Full wwPDB X-ray Structure Validation Report

Oct 30, 2023 – 02:59 PM JST

PDB ID	:	5B1B
Title	:	Bovine heart cytochrome c oxidase in the fully reduced state at 1.6 angstrom resolution
Authors	:	Yano, N.; Muramoto, K.; Shimada, A.; Takemura, S.; Baba, J.; Fujisawa, H.; Mochizuki, M.; Shinzawa-Itoh, K.; Yamashita, E.; Tsukihara, T.; Yoshikawa, S.
Deposited on	:	2015-12-01
Resolution	:	1.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

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

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

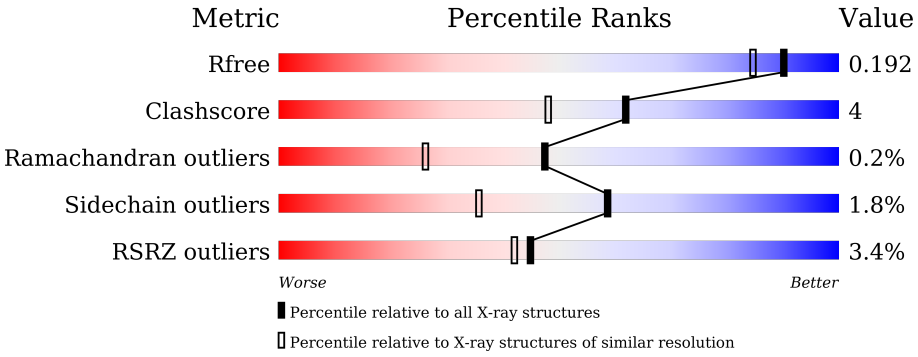
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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	88% 11%
1	N	514	88% 12%
2	B	227	% 86% 12%
2	O	227	2% 85% 15%
3	C	259	93% 7%
3	P	259	93% 7%

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Mol	Chain	Length	Quality of chain
4	D	144	90% 9%
4	Q	144	8% 94% 5%
5	E	105	3% 96%
5	R	105	2% 97%
6	F	98	7% 87% 11%
6	S	98	8% 87% 10%
7	G	84	23% 89% 7%
7	T	84	18% 85% 13%
8	H	79	9% 89% 11%
8	U	79	10% 89% 11%
9	I	73	8% 99%
9	V	73	5% 95% 5%
10	J	58	7% 91% 9%
10	W	58	5% 93% 5%
11	K	49	2% 92% 8%
11	X	49	6% 92% 8%
12	L	46	2% 83% 17%
12	Y	46	2% 91% 7%
13	M	43	9% 93% 7%
13	Z	43	9% 91% 9%

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
23	CHD	J	101	-	-	-	X
24	DMU	D	203	-	-	-	X
24	DMU	K	103	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	DMU	X	101	-	-	-	X
25	CDL	P	305	-	-	-	X
9	SAC	V	1	-	-	-	X

2 Entry composition (i)

There are 29 unique types of molecules in this entry. The entry contains 34425 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	514	Total	C	N	O	S	0	20	0
			4107	2743	633	689	42			
1	N	514	Total	C	N	O	S	0	21	0
			4107	2742	633	689	43			

- 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	6	0
			1844	1198	283	344	19			
2	O	227	Total	C	N	O	S	0	4	0
			1841	1196	284	343	18			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	259	Total	C	N	O	S	0	8	0
			2126	1420	337	356	13			
3	P	259	Total	C	N	O	S	0	8	0
			2129	1423	336	355	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	144	Total	C	N	O	S	0	6	0
			1214	792	200	218	4			
4	Q	144	Total	C	N	O	S	0	1	0
			1196	778	196	218	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	105	Total	C	N	O	S	0	1	0
			858	547	147	162	2			
5	R	105	Total	C	N	O	S	0	0	0
			852	544	144	162	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	98	Total	C	N	O	S	0	4	0
			758	470	136	147	5			
6	S	98	Total	C	N	O	S	0	1	0
			750	465	134	146	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	84	Total	C	N	O	S	0	1	0
			677	437	129	110	1			
7	T	84	Total	C	N	O	S	0	3	0
			687	445	130	111	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	79	Total	C	N	O	S	0	0	0
			662	417	121	119	5			
8	U	79	Total	C	N	O	S	0	0	0
			662	417	121	119	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	73	Total	C	N	O	S	0	0	0
			601	390	107	100	4			
9	V	73	Total	C	N	O	S	0	1	0
			602	391	107	100	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	58	Total	C	N	O	S	0	0	0
			460	297	78	82	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	W	58	Total	C	N	O	S	0	0	0
			460	297	78	82	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	49	Total	C	N	O	S	0	1	0
			386	252	65	67	2			
11	X	49	Total	C	N	O	S	0	1	0
			386	252	65	67	2			

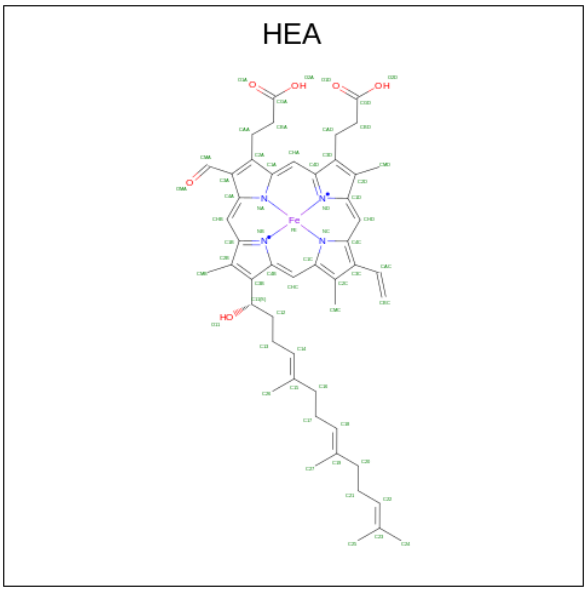
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	0	0
			380	254	64	60	2			
12	Y	46	Total	C	N	O	S	0	0	0
			380	254	64	60	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	43	Total	C	N	O	0	0	0
			335	223	53	59			
13	Z	43	Total	C	N	O	0	0	0
			335	223	53	59			

- Molecule 14 is HEME-A (three-letter code: 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
			70	58	1	4	7		
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
			70	58	1	4	7		
14	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		

- Molecule 15 is COPPER (II) ION (three-letter code: 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		

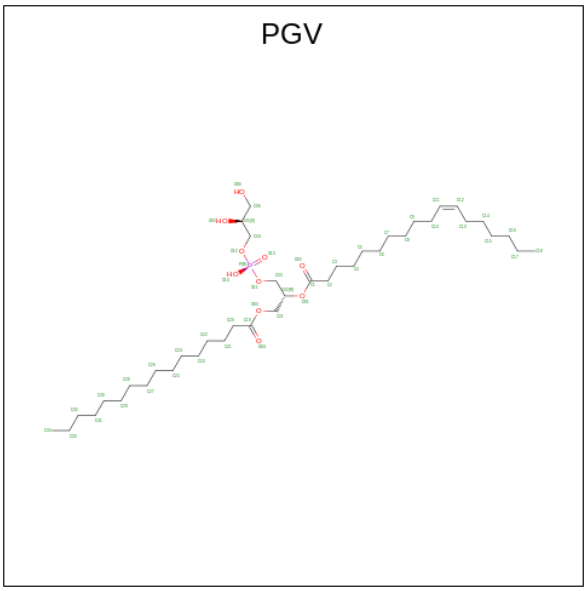
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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 (three-letter code: NA) (formula: Na).

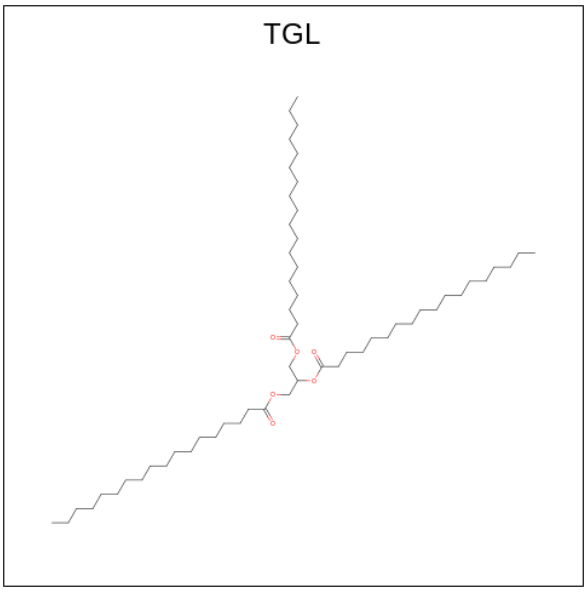
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total Na 1 1	0	0
17	N	1	Total Na 1 1	0	0

- Molecule 18 is (1R)-2-{[{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: $C_{40}H_{77}O_{10}P$).



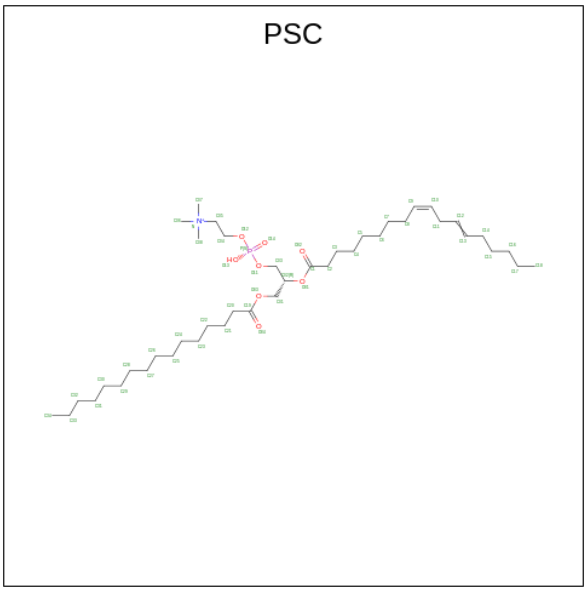
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total C O P 51 40 10 1	0	0
18	A	1	Total C O 37 34 3	0	0
18	C	1	Total C O P 51 40 10 1	0	0
18	C	1	Total C O 36 34 2	0	0
18	N	1	Total C O 40 36 4	0	0
18	N	1	Total C O P 51 40 10 1	0	0
18	P	1	Total C O 41 37 4	0	0
18	P	1	Total C O P 50 39 10 1	0	0

- Molecule 19 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: $C_{57}H_{110}O_6$).



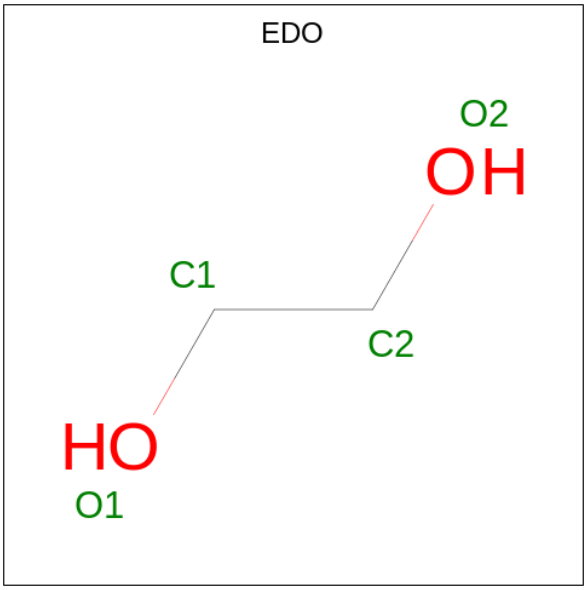
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	A	1	Total C O 62 57 5	0	0
19	D	1	Total C O 63 57 6	0	0
19	L	1	Total C O 59 53 6	0	0
19	N	1	Total C O 57 54 3	0	0
19	O	1	Total C O 58 52 6	0	0
19	Q	1	Total C O 63 57 6	0	0

- Molecule 20 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (three-letter code: PSC) (formula: $C_{42}H_{81}NO_8P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	A	1	Total C 25 25	0	0
20	O	1	Total C 24 24	0	0

- Molecule 21 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	A	1	Total C O 4 2 2	0	0
21	A	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	A	1	Total C O 4 2 2	0	0
21	A	1	Total C O 4 2 2	0	0
21	A	1	Total C O 4 2 2	0	0
21	A	1	Total C O 4 2 2	0	0
21	A	1	Total C O 4 2 2	0	0
21	A	1	Total C O 4 2 2	0	0
21	A	1	Total C O 4 2 2	0	0
21	A	1	Total C O 4 2 2	0	0
21	B	1	Total C O 4 2 2	0	0
21	B	1	Total C O 4 2 2	0	0
21	B	1	Total C O 4 2 2	0	0
21	B	1	Total C O 4 2 2	0	0
21	C	1	Total C O 4 2 2	0	0
21	C	1	Total C O 4 2 2	0	0
21	C	1	Total C O 4 2 2	0	0
21	C	1	Total C O 4 2 2	0	0
21	C	1	Total C O 4 2 2	0	0
21	E	1	Total C O 4 2 2	0	0
21	E	1	Total C O 4 2 2	0	0
21	F	1	Total C O 4 2 2	0	0
21	F	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	F	1	Total C O 4 2 2	0	0
21	F	1	Total C O 4 2 2	0	0
21	F	1	Total C O 4 2 2	0	0
21	G	1	Total C O 4 2 2	0	0
21	J	1	Total C O 4 2 2	0	0
21	J	1	Total C O 4 2 2	0	0
21	N	1	Total C O 4 2 2	0	0
21	N	1	Total C O 4 2 2	0	0
21	N	1	Total C O 4 2 2	0	0
21	N	1	Total C O 4 2 2	0	0
21	N	1	Total C O 4 2 2	0	0
21	N	1	Total C O 4 2 2	0	0
21	N	1	Total C O 4 2 2	0	0
21	N	1	Total C O 4 2 2	0	0
21	N	1	Total C O 4 2 2	0	0
21	N	1	Total C O 4 2 2	0	0
21	N	1	Total C O 4 2 2	0	0
21	N	1	Total C O 4 2 2	0	0
21	N	1	Total C O 4 2 2	0	0
21	O	1	Total C O 4 2 2	0	0
21	O	1	Total C O 4 2 2	0	0

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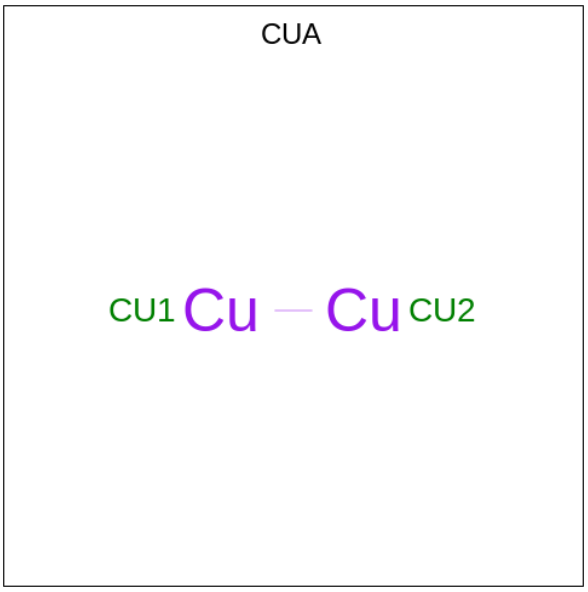
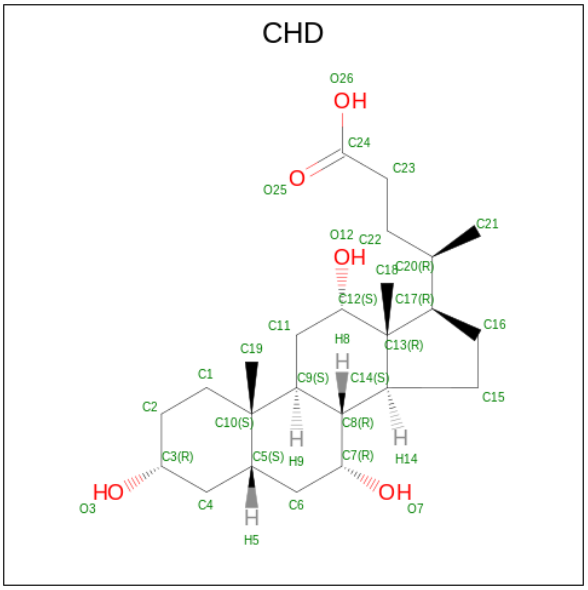
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	O	1	Total	C	O	0	0
			4	2	2		
21	P	1	Total	C	O	0	0
			4	2	2		
21	P	1	Total	C	O	0	0
			4	2	2		
21	P	1	Total	C	O	0	0
			4	2	2		
21	Q	1	Total	C	O	0	0
			4	2	2		
21	Q	1	Total	C	O	0	0
			4	2	2		
21	Q	1	Total	C	O	0	0
			4	2	2		
21	R	1	Total	C	O	0	0
			4	2	2		
21	S	1	Total	C	O	0	0
			4	2	2		
21	S	1	Total	C	O	0	0
			4	2	2		
21	S	1	Total	C	O	0	0
			4	2	2		
21	S	1	Total	C	O	0	0
			4	2	2		
21	S	1	Total	C	O	0	0
			4	2	2		
21	T	1	Total	C	O	0	0
			4	2	2		
21	T	1	Total	C	O	0	0
			4	2	2		
21	W	1	Total	C	O	0	0
			4	2	2		
21	W	1	Total	C	O	0	0
			4	2	2		
21	Y	1	Total	C	O	0	0
			4	2	2		

- Molecule 22 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu_2).



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

- Molecule 23 is CHOLIC ACID (three-letter code: CHD) (formula: $C_{24}H_{40}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	B	1	Total C O 29 24 5	0	0
23	C	1	Total C O 29 24 5	0	0

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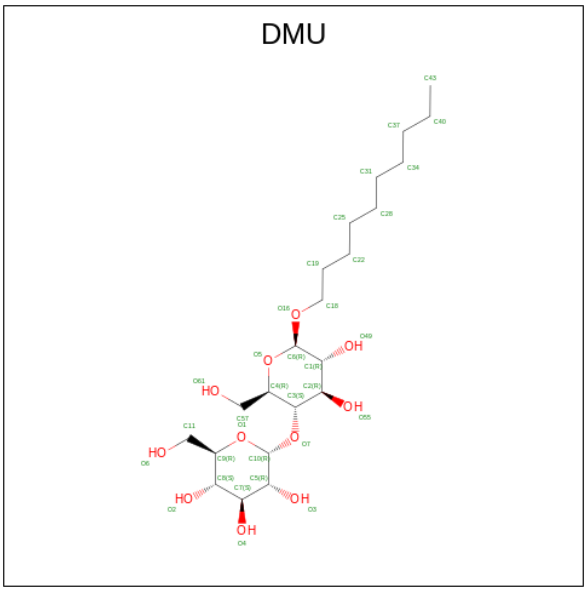
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	G	1	Total C O 29 24 5	0	0
23	J	1	Total C O 29 24 5	0	0
23	P	1	Total C O 29 24 5	0	0
23	P	1	Total C O 29 24 5	0	0

- Molecule 24 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: $C_{22}H_{42}O_{11}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	C	1	Total C 9 9	0	0
24	C	1	Total C O 12 11 1	0	0
24	D	1	Total C O 12 11 1	0	0
24	D	1	Total C 9 9	0	0
24	J	1	Total C O 12 10 2	0	0
24	K	1	Total C O 10 9 1	0	0
24	K	1	Total C 9 9	0	0

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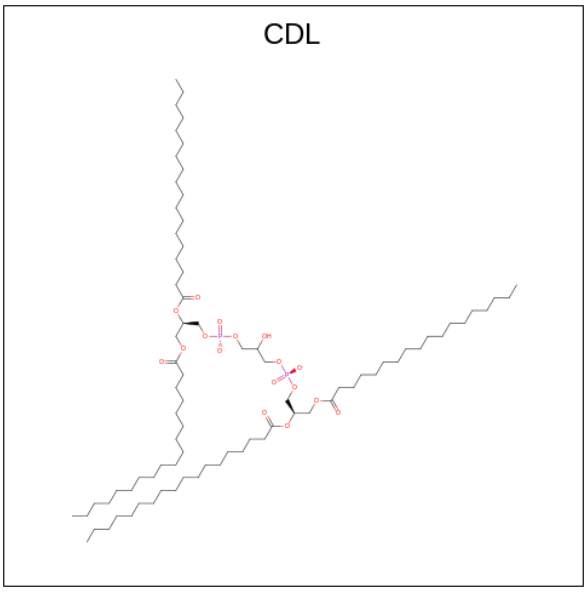
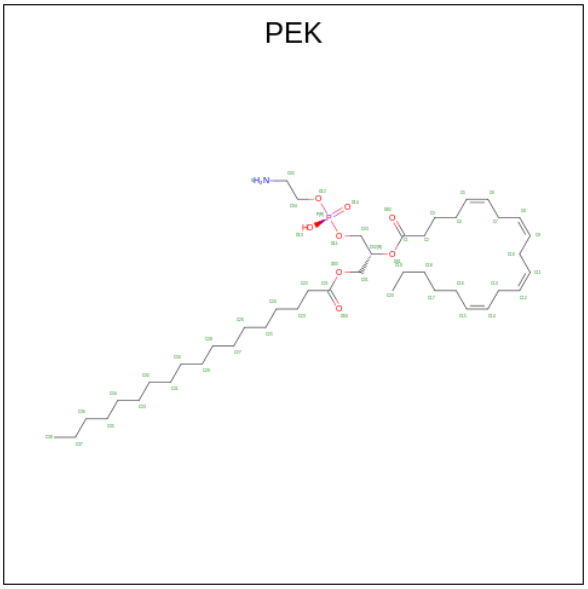
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	K	1	Total C O 33 22 11	0	0
24	K	1	Total C 10 10	0	0
24	K	1	Total C 9 9	0	0
24	K	1	Total C 9 9	0	0
24	L	1	Total C O 21 16 5	0	0
24	M	1	Total C O 33 22 11	0	0
24	O	1	Total C 10 10	0	0
24	P	1	Total C O 33 22 11	0	0
24	P	1	Total C O 11 10 1	0	0
24	W	1	Total C 9 9	0	0
24	X	1	Total C O 33 22 11	0	0
24	X	1	Total C 10 10	0	0
24	X	1	Total C 9 9	0	0
24	X	1	Total C 10 10	0	0
24	X	1	Total C O 11 10 1	0	0
24	Z	1	Total C O 33 22 11	0	0

- Molecule 25 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	C	1	Total C O 56 52 4	0	0
25	G	1	Total C O 64 63 1	0	0
25	P	1	Total C O 69 65 4	0	0
25	T	1	Total C O 79 73 6	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 (three-letter code: PEK) (formula: $C_{43}H_{78}NO_8P$).

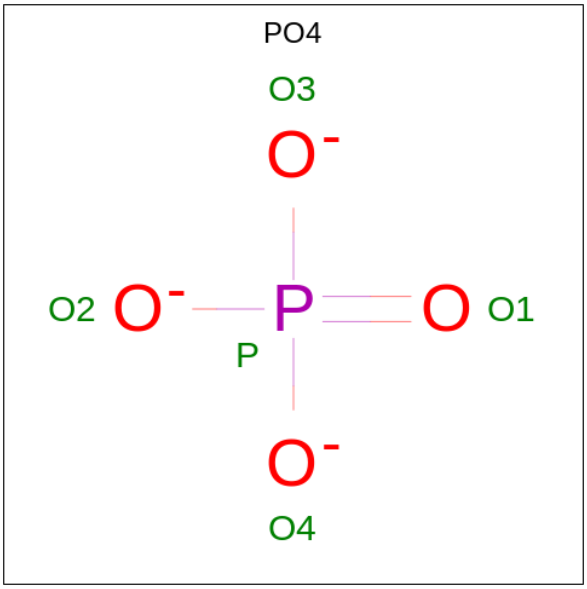


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	C	1	Total C 37 37	0	0
26	C	1	Total C 26 26	0	0
26	G	1	Total C N O P 53 43 1 8 1	0	0
26	P	1	Total C 20 20	0	0
26	P	1	Total C N O P 53 43 1 8 1	0	0
26	P	1	Total C O 39 37 2	0	0

- Molecule 27 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 28 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	H	1	Total O P 5 4 1	0	0
28	U	1	Total O P 5 4 1	0	0

- Molecule 29 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	266	Total O 266 266	0	1
29	B	232	Total O 233 233	0	1
29	C	161	Total O 161 161	0	0
29	D	232	Total O 232 232	0	0
29	E	171	Total O 171 171	0	0
29	F	187	Total O 187 187	0	1
29	G	101	Total O 101 101	0	0
29	H	121	Total O 121 121	0	0
29	I	75	Total O 75 75	0	0
29	J	63	Total O 63 63	0	0
29	K	55	Total O 55 55	0	0
29	L	53	Total O 53 53	0	0
29	M	48	Total O 48 48	0	0
29	N	265	Total O 265 265	0	0
29	O	203	Total O 204 204	0	1
29	P	180	Total O 180 180	0	1
29	Q	133	Total O 133 133	0	0
29	R	148	Total O 148 148	0	0
29	S	174	Total O 174 174	0	0
29	T	84	Total O 84 84	0	0
29	U	103	Total O 103 103	0	0

Continued on next page...

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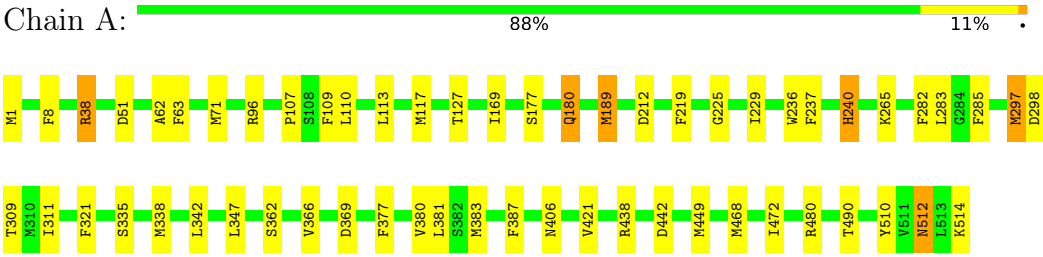
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	V	69	Total O 69 69	0	0
29	W	66	Total O 66 66	0	0
29	X	48	Total O 48 48	0	0
29	Y	35	Total O 35 35	0	0
29	Z	30	Total O 30 30	0	0

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.

