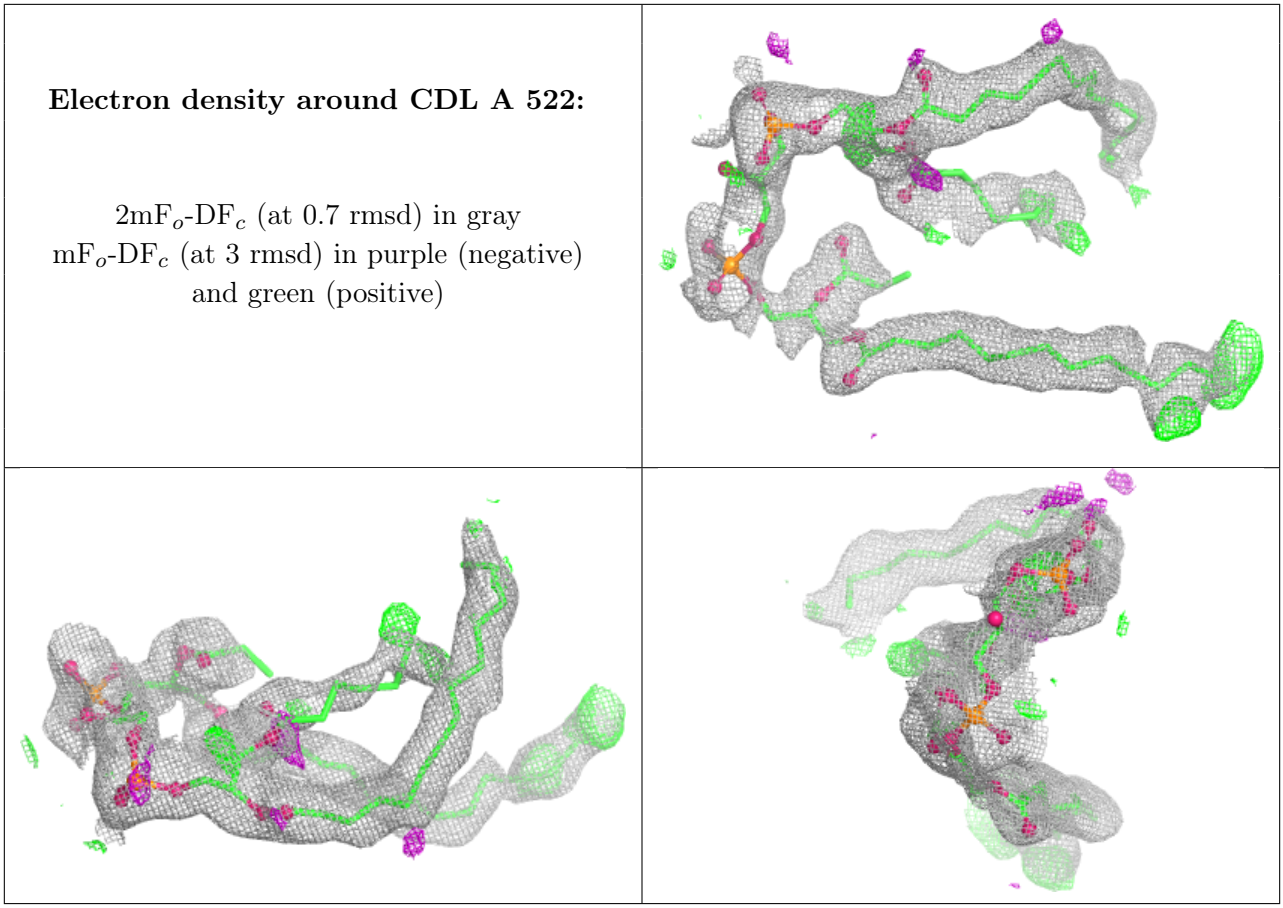
Electron density around LFA N 627:

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



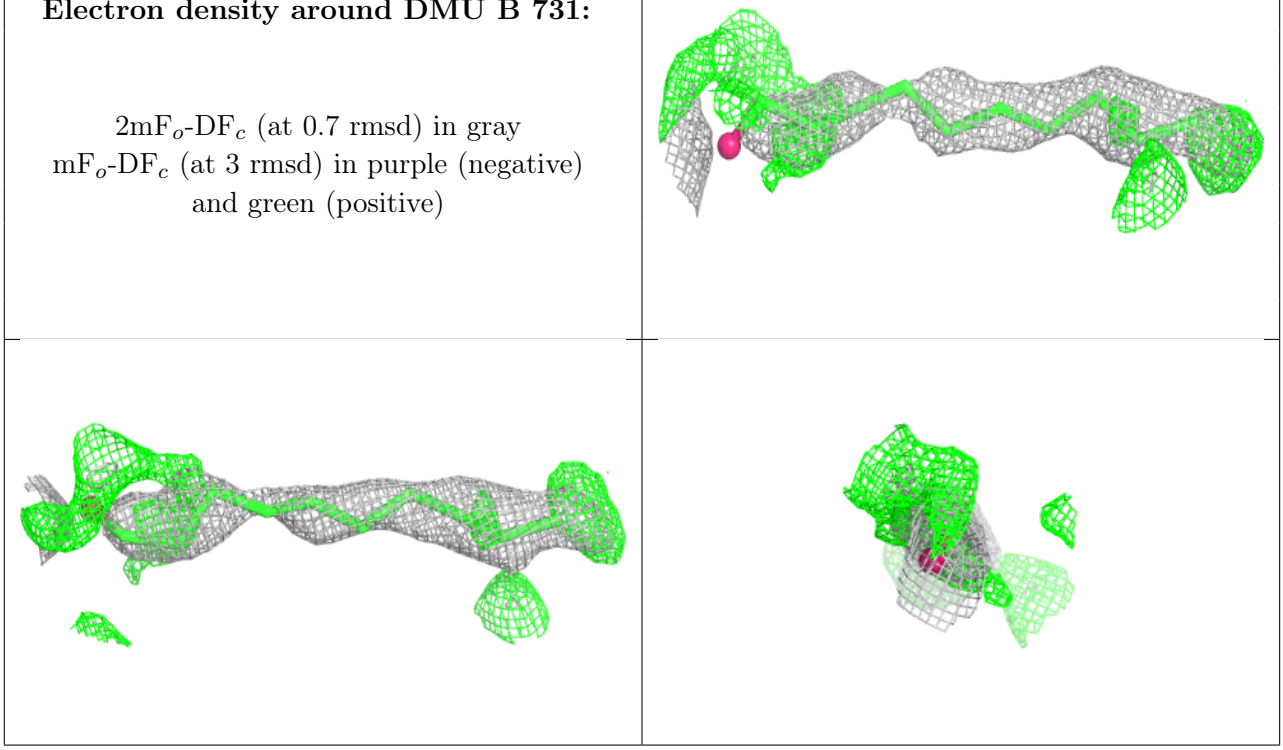
Electron density around CDL A 522:

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



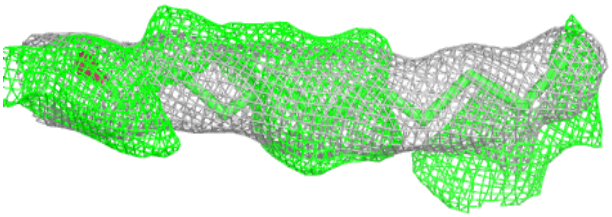
Electron density around DMU B 731:

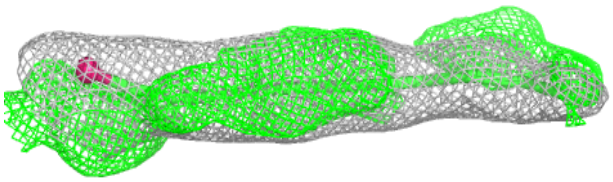
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

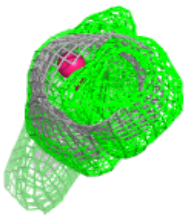


Electron density around DMU P 272:

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

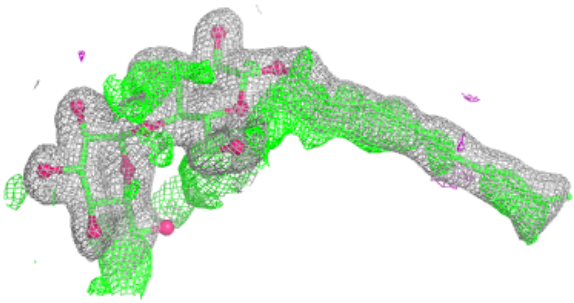


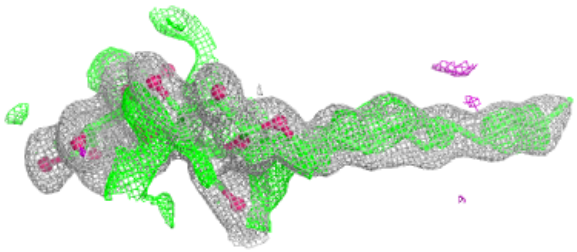


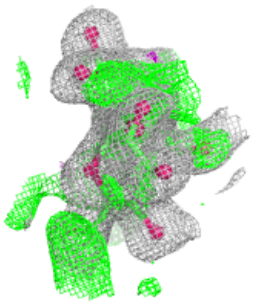


Electron density around DMU A 744:

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

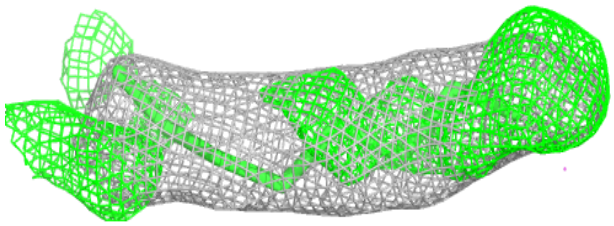


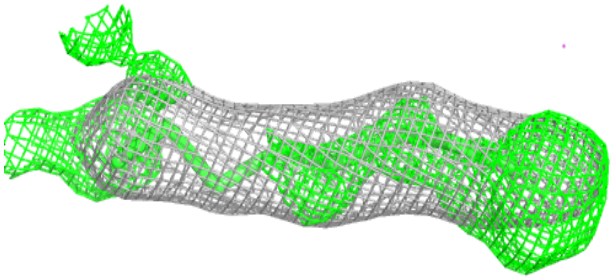


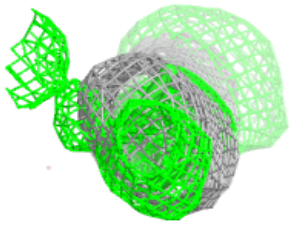


Electron density around DMU Z 746:

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

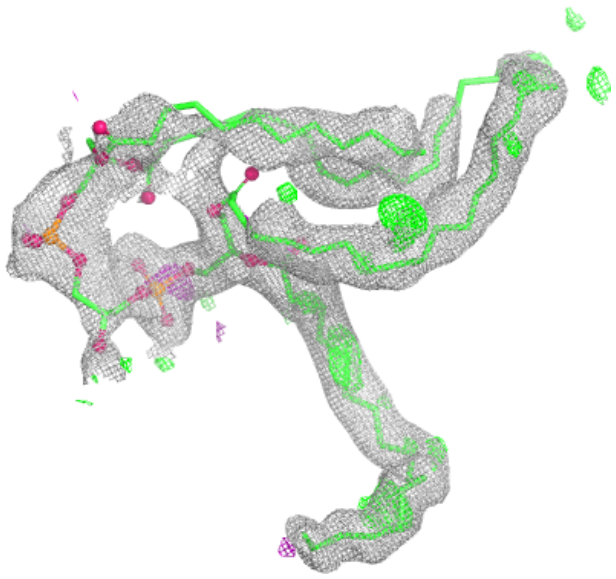


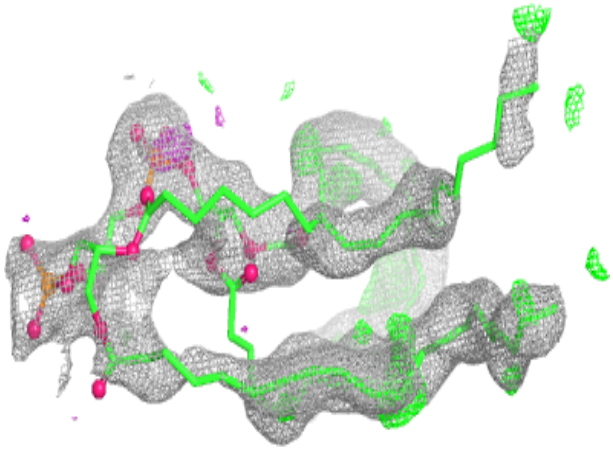


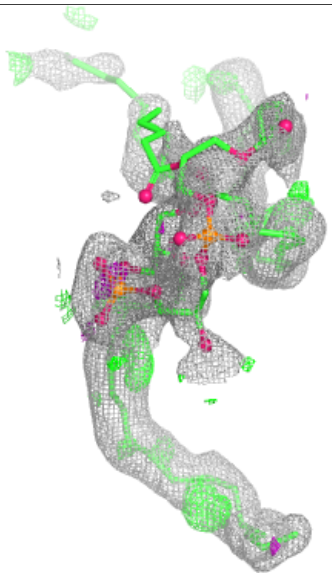


Electron density around CDL A 521:

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

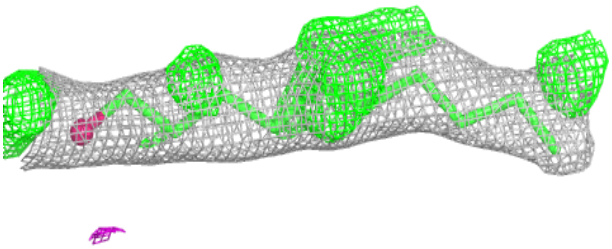


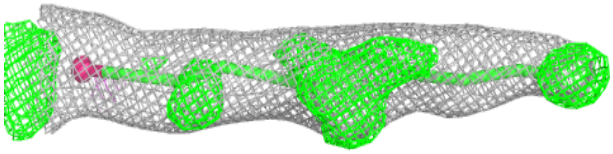


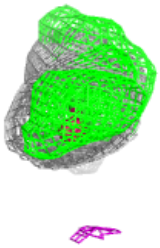


Electron density around DMU C 272:

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

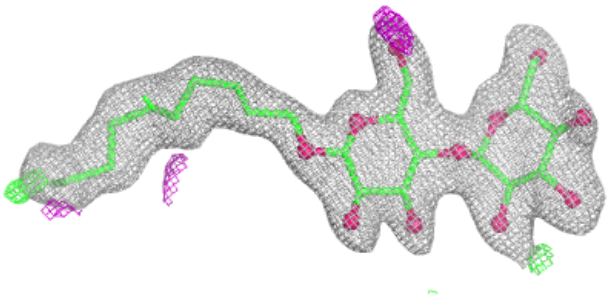


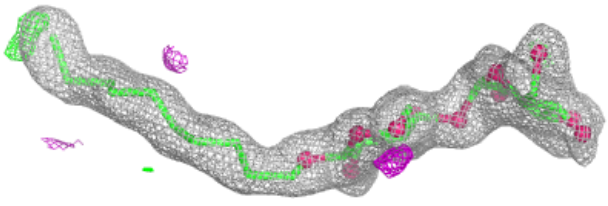


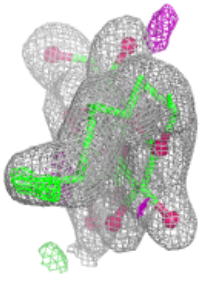


Electron density around DMU N 526:

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

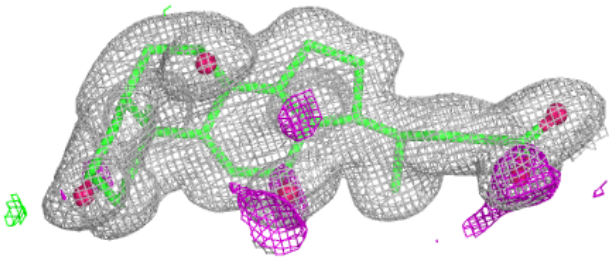


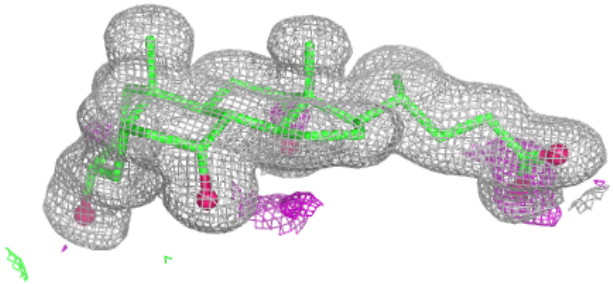


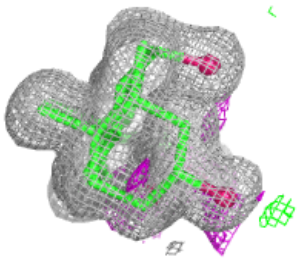


Electron density around CHD A 525:

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

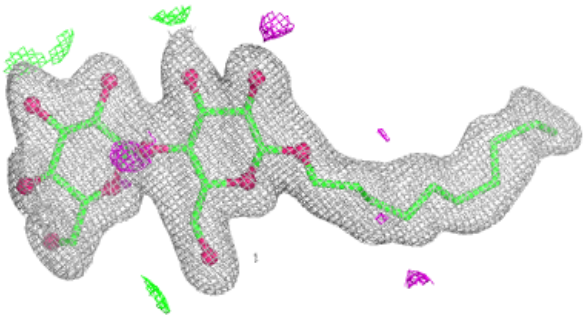


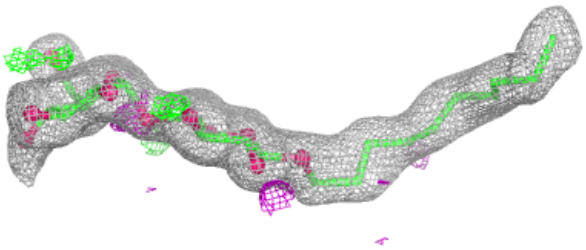


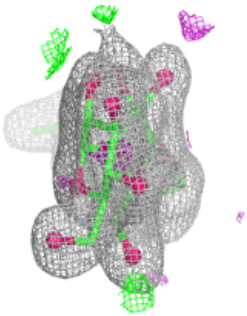


Electron density around DMU A 526:

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

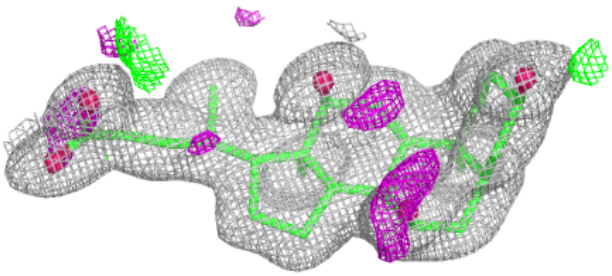


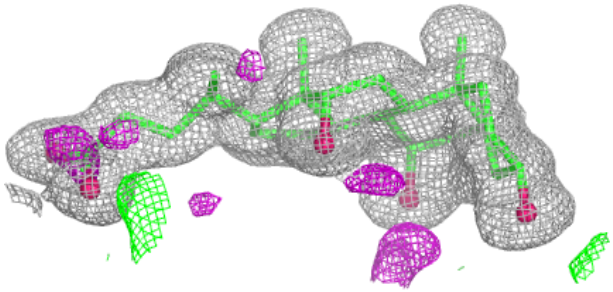


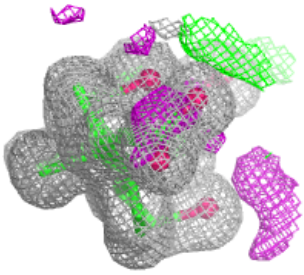


Electron density around CHD N 525:

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

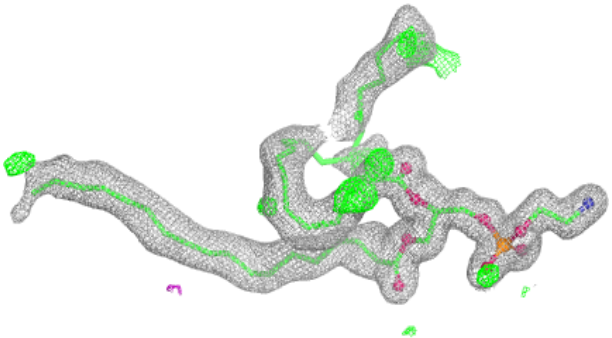


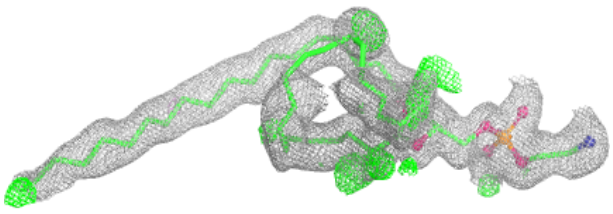


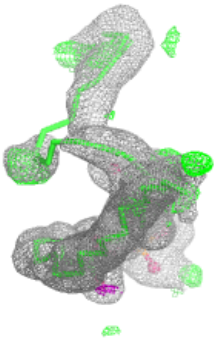


Electron density around PEK P 264:

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

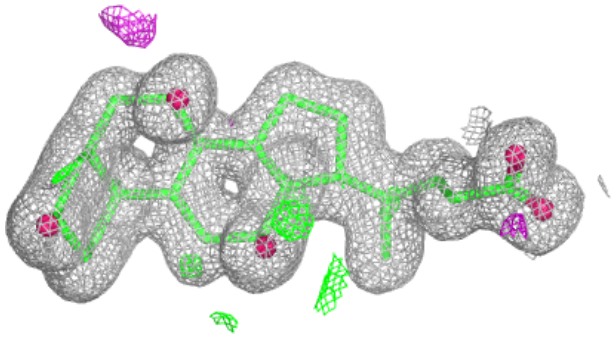


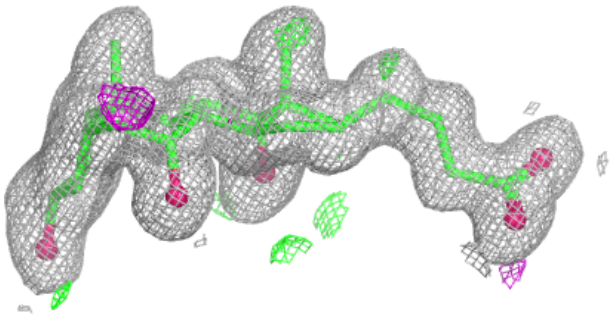


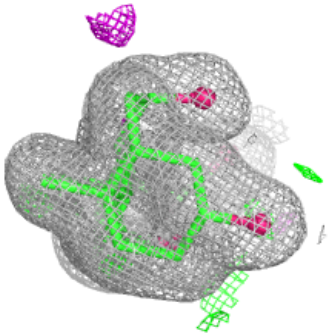


Electron density around CHD G 86:

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

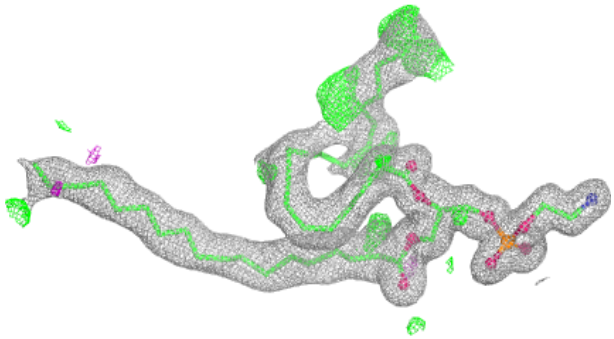


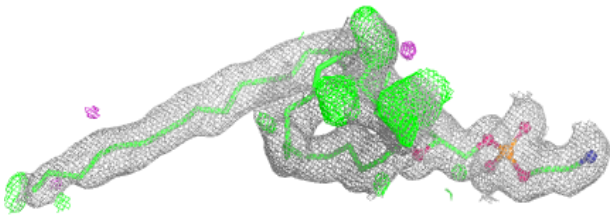


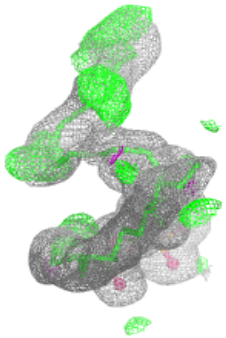


Electron density around PEK C 264:

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

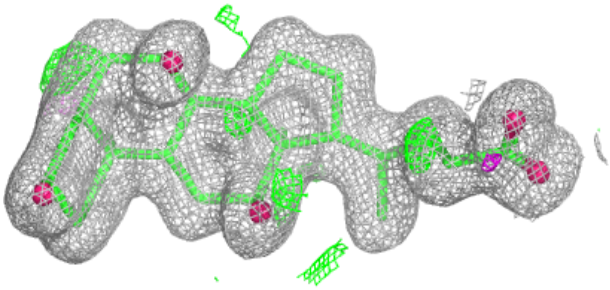


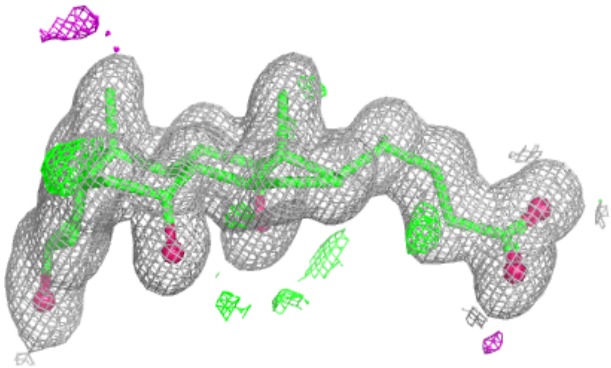


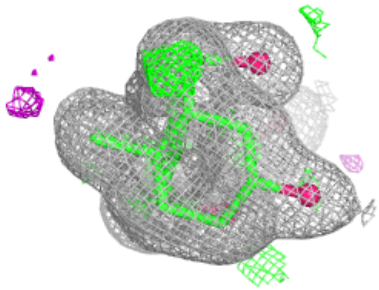


Electron density around CHD T 86:

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

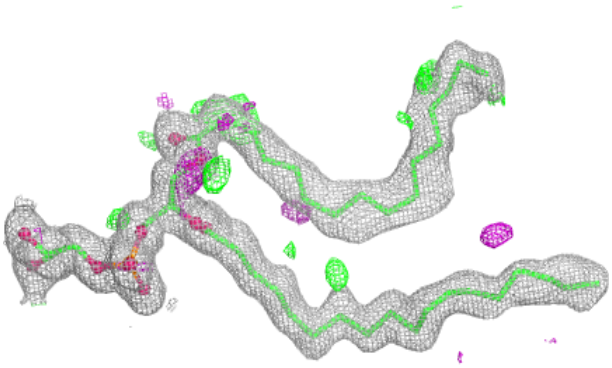


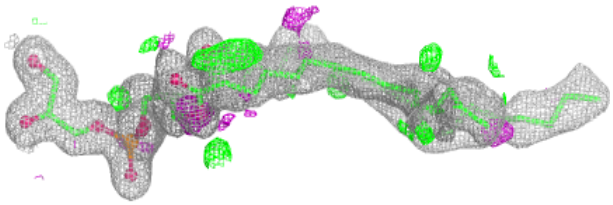


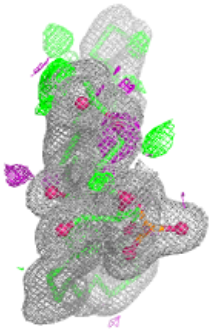


Electron density around PGV P 266:

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

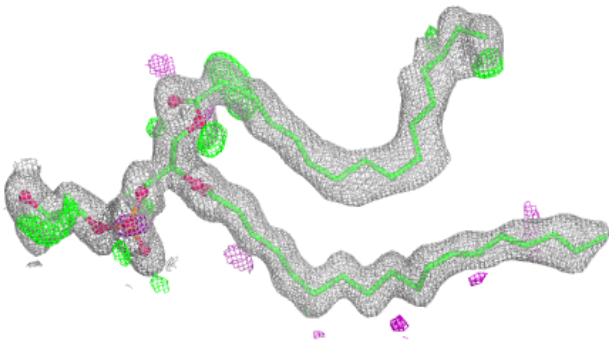


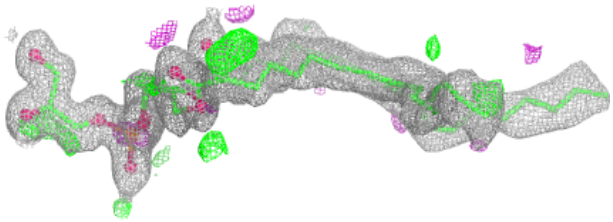


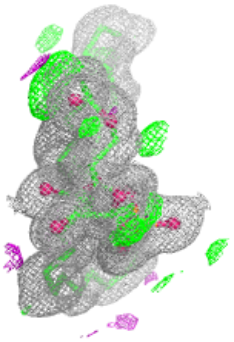


Electron density around PGV C 266:

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

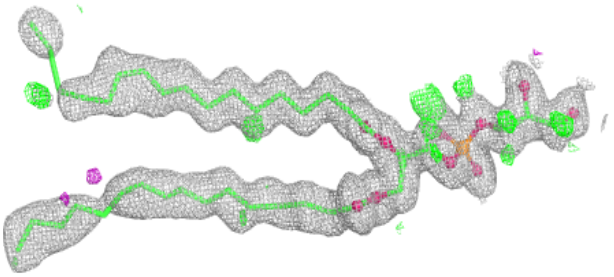


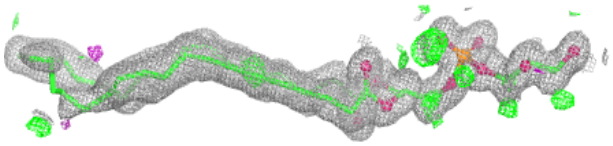


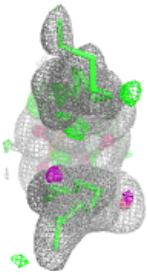


Electron density around PGV C 267:

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

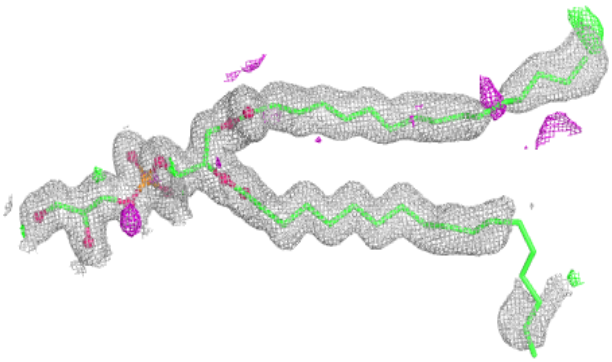


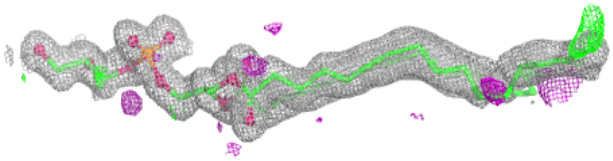


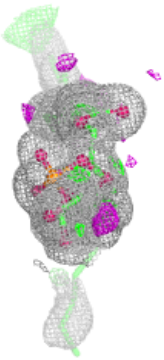


Electron density around PGV P 267:

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

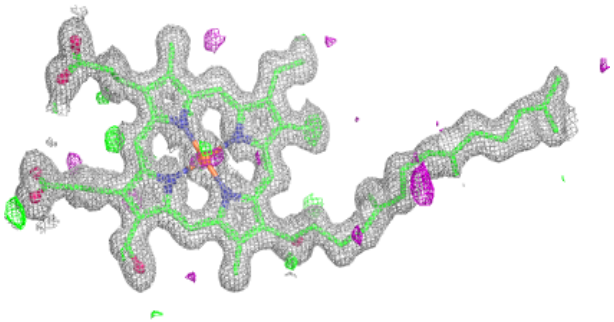


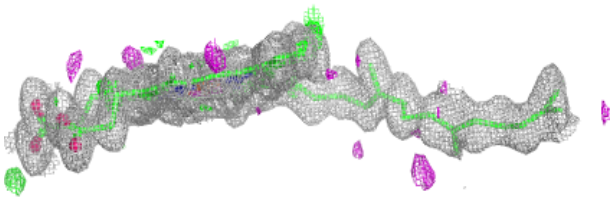


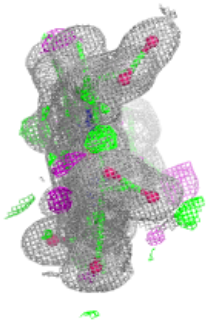


Electron density around HEA A 515 (A):

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

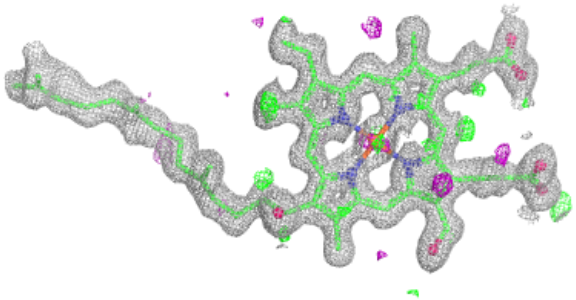


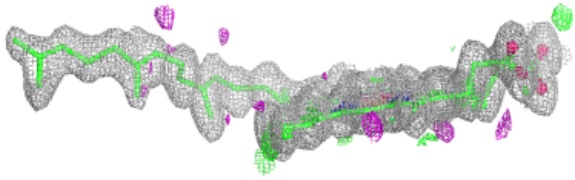


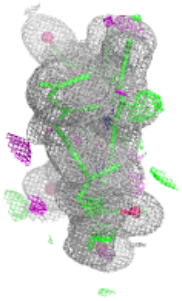


Electron density around HEA A 515 (B):

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

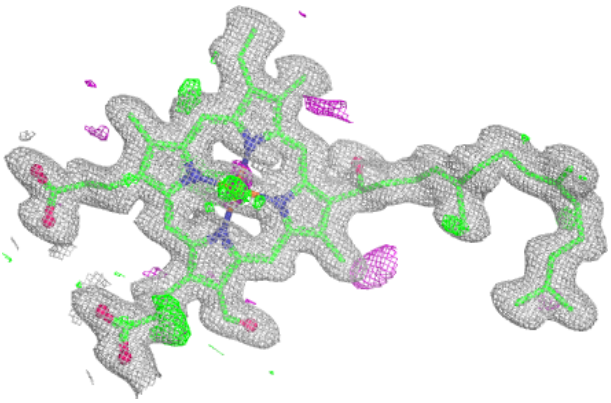


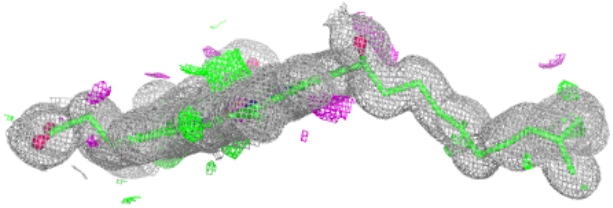


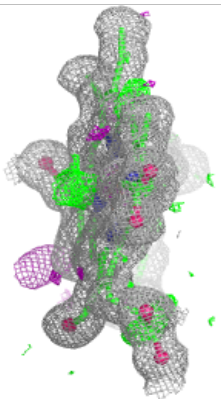


Electron density around HEA A 516:

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

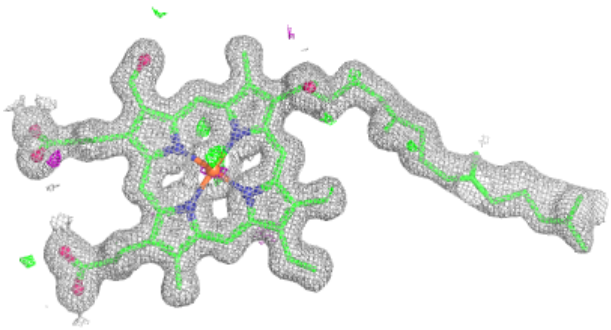


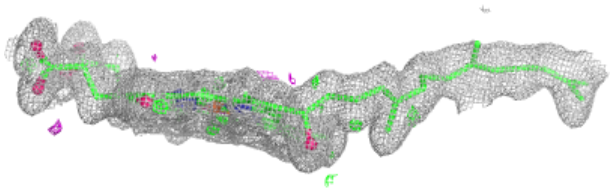


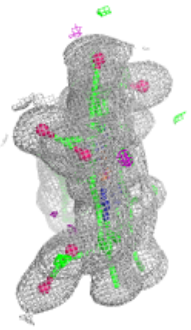


Electron density around HEA N 515 (A):