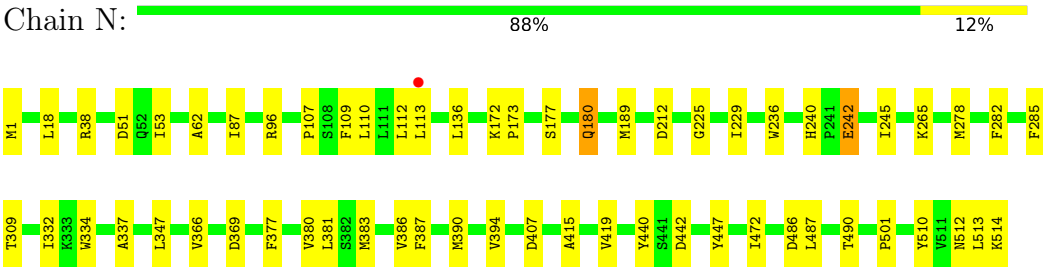
• Molecule 1: Cytochrome c oxidase subunit 1

Chain A:



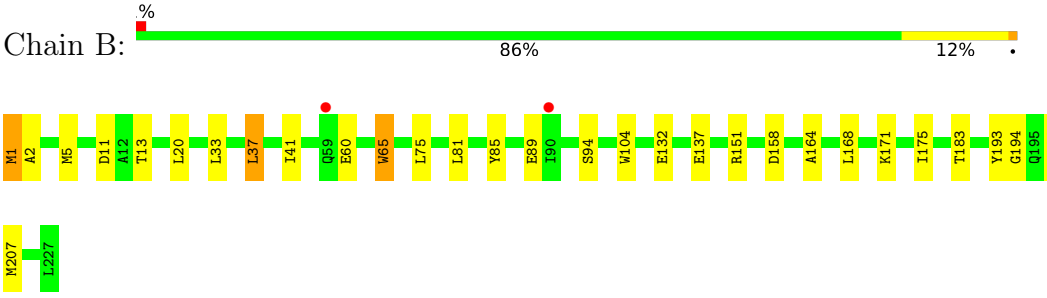
• Molecule 1: Cytochrome c oxidase subunit 1

Chain N:



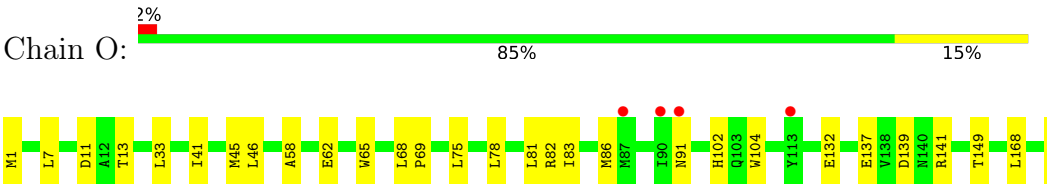
• Molecule 2: Cytochrome c oxidase subunit 2

Chain B:



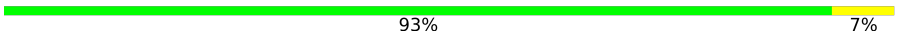
• Molecule 2: Cytochrome c oxidase subunit 2

Chain O:



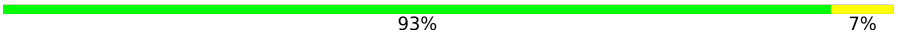
• Molecule 3: Cytochrome c oxidase subunit 3

Chain C:



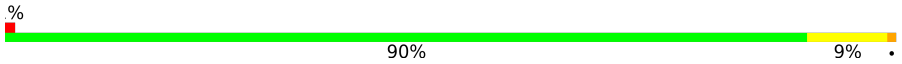
• Molecule 3: Cytochrome c oxidase subunit 3

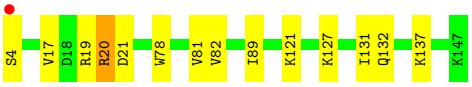
Chain P:



• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

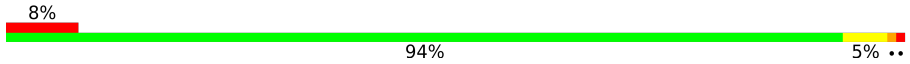
Chain D:

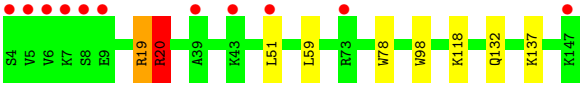




• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

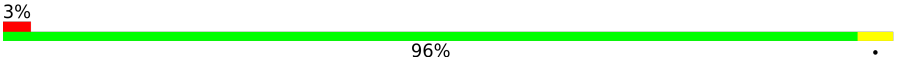
Chain Q:





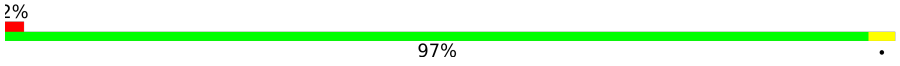
• Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

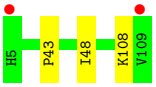
Chain E:



• Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

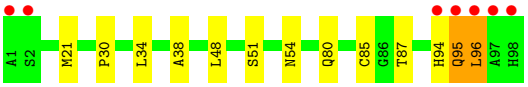
Chain R:





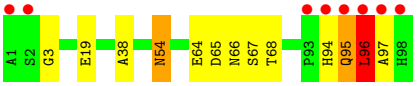
• Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

Chain F:



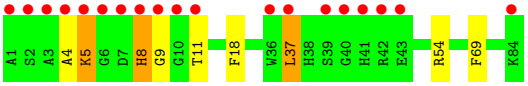
• Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

Chain S:



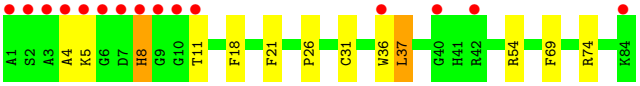
• Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain G:



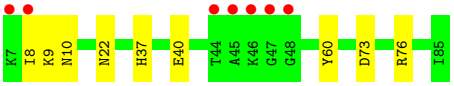
• Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain T:



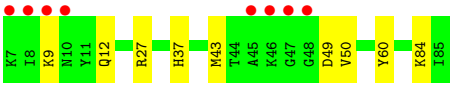
• Molecule 8: Cytochrome c oxidase subunit 6B1

Chain H:



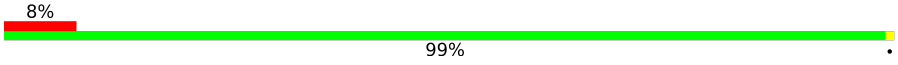
• Molecule 8: Cytochrome c oxidase subunit 6B1

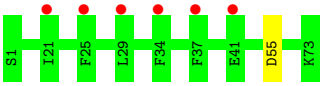
Chain U:



• Molecule 9: Cytochrome c oxidase subunit 6C

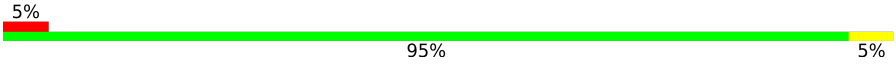
Chain I:

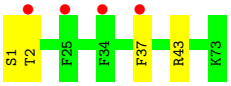




• Molecule 9: Cytochrome c oxidase subunit 6C

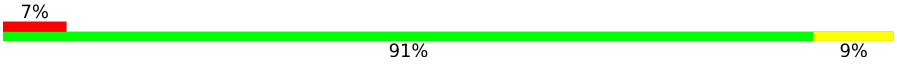
Chain V:

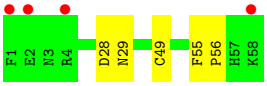




• Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial

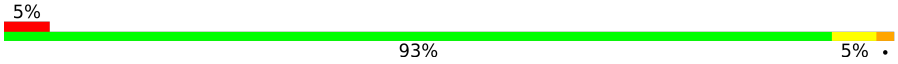
Chain J:

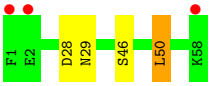




• Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial

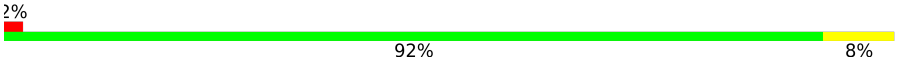
Chain W:





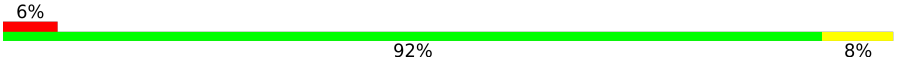
• Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial

Chain K:



• Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial

Chain X:

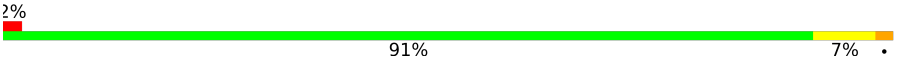


• Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

Chain L:

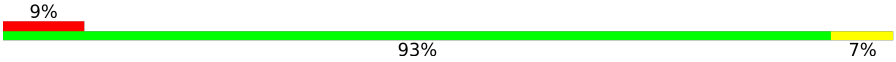
• Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

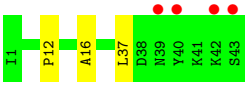
Chain Y:



• Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial

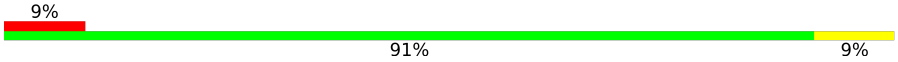
Chain M:

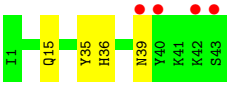




• Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial

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	181.61Å 204.14Å 177.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.90 – 1.60 88.98 – 1.40	Depositor EDS
% Data completeness (in resolution range)	97.5 (39.90-1.60) 96.5 (88.98-1.40)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.61 (at 1.40Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.168 , 0.191 0.169 , 0.192	Depositor DCC
R_{free} test set	61730 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	18.7	Xtriage
Anisotropy	0.588	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 59.8	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	34425	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.58% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, CUA, CHD, NA, TGL, DMU, SAC, PO4, FME, CU, PSC, PEK, MG, CDL, HEA, PGV, ZN

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	1.07	4/4306 (0.1%)	1.06	20/5877 (0.3%)
1	N	1.01	3/4321 (0.1%)	0.99	13/5896 (0.2%)
2	B	0.96	0/1912	1.00	3/2603 (0.1%)
2	O	0.82	1/1900 (0.1%)	0.92	6/2588 (0.2%)
3	C	0.95	1/2261 (0.0%)	0.89	3/3090 (0.1%)
3	P	0.95	1/2260 (0.0%)	0.89	3/3088 (0.1%)
4	D	0.86	1/1284 (0.1%)	1.19	3/1730 (0.2%)
4	Q	0.65	0/1237	0.72	2/1668 (0.1%)
5	E	0.82	1/882 (0.1%)	0.89	2/1196 (0.2%)
5	R	0.71	0/871	0.71	0/1182
6	F	0.84	0/797	0.89	0/1082
6	S	0.76	0/772	0.82	0/1048
7	G	0.80	0/710	0.80	0/966
7	T	0.70	0/732	0.74	0/997
8	H	0.82	0/682	0.89	2/921 (0.2%)
8	U	0.81	0/682	0.76	0/921
9	I	0.67	0/605	0.73	1/802 (0.1%)
9	V	0.63	0/613	0.71	1/812 (0.1%)
10	J	0.62	0/471	0.72	2/636 (0.3%)
10	W	0.60	0/471	0.71	1/636 (0.2%)
11	K	0.80	0/405	0.75	0/556
11	X	0.61	0/405	0.61	0/556
12	L	1.03	0/393	0.85	0/526
12	Y	0.82	0/393	0.71	0/526
13	M	0.85	0/345	0.83	0/470
13	Z	0.84	1/345 (0.3%)	0.68	0/470
All	All	0.90	13/30055 (0.0%)	0.91	62/40843 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected

by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	N	0	1
All	All	0	2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	Z	35	TYR	CD2-CE2	9.30	1.53	1.39
4	D	20	ARG	CZ-NH1	7.52	1.42	1.33
3	C	102	TYR	CG-CD2	-6.33	1.30	1.39
3	P	153	GLU	CG-CD	6.09	1.61	1.51
5	E	70	VAL	CB-CG1	-5.90	1.40	1.52
1	N	242	GLU	CD-OE1	5.70	1.31	1.25
2	O	197	SER	CB-OG	5.66	1.49	1.42
1	A	237	PHE	CD1-CE1	5.53	1.50	1.39
1	A	512	ASN	CB-CG	-5.45	1.38	1.51
1	N	447	TYR	CE1-CZ	5.20	1.45	1.38
1	N	440	TYR	CD1-CE1	5.09	1.47	1.39
1	A	335	SER	CB-OG	5.08	1.48	1.42
1	A	219	PHE	CE2-CZ	5.01	1.46	1.37

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	20	ARG	NE-CZ-NH1	25.98	133.29	120.30
4	D	20	ARG	NE-CZ-NH2	-22.15	109.23	120.30
1	N	189	MET	CG-SD-CE	-11.60	81.63	100.20
4	Q	20	ARG	NE-CZ-NH1	10.25	125.43	120.30
4	Q	20	ARG	NE-CZ-NH2	-9.69	115.46	120.30
1	A	38	ARG	NE-CZ-NH1	8.74	124.67	120.30
1	A	38	ARG	NE-CZ-NH2	-8.50	116.05	120.30
1	A	442	ASP	CB-CG-OD1	7.84	125.36	118.30
2	O	141	ARG	NE-CZ-NH1	-7.62	116.49	120.30
1	N	96	ARG	NE-CZ-NH2	-7.33	116.64	120.30
3	C	214	PHE	CB-CG-CD2	-6.89	115.97	120.80
10	J	28	ASP	CB-CG-OD2	-6.83	112.15	118.30
1	A	63	PHE	CB-CG-CD2	-6.75	116.08	120.80
4	D	20	ARG	CD-NE-CZ	6.68	132.96	123.60
1	A	480	ARG	NE-CZ-NH1	6.63	123.62	120.30
1	A	300	ASP	CB-CG-OD2	-6.61	112.35	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	V	43	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	N	212	ASP	CB-CG-OD2	-6.45	112.50	118.30
5	E	40	ASP	CB-CG-OD1	6.33	123.99	118.30
2	B	11	ASP	CB-CG-OD1	6.31	123.98	118.30
1	N	440	TYR	CD1-CE1-CZ	-6.29	114.14	119.80
1	A	96	ARG	NE-CZ-NH2	-6.25	117.18	120.30
3	C	214	PHE	CB-CG-CD1	6.24	125.17	120.80
1	A	442	ASP	CB-CG-OD2	-6.09	112.82	118.30
2	O	11	ASP	CB-CG-OD1	6.08	123.77	118.30
1	N	38	ARG	NE-CZ-NH2	-5.93	117.33	120.30
5	E	73	ASP	CB-CG-OD2	-5.88	113.01	118.30
1	A	189[A]	MET	CG-SD-CE	-5.78	90.96	100.20
1	A	189[B]	MET	CG-SD-CE	-5.78	90.96	100.20
10	W	28	ASP	CB-CG-OD2	-5.69	113.18	118.30
1	N	51	ASP	CB-CG-OD2	5.61	123.35	118.30
1	N	212	ASP	CB-CG-OD1	5.59	123.33	118.30
1	A	51	ASP	CB-CG-OD2	-5.58	113.28	118.30
2	O	82	ARG	NE-CZ-NH2	-5.51	117.55	120.30
8	H	76	ARG	NE-CZ-NH1	5.48	123.04	120.30
2	O	65	TRP	CA-CB-CG	5.46	124.07	113.70
8	H	73	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	N	298[A]	ASP	CB-CG-OD1	5.36	123.12	118.30
1	N	298[B]	ASP	CB-CG-OD1	5.36	123.12	118.30
1	N	366	VAL	CG1-CB-CG2	-5.35	102.34	110.90
1	A	366	VAL	CG1-CB-CG2	-5.32	102.38	110.90
2	O	141	ARG	NE-CZ-NH2	5.31	122.95	120.30
1	A	8	PHE	CB-CG-CD2	-5.30	117.09	120.80
1	A	8	PHE	CB-CG-CD1	5.28	124.49	120.80
1	N	38	ARG	NE-CZ-NH1	5.27	122.94	120.30
2	B	151	ARG	NE-CZ-NH2	-5.27	117.67	120.30
9	I	55	ASP	CB-CG-OD1	5.26	123.03	118.30
1	A	71[A]	MET	CG-SD-CE	5.23	108.56	100.20
1	A	71[B]	MET	CG-SD-CE	5.23	108.56	100.20
1	A	438	ARG	NE-CZ-NH1	5.16	122.88	120.30
3	P	241	TYR	CB-CG-CD1	-5.14	117.91	121.00
3	P	153	GLU	OE1-CD-OE2	5.14	129.47	123.30
1	A	212	ASP	CB-CG-OD2	-5.14	113.67	118.30
3	C	80	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	N	407	ASP	CB-CG-OD1	5.08	122.87	118.30
1	A	480	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	N	442	ASP	CB-CG-OD2	-5.02	113.78	118.30
3	P	233	PHE	CB-CG-CD1	-5.02	117.29	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	158	ASP	CB-CG-OD1	5.00	122.80	118.30
10	J	28	ASP	CB-CG-OD1	5.00	122.80	118.30
2	O	139	ASP	CB-CG-OD1	5.00	122.80	118.30
1	A	51	ASP	CB-CG-OD1	5.00	122.80	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
1	N	240	HIS	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4107	0	4099	42	0
1	N	4107	0	4086	47	0
2	B	1844	0	1850	19	0
2	O	1841	0	1841	17	0
3	C	2126	0	2026	17	0
3	P	2129	0	2043	13	0
4	D	1214	0	1203	11	0
4	Q	1196	0	1180	8	0
5	E	858	0	854	0	0
5	R	852	0	845	1	0
6	F	758	0	736	10	0
6	S	750	0	731	10	0
7	G	677	0	650	8	0
7	T	687	0	657	12	0
8	H	662	0	623	6	0
8	U	662	0	623	4	0
9	I	601	0	613	0	0
9	V	602	0	610	1	0
10	J	460	0	459	5	0
10	W	460	0	459	3	0
11	K	386	0	371	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	X	386	0	371	3	0
12	L	380	0	380	8	0
12	Y	380	0	380	3	0
13	M	335	0	352	3	0
13	Z	335	0	352	2	0
14	A	130	0	90	7	0
14	N	130	0	90	7	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	88	0	140	6	0
18	C	87	0	136	5	0
18	N	91	0	142	2	0
18	P	91	0	138	2	0
19	A	62	0	110	1	0
19	D	63	0	110	5	0
19	L	59	0	99	6	0
19	N	57	0	103	5	0
19	O	58	0	96	1	0
19	Q	63	0	110	7	0
20	A	25	0	41	3	0
20	O	24	0	40	0	0
21	A	40	0	59	5	0
21	B	16	0	24	2	0
21	C	20	0	30	0	0
21	E	8	0	12	0	0
21	F	20	0	30	3	0
21	G	4	0	6	0	0
21	J	8	0	12	0	0
21	N	52	0	78	4	0
21	O	12	0	18	1	0
21	P	12	0	18	0	0
21	Q	12	0	18	0	0
21	R	4	0	6	0	0
21	S	20	0	30	3	0
21	T	8	0	12	0	0
21	W	8	0	12	0	0
21	Y	4	0	6	0	0
22	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	O	2	0	0	0	0
23	B	29	0	39	0	0
23	C	29	0	39	0	0
23	G	29	0	39	1	0
23	J	29	0	39	1	0
23	P	58	0	78	1	0
24	C	21	0	38	2	0
24	D	21	0	38	1	0
24	J	12	0	21	0	0
24	K	80	0	127	2	0
24	L	21	0	30	4	0
24	M	33	0	42	0	0
24	O	10	0	19	0	0
24	P	44	0	63	4	0
24	W	9	0	17	0	0
24	X	73	0	116	2	0
24	Z	33	0	42	1	0
25	C	56	0	89	7	0
25	G	64	0	122	9	0
25	P	69	0	121	2	0
25	T	79	0	139	12	0
26	C	63	0	103	3	0
26	G	53	0	77	5	0
26	P	112	0	170	11	0
27	F	1	0	0	0	0
27	S	1	0	0	0	0
28	H	5	0	0	0	0
28	U	5	0	0	0	0
29	A	266	0	0	3	0
29	B	233	0	0	1	0
29	C	161	0	0	0	0
29	D	232	0	0	1	0
29	E	171	0	0	0	0
29	F	187	0	0	4	0
29	G	101	0	0	0	0
29	H	121	0	0	2	0
29	I	75	0	0	1	0
29	J	63	0	0	0	0
29	K	55	0	0	0	0
29	L	53	0	0	2	0
29	M	48	0	0	0	0
29	N	265	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	O	204	0	0	1	0
29	P	180	0	0	2	0
29	Q	133	0	0	0	0
29	R	148	0	0	0	0
29	S	174	0	0	3	0
29	T	84	0	0	1	0
29	U	103	0	0	2	0
29	V	69	0	0	0	0
29	W	66	0	0	0	0
29	X	48	0	0	0	0
29	Y	35	0	0	1	0
29	Z	30	0	0	0	0
All	All	34425	0	31818	275	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (275) 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)
6:S:68:THR:H	21:S:103:EDO:H12	1.43	0.82
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.68	0.76
3:C:213:THR:HG23	25:C:303:CDL:H771	1.68	0.74
25:T:101:CDL:H541	25:T:101:CDL:H231	1.72	0.71
7:G:9:GLY:HA3	29:N:707:HOH:O	1.91	0.70
7:G:4:ALA:HB3	1:N:282:PHE:HA	1.77	0.67
7:G:69:PHE:HB3	26:G:101:PEK:H011	1.78	0.66
20:A:609:PSC:H322	2:B:41:ILE:HD13	1.78	0.66
7:G:37:LEU:HD23	25:G:102:CDL:H391	1.76	0.66
26:C:307:PEK:H282	7:T:8:HIS:HE2	1.62	0.65
1:A:308:ALA:O	1:A:311[B]:ILE:HG12	1.97	0.64
21:O:307:EDO:H12	29:P:459:HOH:O	1.97	0.64
25:T:101:CDL:H181	25:T:101:CDL:H511	1.79	0.63
24:C:301:DMU:H11	10:J:49:CYS:HB3	1.79	0.63
6:F:30:PRO:O	6:F:96:LEU:HD11	1.98	0.63
6:F:51:SER:O	6:F:94:HIS:N	2.29	0.63
26:C:305:PEK:H383	25:G:102:CDL:H273	1.79	0.63
21:A:615:EDO:H11	21:A:616:EDO:H22	1.81	0.62
25:G:102:CDL:H771	25:G:102:CDL:H581	1.82	0.62
1:N:347:LEU:HD13	1:N:383[B]:MET:HB3	1.81	0.61
3:P:99:TRP:CD1	18:P:302:PGV:H211	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:31:CYS:SG	25:T:101:CDL:H551	2.40	0.61
11:K:20:SER:HA	24:K:103:DMU:H1	1.83	0.61
14:A:602:HEA:HBD2	14:A:602:HEA:HMD1	1.83	0.60
25:G:102:CDL:H142	25:G:102:CDL:H412	1.83	0.60
10:J:55:PHE:HE1	24:L:102:DMU:H29	1.67	0.60
2:B:203:ASN:HD22	21:B:304:EDO:H22	1.66	0.59
1:N:337:ALA:HB2	1:N:394[A]:VAL:HG23	1.85	0.59
1:A:468:MET:HG3	29:A:928:HOH:O	2.02	0.59
6:F:54[B]:ASN:ND2	29:F:202:HOH:O	2.36	0.59
1:A:347:LEU:HD13	1:A:383[B]:MET:HB3	1.84	0.58
2:O:83:ILE:HA	2:O:86:MET:HG2	1.84	0.58
1:N:377:PHE:HA	1:N:380[B]:VAL:HG22	1.85	0.58
1:A:406:ASN:HD21	18:A:607:PGV:H21	1.68	0.58
3:C:206:LEU:HD13	26:G:101:PEK:H12	1.86	0.58
7:T:8:HIS:ND1	7:T:8:HIS:N	2.51	0.57
24:L:102:DMU:H6	29:L:210:HOH:O	2.02	0.56
1:A:113[B]:LEU:HD23	12:L:39:ILE:HD11	1.88	0.56
3:C:59:ARG:HB2	25:C:303:CDL:H521	1.88	0.56
18:A:607:PGV:H231	13:M:12:PRO:HG3	1.88	0.55
26:P:308:PEK:H011	7:T:69:PHE:HB3	1.87	0.55
1:A:377:PHE:HA	1:A:380[B]:VAL:HG22	1.87	0.55
3:P:210:ILE:HG12	18:P:304:PGV:H132	1.87	0.55
6:S:66:ASN:HA	21:S:103:EDO:H21	1.88	0.55
7:G:8:HIS:ND1	7:G:8:HIS:N	2.53	0.55
6:S:3:GLY:HA3	29:S:201:HOH:O	2.06	0.55
21:A:615:EDO:C1	21:A:616:EDO:H22	2.37	0.55
18:N:606:PGV:H242	18:N:606:PGV:H41	1.88	0.55
1:A:383[B]:MET:HG2	1:A:421:VAL:HG21	1.87	0.55
23:G:103:CHD:H212	23:G:103:CHD:H12	1.89	0.54
18:A:606:PGV:H12	3:C:24:ALA:HB2	1.89	0.54
3:C:52:LEU:HD23	25:C:303:CDL:H362	1.90	0.54
10:J:55:PHE:CE1	24:L:102:DMU:H29	2.42	0.54
1:N:514:LYS:HA	6:S:38:ALA:HB3	1.90	0.53
1:A:472:ILE:HG21	19:L:101:TGL:HA92	1.89	0.53
18:A:607:PGV:H302	13:M:16:ALA:HA	1.88	0.53
4:D:19[B]:ARG:NH2	4:D:21:ASP:OD1	2.42	0.53
7:G:4:ALA:HB2	1:N:285:PHE:CD2	2.43	0.53
1:A:285:PHE:CD2	7:T:4:ALA:HB2	2.44	0.52
1:A:362:SER:HB3	2:B:20:LEU:HD21	1.92	0.52
3:P:244:PHE:HA	26:P:301:PEK:H101	1.90	0.52
2:O:7:LEU:HD11	19:O:301:TGL:H162	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:P:308:PEK:H262	24:P:310:DMU:H13	1.91	0.52
2:O:13:THR:HB	2:O:168:LEU:HD23	1.92	0.52
21:N:617:EDO:H22	29:N:820:HOH:O	2.10	0.52
29:P:402:HOH:O	7:T:74:ARG:NH2	2.42	0.51
6:F:34:LEU:O	21:F:105:EDO:O2	2.25	0.51
4:Q:118:LYS:HB3	11:X:53:TRP:HB3	1.92	0.51
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.92	0.51
4:D:78:TRP:N	19:D:201:TGL:HB22	2.26	0.51
25:G:102:CDL:H401	2:O:81:LEU:HD12	1.92	0.51
3:C:134:THR:HG21	25:G:102:CDL:H611	1.93	0.51
3:C:210:ILE:HD13	18:C:302:PGV:H302	1.92	0.51
1:N:487:LEU:H	21:N:611:EDO:H12	1.75	0.51
3:P:34:TRP:HZ3	26:P:308:PEK:H261	1.75	0.51
12:L:9:LYS:NZ	29:L:201:HOH:O	2.41	0.51
12:L:20:ARG:HH22	19:L:101:TGL:HC42	1.76	0.51
18:A:607:PGV:H312	18:A:607:PGV:H151	1.93	0.51
2:B:203:ASN:ND2	21:B:304:EDO:H22	2.25	0.51
1:N:332:ILE:H	21:N:621:EDO:H12	1.76	0.50
1:A:309:THR:HG22	14:A:602:HEA:HMB2	1.94	0.50
25:G:102:CDL:H412	25:G:102:CDL:H161	1.93	0.50
1:N:229:ILE:HD11	2:O:175:ILE:HD13	1.93	0.50
4:Q:78:TRP:HA	19:Q:201:TGL:HB22	1.94	0.50
4:D:127:LYS:HD2	29:I:140:HOH:O	2.12	0.49
2:B:81:LEU:HD12	25:T:101:CDL:H371	1.94	0.49
26:G:101:PEK:H8	26:G:101:PEK:H302	1.94	0.49
20:A:609:PSC:C33	20:A:609:PSC:H142	2.43	0.49
1:N:107:PRO:HB3	3:P:25:LEU:HB2	1.94	0.49
11:X:24:PHE:HE1	24:X:105:DMU:H16	1.77	0.49
1:A:342:LEU:HB2	19:D:201:TGL:H202	1.94	0.49
21:A:610:EDO:H11	12:L:10:ASN:HD22	1.77	0.49
18:A:606:PGV:H12	3:C:24:ALA:CB	2.43	0.49
2:O:132:GLU:HB3	2:O:137:GLU:HG3	1.95	0.49
6:F:85:CYS:SG	6:F:87:THR:HG23	2.53	0.49
2:B:183:THR:HG22	29:B:596:HOH:O	2.12	0.48
3:P:206:LEU:HB2	26:P:308:PEK:H12	1.95	0.48
1:A:110:LEU:HD12	1:A:113[B]:LEU:HD12	1.95	0.48
1:A:510:TYR:OH	1:A:512:ASN:ND2	2.43	0.48
25:T:101:CDL:H382	25:T:101:CDL:H131	1.95	0.48
1:N:177:SER:H	1:N:180:GLN:NE2	2.12	0.48
1:N:390:MET:O	1:N:394[A]:VAL:HG22	2.13	0.48
1:A:283:LEU:HD22	1:A:311[B]:ILE:HD11	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:29:PHE:HZ	19:L:101:TGL:HA91	1.77	0.48
1:N:510:TYR:OH	1:N:512:ASN:ND2	2.43	0.48
12:L:20:ARG:HH21	19:L:101:TGL:HC61	1.79	0.47
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.94	0.47
1:A:169:ILE:HG12	1:A:189[B]:MET:CE	2.44	0.47
1:A:177:SER:H	1:A:180:GLN:NE2	2.13	0.47
2:O:102:HIS:O	2:O:104:TRP:HA	2.15	0.47
12:Y:42:HIS:NE2	12:Y:46:LYS:HD2	2.30	0.47
1:A:265:LYS:HB2	1:A:490:THR:HG21	1.97	0.47
3:P:29:SER:HB2	24:P:303:DMU:H19	1.96	0.47
1:N:265:LYS:HB2	1:N:490:THR:HG21	1.97	0.46
26:P:309:PEK:H281	7:T:26:PRO:HG3	1.97	0.46
3:C:210:ILE:HG12	18:C:302:PGV:H132	1.97	0.46
1:A:225:GLY:HA3	3:C:112:LEU:HD21	1.98	0.46
1:A:321:PHE:CD2	2:B:65:TRP:HB2	2.50	0.46
1:A:236:TRP:HH2	14:A:602:HEA:HBD1	1.79	0.46
4:D:4:SER:N	29:D:305:HOH:O	2.49	0.46
26:G:101:PEK:H71	26:G:101:PEK:H42	1.67	0.46
1:A:449[A]:MET:SD	2:B:5:MET:HG2	2.56	0.46
2:B:37:LEU:HD22	2:B:37:LEU:HA	1.78	0.46
3:C:99:TRP:CE3	18:C:306:PGV:H271	2.50	0.46
8:H:40:GLU:OE2	29:H:201:HOH:O	2.21	0.46
4:Q:98:TRP:CE3	24:Z:101:DMU:H12	2.51	0.46
2:B:13:THR:HB	2:B:168:LEU:HD23	1.98	0.46
1:N:236:TRP:CH2	14:N:602:HEA:HBD1	2.51	0.46
3:P:34:TRP:CZ3	26:P:308:PEK:H261	2.51	0.46
2:B:196:CYS:HB2	2:B:207:MET:HG3	1.96	0.46
10:J:29:ASN:HD22	10:J:29:ASN:H	1.61	0.46
6:S:96:LEU:HB3	6:S:97:ALA:H	1.42	0.46
1:N:472:ILE:HG21	19:N:608:TGL:HA82	1.97	0.45
26:P:309:PEK:H241	7:T:21:PHE:CD1	2.51	0.45
1:N:87:ILE:O	1:N:173:PRO:HD3	2.16	0.45
4:D:82:VAL:HG21	24:D:203:DMU:H14	1.98	0.45
1:N:377:PHE:CD2	14:N:602:HEA:HAD1	2.52	0.45
1:N:347:LEU:CD1	1:N:383[B]:MET:HB3	2.47	0.45
7:T:37:LEU:HD23	25:T:101:CDL:H361	1.99	0.45
6:F:95:GLN:NE2	29:F:205:HOH:O	2.50	0.45
18:N:606:PGV:H222	13:Z:15:GLN:HE22	1.81	0.45
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.52	0.45
3:P:47:LEU:O	3:P:51[B]:MET:HG3	2.17	0.45
11:X:34:THR:HA	24:X:103:DMU:H11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298[A]:ASP:OD1	8:H:22:ASN:HB3	2.16	0.44
26:P:308:PEK:H221	26:P:308:PEK:H251	1.65	0.44
3:C:210:ILE:HG23	18:C:302:PGV:H91	1.98	0.44
3:C:244:PHE:HA	26:C:307:PEK:H101	1.99	0.44
4:D:132:GLN:O	4:D:137[B]:LYS:NZ	2.50	0.44
2:O:168:LEU:HD13	2:O:184:LEU:HG	2.00	0.44
1:A:311[B]:ILE:HG22	25:T:101:CDL:H441	1.99	0.44
26:P:308:PEK:H291	26:P:308:PEK:H8	1.99	0.44
25:P:305:CDL:H382	25:P:305:CDL:H351	1.70	0.44
1:N:486:ASP:OD2	4:Q:19:ARG:HD2	2.18	0.44
10:W:29:ASN:HD22	10:W:29:ASN:H	1.65	0.44
6:S:19:GLU:HG2	29:S:301:HOH:O	2.18	0.44
26:P:309:PEK:H383	25:T:101:CDL:H272	2.00	0.44
7:T:31:CYS:SG	25:T:101:CDL:H532	2.58	0.44
1:A:347:LEU:HD22	1:A:383[B]:MET:SD	2.58	0.44
4:Q:78:TRP:CA	19:Q:201:TGL:HB22	2.48	0.44
6:S:64:GLU:O	6:S:65:ASP:HB2	2.17	0.44
1:A:381[A]:LEU:HB2	14:A:602:HEA:CAC	2.47	0.44
7:G:5:LYS:HB3	1:N:278[B]:MET:HE3	1.99	0.44
19:D:201:TGL:OA1	19:D:201:TGL:HC52	2.18	0.43
1:N:419:VAL:HG21	19:Q:201:TGL:H301	2.00	0.43
6:S:67:SER:H	21:S:103:EDO:C2	2.31	0.43
1:N:513:LEU:HA	1:N:513:LEU:HD23	1.67	0.43
24:K:103:DMU:H2	24:K:103:DMU:H36	1.78	0.43
1:N:136[B]:LEU:HD11	29:T:267:HOH:O	2.19	0.43
2:O:41:ILE:O	2:O:45:MET:HG2	2.19	0.43
19:Q:201:TGL:H221	19:Q:201:TGL:HA81	2.01	0.43
1:A:514:LYS:HA	6:F:38:ALA:HB3	1.99	0.43
1:A:309:THR:CG2	14:A:602:HEA:HMB2	2.49	0.43
3:C:51[A]:MET:SD	25:C:303:CDL:H611	2.58	0.43
12:L:9:LYS:HA	12:L:9:LYS:HD2	1.76	0.43
1:N:172:LYS:NZ	29:N:707:HOH:O	2.51	0.43
6:S:54:ASN:HD22	6:S:54:ASN:C	2.22	0.43
25:T:101:CDL:H762	25:T:101:CDL:H561	2.00	0.43
20:A:609:PSC:H242	20:A:609:PSC:H82	2.01	0.43
2:O:68:LEU:HB3	2:O:69:PRO:HD3	2.01	0.43
3:P:47:LEU:O	3:P:51[A]:MET:HG2	2.18	0.43
2:O:58:ALA:O	2:O:62:GLU:HG3	2.19	0.43
3:P:213:THR:HG23	25:P:305:CDL:C77	2.49	0.43
2:B:85:TYR:O	2:B:89:GLU:HG3	2.19	0.43
4:D:81:VAL:HG11	19:D:201:TGL:HB62	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:131[A]:ILE:HG22	4:D:132:GLN:HG3	1.99	0.43
19:Q:201:TGL:HA52	19:Q:201:TGL:HB72	2.01	0.43
8:U:12:GLN:HE21	8:U:12:GLN:HB3	1.59	0.43
1:A:285:PHE:CE2	7:T:4:ALA:HB2	2.54	0.42
2:B:1:FME:HE2	2:B:2:ALA:O	2.19	0.42
2:B:164:ALA:O	2:B:194:GLY:HA3	2.18	0.42
8:H:37:HIS:HD2	8:H:40:GLU:OE2	2.02	0.42
8:U:37:HIS:HE1	29:U:218:HOH:O	2.02	0.42
21:A:614:EDO:H21	29:A:921:HOH:O	2.19	0.42
8:H:9:LYS:HB3	8:H:10:ASN:H	1.67	0.42
3:C:175:LEU:HD21	25:C:303:CDL:H873	2.01	0.42
4:D:89:ILE:HD13	19:D:201:TGL:H312	2.01	0.42
23:J:101:CHD:H183	23:J:101:CHD:H221	2.00	0.42
25:G:102:CDL:H761	1:N:282:PHE:HZ	1.85	0.42
2:O:91:ASN:HB3	2:O:149:THR:HG21	2.02	0.42
3:P:156:ARG:HE	23:P:306:CHD:C24	2.33	0.42
13:Z:36:HIS:HB3	13:Z:39:ASN:HD21	1.85	0.42
1:A:383[B]:MET:HA	1:A:387:PHE:CD1	2.54	0.42
19:A:608:TGL:H282	19:A:608:TGL:H251	1.83	0.42
1:N:415:ALA:HB1	19:Q:201:TGL:H132	2.01	0.42
12:Y:2:HIS:N	29:Y:201:HOH:O	2.53	0.42
1:A:229:ILE:HD11	2:B:175:ILE:HD13	2.01	0.42
2:B:104:TRP:CD2	2:B:203:ASN:HB2	2.55	0.42
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.54	0.42
1:N:381[A]:LEU:HB2	14:N:602:HEA:CAC	2.50	0.42
8:U:43:MET:HE3	8:U:49:ASP:N	2.35	0.42
2:B:1:FME:O1	2:B:193:TYR:HB2	2.19	0.42
26:G:101:PEK:H8	26:G:101:PEK:C30	2.50	0.42
1:A:117[A]:MET:HE1	24:L:102:DMU:H10	2.01	0.41
18:C:306:PGV:H241	18:C:306:PGV:H272	1.84	0.41
1:N:110:LEU:HD13	19:N:608:TGL:H311	2.00	0.41
14:N:602:HEA:HBC1	14:N:602:HEA:HMC1	2.02	0.41
1:A:311[B]:ILE:CD1	25:T:101:CDL:H221	2.49	0.41
25:C:303:CDL:H131	25:C:303:CDL:H162	1.88	0.41
6:F:80[A]:GLN:HE21	21:F:103:EDO:H21	1.85	0.41
1:N:377:PHE:HA	1:N:380[A]:VAL:HG12	2.01	0.41
24:P:303:DMU:H21	10:W:50:LEU:HG	2.02	0.41
7:G:4:ALA:HB2	1:N:285:PHE:CE2	2.54	0.41
25:G:102:CDL:H382	2:O:78:LEU:HD12	2.03	0.41
1:N:236:TRP:HH2	14:N:602:HEA:HBD1	1.84	0.41
5:R:43:PRO:HB2	5:R:48:ILE:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:334:TRP:CZ2	2:O:46:LEU:HB3	2.56	0.41
1:N:501:PRO:HB3	12:Y:5:GLU:OE2	2.20	0.41
1:A:240:HIS:CD2	1:A:240:HIS:C	2.93	0.41
3:C:33:MET:HB2	24:C:301:DMU:C19	2.50	0.41
6:S:95:GLN:NE2	29:S:204:HOH:O	2.53	0.41
4:D:17[B]:VAL:HG22	4:D:19[B]:ARG:HG3	2.03	0.41
1:N:18:LEU:CD2	19:N:608:TGL:HB21	2.50	0.41
25:C:303:CDL:H762	25:C:303:CDL:H732	1.88	0.41
6:F:80[A]:GLN:NE2	29:F:207:HOH:O	2.54	0.41
4:Q:132:GLN:O	4:Q:137:LYS:NZ	2.54	0.41
1:A:113[A]:LEU:HD12	19:L:101:TGL:H131	2.02	0.41
1:A:177:SER:H	1:A:180:GLN:HE21	1.66	0.41
1:N:225:GLY:HA3	3:P:112:LEU:HD21	2.03	0.41
1:N:386[B]:VAL:HG21	14:N:601[B]:HEA:H261	2.02	0.41
4:Q:20:ARG:H	4:Q:20:ARG:HG2	1.57	0.41
9:V:1:SAC:H2A1	9:V:2:THR:H	1.86	0.41
21:F:105:EDO:H22	29:F:239:HOH:O	2.21	0.41
8:H:9:LYS:HD3	8:H:9:LYS:HA	1.77	0.41
11:K:7:PRO:O	11:K:12:LYS:NZ	2.53	0.41
8:U:50:VAL:HG23	29:U:249:HOH:O	2.20	0.41
1:A:377:PHE:HA	1:A:380[A]:VAL:HG12	2.03	0.40
8:H:37:HIS:HE1	29:H:213:HOH:O	2.04	0.40
1:N:53:ILE:HG12	29:N:889:HOH:O	2.20	0.40
1:N:112:LEU:HD23	1:N:112:LEU:C	2.42	0.40
1:N:309:THR:HG22	14:N:602:HEA:HMB2	2.02	0.40
14:A:602:HEA:HBC1	14:A:602:HEA:HMC1	2.02	0.40
21:A:615:EDO:H22	29:A:939:HOH:O	2.20	0.40
4:D:121:LYS:HD3	11:K:52:GLU:HA	2.03	0.40
10:J:55:PHE:HA	10:J:56:PRO:HD3	1.96	0.40
12:L:25:MET:HG2	19:L:101:TGL:HA41	2.04	0.40
13:M:37:LEU:HD23	13:M:37:LEU:HA	1.95	0.40
1:N:113[A]:LEU:HD12	19:N:608:TGL:H132	2.03	0.40
19:Q:201:TGL:HA32	19:Q:201:TGL:HB52	2.02	0.40
1:A:236:TRP:CH2	14:A:602:HEA:HBD1	2.56	0.40
1:N:242:GLU:HA	1:N:245:ILE:HD12	2.04	0.40
1:N:383[B]:MET:HA	1:N:387:PHE:CD1	2.57	0.40
19:N:608:TGL:HA91	19:N:608:TGL:H221	1.85	0.40
21:N:621:EDO:H11	29:O:454:HOH:O	2.22	0.40
24:P:303:DMU:H25	10:W:46:SER:HB2	2.03	0.40
4:Q:51:LEU:HD21	4:Q:59:LEU:HD12	2.03	0.40
25:T:101:CDL:H202	25:T:101:CDL:H531	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	532/514 (104%)	517 (97%)	15 (3%)	0	100	100
1	N	534/514 (104%)	522 (98%)	12 (2%)	0	100	100
2	B	231/227 (102%)	226 (98%)	5 (2%)	0	100	100
2	O	229/227 (101%)	222 (97%)	7 (3%)	0	100	100
3	C	265/259 (102%)	260 (98%)	5 (2%)	0	100	100
3	P	265/259 (102%)	260 (98%)	5 (2%)	0	100	100
4	D	148/144 (103%)	145 (98%)	3 (2%)	0	100	100
4	Q	143/144 (99%)	138 (96%)	5 (4%)	0	100	100
5	E	104/105 (99%)	104 (100%)	0	0	100	100
5	R	103/105 (98%)	103 (100%)	0	0	100	100
6	F	100/98 (102%)	95 (95%)	3 (3%)	2 (2%)	7	1
6	S	97/98 (99%)	90 (93%)	4 (4%)	3 (3%)	4	0
7	G	83/84 (99%)	72 (87%)	10 (12%)	1 (1%)	13	2
7	T	85/84 (101%)	75 (88%)	9 (11%)	1 (1%)	13	2
8	H	77/79 (98%)	72 (94%)	4 (5%)	1 (1%)	12	2
8	U	77/79 (98%)	74 (96%)	3 (4%)	0	100	100
9	I	71/73 (97%)	70 (99%)	1 (1%)	0	100	100
9	V	72/73 (99%)	69 (96%)	3 (4%)	0	100	100
10	J	56/58 (97%)	56 (100%)	0	0	100	100
10	W	56/58 (97%)	56 (100%)	0	0	100	100
11	K	48/49 (98%)	46 (96%)	2 (4%)	0	100	100
11	X	48/49 (98%)	47 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	L	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
12	Y	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
13	M	41/43 (95%)	40 (98%)	1 (2%)	0	100	100
13	Z	41/43 (95%)	41 (100%)	0	0	100	100
All	All	3594/3558 (101%)	3486 (97%)	100 (3%)	8 (0%)	47	26

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	S	96	LEU
6	F	96	LEU
6	F	95	GLN
6	S	95	GLN
7	G	5	LYS
6	S	94	HIS
7	T	5	LYS
8	H	8	ILE

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	444/426 (104%)	436 (98%)	8 (2%)	59	36
1	N	446/426 (105%)	443 (99%)	3 (1%)	84	73
2	B	216/210 (103%)	209 (97%)	7 (3%)	39	15
2	O	214/210 (102%)	210 (98%)	4 (2%)	57	34
3	C	232/224 (104%)	230 (99%)	2 (1%)	78	65
3	P	232/224 (104%)	230 (99%)	2 (1%)	78	65
4	D	134/128 (105%)	133 (99%)	1 (1%)	84	73
4	Q	129/128 (101%)	127 (98%)	2 (2%)	62	41
5	E	93/92 (101%)	92 (99%)	1 (1%)	73	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	R	92/92 (100%)	91 (99%)	1 (1%)	73 57
6	F	85/81 (105%)	84 (99%)	1 (1%)	71 54
6	S	82/81 (101%)	80 (98%)	2 (2%)	49 24
7	G	69/68 (102%)	63 (91%)	6 (9%)	10 1
7	T	71/68 (104%)	64 (90%)	7 (10%)	8 1
8	H	71/71 (100%)	70 (99%)	1 (1%)	67 47
8	U	71/71 (100%)	67 (94%)	4 (6%)	21 5
9	I	57/57 (100%)	57 (100%)	0	100 100
9	V	58/57 (102%)	57 (98%)	1 (2%)	60 38
10	J	49/49 (100%)	49 (100%)	0	100 100
10	W	49/49 (100%)	48 (98%)	1 (2%)	55 31
11	K	40/39 (103%)	40 (100%)	0	100 100
11	X	40/39 (103%)	39 (98%)	1 (2%)	47 22
12	L	39/39 (100%)	37 (95%)	2 (5%)	24 6
12	Y	39/39 (100%)	38 (97%)	1 (3%)	46 21
13	M	37/37 (100%)	37 (100%)	0	100 100
13	Z	37/37 (100%)	37 (100%)	0	100 100
All	All	3126/3042 (103%)	3068 (98%)	58 (2%)	59 34

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	109	PHE
1	A	127	THR
1	A	180	GLN
1	A	297[A]	MET
1	A	297[B]	MET
1	A	338	MET
1	A	369	ASP
2	B	33	LEU
2	B	37	LEU
2	B	60	GLU
2	B	65	TRP
2	B	75	LEU
2	B	94	SER

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Mol	Chain	Res	Type
2	B	171	LYS
3	C	159	MET
3	C	214	PHE
4	D	20	ARG
5	E	90	ARG
6	F	48	LEU
7	G	8	HIS
7	G	11	THR
7	G	18[A]	PHE
7	G	18[B]	PHE
7	G	37	LEU
7	G	54	ARG
8	H	60	TYR
12	L	2	HIS
12	L	47	LYS
1	N	109	PHE
1	N	180	GLN
1	N	369	ASP
2	O	33	LEU
2	O	75	LEU
2	O	171	LYS
2	O	217	LYS
3	P	159	MET
3	P	214	PHE
4	Q	19	ARG
4	Q	20	ARG
5	R	108	LYS
6	S	54	ASN
6	S	96	LEU
7	T	8	HIS
7	T	11	THR
7	T	18	PHE
7	T	36[A]	TRP
7	T	36[B]	TRP
7	T	37	LEU
7	T	54	ARG
8	U	9	LYS
8	U	27	ARG
8	U	60	TYR
8	U	84	LYS
9	V	37	PHE
10	W	50	LEU

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Mol	Chain	Res	Type
11	X	52	GLU
12	Y	2	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	ASN
1	A	98	ASN
1	A	178	GLN
1	A	180	GLN
1	A	512	ASN
2	B	10	GLN
2	B	59	GLN
2	B	91	ASN
2	B	195	GLN
3	C	68	GLN
4	D	101	HIS
5	E	94	ASN
8	H	37	HIS
10	J	29	ASN
11	K	35	GLN
1	N	80	ASN
1	N	98	ASN
1	N	180	GLN
1	N	512	ASN
2	O	10	GLN
2	O	59	GLN
2	O	91	ASN
2	O	181	GLN
2	O	195	GLN
3	P	68	GLN
4	Q	109	HIS
5	R	94	ASN
6	S	54	ASN
8	U	12	GLN
8	U	23	GLN
8	U	37	HIS
10	W	29	ASN
11	X	15	ASN
11	X	35	GLN
13	Z	39	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

6 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	$\#\|Z\| > 2$
9	SAC	V	1	9	7,8,9	0.59	0	8,9,11	0.81	0
1	FME	N	1	1	8,9,10	0.52	0	7,9,11	1.51	2 (28%)
9	SAC	I	1	9	7,8,9	0.64	0	8,9,11	0.79	0
1	FME	A	1	1	8,9,10	0.57	0	7,9,11	1.52	2 (28%)
2	FME	O	1	2	8,9,10	0.95	0	7,9,11	1.05	1 (14%)
2	FME	B	1	2	8,9,10	2.48	2 (25%)	7,9,11	2.87	3 (42%)

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
9	SAC	V	1	9	-	3/7/8/10	-
1	FME	N	1	1	-	2/7/9/11	-
9	SAC	I	1	9	-	3/7/8/10	-
1	FME	A	1	1	-	5/7/9/11	-
2	FME	O	1	2	-	0/7/9/11	-
2	FME	B	1	2	-	0/7/9/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	FME	CN-N	5.96	1.53	1.33
2	B	1	FME	CG-SD	-2.01	1.70	1.81

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1	FME	CA-N-CN	-5.90	113.75	122.82
2	B	1	FME	C-CA-N	3.91	116.80	109.73
1	N	1	FME	O-C-CA	-2.68	117.76	124.78
2	O	1	FME	O-C-CA	-2.31	118.71	124.78
1	N	1	FME	CG-CB-CA	-2.25	106.69	112.95
2	B	1	FME	O-C-CA	-2.09	119.30	124.78
1	A	1	FME	C-CA-N	2.08	113.49	109.73
1	A	1	FME	O1-CN-N	-2.02	119.94	125.27

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	O1-CN-N-CA
1	A	1	FME	N-CA-CB-CG
9	I	1	SAC	C2A-C1A-N-CA
9	I	1	SAC	OAC-C1A-N-CA
9	I	1	SAC	C-CA-N-C1A
1	N	1	FME	O1-CN-N-CA
9	V	1	SAC	C2A-C1A-N-CA
9	V	1	SAC	OAC-C1A-N-CA
9	V	1	SAC	O-C-CA-CB
1	A	1	FME	CA-CB-CG-SD
1	A	1	FME	C-CA-CB-CG
1	A	1	FME	CB-CA-N-CN
1	N	1	FME	CB-CG-SD-CE

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	V	1	SAC	1	0
2	B	1	FME	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 135 ligands modelled in this entry, 8 are monoatomic - leaving 127 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
21	EDO	E	201	-	3,3,3	0.57	0	2,2,2	0.46	0
21	EDO	G	104	-	3,3,3	0.76	0	2,2,2	0.53	0
21	EDO	N	612	-	3,3,3	0.52	0	2,2,2	0.44	0
21	EDO	N	619	-	3,3,3	0.30	0	2,2,2	1.47	0
25	CDL	P	305	-	66,66,99	1.37	9 (13%)	65,65,111	1.00	1 (1%)
21	EDO	S	103	-	3,3,3	0.67	0	2,2,2	0.77	0
21	EDO	T	102	-	3,3,3	0.64	0	2,2,2	0.28	0
19	TGL	D	201	-	62,62,62	1.08	3 (4%)	65,65,65	1.15	6 (9%)
23	CHD	C	304	-	32,32,32	1.06	1 (3%)	51,51,51	1.82	16 (31%)
21	EDO	Q	203	-	3,3,3	0.34	0	2,2,2	0.73	0
21	EDO	A	617	-	3,3,3	0.51	0	2,2,2	0.56	0
24	DMU	Z	101	-	34,34,34	0.55	1 (2%)	45,45,45	0.83	0
24	DMU	X	105	-	9,9,34	0.22	0	8,8,45	0.56	0
21	EDO	P	312	-	3,3,3	0.33	0	2,2,2	0.75	0
21	EDO	S	106	-	3,3,3	0.34	0	2,2,2	0.19	0
18	PGV	C	302	-	50,50,50	0.81	1 (2%)	53,56,56	0.87	1 (1%)
26	PEK	G	101	-	52,52,52	0.97	4 (7%)	55,57,57	1.60	8 (14%)
26	PEK	C	307	-	24,24,52	0.29	0	22,22,57	0.45	0
24	DMU	D	202	-	11,11,34	0.29	0	10,10,45	0.30	0
14	HEA	N	601[A]	-	57,67,67	1.54	12 (21%)	61,103,103	1.91	20 (32%)
18	PGV	P	302	-	40,40,50	1.12	2 (5%)	42,42,56	1.45	6 (14%)
21	EDO	R	201	-	3,3,3	0.81	0	2,2,2	0.42	0
23	CHD	P	307	-	32,32,32	0.95	1 (3%)	51,51,51	1.26	6 (11%)
18	PGV	P	304	-	49,49,50	1.06	4 (8%)	52,55,56	2.06	7 (13%)
24	DMU	K	105	-	8,8,34	0.24	0	7,7,45	0.56	0
21	EDO	N	610	-	3,3,3	1.04	0	2,2,2	0.60	0
21	EDO	O	307	-	3,3,3	0.63	0	2,2,2	0.24	0
21	EDO	C	309	-	3,3,3	0.62	0	2,2,2	1.06	0
21	EDO	F	104	-	3,3,3	0.93	0	2,2,2	0.32	0
21	EDO	N	611	-	3,3,3	0.66	0	2,2,2	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	EDO	F	103	-	3,3,3	0.61	0	2,2,2	0.35	0
24	DMU	X	103	-	8,8,34	0.27	0	7,7,45	0.50	0
24	DMU	C	301	-	8,8,34	0.33	0	7,7,45	0.36	0
18	PGV	N	606	-	39,39,50	1.09	2 (5%)	40,40,56	1.15	4 (10%)
23	CHD	B	302	-	32,32,32	1.20	3 (9%)	51,51,51	1.76	14 (27%)
21	EDO	N	614	-	3,3,3	0.49	0	2,2,2	0.31	0
21	EDO	B	303	-	3,3,3	0.57	0	2,2,2	0.35	0
14	HEA	A	601[B]	-	57,67,67	1.56	11 (19%)	61,103,103	1.97	19 (31%)
21	EDO	A	611	-	3,3,3	0.55	0	2,2,2	0.63	0
24	DMU	P	310	-	10,10,34	0.28	0	9,9,45	0.53	0
21	EDO	J	103	-	3,3,3	0.59	0	2,2,2	0.16	0
21	EDO	N	616	-	3,3,3	1.02	0	2,2,2	0.93	0
24	DMU	X	101	-	34,34,34	0.42	0	45,45,45	0.80	1 (2%)
21	EDO	E	202	-	3,3,3	0.58	0	2,2,2	0.33	0
21	EDO	P	311	-	3,3,3	0.57	0	2,2,2	0.30	0
21	EDO	N	621	-	3,3,3	0.78	0	2,2,2	0.23	0
21	EDO	A	619	-	3,3,3	1.19	0	2,2,2	0.90	0
19	TGL	Q	201	-	62,62,62	1.00	3 (4%)	65,65,65	1.04	6 (9%)
20	PSC	O	303	-	22,22,51	0.81	1 (4%)	20,20,59	0.85	0
18	PGV	N	607	-	50,50,50	1.06	4 (8%)	53,56,56	1.11	4 (7%)
19	TGL	L	101	-	58,58,62	1.08	3 (5%)	61,61,65	1.33	8 (13%)
24	DMU	O	304	-	9,9,34	0.22	0	8,8,45	0.47	0
21	EDO	A	615	-	3,3,3	0.70	0	2,2,2	0.78	0
24	DMU	D	203	-	8,8,34	0.28	0	7,7,45	0.48	0
21	EDO	N	615	-	3,3,3	0.53	0	2,2,2	0.71	0
21	EDO	W	102	-	3,3,3	0.47	0	2,2,2	1.02	0
14	HEA	A	602	1	57,67,67	1.61	9 (15%)	61,103,103	2.24	25 (40%)
19	TGL	N	608	-	54,54,62	0.65	1 (1%)	52,52,65	0.79	1 (1%)
21	EDO	J	104	-	3,3,3	0.38	0	2,2,2	0.48	0
26	PEK	P	309	-	37,37,52	0.74	1 (2%)	35,36,57	0.83	1 (2%)
21	EDO	S	104	-	3,3,3	0.57	0	2,2,2	0.73	0
23	CHD	P	306	-	32,32,32	0.74	0	51,51,51	1.33	8 (15%)
21	EDO	F	106	-	3,3,3	0.84	0	2,2,2	0.45	0
21	EDO	Q	202	-	3,3,3	0.53	0	2,2,2	0.13	0
22	CUA	B	301	2	0,1,1	-	-	-		
24	DMU	C	308	-	11,11,34	0.33	0	10,10,45	0.51	0
21	EDO	B	304	-	3,3,3	0.61	0	2,2,2	0.64	0
21	EDO	B	306	-	3,3,3	0.88	0	2,2,2	0.60	0
25	CDL	G	102	-	60,60,99	1.19	8 (13%)	56,56,111	0.77	0
26	PEK	C	305	-	35,35,52	0.24	0	33,33,57	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	HEA	N	601[B]	-	57,67,67	1.50	11 (19%)	61,103,103	1.97	17 (27%)
24	DMU	J	102	-	10,10,34	0.24	0	9,9,45	0.60	0
24	DMU	P	303	-	34,34,34	0.52	1 (2%)	45,45,45	0.79	0
21	EDO	A	614	-	3,3,3	0.84	0	2,2,2	0.81	0
21	EDO	S	105	-	3,3,3	0.67	0	2,2,2	0.53	0
28	PO4	U	101	-	4,4,4	1.02	0	6,6,6	0.35	0
26	PEK	P	308	-	52,52,52	0.73	2 (3%)	55,57,57	1.53	7 (12%)
21	EDO	A	616	-	3,3,3	0.50	0	2,2,2	0.47	0
23	CHD	J	101	-	32,32,32	0.66	0	51,51,51	1.24	5 (9%)
21	EDO	S	102	-	3,3,3	0.51	0	2,2,2	0.74	0
24	DMU	K	103	-	34,34,34	0.54	1 (2%)	45,45,45	0.97	2 (4%)
24	DMU	L	102	-	21,21,34	0.50	0	24,25,45	1.13	3 (12%)
21	EDO	C	311	-	3,3,3	0.70	0	2,2,2	0.23	0
21	EDO	N	617	-	3,3,3	0.49	0	2,2,2	0.21	0
24	DMU	K	104	-	8,8,34	0.24	0	7,7,45	0.43	0
21	EDO	Q	204	-	3,3,3	0.48	0	2,2,2	0.42	0
18	PGV	A	606	-	50,50,50	0.89	2 (4%)	53,56,56	0.86	1 (1%)
24	DMU	M	101	-	34,34,34	0.46	0	45,45,45	1.17	3 (6%)
14	HEA	N	602	1	57,67,67	1.52	10 (17%)	61,103,103	2.03	20 (32%)
21	EDO	T	103	-	3,3,3	0.42	0	2,2,2	0.51	0
19	TGL	O	301	-	56,56,62	1.07	3 (5%)	58,58,65	1.30	5 (8%)
21	EDO	A	613	-	3,3,3	0.64	0	2,2,2	0.58	0
21	EDO	F	105	-	3,3,3	0.55	0	2,2,2	0.68	0
21	EDO	N	613	-	3,3,3	0.65	0	2,2,2	0.40	0
24	DMU	K	101	-	8,8,34	0.23	0	7,7,45	0.58	0
21	EDO	F	102	-	3,3,3	0.67	0	2,2,2	0.51	0
24	DMU	W	101	-	8,8,34	0.21	0	7,7,45	0.51	0
24	DMU	X	104	-	9,9,34	0.30	0	8,8,45	0.50	0
25	CDL	T	101	-	76,76,99	1.42	12 (15%)	77,77,111	1.38	3 (3%)
21	EDO	Y	101	-	3,3,3	0.55	0	2,2,2	0.43	0
23	CHD	G	103	-	32,32,32	0.87	1 (3%)	51,51,51	1.45	6 (11%)
24	DMU	K	106	-	8,8,34	0.26	0	7,7,45	0.52	0
28	PO4	H	101	-	4,4,4	1.10	0	6,6,6	0.48	0
26	PEK	P	301	-	19,19,52	0.23	0	18,18,57	0.52	0
18	PGV	C	306	-	34,34,50	0.93	1 (2%)	33,33,56	1.06	2 (6%)
21	EDO	C	312	-	3,3,3	0.61	0	2,2,2	0.10	0
21	EDO	N	620	-	3,3,3	0.42	0	2,2,2	0.61	0
18	PGV	A	607	-	35,35,50	0.92	1 (2%)	34,34,56	0.87	0
22	CUA	O	302	2	0,1,1	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CDL	C	303	-	52,52,99	1.14	5 (9%)	50,50,111	1.06	2 (4%)
21	EDO	C	310	-	3,3,3	0.79	0	2,2,2	0.30	0
21	EDO	O	306	-	3,3,3	0.62	0	2,2,2	0.13	0
24	DMU	K	102	-	8,8,34	0.26	0	7,7,45	0.48	0
21	EDO	C	313	-	3,3,3	0.66	0	2,2,2	0.48	0
21	EDO	B	305	-	3,3,3	0.63	0	2,2,2	0.37	0
20	PSC	A	609	-	23,23,51	0.81	1 (4%)	20,21,59	0.77	0
19	TGL	A	608	-	61,61,62	0.85	2 (3%)	63,63,65	1.23	4 (6%)
24	DMU	X	102	-	9,9,34	0.24	0	8,8,45	0.50	0
21	EDO	O	305	-	3,3,3	0.69	0	2,2,2	0.44	0
21	EDO	P	313	-	3,3,3	0.82	0	2,2,2	0.44	0
21	EDO	A	612	-	3,3,3	0.64	0	2,2,2	0.24	0
21	EDO	A	610	-	3,3,3	0.93	0	2,2,2	1.20	0
21	EDO	N	618	-	3,3,3	0.44	0	2,2,2	0.41	0
14	HEA	A	601[A]	-	57,67,67	1.66	13 (22%)	61,103,103	1.90	18 (29%)
21	EDO	N	609	-	3,3,3	0.73	0	2,2,2	0.11	0
21	EDO	W	103	-	3,3,3	0.46	0	2,2,2	0.19	0
21	EDO	A	618	-	3,3,3	0.38	0	2,2,2	0.60	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
21	EDO	E	201	-	-	0/1/1/1	-
21	EDO	G	104	-	-	0/1/1/1	-
21	EDO	N	612	-	-	0/1/1/1	-
21	EDO	N	619	-	-	1/1/1/1	-
25	CDL	P	305	-	-	11/62/62/110	-
21	EDO	S	103	-	-	0/1/1/1	-
21	EDO	T	102	-	-	1/1/1/1	-
19	TGL	D	201	-	-	15/65/65/65	-
23	CHD	C	304	-	-	2/9/74/74	0/4/4/4
21	EDO	Q	203	-	-	0/1/1/1	-
21	EDO	A	617	-	-	0/1/1/1	-
24	DMU	Z	101	-	-	5/19/59/59	0/2/2/2
24	DMU	X	105	-	-	2/7/7/59	-
21	EDO	P	312	-	-	1/1/1/1	-
21	EDO	S	106	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	PGV	C	302	-	-	7/55/55/55	-
26	PEK	G	101	-	-	14/56/56/56	-
26	PEK	C	307	-	-	10/20/20/56	-
24	DMU	D	202	-	-	5/9/9/59	-
14	HEA	N	601[A]	-	-	6/32/76/76	-
18	PGV	P	302	-	-	8/41/41/55	-
21	EDO	R	201	-	-	0/1/1/1	-
23	CHD	P	307	-	-	2/9/74/74	0/4/4/4
18	PGV	P	304	-	-	9/54/54/55	-
24	DMU	K	105	-	-	0/6/6/59	-
21	EDO	N	610	-	-	0/1/1/1	-
21	EDO	O	307	-	-	0/1/1/1	-
21	EDO	C	309	-	-	0/1/1/1	-
21	EDO	F	104	-	-	0/1/1/1	-
21	EDO	N	611	-	-	0/1/1/1	-
21	EDO	F	103	-	-	0/1/1/1	-
24	DMU	X	103	-	-	1/6/6/59	-
24	DMU	C	301	-	-	3/6/6/59	-
18	PGV	N	606	-	-	11/39/39/55	-
23	CHD	B	302	-	-	2/9/74/74	0/4/4/4
21	EDO	N	614	-	-	0/1/1/1	-
21	EDO	B	303	-	-	0/1/1/1	-
14	HEA	A	601[B]	-	-	8/32/76/76	-
21	EDO	A	611	-	-	0/1/1/1	-
24	DMU	P	310	-	-	0/8/8/59	-
21	EDO	J	103	-	-	0/1/1/1	-
21	EDO	N	616	-	-	0/1/1/1	-
24	DMU	X	101	-	-	1/19/59/59	0/2/2/2
21	EDO	E	202	-	-	1/1/1/1	-
21	EDO	P	311	-	-	0/1/1/1	-
21	EDO	N	621	-	-	0/1/1/1	-
21	EDO	A	619	-	-	1/1/1/1	-
19	TGL	Q	201	-	-	17/65/65/65	-
20	PSC	O	303	-	-	5/18/18/55	-
18	PGV	N	607	-	-	4/55/55/55	-
19	TGL	L	101	-	-	21/61/61/65	-
24	DMU	O	304	-	-	2/7/7/59	-
21	EDO	A	615	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	DMU	D	203	-	-	1/6/6/59	-
21	EDO	N	615	-	-	0/1/1/1	-
21	EDO	W	102	-	-	0/1/1/1	-
14	HEA	A	602	1	-	6/32/76/76	-
19	TGL	N	608	-	-	14/48/49/65	-
21	EDO	J	104	-	-	0/1/1/1	-
26	PEK	P	309	-	-	16/34/34/56	-
21	EDO	S	104	-	-	0/1/1/1	-
23	CHD	P	306	-	-	0/9/74/74	0/4/4/4
21	EDO	F	106	-	-	0/1/1/1	-
21	EDO	Q	202	-	-	1/1/1/1	-
24	DMU	C	308	-	-	0/9/9/59	-
21	EDO	B	304	-	-	0/1/1/1	-
21	EDO	B	306	-	-	0/1/1/1	-
25	CDL	G	102	-	-	8/51/52/110	-
26	PEK	C	305	-	-	13/31/31/56	-
14	HEA	N	601[B]	-	-	7/32/76/76	-
24	DMU	J	102	-	-	2/8/8/59	-
24	DMU	P	303	-	-	5/19/59/59	0/2/2/2
21	EDO	A	614	-	-	0/1/1/1	-
21	EDO	S	105	-	-	0/1/1/1	-
26	PEK	P	308	-	-	16/56/56/56	-
21	EDO	A	616	-	-	0/1/1/1	-
23	CHD	J	101	-	-	5/9/74/74	0/4/4/4
21	EDO	S	102	-	-	0/1/1/1	-
24	DMU	K	103	-	-	9/19/59/59	0/2/2/2
24	DMU	L	102	-	-	7/13/29/59	0/1/1/2
21	EDO	C	311	-	-	1/1/1/1	-
21	EDO	N	617	-	-	0/1/1/1	-
24	DMU	K	104	-	-	1/6/6/59	-
21	EDO	Q	204	-	-	1/1/1/1	-
18	PGV	A	606	-	-	7/55/55/55	-
24	DMU	M	101	-	-	4/19/59/59	0/2/2/2
14	HEA	N	602	1	-	7/32/76/76	-
21	EDO	T	103	-	-	0/1/1/1	-
19	TGL	O	301	-	-	14/57/57/65	-
21	EDO	A	613	-	-	1/1/1/1	-
21	EDO	F	105	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	EDO	N	613	-	-	1/1/1/1	-
24	DMU	K	101	-	-	1/6/6/59	-
21	EDO	F	102	-	-	0/1/1/1	-
24	DMU	W	101	-	-	1/6/6/59	-
24	DMU	X	104	-	-	1/7/7/59	-
25	CDL	T	101	-	-	18/73/73/110	-
21	EDO	Y	101	-	-	0/1/1/1	-
23	CHD	G	103	-	-	2/9/74/74	0/4/4/4
24	DMU	K	106	-	-	1/6/6/59	-
26	PEK	P	301	-	-	11/17/17/56	-
18	PGV	C	306	-	-	6/31/31/55	-
21	EDO	C	312	-	-	0/1/1/1	-
21	EDO	N	620	-	-	0/1/1/1	-
18	PGV	A	607	-	-	9/30/31/55	-
25	CDL	C	303	-	-	6/47/47/110	-
21	EDO	C	310	-	-	0/1/1/1	-
21	EDO	O	306	-	-	0/1/1/1	-
24	DMU	K	102	-	-	3/6/6/59	-
21	EDO	C	313	-	-	0/1/1/1	-
21	EDO	B	305	-	-	0/1/1/1	-
20	PSC	A	609	-	-	4/19/19/55	-
19	TGL	A	608	-	-	17/63/63/65	-
24	DMU	X	102	-	-	1/7/7/59	-
21	EDO	O	305	-	-	0/1/1/1	-
21	EDO	P	313	-	-	0/1/1/1	-
21	EDO	A	612	-	-	0/1/1/1	-
21	EDO	A	610	-	-	1/1/1/1	-
21	EDO	N	618	-	-	0/1/1/1	-
14	HEA	A	601[A]	-	-	6/32/76/76	-
21	EDO	N	609	-	-	0/1/1/1	-
21	EDO	W	103	-	-	1/1/1/1	-
21	EDO	A	618	-	-	1/1/1/1	-