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

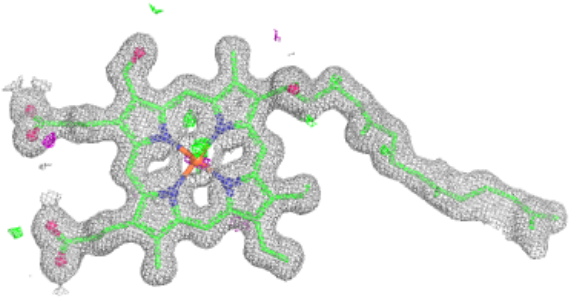


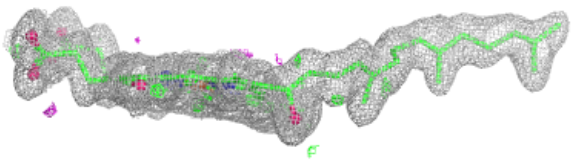


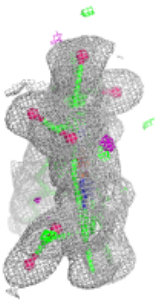


Electron density around HEA N 515 (B):

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

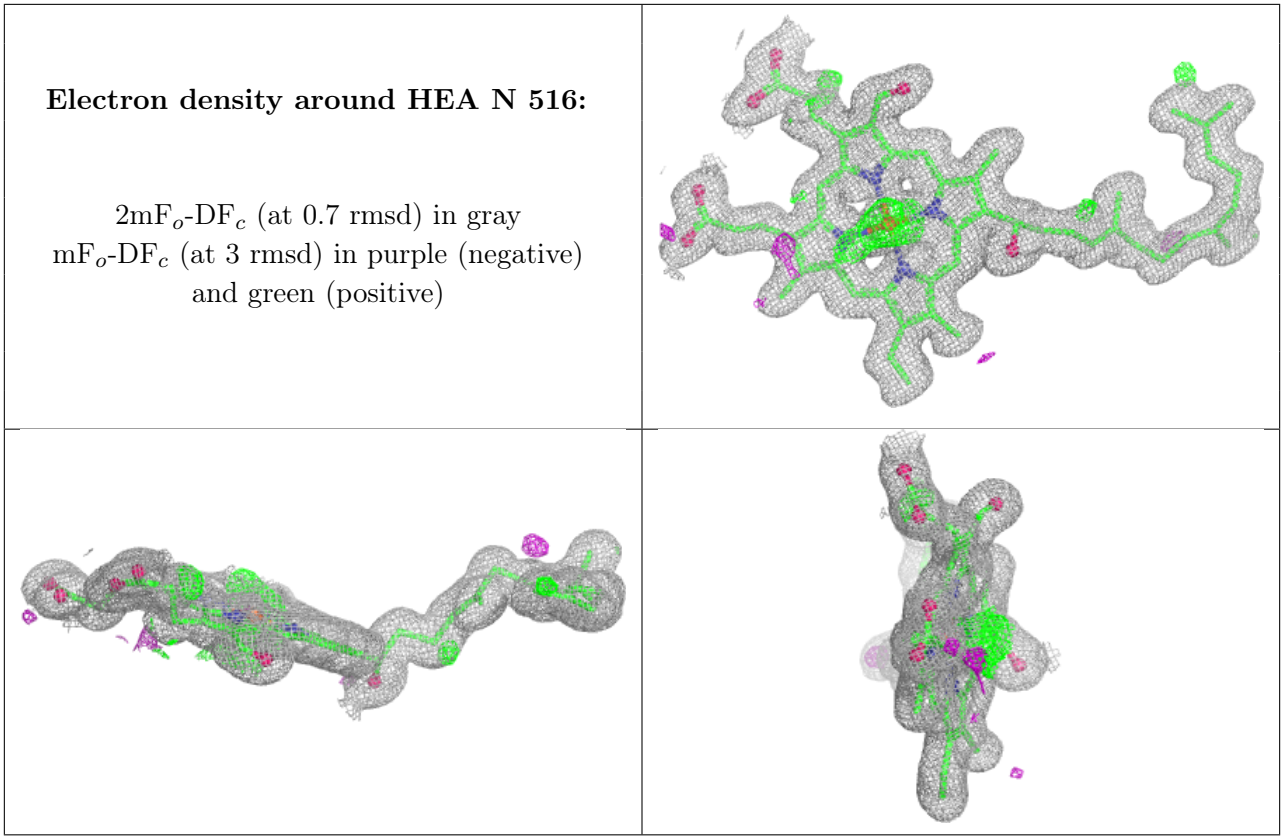






Electron density around HEA N 516:

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



6.5 Other polymers (i)

There are no such residues in this entry.