All (150) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	C	306	PGV	O03-C19	5.09	1.48	1.33
25	P	305	CDL	OB6-CB5	4.92	1.47	1.33
25	P	305	CDL	OB8-CB7	4.92	1.47	1.33
18	A	607	PGV	O01-C1	4.90	1.47	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	D	201	TGL	OG3-CC1	4.86	1.47	1.33
25	T	101	CDL	OB8-CB7	4.73	1.47	1.33
18	N	606	PGV	O03-C19	4.73	1.47	1.33
19	L	101	TGL	OG3-CC1	4.69	1.47	1.33
25	T	101	CDL	OA8-CA7	4.68	1.46	1.30
19	O	301	TGL	OG1-CA1	4.66	1.46	1.33
18	P	302	PGV	O01-C1	4.64	1.47	1.34
14	A	602	HEA	CHD-C1D	4.60	1.46	1.35
19	A	608	TGL	OG2-CB1	4.53	1.47	1.34
25	C	303	CDL	OB6-CB5	4.51	1.46	1.33
14	A	602	HEA	CHC-C4B	4.48	1.46	1.35
18	P	302	PGV	O03-C19	4.46	1.46	1.33
18	P	304	PGV	O03-C01	-4.46	1.35	1.45
18	N	606	PGV	O01-C1	4.40	1.46	1.33
19	O	301	TGL	OG3-CC1	4.32	1.46	1.33
19	L	101	TGL	OG2-CB1	4.27	1.46	1.34
19	L	101	TGL	OG1-CA1	4.26	1.45	1.33
19	D	201	TGL	OG2-CB1	4.25	1.46	1.34
19	Q	201	TGL	OG1-CA1	4.25	1.45	1.33
19	O	301	TGL	OG2-CB1	4.24	1.46	1.34
19	D	201	TGL	OG1-CA1	4.22	1.45	1.33
19	Q	201	TGL	OG2-CB1	4.19	1.46	1.34
19	Q	201	TGL	OG3-CC1	4.19	1.45	1.33
19	N	608	TGL	OG3-CC1	4.15	1.46	1.33
25	T	101	CDL	OB6-CB5	4.08	1.45	1.34
19	A	608	TGL	OG3-CC1	4.06	1.45	1.33
14	N	602	HEA	C1D-ND	-4.04	1.33	1.40
14	A	601[A]	HEA	C3C-C2C	-4.04	1.34	1.40
14	A	601[B]	HEA	C3C-C2C	-4.04	1.34	1.40
26	P	309	PEK	O03-C21	4.00	1.45	1.33
14	N	601[A]	HEA	CHC-C4B	3.74	1.44	1.35
14	N	601[B]	HEA	CHC-C4B	3.74	1.44	1.35
20	A	609	PSC	C13-C12	3.70	1.53	1.31
14	N	602	HEA	CHD-C1D	3.67	1.44	1.35
14	A	601[A]	HEA	C4D-C3D	-3.63	1.38	1.45
14	A	601[B]	HEA	C4D-C3D	-3.63	1.38	1.45
14	A	602	HEA	C1D-C2D	-3.59	1.37	1.44
20	O	303	PSC	C13-C12	3.52	1.52	1.31
14	A	601[A]	HEA	CHC-C4B	3.52	1.44	1.35
14	A	601[B]	HEA	CHC-C4B	3.52	1.44	1.35
26	G	101	PEK	O04-C21	3.50	1.32	1.22
14	A	601[A]	HEA	CHD-C1D	3.48	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	601[B]	HEA	CHD-C1D	3.48	1.43	1.35
25	P	305	CDL	C82-C81	-3.46	1.32	1.51
26	G	101	PEK	O03-C01	-3.40	1.37	1.45
25	C	303	CDL	C82-C81	-3.37	1.32	1.51
25	G	102	CDL	C59-C58	-3.35	1.32	1.51
14	N	601[A]	HEA	CMD-C2D	3.30	1.57	1.50
14	N	601[B]	HEA	CMD-C2D	3.30	1.57	1.50
18	P	304	PGV	O03-C19	3.30	1.43	1.33
25	C	303	CDL	C79-C78	-3.29	1.33	1.51
14	N	601[A]	HEA	C4B-NB	-3.26	1.34	1.40
14	N	601[B]	HEA	C4B-NB	-3.26	1.34	1.40
25	T	101	CDL	C62-C61	-3.26	1.33	1.51
25	P	305	CDL	C79-C78	-3.26	1.33	1.51
14	A	601[A]	HEA	O11-C11	3.26	1.49	1.42
14	N	601[A]	HEA	O11-C11	3.24	1.49	1.42
25	P	305	CDL	C22-C21	-3.24	1.33	1.51
25	P	305	CDL	C19-C18	-3.23	1.33	1.51
25	G	102	CDL	C22-C21	-3.22	1.33	1.51
25	T	101	CDL	C82-C81	-3.21	1.33	1.51
25	G	102	CDL	C19-C18	-3.18	1.33	1.51
25	G	102	CDL	C62-C61	-3.18	1.33	1.51
25	P	305	CDL	C42-C41	-3.17	1.33	1.51
25	P	305	CDL	C39-C38	-3.16	1.33	1.51
25	G	102	CDL	C39-C38	-3.16	1.33	1.51
25	T	101	CDL	C19-C18	-3.16	1.33	1.51
25	G	102	CDL	C42-C41	-3.15	1.33	1.51
25	T	101	CDL	C59-C58	-3.15	1.33	1.51
14	N	602	HEA	O11-C11	3.14	1.49	1.42
25	G	102	CDL	C82-C81	-3.14	1.34	1.51
25	T	101	CDL	C22-C21	-3.13	1.34	1.51
25	T	101	CDL	C39-C38	-3.13	1.34	1.51
25	T	101	CDL	C79-C78	-3.12	1.34	1.51
25	T	101	CDL	C42-C41	-3.07	1.34	1.51
25	C	303	CDL	C59-C58	-3.07	1.34	1.51
25	G	102	CDL	C79-C78	-3.06	1.34	1.51
18	N	607	PGV	O01-C1	2.98	1.42	1.34
14	A	602	HEA	C3C-C2C	-2.89	1.36	1.40
18	N	607	PGV	O01-C02	-2.89	1.39	1.46
14	N	602	HEA	C1D-C2D	-2.81	1.39	1.44
23	C	304	CHD	O12-C12	2.75	1.48	1.43
18	N	607	PGV	O03-C01	2.74	1.51	1.45
14	N	601[A]	HEA	CMB-C2B	2.71	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	601[B]	HEA	CMB-C2B	2.71	1.56	1.50
23	B	302	CHD	C11-C12	2.70	1.57	1.53
14	A	602	HEA	C1D-ND	-2.59	1.35	1.40
14	N	601[A]	HEA	C1D-C2D	-2.57	1.39	1.44
14	N	601[B]	HEA	C1D-C2D	-2.57	1.39	1.44
14	N	601[A]	HEA	O1A-CGA	2.56	1.30	1.22
14	N	601[B]	HEA	O1A-CGA	2.56	1.30	1.22
18	C	302	PGV	O03-C01	2.52	1.50	1.45
14	N	601[A]	HEA	C3C-C2C	-2.51	1.36	1.40
14	N	601[B]	HEA	C3C-C2C	-2.51	1.36	1.40
25	P	305	CDL	C59-C58	-2.51	1.33	1.51
26	P	308	PEK	O03-C21	2.50	1.40	1.33
18	N	607	PGV	C03-C02	2.44	1.58	1.50
18	P	304	PGV	P-O14	-2.44	1.43	1.55
26	G	101	PEK	O03-C21	2.41	1.40	1.33
14	N	602	HEA	CHC-C4B	2.41	1.41	1.35
14	A	601[A]	HEA	C4B-NB	-2.39	1.36	1.40
14	A	601[B]	HEA	C4B-NB	-2.39	1.36	1.40
23	B	302	CHD	C10-C9	-2.38	1.51	1.56
23	B	302	CHD	O12-C12	2.38	1.47	1.43
14	N	602	HEA	C4B-C3B	-2.36	1.40	1.44
14	N	601[A]	HEA	CBD-CGD	2.35	1.56	1.50
14	N	601[B]	HEA	CBD-CGD	2.35	1.56	1.50
14	A	601[A]	HEA	CBD-CGD	2.32	1.56	1.50
14	A	601[B]	HEA	CBD-CGD	2.32	1.56	1.50
14	A	601[A]	HEA	C12-C13	2.31	1.61	1.53
14	A	602	HEA	O11-C11	2.31	1.47	1.42
26	G	101	PEK	O01-C1	2.30	1.40	1.34
25	T	101	CDL	OB6-CB4	-2.30	1.43	1.47
23	P	307	CHD	O12-C12	2.28	1.47	1.43
18	A	606	PGV	O01-C1	2.24	1.40	1.34
24	Z	101	DMU	O16-C6	2.23	1.44	1.40
26	P	308	PEK	C05-C04	2.21	1.59	1.50
14	N	601[A]	HEA	CHD-C1D	2.20	1.40	1.35
14	N	601[B]	HEA	CHD-C1D	2.20	1.40	1.35
24	P	303	DMU	O16-C6	2.19	1.43	1.40
14	N	602	HEA	C12-C11	2.17	1.56	1.52
18	A	606	PGV	O01-C02	-2.16	1.41	1.46
18	P	304	PGV	C20-C19	2.16	1.57	1.50
14	N	602	HEA	C1B-C2B	-2.14	1.40	1.44
14	A	601[A]	HEA	CMB-C2B	2.14	1.55	1.50
14	A	601[B]	HEA	CMB-C2B	2.14	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	601[A]	HEA	C3C-CAC	2.13	1.52	1.47
14	N	601[B]	HEA	C3C-CAC	2.13	1.52	1.47
24	K	103	DMU	O16-C6	2.13	1.43	1.40
14	N	601[A]	HEA	C1D-ND	-2.13	1.36	1.40
14	N	601[B]	HEA	C1D-ND	-2.13	1.36	1.40
14	A	602	HEA	O2D-CGD	-2.11	1.23	1.30
14	A	601[A]	HEA	C2A-C1A	-2.09	1.37	1.42
14	A	601[B]	HEA	C2A-C1A	-2.09	1.37	1.42
14	A	601[A]	HEA	C1B-C2B	-2.09	1.40	1.44
14	A	601[B]	HEA	C1B-C2B	-2.09	1.40	1.44
14	N	602	HEA	C4D-C3D	-2.07	1.41	1.45
14	A	602	HEA	C12-C11	2.03	1.56	1.52
14	A	602	HEA	O1A-CGA	2.03	1.28	1.22
14	A	601[A]	HEA	C4C-CHD	2.03	1.46	1.41
14	A	601[B]	HEA	C4C-CHD	2.03	1.46	1.41
14	N	602	HEA	CBA-CGA	2.02	1.55	1.50
23	G	103	CHD	C10-C9	-2.02	1.52	1.56
14	A	601[A]	HEA	CAD-C3D	2.01	1.56	1.51
14	A	601[B]	HEA	CAD-C3D	2.01	1.56	1.51
25	C	303	CDL	C39-C38	-2.00	1.33	1.49

All (260) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	P	304	PGV	O03-C19-O04	-8.99	100.89	123.59
18	P	304	PGV	O03-C19-C20	7.92	136.76	111.91
25	T	101	CDL	CB4-OB6-CB5	-6.66	109.31	117.88
14	A	602	HEA	C2D-C1D-ND	6.64	117.71	109.84
14	N	601[B]	HEA	C13-C12-C11	-6.43	104.70	114.35
14	N	602	HEA	O2D-CGD-O1D	6.28	138.95	123.30
19	A	608	TGL	OG2-CB1-CB2	6.10	124.66	111.50
19	O	301	TGL	OG2-CB1-CB2	5.99	124.40	111.50
26	G	101	PEK	O03-C21-C22	5.41	128.90	111.91
25	T	101	CDL	OB6-CB5-C51	5.33	123.00	111.50
19	L	101	TGL	OG2-CB1-CB2	4.96	122.20	111.50
26	G	101	PEK	O03-C21-O04	-4.95	111.10	123.59
14	N	602	HEA	CBD-CAD-C3D	4.76	125.84	112.63
23	B	302	CHD	C11-C9-C10	-4.64	108.94	113.73
18	P	304	PGV	C03-C02-C01	4.61	122.68	111.79
18	P	302	PGV	O01-C1-C2	4.61	121.43	111.50
19	D	201	TGL	OG3-CC1-CC2	4.55	126.18	111.91
26	P	308	PEK	O03-C21-C22	4.52	126.09	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	P	308	PEK	C02-O01-C1	-4.47	106.79	117.79
14	A	601[A]	HEA	C3D-C4D-ND	4.45	114.67	110.36
14	A	601[B]	HEA	C3D-C4D-ND	4.45	114.67	110.36
14	A	602	HEA	C13-C12-C11	-4.44	107.67	114.35
26	G	101	PEK	C02-O01-C1	-4.41	106.94	117.79
14	A	602	HEA	CMD-C2D-C1D	4.29	131.56	125.04
14	N	601[A]	HEA	C3C-C4C-NC	4.28	114.74	109.21
14	N	601[B]	HEA	C3C-C4C-NC	4.28	114.74	109.21
14	A	601[B]	HEA	C13-C12-C11	-4.22	108.00	114.35
14	N	602	HEA	C2D-C1D-ND	4.22	114.84	109.84
14	N	602	HEA	C2B-C1B-NB	4.17	114.88	109.88
14	A	601[A]	HEA	CMB-C2B-C1B	-4.15	118.71	125.04
14	A	601[B]	HEA	CMB-C2B-C1B	-4.15	118.71	125.04
14	A	601[A]	HEA	C17-C18-C19	-4.04	117.92	127.66
26	P	308	PEK	C01-O03-C21	4.04	132.06	117.12
23	C	304	CHD	C14-C8-C7	-3.98	106.52	111.81
14	A	602	HEA	O2D-CGD-O1D	3.98	133.21	123.30
18	P	302	PGV	O03-C19-C20	3.84	123.95	111.91
23	G	103	CHD	C4-C3-C2	-3.82	106.00	110.55
23	C	304	CHD	C1-C2-C3	-3.82	105.57	110.47
14	A	602	HEA	C2B-C1B-NB	3.80	114.43	109.88
14	N	601[A]	HEA	CAA-CBA-CGA	-3.77	103.19	113.76
14	N	601[B]	HEA	CAA-CBA-CGA	-3.77	103.19	113.76
26	P	308	PEK	O03-C21-O04	-3.75	114.14	123.59
23	B	302	CHD	C19-C10-C5	-3.69	104.10	110.36
14	A	602	HEA	C4D-CHA-C1A	3.65	127.38	122.56
19	Q	201	TGL	OG2-CB1-CB2	3.62	119.29	111.50
18	C	306	PGV	O03-C19-C20	3.61	123.24	111.91
26	P	308	PEK	C03-C02-C01	3.60	120.31	111.79
23	B	302	CHD	C6-C5-C4	-3.59	107.06	111.19
19	D	201	TGL	OG3-CC1-OC1	-3.57	114.58	123.59
18	N	607	PGV	O01-C1-O02	-3.56	115.11	123.70
14	A	602	HEA	C3C-C4C-NC	3.49	113.72	109.21
18	P	302	PGV	O01-C02-C01	3.48	114.19	106.13
24	M	101	DMU	C18-O16-C6	-3.48	108.07	113.84
14	A	601[B]	HEA	C17-C18-C19	-3.46	119.32	127.66
14	A	601[A]	HEA	C3B-C4B-NB	3.46	113.94	109.84
14	A	601[B]	HEA	C3B-C4B-NB	3.46	113.94	109.84
23	P	306	CHD	C13-C17-C20	-3.45	115.37	119.50
14	N	601[A]	HEA	C27-C19-C20	3.45	121.08	115.27
14	N	601[B]	HEA	C27-C19-C20	3.45	121.08	115.27
18	P	304	PGV	C01-O03-C19	3.45	129.88	117.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	601[A]	HEA	C4B-NB-C1B	-3.42	101.54	105.07
14	A	601[B]	HEA	C4B-NB-C1B	-3.42	101.54	105.07
23	J	101	CHD	C22-C20-C17	3.42	117.34	110.28
18	N	606	PGV	O01-C1-C2	3.41	122.62	111.91
14	A	601[A]	HEA	CMC-C2C-C1C	-3.41	123.22	128.46
14	A	601[B]	HEA	CMC-C2C-C1C	-3.41	123.22	128.46
14	N	602	HEA	C4B-NB-C1B	-3.33	101.64	105.07
14	N	601[A]	HEA	O2A-CGA-CBA	3.21	124.35	114.03
14	N	601[B]	HEA	O2A-CGA-CBA	3.21	124.35	114.03
23	G	103	CHD	C21-C20-C17	-3.19	108.04	112.92
25	C	303	CDL	OB6-CB5-C51	3.18	121.88	111.91
23	C	304	CHD	C6-C7-C8	-3.17	108.10	111.48
23	P	306	CHD	C17-C13-C14	3.15	103.27	100.09
23	C	304	CHD	C1-C10-C5	3.15	112.42	107.77
24	K	103	DMU	C10-O7-C3	-3.14	110.19	117.96
23	C	304	CHD	C14-C13-C12	3.13	110.32	107.40
26	G	101	PEK	O03-C01-C02	-3.12	99.35	108.43
23	P	307	CHD	C22-C20-C17	-3.11	103.85	110.28
24	K	103	DMU	C7-C8-C9	-3.11	104.69	110.24
23	P	307	CHD	C22-C23-C24	-3.10	104.28	112.51
23	G	103	CHD	C6-C5-C4	-3.10	107.63	111.19
23	G	103	CHD	C2-C1-C10	-3.08	107.50	112.78
14	A	602	HEA	C1D-C2D-C3D	-3.07	103.73	106.96
14	N	601[A]	HEA	C27-C19-C18	-3.05	115.85	123.68
23	C	304	CHD	C4-C3-C2	3.05	114.19	110.55
14	N	601[A]	HEA	OMA-CMA-C3A	-3.05	118.28	124.91
14	N	601[B]	HEA	OMA-CMA-C3A	-3.05	118.28	124.91
14	A	602	HEA	CBA-CAA-C2A	-3.03	107.49	112.60
14	N	602	HEA	C27-C19-C20	3.03	120.36	115.27
26	P	308	PEK	O11-P-O14	-3.02	97.25	109.07
14	N	601[A]	HEA	C4D-CHA-C1A	-3.02	118.57	122.56
14	N	601[B]	HEA	C4D-CHA-C1A	-3.02	118.57	122.56
14	A	602	HEA	CMC-C2C-C1C	-3.02	123.81	128.46
14	A	602	HEA	C1D-ND-C4D	-3.00	101.98	105.07
14	A	601[A]	HEA	CHA-C4D-C3D	-2.99	120.44	124.84
14	A	601[B]	HEA	CHA-C4D-C3D	-2.99	120.44	124.84
14	N	601[A]	HEA	C13-C12-C11	-2.97	109.89	114.35
24	L	102	DMU	C3-C4-C57	-2.97	107.40	112.60
19	Q	201	TGL	OG1-CA1-CA2	2.96	121.21	111.91
14	A	602	HEA	C25-C23-C22	-2.95	114.13	122.65
23	B	302	CHD	C16-C17-C20	-2.94	107.59	112.15
23	J	101	CHD	C15-C14-C13	2.94	106.43	103.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	304	CHD	C4-C5-C10	-2.92	109.56	112.66
25	P	305	CDL	OB8-CB7-C71	2.91	121.05	111.91
14	N	602	HEA	O2D-CGD-CBD	-2.90	104.72	114.03
18	C	306	PGV	O03-C19-O04	-2.88	116.31	123.59
19	Q	201	TGL	CG2-OG2-CB1	-2.87	110.72	117.79
23	P	306	CHD	C13-C14-C8	-2.87	111.08	114.74
14	A	601[A]	HEA	C2B-C1B-NB	2.86	113.31	109.88
14	A	601[B]	HEA	C2B-C1B-NB	2.86	113.31	109.88
19	A	608	TGL	OG3-CC1-CC2	2.86	120.88	111.91
23	C	304	CHD	C18-C13-C12	2.84	111.96	109.07
14	A	602	HEA	CHB-C1B-NB	-2.84	121.34	124.43
23	P	306	CHD	C11-C9-C10	-2.83	110.80	113.73
14	A	602	HEA	C4B-NB-C1B	-2.82	102.17	105.07
24	M	101	DMU	O5-C6-O16	-2.82	103.31	109.97
14	N	601[A]	HEA	C3B-C4B-NB	2.80	113.15	109.84
14	N	601[B]	HEA	C3B-C4B-NB	2.80	113.15	109.84
14	A	602	HEA	CBD-CAD-C3D	2.79	120.39	112.63
18	N	606	PGV	O03-C19-C20	2.78	120.63	111.91
19	O	301	TGL	OG3-CC1-CC2	2.78	120.62	111.91
19	L	101	TGL	OG1-CA1-CA2	2.77	120.59	111.91
14	A	601[A]	HEA	C20-C21-C22	-2.76	102.82	111.88
14	A	601[B]	HEA	C20-C21-C22	-2.76	102.82	111.88
23	P	307	CHD	C21-C20-C22	-2.75	106.05	110.36
19	D	201	TGL	CG2-OG2-CB1	-2.74	111.05	117.79
23	B	302	CHD	O12-C12-C13	-2.74	106.41	111.03
14	N	602	HEA	C3C-C4C-NC	2.73	112.74	109.21
14	N	601[A]	HEA	C26-C15-C14	-2.73	116.69	123.68
23	C	304	CHD	C13-C14-C8	-2.72	111.27	114.74
18	C	302	PGV	C21-C20-C19	-2.72	103.74	113.62
14	N	601[A]	HEA	C20-C21-C22	-2.69	103.03	111.88
14	N	601[B]	HEA	C20-C21-C22	-2.69	103.03	111.88
14	N	601[A]	HEA	C17-C18-C19	-2.69	121.18	127.66
23	B	302	CHD	C10-C9-C8	2.69	114.71	111.82
19	O	301	TGL	CG2-OG2-CB1	-2.69	111.17	117.79
14	N	602	HEA	CMD-C2D-C1D	2.68	129.12	125.04
14	N	601[A]	HEA	CHA-C4D-C3D	-2.68	120.91	124.84
14	N	601[B]	HEA	CHA-C4D-C3D	-2.68	120.91	124.84
14	A	601[A]	HEA	CHB-C1B-NB	-2.67	121.53	124.43
14	A	601[B]	HEA	CHB-C1B-NB	-2.67	121.53	124.43
18	P	302	PGV	O03-C19-O04	-2.66	116.87	123.59
14	A	602	HEA	CAD-C3D-C4D	-2.66	120.01	124.66
14	A	602	HEA	CAD-C3D-C2D	2.66	132.83	127.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	N	602	HEA	CMB-C2B-C1B	2.64	129.06	125.04
19	O	301	TGL	OG1-CA1-CA2	2.63	120.16	111.91
18	P	302	PGV	C01-O03-C19	2.63	126.85	117.12
14	A	601[A]	HEA	CAA-CBA-CGA	-2.62	106.41	113.76
14	A	601[B]	HEA	CAA-CBA-CGA	-2.62	106.41	113.76
19	D	201	TGL	OG1-CA1-CA2	2.60	120.08	111.91
14	A	601[A]	HEA	C1D-ND-C4D	-2.60	102.39	105.07
14	A	601[B]	HEA	C1D-ND-C4D	-2.60	102.39	105.07
23	B	302	CHD	C19-C10-C9	2.60	114.76	111.18
19	A	608	TGL	OG3-CC1-OC1	-2.59	117.04	123.59
23	P	306	CHD	C22-C23-C24	-2.59	105.62	112.51
18	N	606	PGV	O01-C1-O02	-2.59	117.06	123.59
23	P	306	CHD	C16-C17-C13	2.57	106.08	103.55
14	A	601[A]	HEA	C3C-C4C-NC	2.57	112.53	109.21
14	A	601[B]	HEA	C3C-C4C-NC	2.57	112.53	109.21
14	A	601[A]	HEA	C13-C12-C11	-2.55	110.52	114.35
14	N	601[A]	HEA	CHA-C4D-ND	2.55	127.20	124.43
14	N	601[B]	HEA	CHA-C4D-ND	2.55	127.20	124.43
19	O	301	TGL	OG2-CB1-OB1	-2.55	117.55	123.70
25	T	101	CDL	OB6-CB5-OB7	-2.55	117.55	123.70
26	G	101	PEK	C23-C22-C21	-2.54	104.38	113.62
14	N	602	HEA	CHA-C4D-ND	2.53	127.19	124.43
18	P	304	PGV	O03-C01-C02	-2.52	101.08	108.43
14	N	601[A]	HEA	CMB-C2B-C1B	-2.52	121.20	125.04
14	N	601[B]	HEA	CMB-C2B-C1B	-2.52	121.20	125.04
23	P	307	CHD	C19-C10-C1	-2.52	104.21	108.26
23	G	103	CHD	C4-C5-C10	-2.52	109.99	112.66
23	P	307	CHD	O12-C12-C13	-2.50	106.80	111.03
19	L	101	TGL	CB3-CB2-CB1	-2.50	104.54	113.62
19	L	101	TGL	CG2-OG2-CB1	-2.50	111.64	117.79
14	A	601[A]	HEA	CHC-C4B-C3B	-2.49	119.39	125.80
14	A	601[B]	HEA	CHC-C4B-C3B	-2.49	119.39	125.80
14	A	602	HEA	C27-C19-C20	2.49	119.45	115.27
14	N	602	HEA	CHB-C1B-NB	-2.48	121.74	124.43
26	P	308	PEK	C23-C22-C21	-2.48	104.61	113.62
18	P	302	PGV	C03-C02-C01	-2.46	105.55	112.63
14	N	601[B]	HEA	C16-C17-C18	-2.46	103.79	111.88
14	A	601[B]	HEA	C26-C15-C16	2.46	119.41	115.27
19	L	101	TGL	OG3-CC1-CC2	2.44	119.58	111.91
25	C	303	CDL	CB7-OB8-CB6	2.44	123.84	113.29
14	A	602	HEA	CHD-C1D-C2D	-2.43	120.01	126.72
14	N	602	HEA	C13-C12-C11	-2.42	110.72	114.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	302	CHD	C13-C14-C8	-2.41	111.66	114.74
23	C	304	CHD	C19-C10-C1	-2.40	104.39	108.26
14	N	602	HEA	C4D-CHA-C1A	2.38	125.70	122.56
26	G	101	PEK	C03-C02-C01	2.38	117.42	111.79
14	A	601[A]	HEA	O2A-CGA-CBA	2.38	121.67	114.03
14	A	601[B]	HEA	O2A-CGA-CBA	2.38	121.67	114.03
26	P	309	PEK	O03-C21-C22	2.37	121.61	112.23
26	G	101	PEK	O11-P-O14	-2.37	99.80	109.07
19	D	201	TGL	CG3-CG2-CG1	-2.37	106.19	111.79
18	A	606	PGV	C4-C3-C2	-2.35	104.73	113.19
14	N	601[B]	HEA	C17-C18-C19	-2.35	122.00	127.66
14	N	601[A]	HEA	O1D-CGD-CBD	-2.34	115.57	123.08
14	N	601[B]	HEA	O1D-CGD-CBD	-2.34	115.57	123.08
23	J	101	CHD	C13-C14-C8	-2.34	111.76	114.74
18	P	304	PGV	C22-C21-C20	-2.32	104.86	113.19
14	A	602	HEA	O2A-CGA-CBA	2.31	121.47	114.03
24	L	102	DMU	O5-C4-C57	2.31	110.54	106.83
14	N	602	HEA	CHD-C1D-ND	-2.31	121.53	124.38
23	B	302	CHD	C5-C4-C3	-2.30	109.38	112.76
24	M	101	DMU	C11-C9-C8	-2.29	107.64	113.00
19	L	101	TGL	CG3-CG2-CG1	-2.29	106.37	111.79
23	G	103	CHD	C19-C10-C5	-2.28	106.49	110.36
23	C	304	CHD	C21-C20-C17	2.28	116.41	112.92
23	B	302	CHD	C17-C13-C12	2.27	119.74	117.67
14	A	601[B]	HEA	C16-C17-C18	-2.27	104.42	111.88
14	A	602	HEA	C13-C14-C15	-2.27	122.21	127.66
14	A	601[A]	HEA	C4B-C3B-C2B	-2.26	103.55	107.41
14	A	601[B]	HEA	C4B-C3B-C2B	-2.26	103.55	107.41
23	C	304	CHD	C21-C20-C22	-2.24	106.84	110.36
14	N	601[A]	HEA	C13-C14-C15	-2.23	122.28	127.66
23	J	101	CHD	C16-C17-C13	2.23	105.74	103.55
19	Q	201	TGL	OG3-CC1-CC2	2.22	118.88	111.91
23	C	304	CHD	C11-C9-C10	-2.22	111.44	113.73
14	N	602	HEA	C1D-C2D-C3D	-2.22	104.62	106.96
19	L	101	TGL	C20-CA9-CA8	-2.22	103.17	114.42
14	A	601[A]	HEA	C13-C14-C15	-2.21	122.33	127.66
23	B	302	CHD	C16-C17-C13	2.21	105.72	103.55
23	P	306	CHD	C19-C10-C9	-2.20	108.15	111.18
14	N	602	HEA	C3B-C4B-NB	2.20	112.45	109.84
19	D	201	TGL	OG1-CA1-OA1	-2.20	118.04	123.59
23	B	302	CHD	C22-C23-C24	-2.18	106.71	112.51
19	Q	201	TGL	OG1-CA1-OA1	-2.18	118.10	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	N	607	PGV	C4-C3-C2	-2.18	105.36	113.19
14	N	602	HEA	C1B-C2B-C3B	-2.18	104.20	106.80
26	G	101	PEK	O12-C04-C05	-2.16	101.01	109.10
18	P	304	PGV	C24-C23-C22	-2.16	103.48	114.42
23	C	304	CHD	O3-C3-C2	-2.15	104.69	110.16
23	B	302	CHD	C1-C10-C5	2.14	110.93	107.77
14	A	602	HEA	O1A-CGA-CBA	-2.13	116.22	123.08
23	J	101	CHD	C13-C17-C20	2.13	122.04	119.50
18	N	607	PGV	C01-O03-C19	-2.13	109.24	117.12
23	P	307	CHD	O7-C7-C8	2.12	114.16	109.43
14	N	601[A]	HEA	C26-C15-C16	2.11	118.83	115.27
19	L	101	TGL	OG1-CA1-OA1	-2.10	118.28	123.59
19	A	608	TGL	OG2-CB1-OB1	-2.10	118.62	123.70
14	N	602	HEA	O1D-CGD-CBD	-2.10	116.33	123.08
14	A	602	HEA	C21-C20-C19	2.10	119.88	112.98
24	X	101	DMU	C10-O7-C3	-2.09	112.78	117.96
24	L	102	DMU	C6-O5-C4	2.08	115.44	113.13
19	Q	201	TGL	OG2-CB1-OB1	-2.08	118.68	123.70
14	A	602	HEA	C12-C13-C14	-2.08	106.75	112.23
23	C	304	CHD	C22-C20-C17	-2.08	105.99	110.28
14	N	601[A]	HEA	CMC-C2C-C1C	-2.05	125.32	128.46
14	N	601[B]	HEA	CMC-C2C-C1C	-2.05	125.32	128.46
18	N	606	PGV	C02-O01-C1	-2.04	110.31	116.92
23	C	304	CHD	C22-C23-C24	-2.04	107.09	112.51
14	A	602	HEA	CAA-CBA-CGA	-2.04	108.04	113.76
23	P	306	CHD	O25-C24-C23	-2.04	116.53	123.08
19	N	608	TGL	OG3-CC1-CC2	2.03	120.26	112.23
18	N	607	PGV	O02-C1-C2	2.03	131.65	123.73
23	B	302	CHD	C14-C8-C9	2.02	112.49	109.71
14	N	602	HEA	C16-C15-C14	-2.02	117.03	121.12
14	N	601[A]	HEA	CHC-C4B-C3B	-2.02	120.60	125.80
14	N	601[B]	HEA	CHC-C4B-C3B	-2.02	120.60	125.80

There are no chirality outliers.

All (413) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	601[A]	HEA	C14-C15-C16-C17
14	A	601[A]	HEA	C26-C15-C16-C17
14	A	602	HEA	C2D-C3D-CAD-CBD
14	A	602	HEA	C4D-C3D-CAD-CBD
14	N	601[A]	HEA	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
14	N	601[A]	HEA	C26-C15-C16-C17
18	A	606	PGV	C10-C11-C12-C13
18	C	302	PGV	C10-C11-C12-C13
18	C	306	PGV	O04-C19-O03-C01
18	C	306	PGV	C20-C19-O03-C01
18	N	606	PGV	O04-C19-O03-C01
18	N	606	PGV	C20-C19-O03-C01
18	P	302	PGV	O04-C19-O03-C01
18	P	302	PGV	C20-C19-O03-C01
18	P	302	PGV	C10-C11-C12-C13
18	P	304	PGV	O04-C19-O03-C01
18	P	304	PGV	C20-C19-O03-C01
23	J	101	CHD	C13-C17-C20-C22
24	L	102	DMU	C1-C6-O16-C18
24	L	102	DMU	O5-C6-O16-C18
25	T	101	CDL	OB6-CB4-CB6-OB8
26	C	307	PEK	C9-C10-C11-C12
26	G	101	PEK	C22-C21-O03-C01
26	P	301	PEK	C4-C5-C6-C7
26	P	301	PEK	C9-C10-C11-C12
26	G	101	PEK	O04-C21-O03-C01
26	P	308	PEK	O04-C21-O03-C01
26	P	309	PEK	O04-C21-O03-C01
24	K	103	DMU	O5-C4-C57-O61
26	P	309	PEK	C22-C21-O03-C01
26	P	308	PEK	C22-C21-O03-C01
18	A	607	PGV	C10-C11-C12-C13
18	P	304	PGV	C10-C11-C12-C13
26	G	101	PEK	C10-C11-C12-C13
26	P	309	PEK	C4-C5-C6-C7
26	P	309	PEK	C7-C8-C9-C10
24	K	103	DMU	C3-C4-C57-O61
14	A	601[B]	HEA	C15-C16-C17-C18
24	M	101	DMU	C28-C31-C34-C37
24	Z	101	DMU	C19-C22-C25-C28
23	J	101	CHD	C16-C17-C20-C22
19	D	201	TGL	C21-C22-C23-C24
23	J	101	CHD	C16-C17-C20-C21
25	T	101	CDL	C40-C41-C42-C43
19	Q	201	TGL	CC5-CC6-CC7-CC8
26	C	305	PEK	C13-C14-C15-C16
19	L	101	TGL	CA1-CA2-CA3-CA4

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Mol	Chain	Res	Type	Atoms
19	O	301	TGL	CC1-CC2-CC3-CC4
18	P	302	PGV	C1-C2-C3-C4
18	N	606	PGV	O03-C01-C02-O01
14	N	601[B]	HEA	C15-C16-C17-C18
23	J	101	CHD	C13-C17-C20-C21
19	A	608	TGL	CB1-CB2-CB3-CB4
26	C	305	PEK	C7-C8-C9-C10
19	L	101	TGL	CB2-CB3-CB4-CB5
24	K	106	DMU	C28-C31-C34-C37
26	P	308	PEK	C23-C24-C25-C26
19	N	608	TGL	C12-C13-C14-C29
19	O	301	TGL	C18-C19-C33-C34
24	J	102	DMU	C31-C34-C37-C40
25	C	303	CDL	C80-C81-C82-C83
25	G	102	CDL	C40-C41-C42-C43
25	T	101	CDL	C20-C21-C22-C23
25	T	101	CDL	C60-C61-C62-C63
26	C	305	PEK	C10-C11-C12-C13
26	C	307	PEK	C7-C8-C9-C10
19	D	201	TGL	CA7-CA8-CA9-C20
25	T	101	CDL	C77-C78-C79-C80
19	Q	201	TGL	CC2-CC3-CC4-CC5
19	D	201	TGL	C22-C23-C24-C25
24	M	101	DMU	C19-C22-C25-C28
25	P	305	CDL	C20-C21-C22-C23
19	Q	201	TGL	CC7-CC8-CC9-C15
19	Q	201	TGL	C21-C20-CA9-CA8
25	G	102	CDL	C57-C58-C59-C60
19	L	101	TGL	CC9-C15-C16-C17
24	P	303	DMU	C22-C25-C28-C31
24	K	103	DMU	C22-C25-C28-C31
25	P	305	CDL	C77-C78-C79-C80
19	D	201	TGL	C20-C21-C22-C23
19	O	301	TGL	CB9-C10-C11-C12
24	O	304	DMU	C22-C25-C28-C31
18	N	607	PGV	C10-C11-C12-C13
20	O	303	PSC	C22-C23-C24-C25
25	C	303	CDL	OB6-CB4-CB6-OB8
25	P	305	CDL	C37-C38-C39-C40
24	L	102	DMU	C18-C19-C22-C25
25	G	102	CDL	C37-C38-C39-C40
19	L	101	TGL	CA3-CA4-CA5-CA6

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Mol	Chain	Res	Type	Atoms
19	N	608	TGL	CC5-CC6-CC7-CC8
20	O	303	PSC	C23-C24-C25-C26
26	P	309	PEK	C25-C26-C27-C28
19	A	608	TGL	CA2-CA3-CA4-CA5
19	L	101	TGL	CB5-CB6-CB7-CB8
19	O	301	TGL	CB7-CB8-CB9-C10
21	A	610	EDO	O1-C1-C2-O2
19	Q	201	TGL	C20-C21-C22-C23
19	L	101	TGL	CA5-CA6-CA7-CA8
24	K	103	DMU	O16-C18-C19-C22
25	P	305	CDL	C17-C18-C19-C20
18	N	606	PGV	C01-C02-O01-C1
26	C	307	PEK	C4-C5-C6-C7
19	L	101	TGL	CB7-CB8-CB9-C10
18	N	606	PGV	C2-C1-O01-C02
18	P	304	PGV	C7-C8-C9-C10
19	N	608	TGL	CB9-C10-C11-C12
24	P	303	DMU	O16-C18-C19-C22
25	T	101	CDL	C80-C81-C82-C83
24	J	102	DMU	C28-C31-C34-C37
18	N	606	PGV	O02-C1-O01-C02
18	A	607	PGV	C2-C3-C4-C5
24	K	103	DMU	C2-C3-O7-C10
19	Q	201	TGL	CB2-CB1-OG2-CG2
24	K	103	DMU	C4-C3-O7-C10
25	C	303	CDL	C72-C73-C74-C75
19	A	608	TGL	C25-C26-C27-C28
25	G	102	CDL	C60-C61-C62-C63
19	O	301	TGL	CC9-C15-C16-C17
24	P	303	DMU	O6-C11-C9-O1
19	O	301	TGL	OG1-CG1-CG2-CG3
26	P	308	PEK	C7-C8-C9-C10
24	K	103	DMU	C18-C19-C22-C25
19	Q	201	TGL	CB7-CB8-CB9-C10
14	N	602	HEA	C4D-C3D-CAD-CBD
18	C	306	PGV	C24-C25-C26-C27
19	Q	201	TGL	C29-C30-C31-C32
24	Z	101	DMU	C34-C37-C40-C43
19	Q	201	TGL	CA1-CA2-CA3-CA4
18	N	606	PGV	C10-C11-C12-C13
26	G	101	PEK	C7-C8-C9-C10
26	P	309	PEK	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
19	L	101	TGL	C21-C22-C23-C24
18	A	607	PGV	C3-C4-C5-C6
19	A	608	TGL	C15-C16-C17-C18
19	D	201	TGL	CB2-CB3-CB4-CB5
24	D	202	DMU	C28-C31-C34-C37
24	X	102	DMU	C34-C37-C40-C43
25	P	305	CDL	OB6-CB4-CB6-OB8
19	L	101	TGL	CC2-CC3-CC4-CC5
24	K	104	DMU	C28-C31-C34-C37
19	Q	201	TGL	CB9-C10-C11-C12
19	Q	201	TGL	CA6-CA7-CA8-CA9
19	Q	201	TGL	OB1-CB1-OG2-CG2
26	G	101	PEK	C4-C5-C6-C7
26	P	308	PEK	C10-C11-C12-C13
25	T	101	CDL	C37-C38-C39-C40
24	X	104	DMU	C31-C34-C37-C40
25	C	303	CDL	C57-C58-C59-C60
25	T	101	CDL	CA7-C31-C32-C33
19	N	608	TGL	CB2-CB3-CB4-CB5
24	C	301	DMU	C22-C25-C28-C31
18	P	304	PGV	C02-C03-O11-P
25	T	101	CDL	CB3-CB4-CB6-OB8
26	P	308	PEK	O03-C01-C02-C03
26	P	308	PEK	C4-C5-C6-C7
24	K	102	DMU	C31-C34-C37-C40
20	A	609	PSC	C9-C10-C11-C12
20	A	609	PSC	C10-C11-C12-C13
20	O	303	PSC	C10-C11-C12-C13
26	C	305	PEK	C5-C6-C7-C8
26	C	305	PEK	C6-C7-C8-C9
26	C	305	PEK	C11-C10-C9-C8
26	C	305	PEK	C9-C10-C11-C12
26	C	305	PEK	C11-C12-C13-C14
26	C	305	PEK	C12-C13-C14-C15
26	C	307	PEK	C5-C6-C7-C8
26	C	307	PEK	C6-C7-C8-C9
26	C	307	PEK	C11-C10-C9-C8
26	C	307	PEK	C11-C12-C13-C14
26	C	307	PEK	C12-C13-C14-C15
26	G	101	PEK	C6-C7-C8-C9
26	G	101	PEK	C9-C10-C11-C12
26	G	101	PEK	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
26	G	101	PEK	C12-C13-C14-C15
26	P	301	PEK	C5-C6-C7-C8
26	P	301	PEK	C6-C7-C8-C9
26	P	301	PEK	C11-C10-C9-C8
26	P	301	PEK	C11-C12-C13-C14
26	P	301	PEK	C12-C13-C14-C15
26	P	308	PEK	C9-C10-C11-C12
26	P	308	PEK	C11-C12-C13-C14
26	P	308	PEK	C12-C13-C14-C15
26	P	309	PEK	C5-C6-C7-C8
26	P	309	PEK	C6-C7-C8-C9
26	P	309	PEK	C11-C10-C9-C8
26	P	309	PEK	C9-C10-C11-C12
26	P	309	PEK	C11-C12-C13-C14
26	P	309	PEK	C12-C13-C14-C15
25	C	303	CDL	C82-C83-C84-C85
19	A	608	TGL	OG1-CG1-CG2-OG2
26	P	308	PEK	O03-C01-C02-O01
19	D	201	TGL	C23-C24-C25-C26
19	L	101	TGL	C17-C18-C19-C33
14	N	602	HEA	C2D-C3D-CAD-CBD
24	L	102	DMU	O16-C18-C19-C22
24	O	304	DMU	C18-C19-C22-C25
19	O	301	TGL	C11-C10-CB9-CB8
20	A	609	PSC	C7-C8-C9-C10
26	P	309	PEK	C3-C4-C5-C6
18	N	607	PGV	C26-C27-C28-C29
19	N	608	TGL	C25-C26-C27-C28
26	P	309	PEK	C30-C31-C32-C33
19	L	101	TGL	CA2-CA3-CA4-CA5
19	A	608	TGL	CG1-CG2-CG3-OG3
20	O	303	PSC	C9-C10-C11-C12
25	G	102	CDL	C77-C78-C79-C80
19	Q	201	TGL	CA3-CA4-CA5-CA6
19	D	201	TGL	C11-C10-CB9-CB8
19	N	608	TGL	CA2-CA3-CA4-CA5
18	A	606	PGV	C29-C30-C31-C32
18	P	302	PGV	C14-C15-C16-C17
19	A	608	TGL	OG2-CG2-CG3-OG3
26	P	309	PEK	C33-C34-C35-C36
24	W	101	DMU	C28-C31-C34-C37
24	K	101	DMU	C22-C25-C28-C31

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Mol	Chain	Res	Type	Atoms
25	P	305	CDL	C57-C58-C59-C60
19	D	201	TGL	C21-C20-CA9-CA8
19	D	201	TGL	C24-C25-C26-C27
24	L	102	DMU	C31-C34-C37-C40
19	O	301	TGL	C17-C18-C19-C33
18	C	302	PGV	C02-C03-O11-P
25	T	101	CDL	OB9-CB7-OB8-CB6
26	P	308	PEK	C27-C28-C29-C30
19	N	608	TGL	CA6-CA7-CA8-CA9
24	D	202	DMU	C18-C19-C22-C25
19	Q	201	TGL	CB1-CB2-CB3-CB4
20	O	303	PSC	C12-C13-C14-C15
24	Z	101	DMU	C18-C19-C22-C25
18	P	304	PGV	O03-C01-C02-C03
19	A	608	TGL	OG1-CG1-CG2-CG3
19	O	301	TGL	OG1-CG1-CG2-OG2
19	D	201	TGL	CC3-CC4-CC5-CC6
24	Z	101	DMU	C28-C31-C34-C37
19	A	608	TGL	CC9-C15-C16-C17
24	K	103	DMU	C19-C22-C25-C28
26	C	305	PEK	C29-C30-C31-C32
14	N	601[B]	HEA	C26-C15-C16-C17
25	T	101	CDL	C71-CB7-OB8-CB6
19	Q	201	TGL	C16-C15-CC9-CC8
19	N	608	TGL	C23-C24-C25-C26
24	P	303	DMU	C19-C22-C25-C28
21	A	613	EDO	O1-C1-C2-O2
21	A	618	EDO	O1-C1-C2-O2
21	N	619	EDO	O1-C1-C2-O2
18	N	606	PGV	C11-C12-C13-C14
26	C	305	PEK	C3-C4-C5-C6
24	D	202	DMU	C31-C34-C37-C40
25	T	101	CDL	C53-C54-C55-C56
25	T	101	CDL	C17-C18-C19-C20
19	D	201	TGL	OG1-CG1-CG2-CG3
18	P	302	PGV	C23-C24-C25-C26
24	M	101	DMU	C34-C37-C40-C43
24	X	105	DMU	C25-C28-C31-C34
14	A	601[B]	HEA	C12-C13-C14-C15
19	N	608	TGL	CA7-CA8-CA9-C20
24	X	105	DMU	C31-C34-C37-C40
24	P	303	DMU	C34-C37-C40-C43

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Mol	Chain	Res	Type	Atoms
18	C	306	PGV	C11-C12-C13-C14
18	N	607	PGV	C11-C12-C13-C14
19	A	608	TGL	OB1-CB1-OG2-CG2
25	G	102	CDL	C43-C44-C45-C46
26	P	301	PEK	C7-C8-C9-C10
26	P	301	PEK	C13-C14-C15-C16
19	Q	201	TGL	CB3-CB4-CB5-CB6
14	A	601[A]	HEA	CAD-CBD-CGD-O1D
14	A	601[B]	HEA	CAD-CBD-CGD-O1D
14	N	601[A]	HEA	CAD-CBD-CGD-O1D
14	N	601[B]	HEA	CAD-CBD-CGD-O1D
14	N	602	HEA	CAA-CBA-CGA-O1A
19	D	201	TGL	CB6-CB7-CB8-CB9
19	O	301	TGL	C16-C15-CC9-CC8
24	K	103	DMU	C25-C28-C31-C34
25	P	305	CDL	OB7-CB5-OB6-CB4
25	T	101	CDL	OB7-CB5-OB6-CB4
18	C	302	PGV	C20-C21-C22-C23
18	N	606	PGV	C20-C21-C22-C23
23	G	103	CHD	C22-C23-C24-O25
19	D	201	TGL	OG1-CG1-CG2-OG2
19	O	301	TGL	OG2-CG2-CG3-OG3
24	K	102	DMU	C19-C22-C25-C28
20	A	609	PSC	C12-C13-C14-C15
26	P	308	PEK	C14-C15-C16-C17
24	L	102	DMU	C19-C22-C25-C28
26	G	101	PEK	C22-C23-C24-C25
14	N	601[B]	HEA	C14-C15-C16-C17
14	A	602	HEA	CAA-CBA-CGA-O1A
14	N	601[A]	HEA	CAD-CBD-CGD-O2D
14	N	601[B]	HEA	CAD-CBD-CGD-O2D
19	L	101	TGL	CA4-CA5-CA6-CA7
19	L	101	TGL	CB1-CB2-CB3-CB4
26	C	305	PEK	C26-C27-C28-C29
23	B	302	CHD	C22-C23-C24-O26
14	A	601[B]	HEA	C26-C15-C16-C17
14	A	601[A]	HEA	CAD-CBD-CGD-O2D
14	A	601[B]	HEA	CAD-CBD-CGD-O2D
26	G	101	PEK	C5-C6-C7-C8
26	G	101	PEK	C11-C10-C9-C8
26	P	308	PEK	C6-C7-C8-C9
26	P	308	PEK	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
19	O	301	TGL	CC2-CC1-OG3-CG3
18	C	306	PGV	C10-C11-C12-C13
14	N	602	HEA	CAA-CBA-CGA-O2A
23	B	302	CHD	C22-C23-C24-O25
23	G	103	CHD	C22-C23-C24-O26
19	N	608	TGL	C21-C22-C23-C24
19	Q	201	TGL	C21-C22-C23-C24
26	P	309	PEK	C14-C15-C16-C17
19	A	608	TGL	C11-C12-C13-C14
19	L	101	TGL	CB4-CB5-CB6-CB7
18	A	607	PGV	C7-C8-C9-C10
25	T	101	CDL	C57-C58-C59-C60
18	P	304	PGV	O03-C01-C02-O01
18	C	302	PGV	C11-C12-C13-C14
24	K	102	DMU	C28-C31-C34-C37
25	C	303	CDL	C77-C78-C79-C80
25	G	102	CDL	C80-C81-C82-C83
19	A	608	TGL	C21-C20-CA9-CA8
24	C	301	DMU	C25-C28-C31-C34
18	N	607	PGV	O03-C19-C20-C21
21	C	311	EDO	O1-C1-C2-O2
21	N	613	EDO	O1-C1-C2-O2
21	T	102	EDO	O1-C1-C2-O2
21	W	103	EDO	O1-C1-C2-O2
25	P	305	CDL	C81-C82-C83-C84
19	N	608	TGL	C24-C25-C26-C27
24	Z	101	DMU	O16-C18-C19-C22
23	J	101	CHD	C21-C20-C22-C23
18	A	607	PGV	C9-C10-C11-C12
26	P	301	PEK	C14-C15-C16-C17
25	P	305	CDL	C53-C54-C55-C56
14	N	602	HEA	CAD-CBD-CGD-O2D
23	P	307	CHD	C22-C23-C24-O25
24	D	203	DMU	C25-C28-C31-C34
14	N	602	HEA	C26-C15-C16-C17
18	A	607	PGV	C21-C22-C23-C24
14	A	601[B]	HEA	C14-C15-C16-C17
14	A	602	HEA	CAA-CBA-CGA-O2A
18	P	302	PGV	C9-C10-C11-C12
18	A	606	PGV	O03-C19-C20-C21
18	A	606	PGV	C23-C24-C25-C26
14	N	601[B]	HEA	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
18	A	606	PGV	C11-C12-C13-C14
18	A	607	PGV	C11-C12-C13-C14
18	N	606	PGV	C9-C10-C11-C12
18	P	302	PGV	C11-C12-C13-C14
26	C	307	PEK	C3-C4-C5-C6
26	G	101	PEK	C14-C15-C16-C17
25	G	102	CDL	C72-C73-C74-C75
14	A	602	HEA	CAD-CBD-CGD-O2D
18	A	607	PGV	O01-C1-C2-C3
18	A	607	PGV	O02-C1-C2-C3
19	A	608	TGL	CB6-CB7-CB8-CB9
18	P	304	PGV	C9-C10-C11-C12
18	P	304	PGV	C11-C12-C13-C14
26	C	307	PEK	C14-C15-C16-C17
26	P	301	PEK	C3-C4-C5-C6
18	C	302	PGV	C25-C26-C27-C28
25	P	305	CDL	C51-CB5-OB6-CB4
21	E	202	EDO	O1-C1-C2-O2
21	Q	204	EDO	O1-C1-C2-O2
14	A	602	HEA	CAD-CBD-CGD-O1D
14	N	602	HEA	CAD-CBD-CGD-O1D
23	C	304	CHD	C22-C23-C24-O25
25	T	101	CDL	C32-C31-CA7-OA8
23	C	304	CHD	C22-C23-C24-O26
19	D	201	TGL	OG1-CA1-CA2-CA3
24	X	101	DMU	C34-C37-C40-C43
25	T	101	CDL	C51-CB5-OB6-CB4
25	P	305	CDL	C14-C15-C16-C17
24	X	103	DMU	C34-C37-C40-C43
14	N	601[A]	HEA	C15-C16-C17-C18
19	A	608	TGL	C24-C25-C26-C27
19	A	608	TGL	C29-C30-C31-C32
24	C	301	DMU	C19-C22-C25-C28
18	C	306	PGV	C9-C10-C11-C12
24	D	202	DMU	C22-C25-C28-C31
18	A	606	PGV	C26-C27-C28-C29
19	L	101	TGL	C16-C17-C18-C19
25	T	101	CDL	C32-C31-CA7-OA9
19	O	301	TGL	OC1-CC1-OG3-CG3
26	C	305	PEK	C14-C15-C16-C17
19	L	101	TGL	C18-C19-C33-C34
19	O	301	TGL	CG1-CG2-CG3-OG3

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Mol	Chain	Res	Type	Atoms
26	G	101	PEK	O03-C01-C02-C03
19	A	608	TGL	CB2-CB3-CB4-CB5
23	P	307	CHD	C22-C23-C24-O26
19	N	608	TGL	CB3-CB4-CB5-CB6
14	N	601[A]	HEA	CAA-CBA-CGA-O2A
14	N	601[B]	HEA	CAA-CBA-CGA-O2A
18	C	302	PGV	C9-C10-C11-C12
24	M	101	DMU	O6-C11-C9-O1
21	A	619	EDO	O1-C1-C2-O2
21	P	312	EDO	O1-C1-C2-O2
21	Q	202	EDO	O1-C1-C2-O2
14	A	601[A]	HEA	CAA-CBA-CGA-O2A
14	A	601[B]	HEA	CAA-CBA-CGA-O2A
19	L	101	TGL	C20-C21-C22-C23
19	A	608	TGL	CC2-CC1-OG3-CG3
18	C	302	PGV	C24-C25-C26-C27
19	D	201	TGL	OA1-CA1-CA2-CA3
19	L	101	TGL	CC6-CC7-CC8-CC9
24	D	202	DMU	C34-C37-C40-C43
18	A	606	PGV	C31-C32-C33-C34
26	P	308	PEK	C22-C23-C24-C25
19	L	101	TGL	CC1-CC2-CC3-CC4
14	A	601[A]	HEA	CAA-CBA-CGA-O1A
14	A	601[B]	HEA	CAA-CBA-CGA-O1A
24	L	102	DMU	C34-C37-C40-C43
19	L	101	TGL	OG3-CC1-CC2-CC3
19	N	608	TGL	CB6-CB7-CB8-CB9
18	N	606	PGV	O03-C19-C20-C21
19	N	608	TGL	CB5-CB6-CB7-CB8
19	L	101	TGL	C22-C23-C24-C25

There are no ring outliers.

51 monomers are involved in 140 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	P	305	CDL	2	0
21	S	103	EDO	3	0
19	D	201	TGL	5	0
24	Z	101	DMU	1	0
24	X	105	DMU	1	0
18	C	302	PGV	3	0
26	G	101	PEK	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	C	307	PEK	2	0
18	P	302	PGV	1	0
18	P	304	PGV	1	0
21	O	307	EDO	1	0
21	N	611	EDO	1	0
21	F	103	EDO	1	0
24	X	103	DMU	1	0
24	C	301	DMU	2	0
18	N	606	PGV	2	0
24	P	310	DMU	1	0
21	N	621	EDO	2	0
19	Q	201	TGL	7	0
19	L	101	TGL	6	0
21	A	615	EDO	3	0
24	D	203	DMU	1	0
14	A	602	HEA	7	0
19	N	608	TGL	5	0
26	P	309	PEK	3	0
23	P	306	CHD	1	0
21	B	304	EDO	2	0
25	G	102	CDL	9	0
26	C	305	PEK	1	0
14	N	601[B]	HEA	1	0
24	P	303	DMU	3	0
21	A	614	EDO	1	0
26	P	308	PEK	7	0
21	A	616	EDO	2	0
23	J	101	CHD	1	0
24	K	103	DMU	2	0
24	L	102	DMU	4	0
21	N	617	EDO	1	0
18	A	606	PGV	2	0
14	N	602	HEA	6	0
19	O	301	TGL	1	0
21	F	105	EDO	2	0
25	T	101	CDL	12	0
23	G	103	CHD	1	0
26	P	301	PEK	1	0
18	C	306	PGV	2	0
18	A	607	PGV	4	0
25	C	303	CDL	7	0
20	A	609	PSC	3	0

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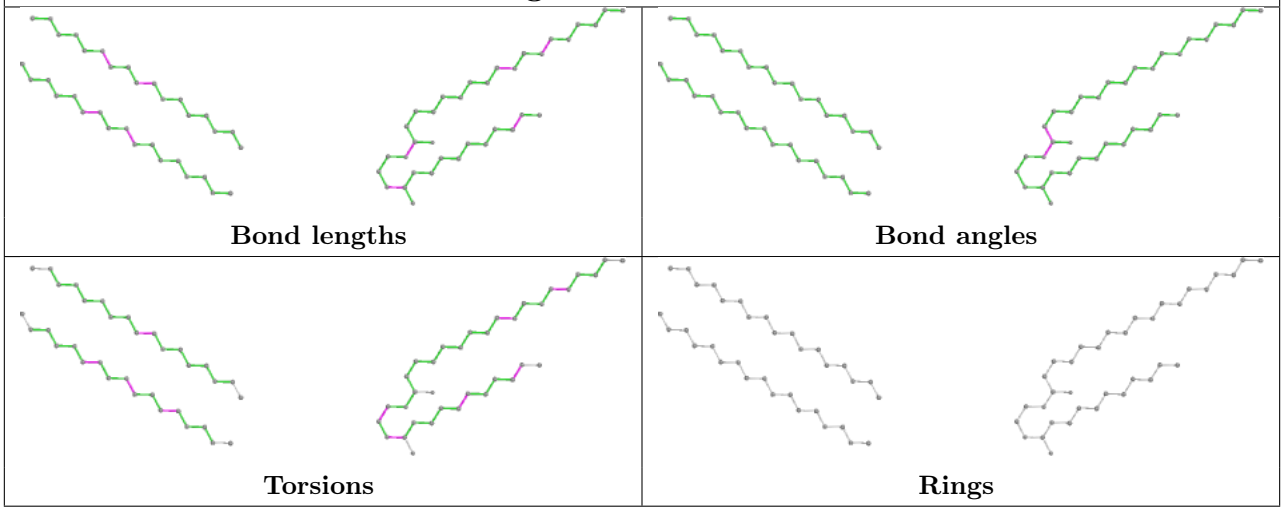
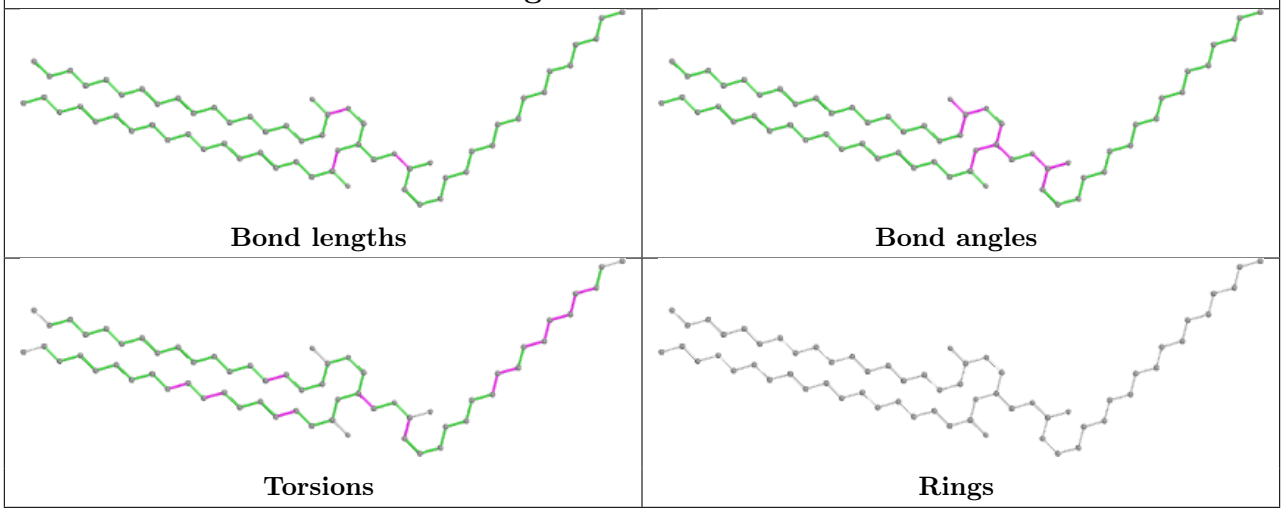
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	608	TGL	1	0
21	A	610	EDO	1	0

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.

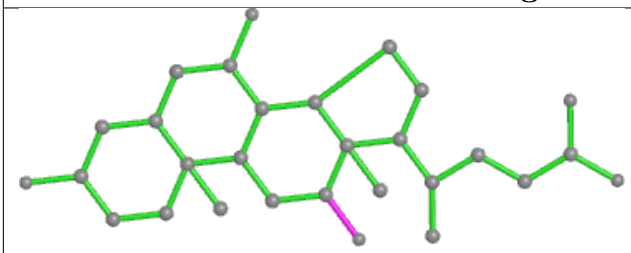
Ligand CDL P 305



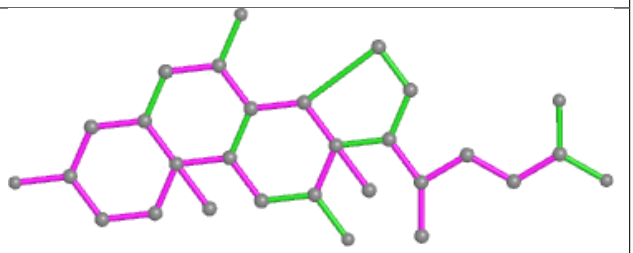
Ligand TGL D 201



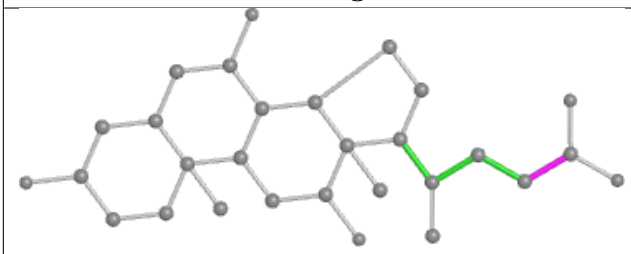
Ligand CHD C 304



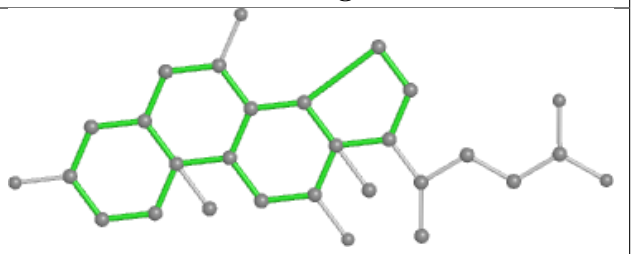
Bond lengths



Bond angles

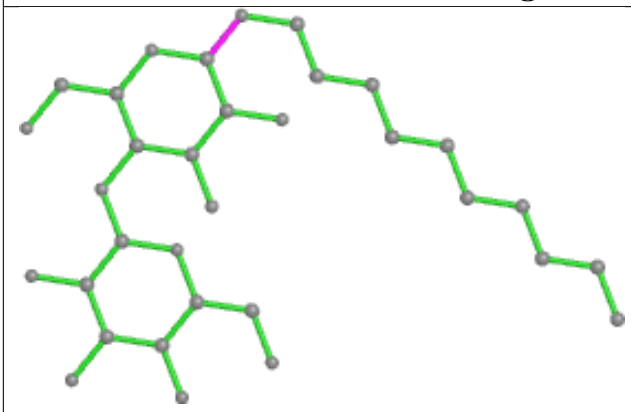


Torsions

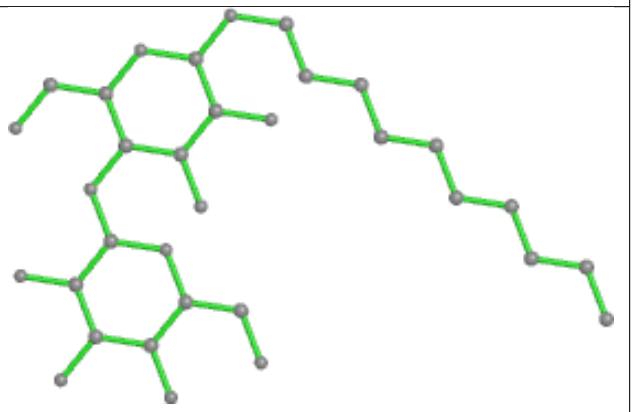


Rings

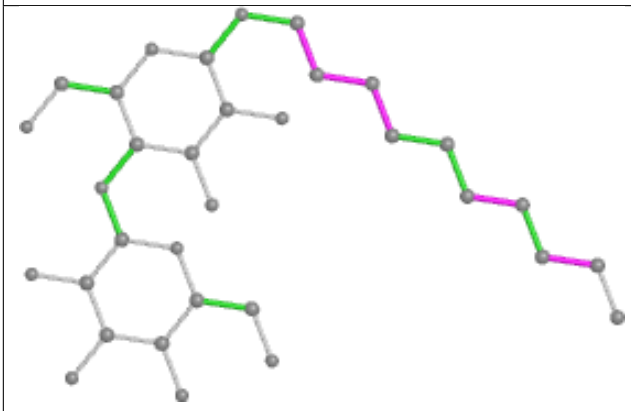
Ligand DMU Z 101



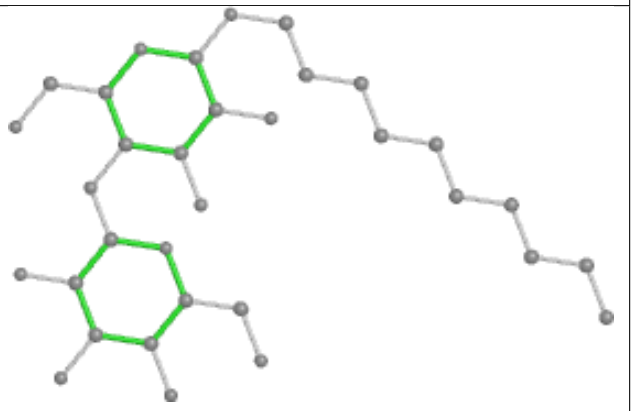
Bond lengths



Bond angles

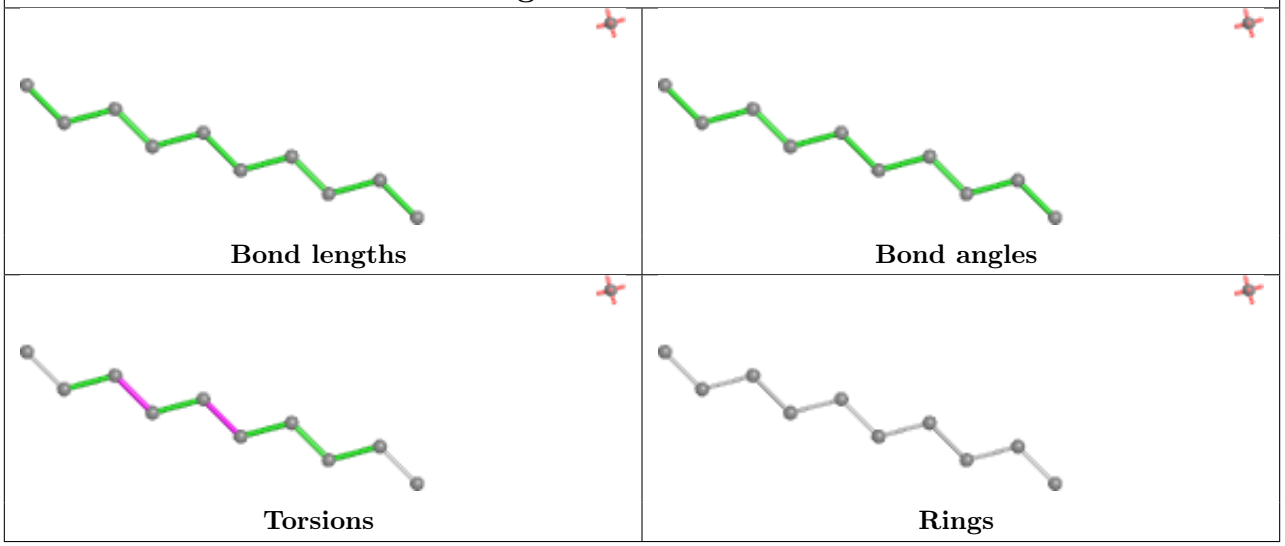


Torsions

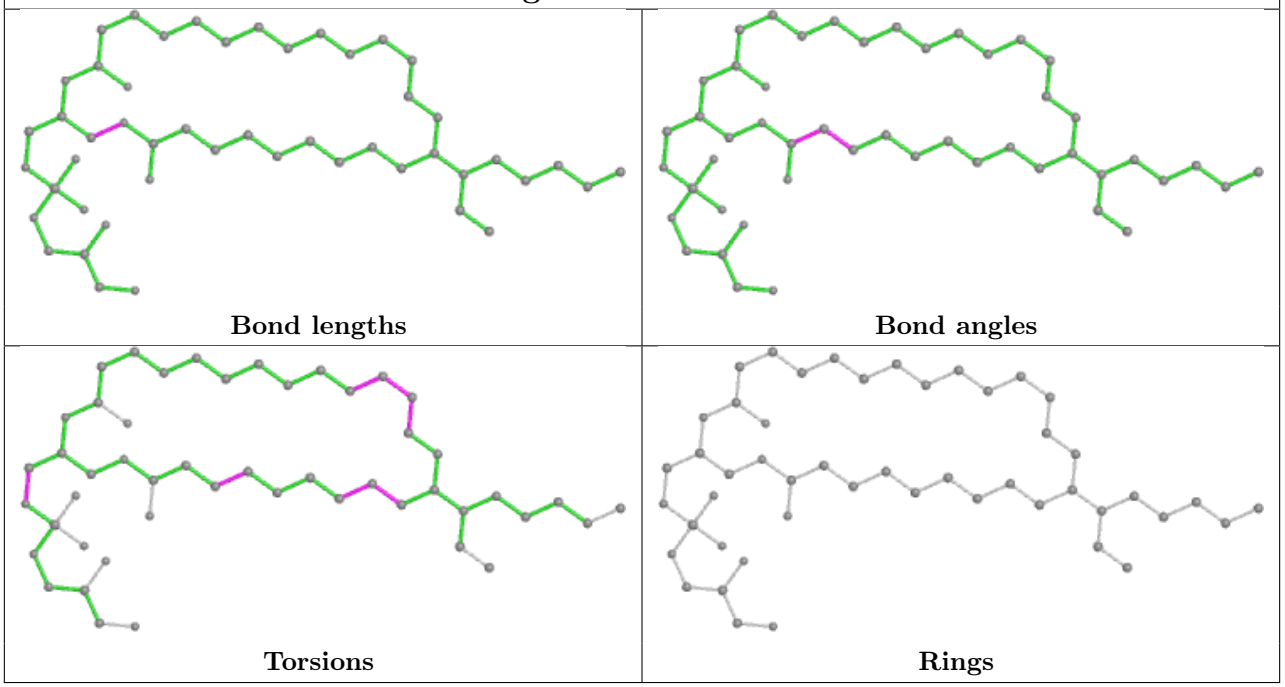


Rings

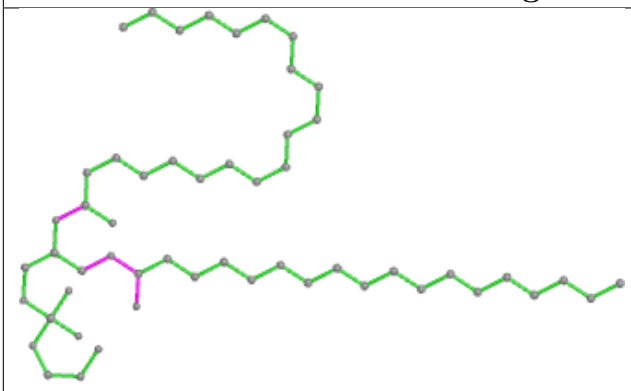
Ligand DMU X 105



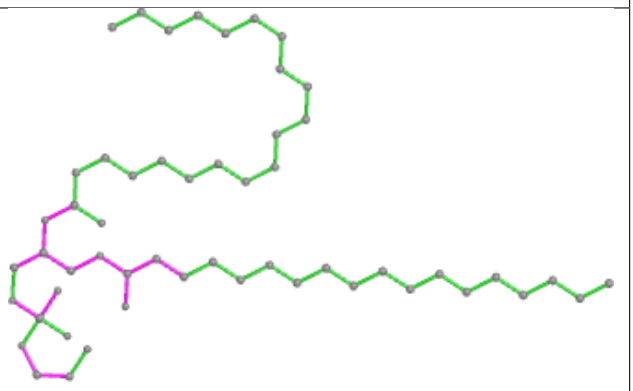
Ligand PGV C 302



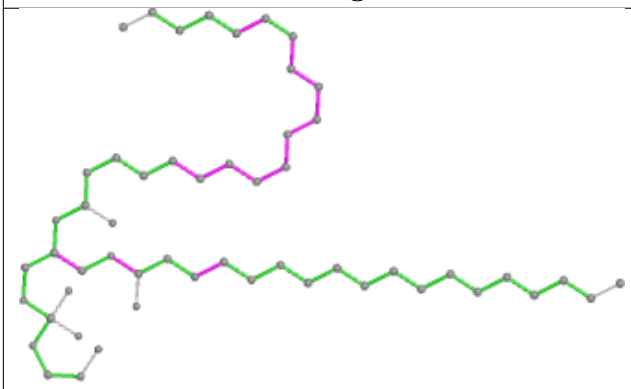
Ligand PEK G 101



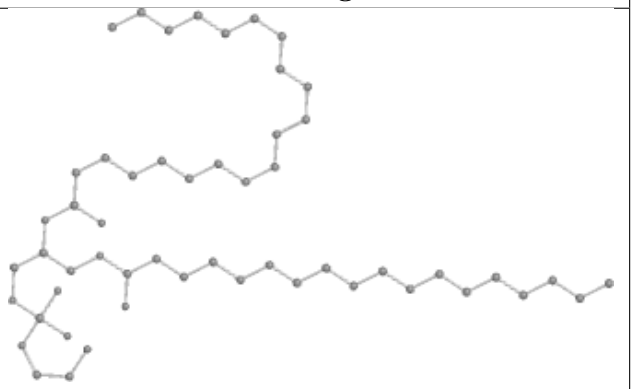
Bond lengths



Bond angles

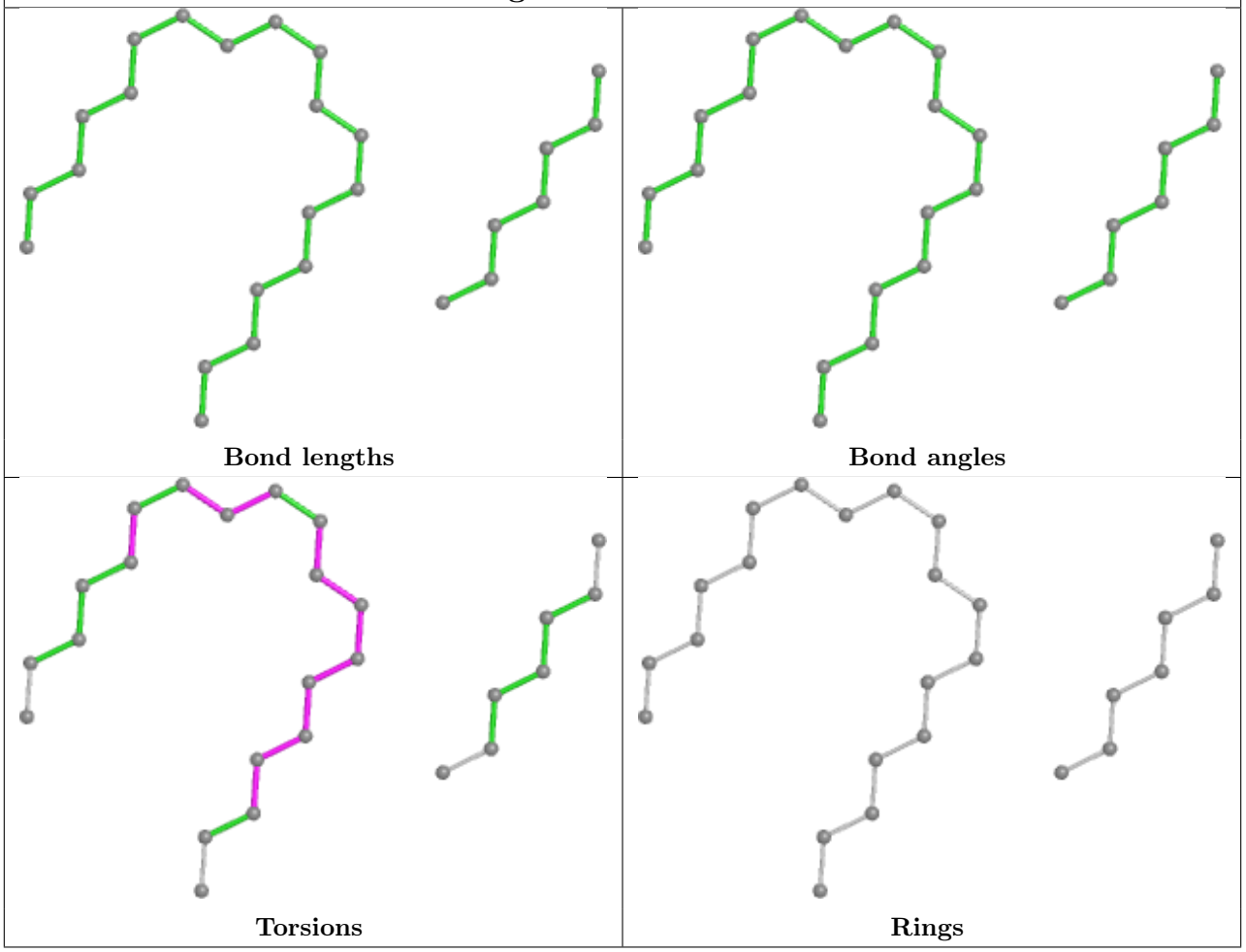


Torsions

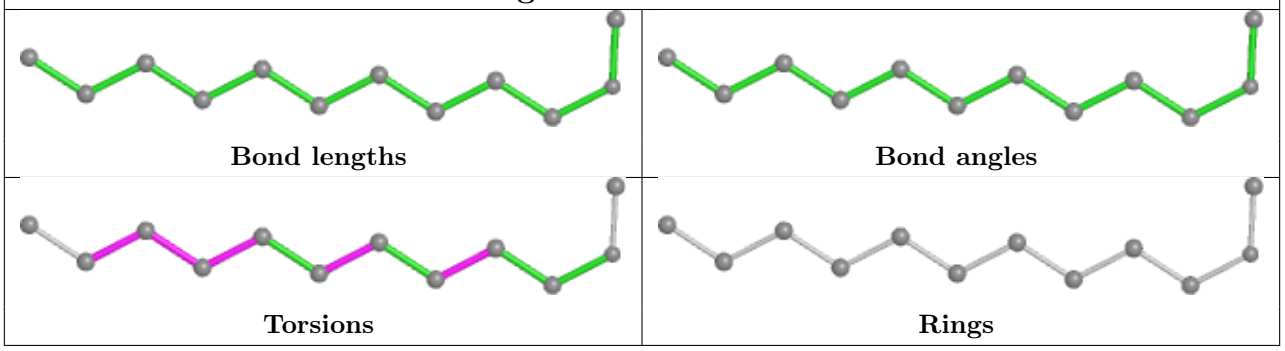


Rings

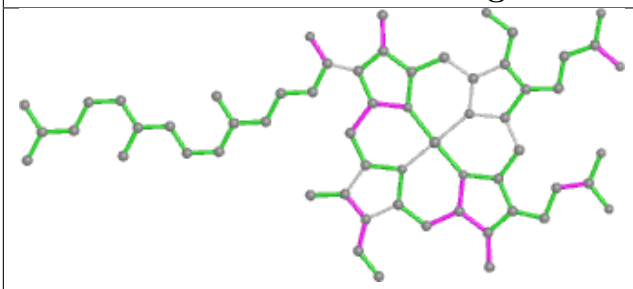
Ligand PEK C 307



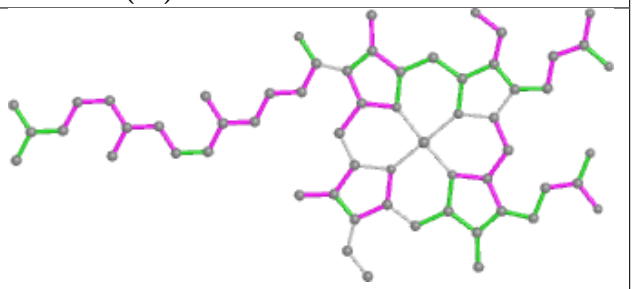
Ligand DMU D 202



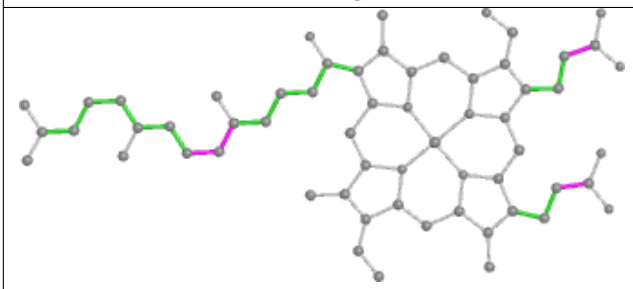
Ligand HEA N 601 (A)



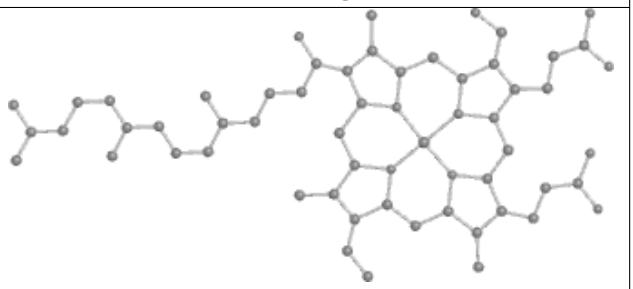
Bond lengths



Bond angles

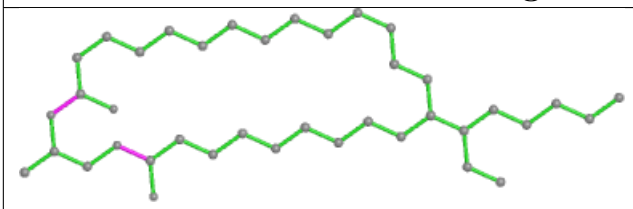


Torsions

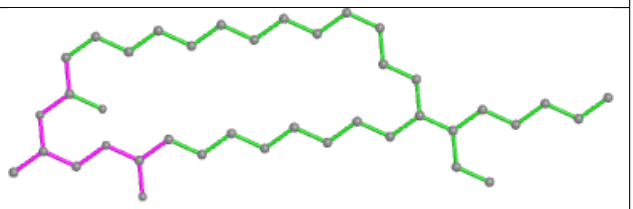


Rings

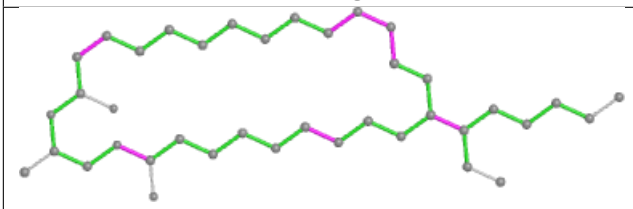
Ligand PGV P 302



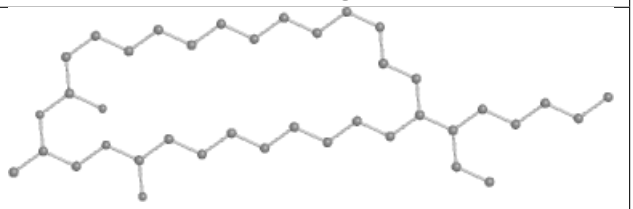
Bond lengths



Bond angles

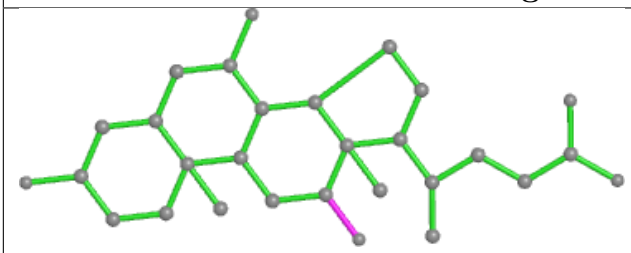


Torsions

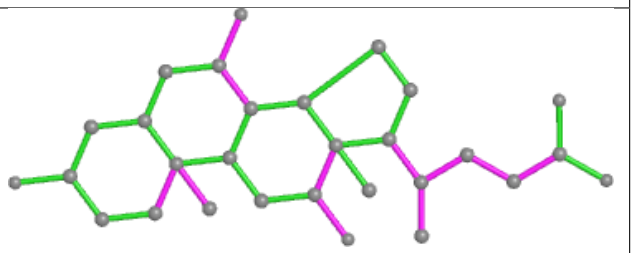


Rings

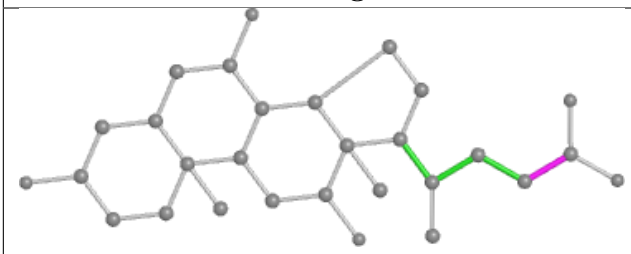
Ligand CHD P 307



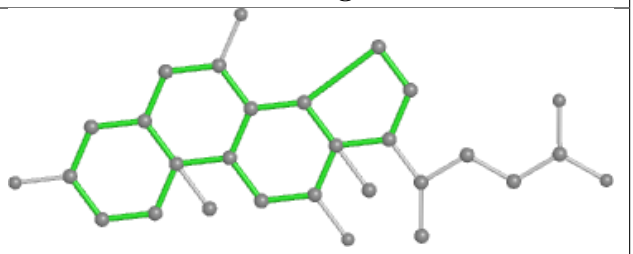
Bond lengths



Bond angles

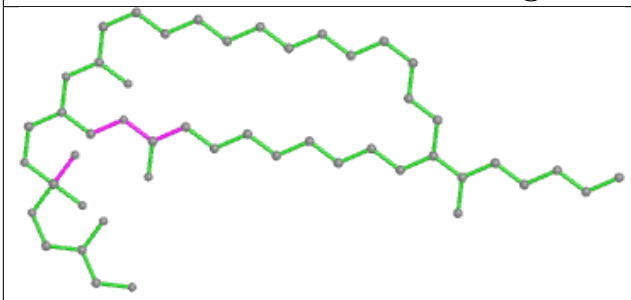


Torsions

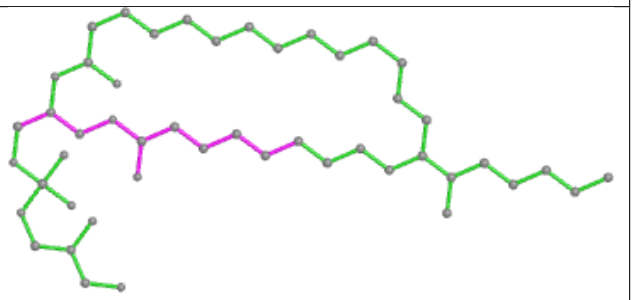


Rings

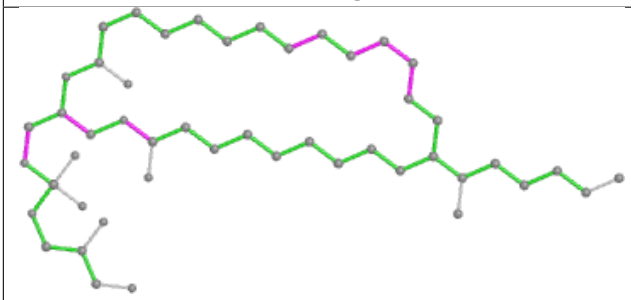
Ligand PGV P 304



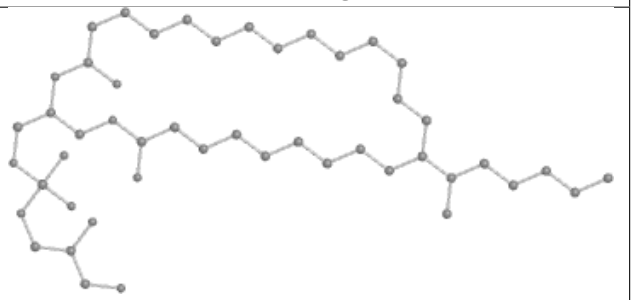
Bond lengths



Bond angles

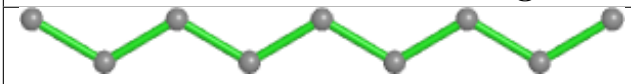


Torsions

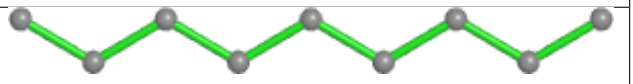


Rings

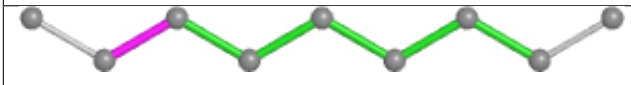
Ligand DMU X 103



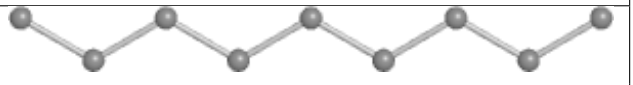
Bond lengths



Bond angles

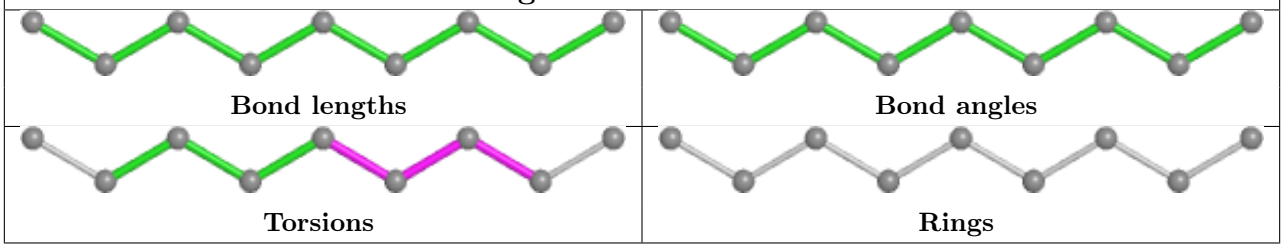


Torsions

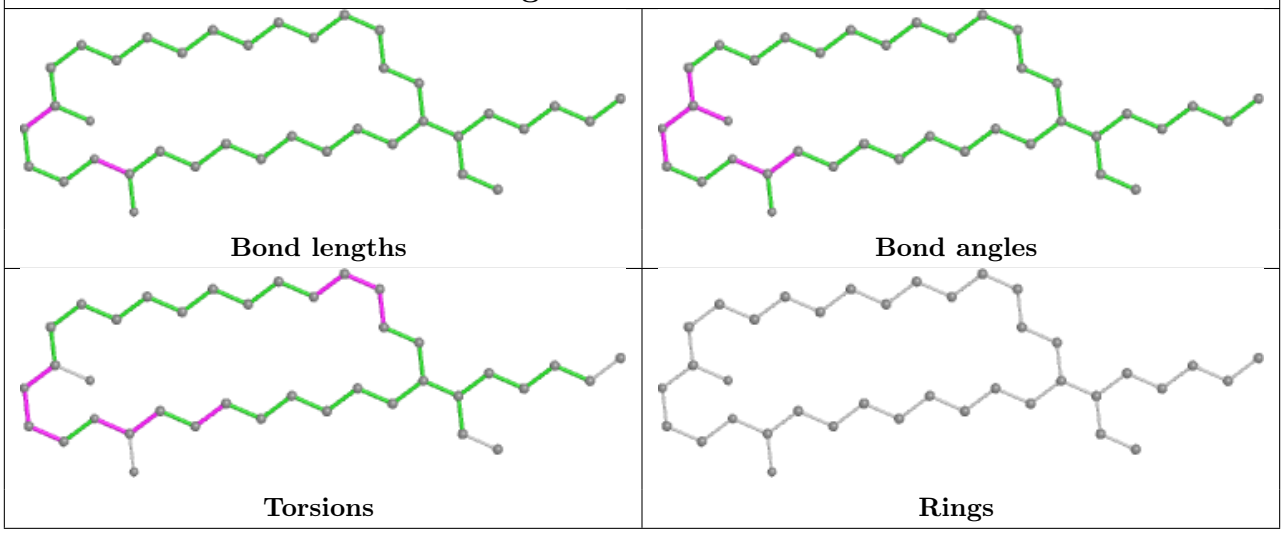


Rings

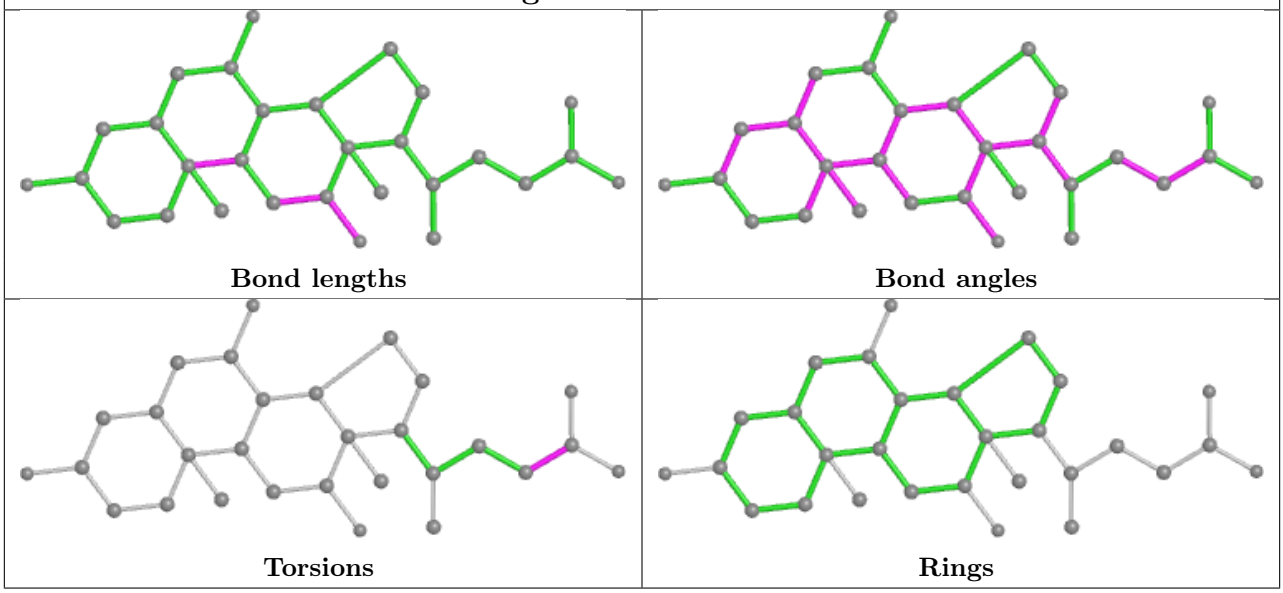
Ligand DMU C 301



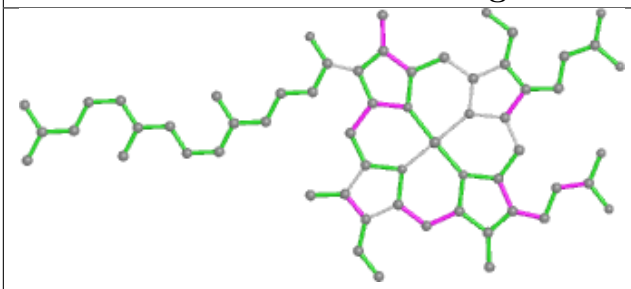
Ligand PGV N 606



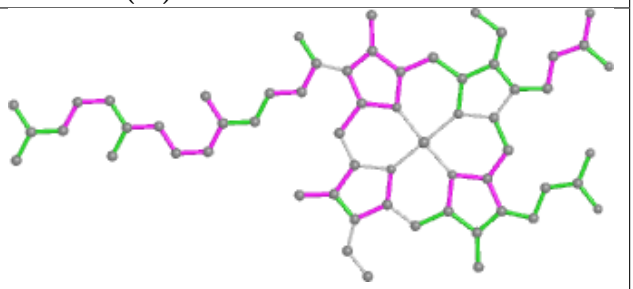
Ligand CHD B 302



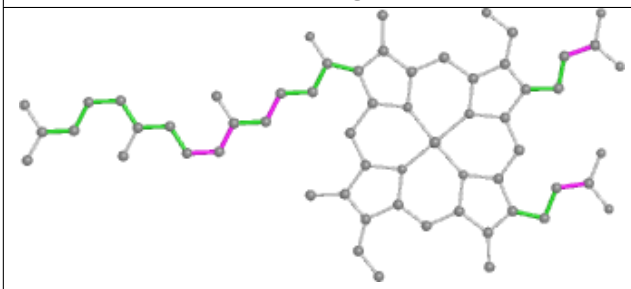
Ligand HEA A 601 (B)



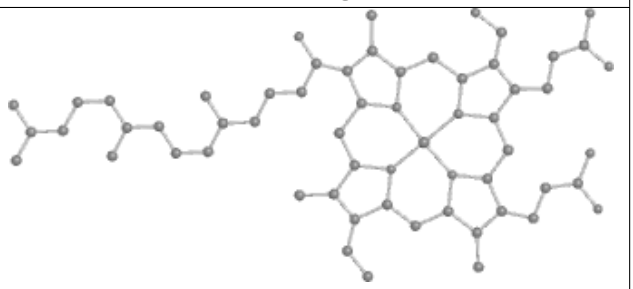
Bond lengths



Bond angles

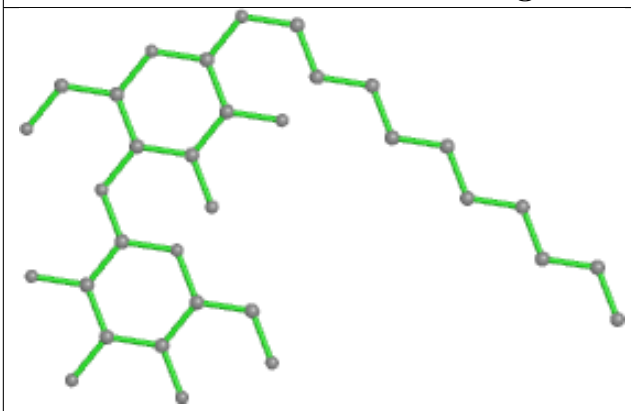


Torsions

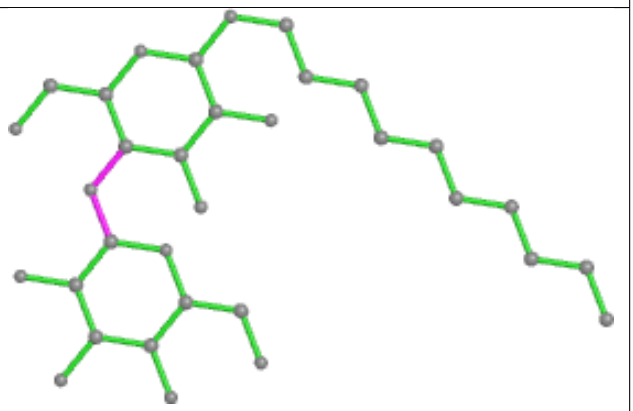


Rings

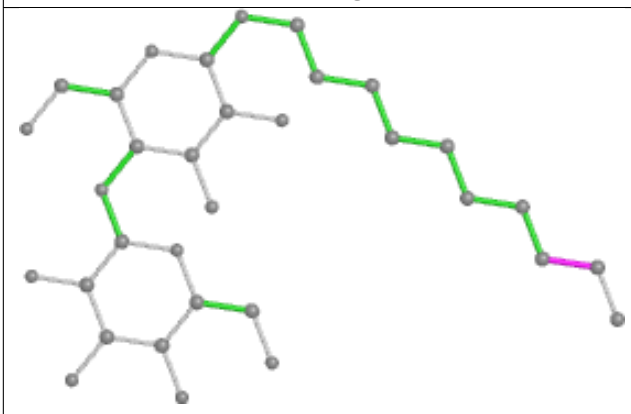
Ligand DMU X 101



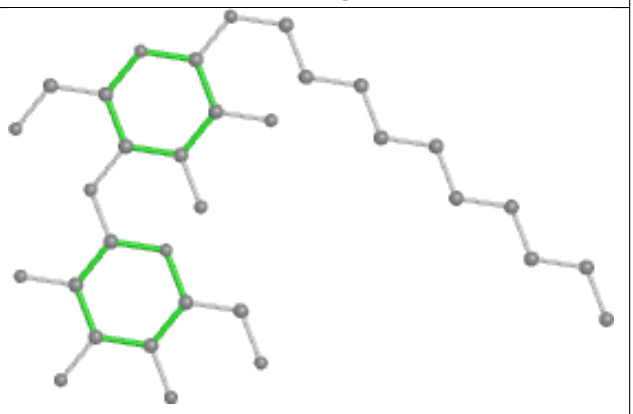
Bond lengths



Bond angles

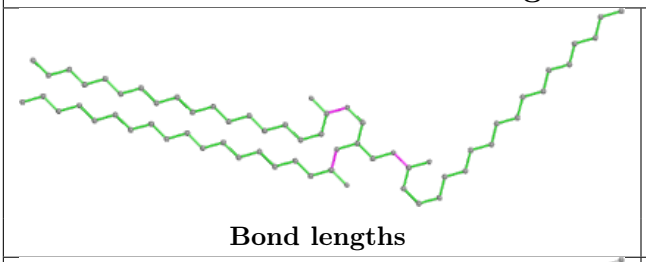


Torsions

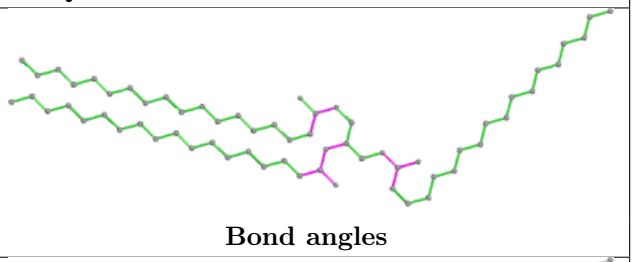


Rings

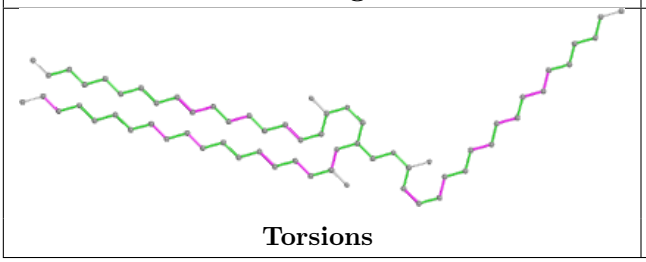
Ligand TGL Q 201



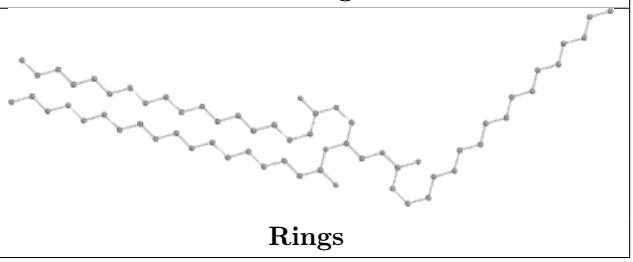
Bond lengths



Bond angles

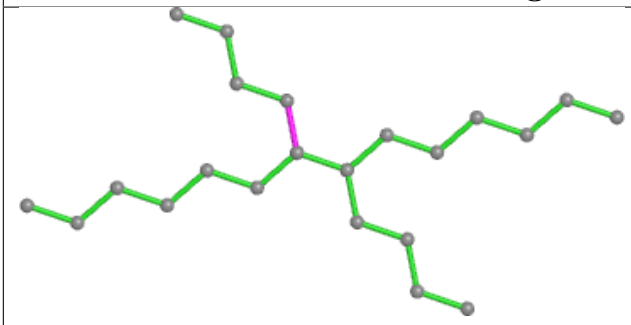


Torsions

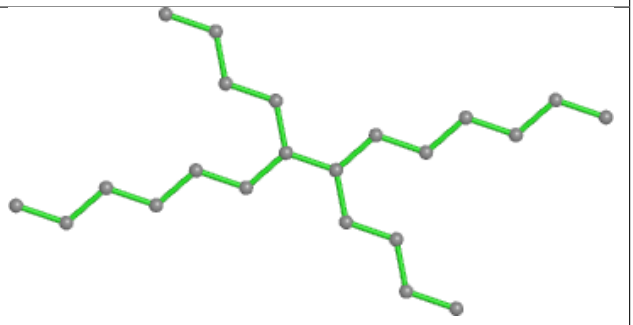


Rings

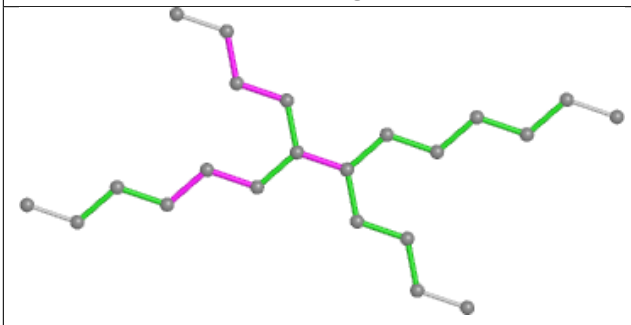
Ligand PSC O 303



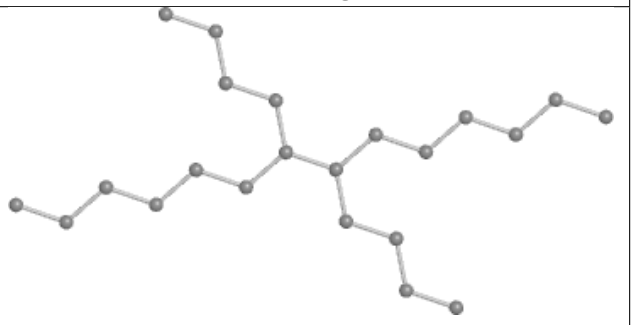
Bond lengths



Bond angles

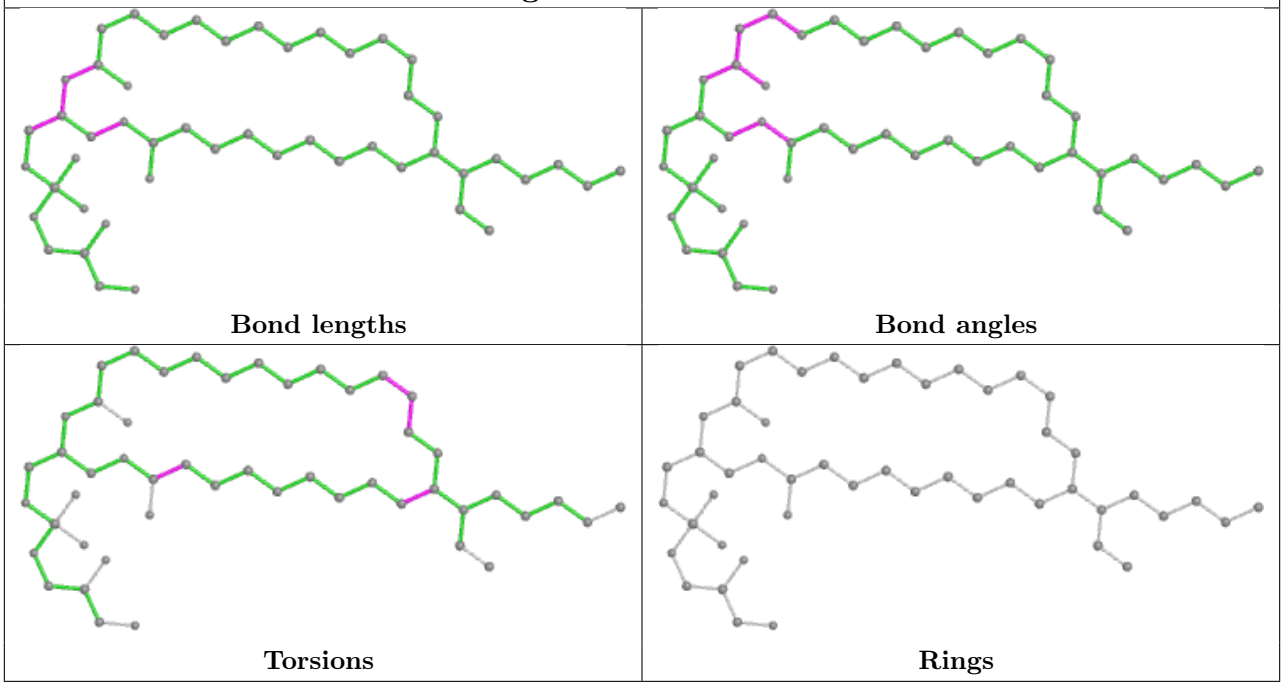


Torsions

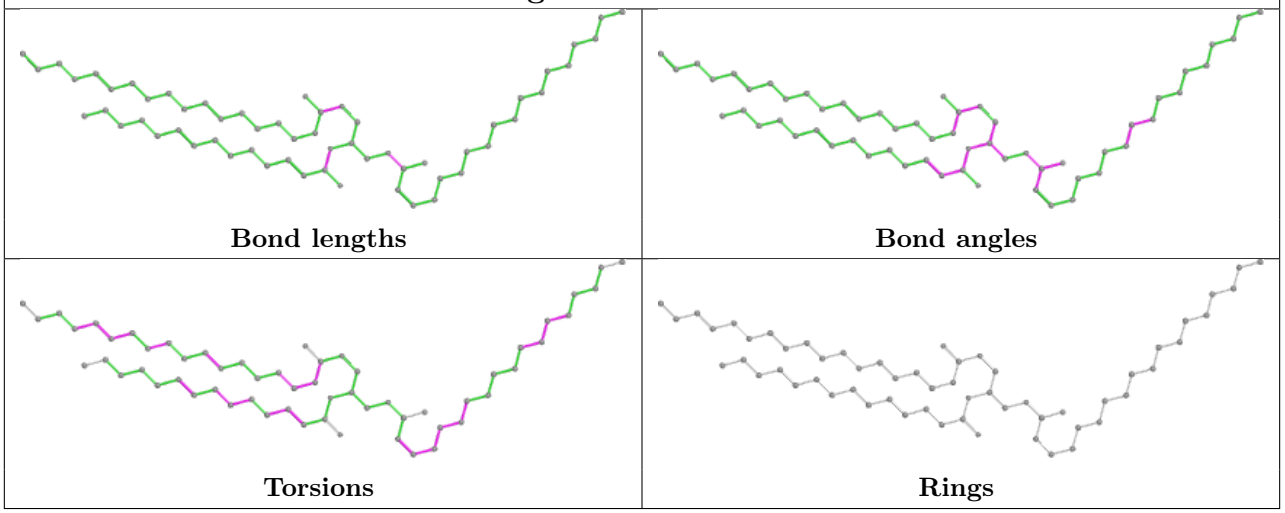


Rings

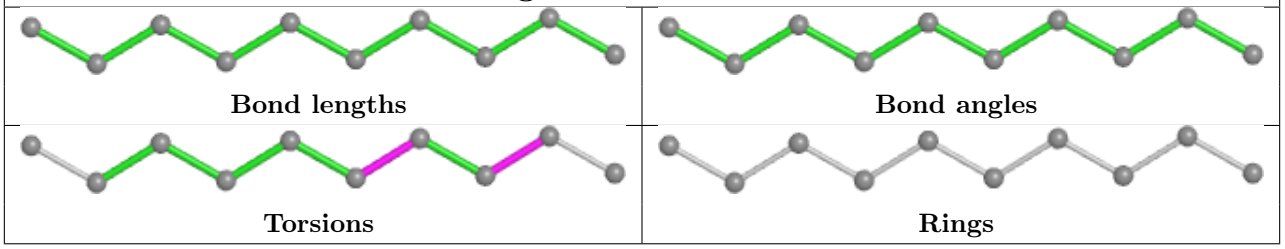
Ligand PGV N 607



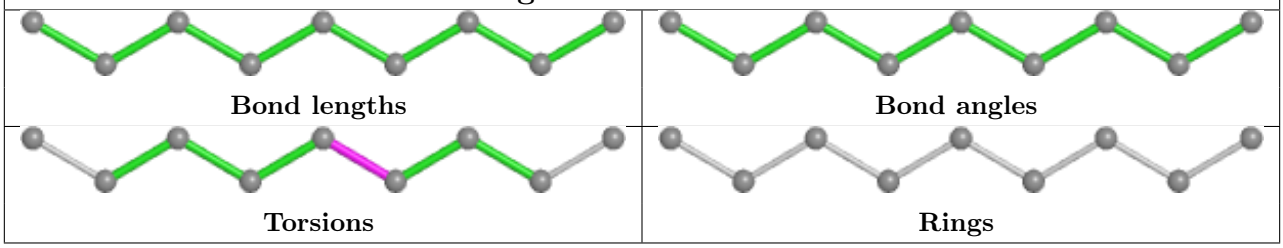
Ligand TGL L 101



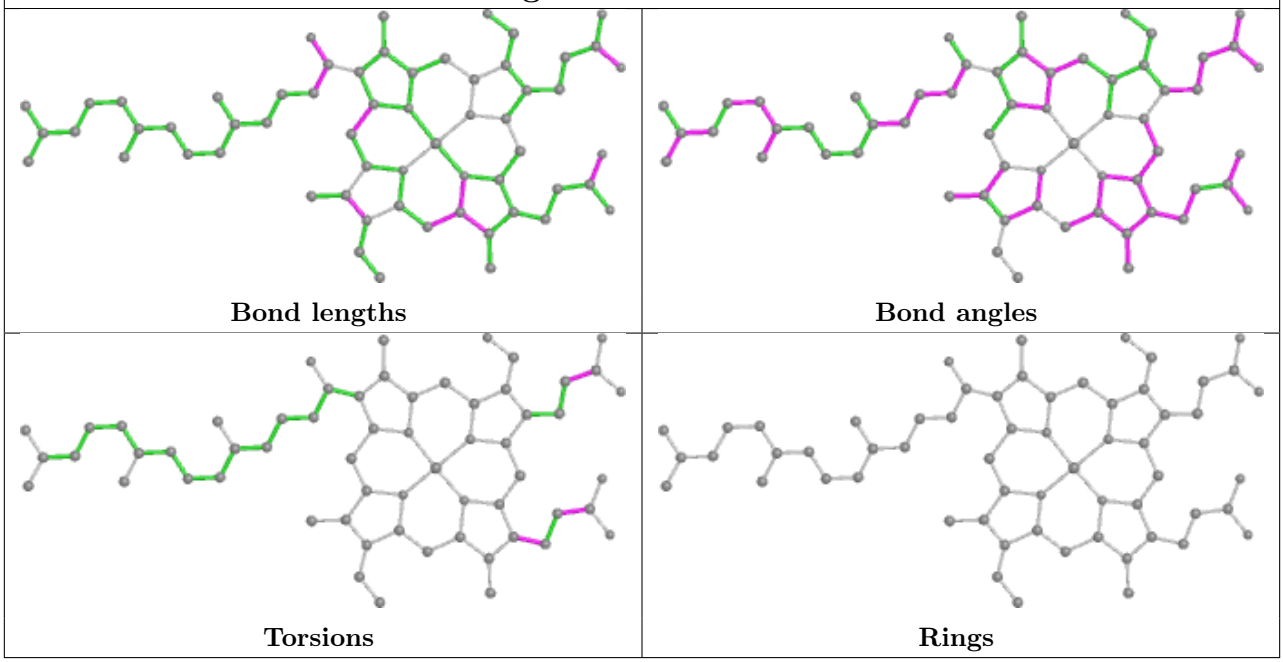
Ligand DMU O 304



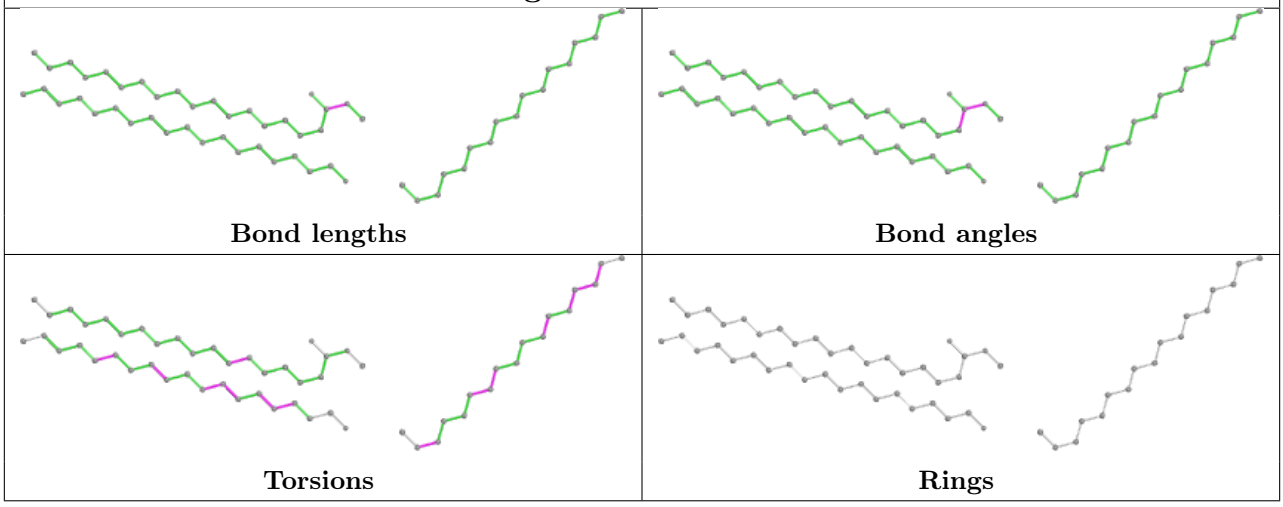
Ligand DMU D 203



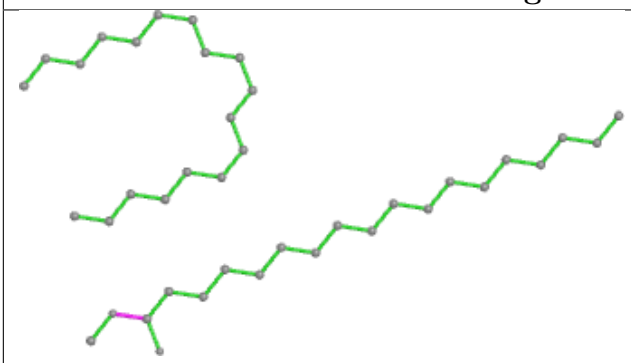
Ligand HEA A 602



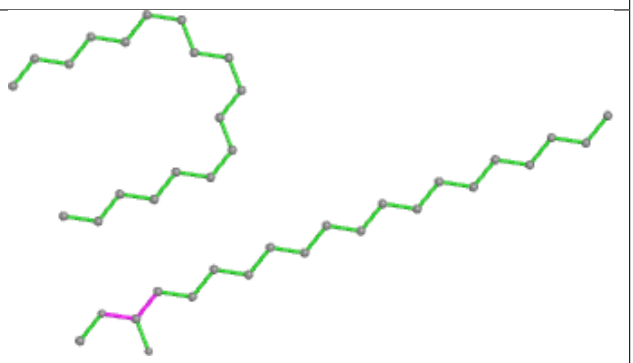
Ligand TGL N 608



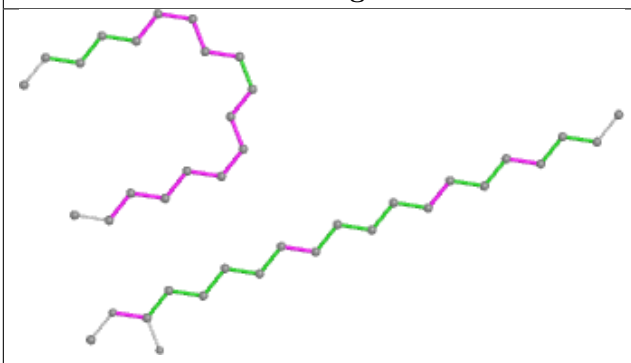
Ligand PEK P 309



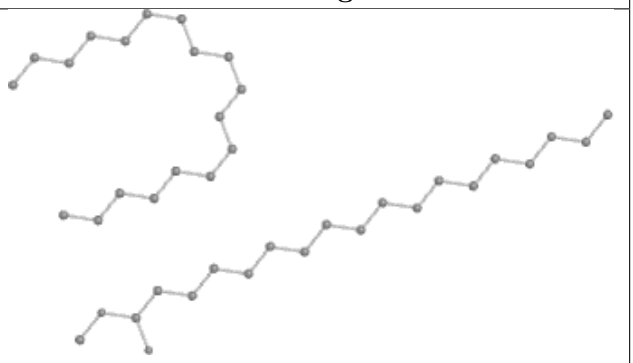
Bond lengths



Bond angles

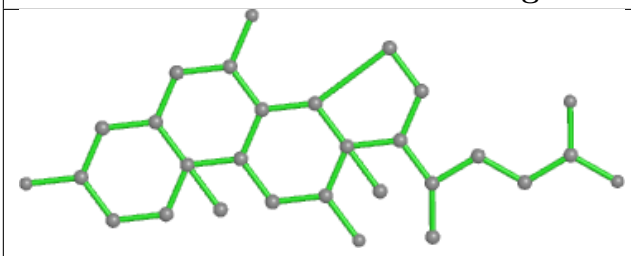


Torsions

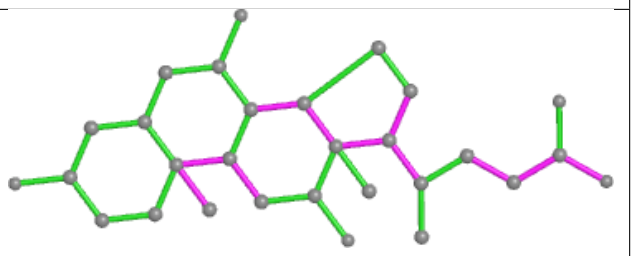


Rings

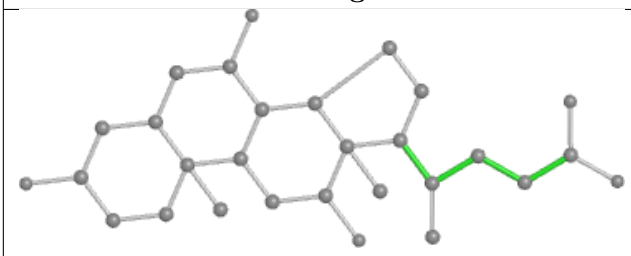
Ligand CHD P 306



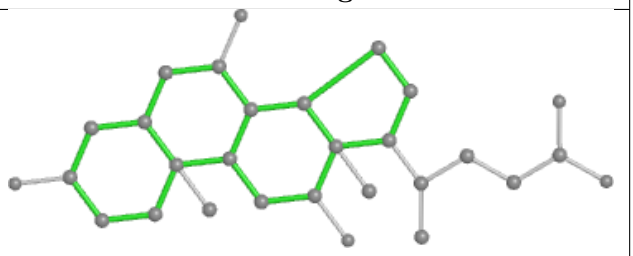
Bond lengths



Bond angles

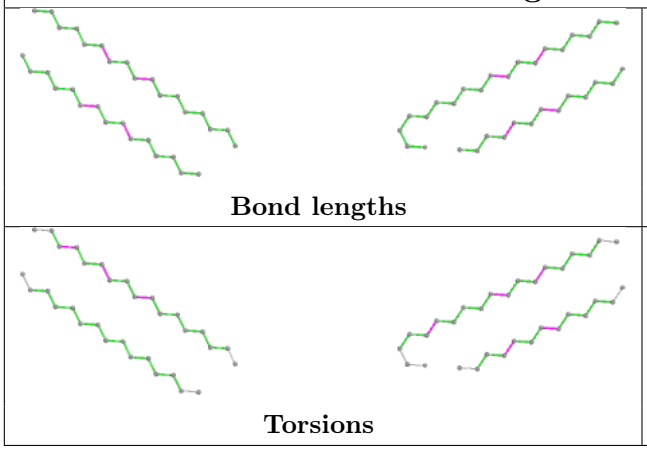


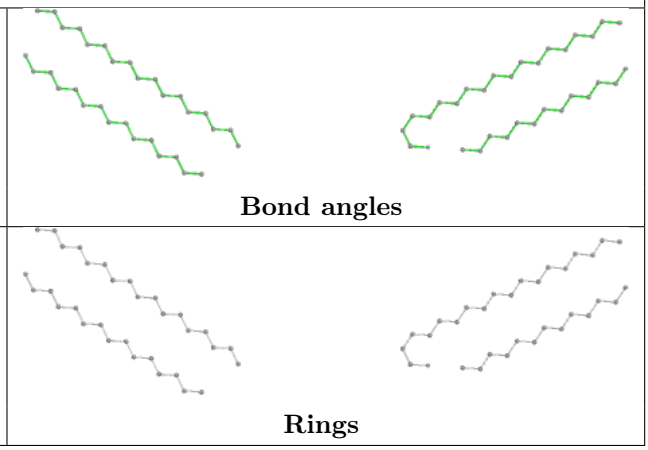
Torsions



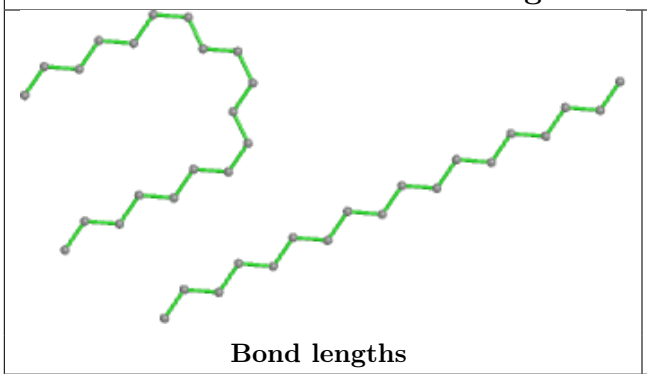
Rings

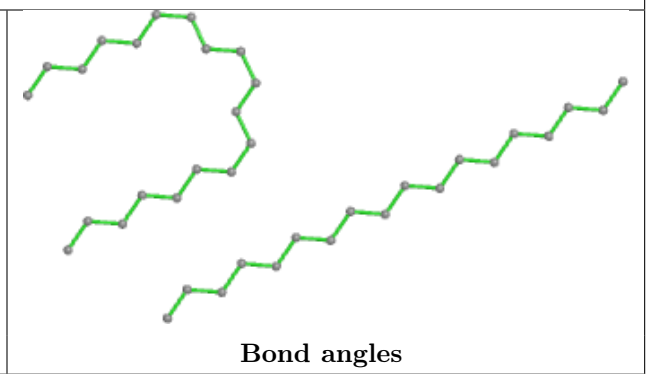
Ligand CDL G 102

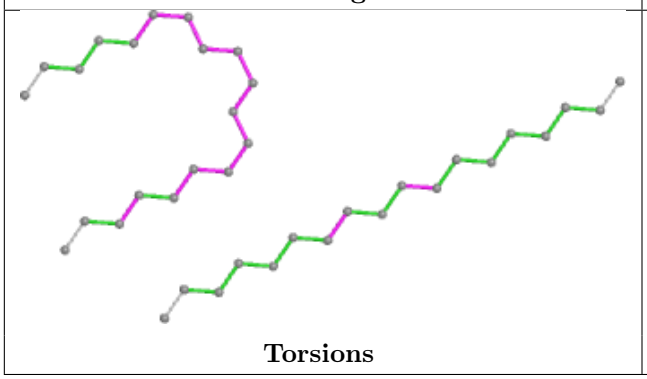


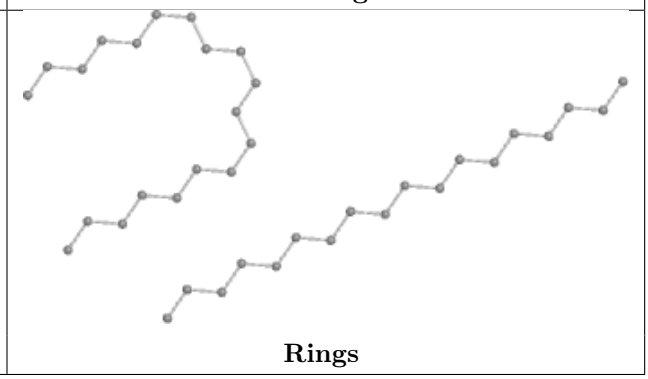


Ligand PEK C 305

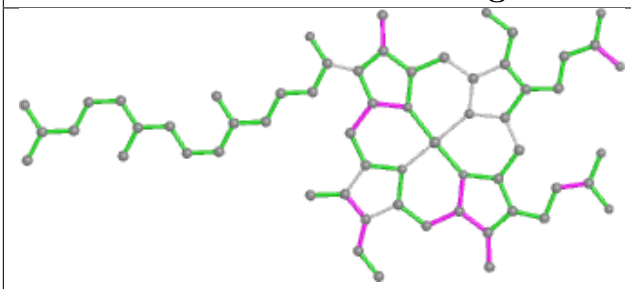




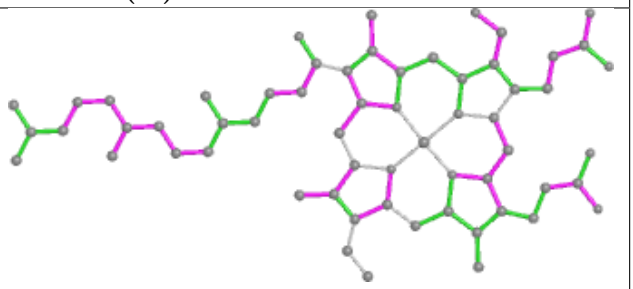




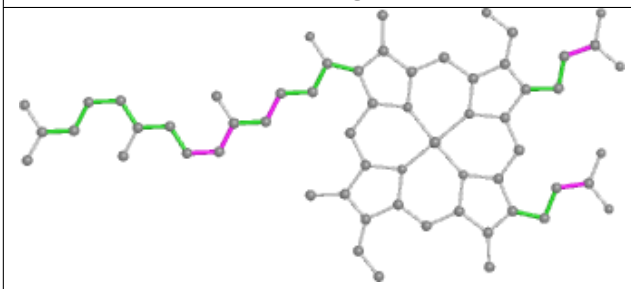
Ligand HEA N 601 (B)



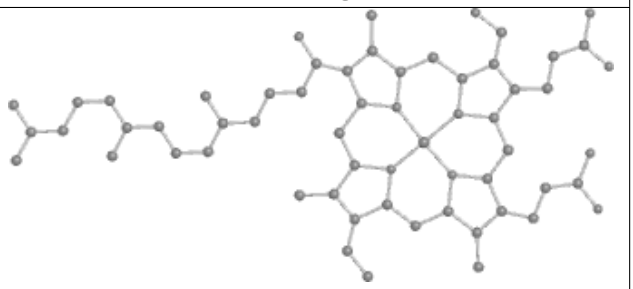
Bond lengths



Bond angles

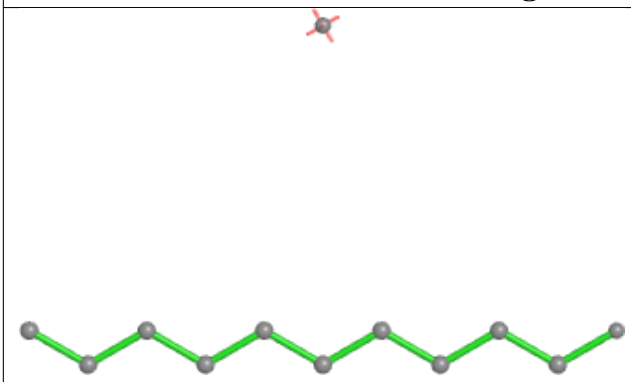


Torsions

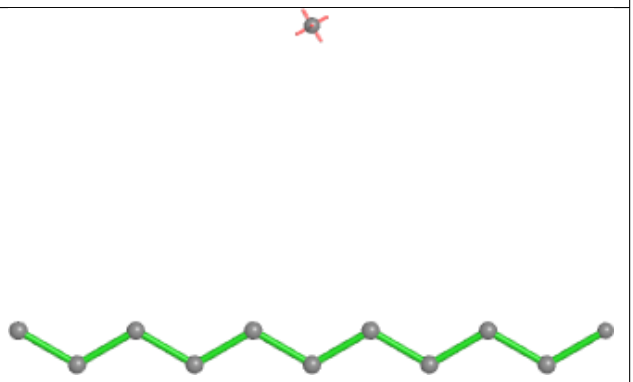


Rings

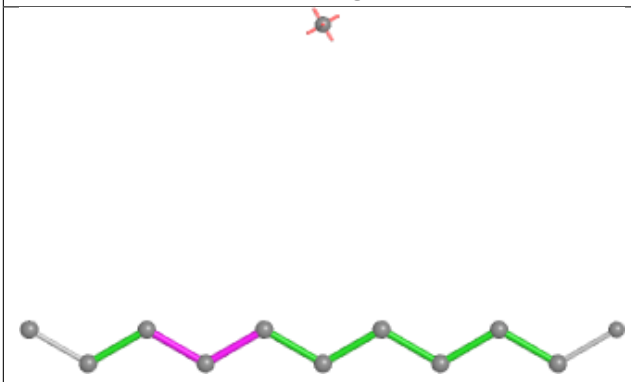
Ligand DMU J 102



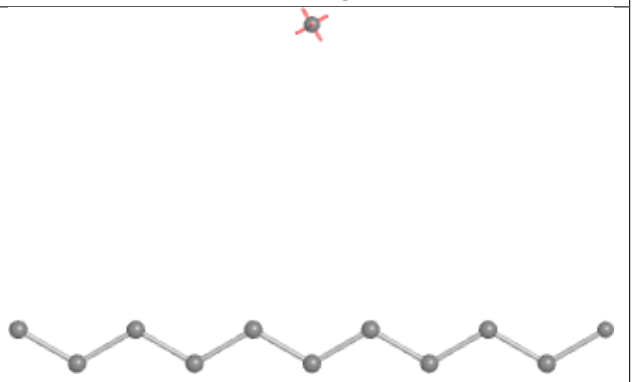
Bond lengths



Bond angles

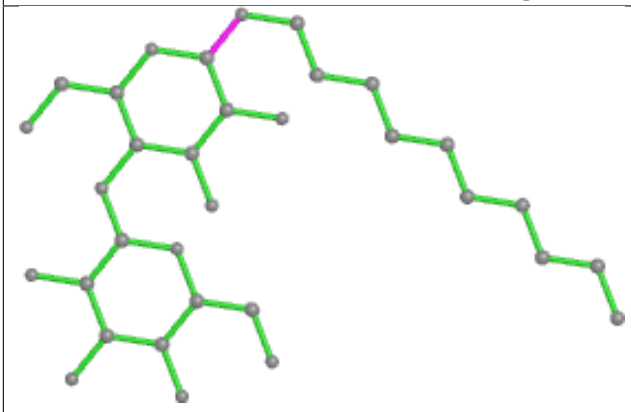


Torsions

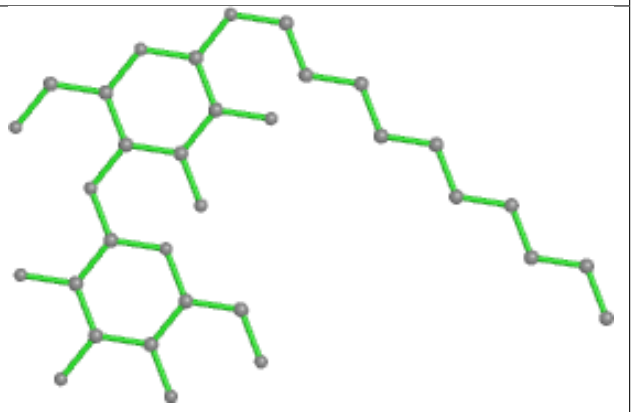


Rings

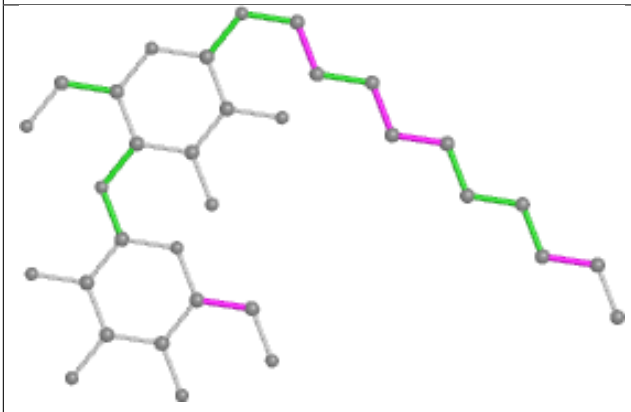
Ligand DMU P 303



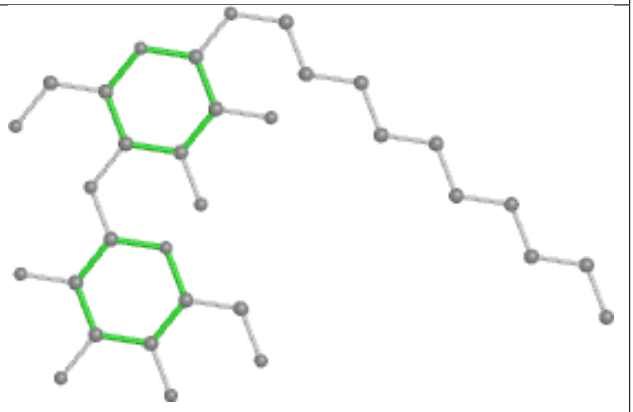
Bond lengths



Bond angles

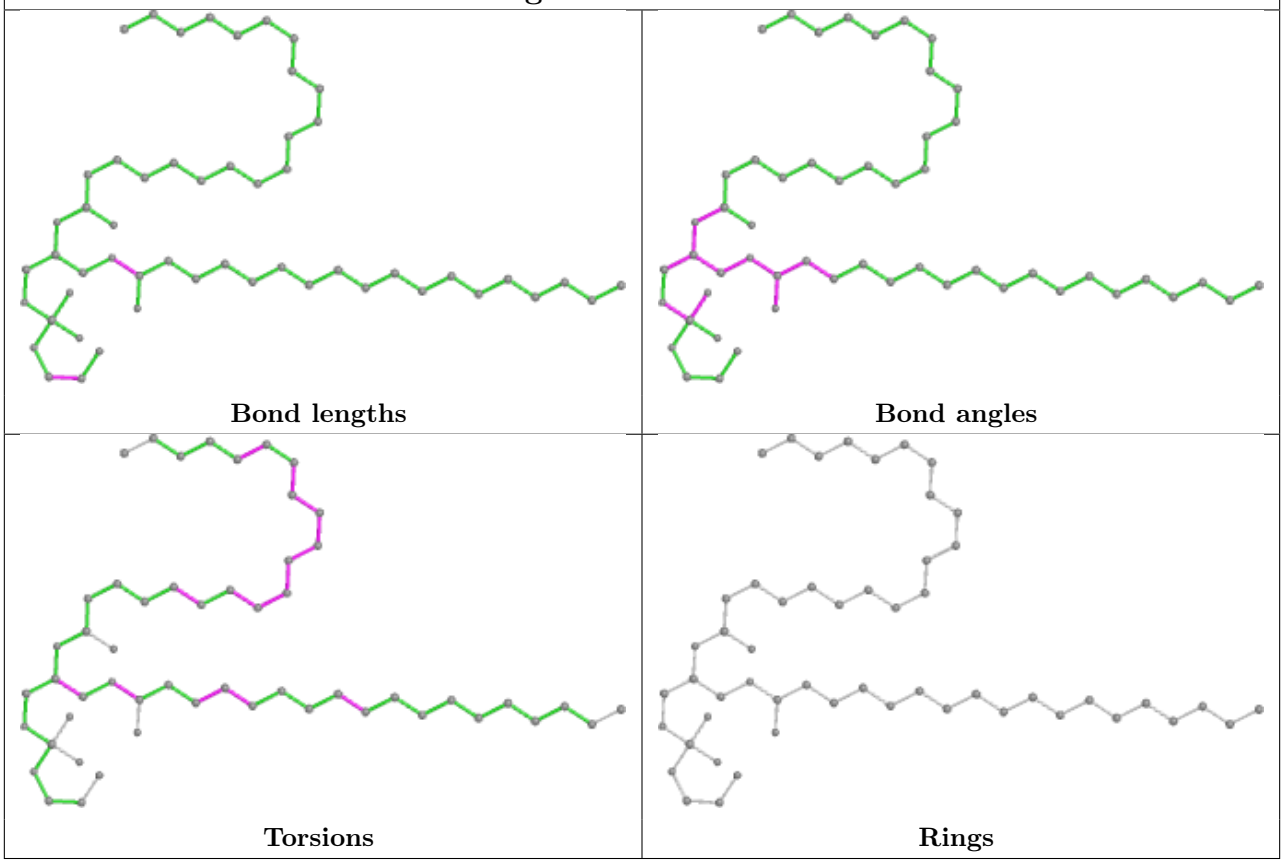


Torsions

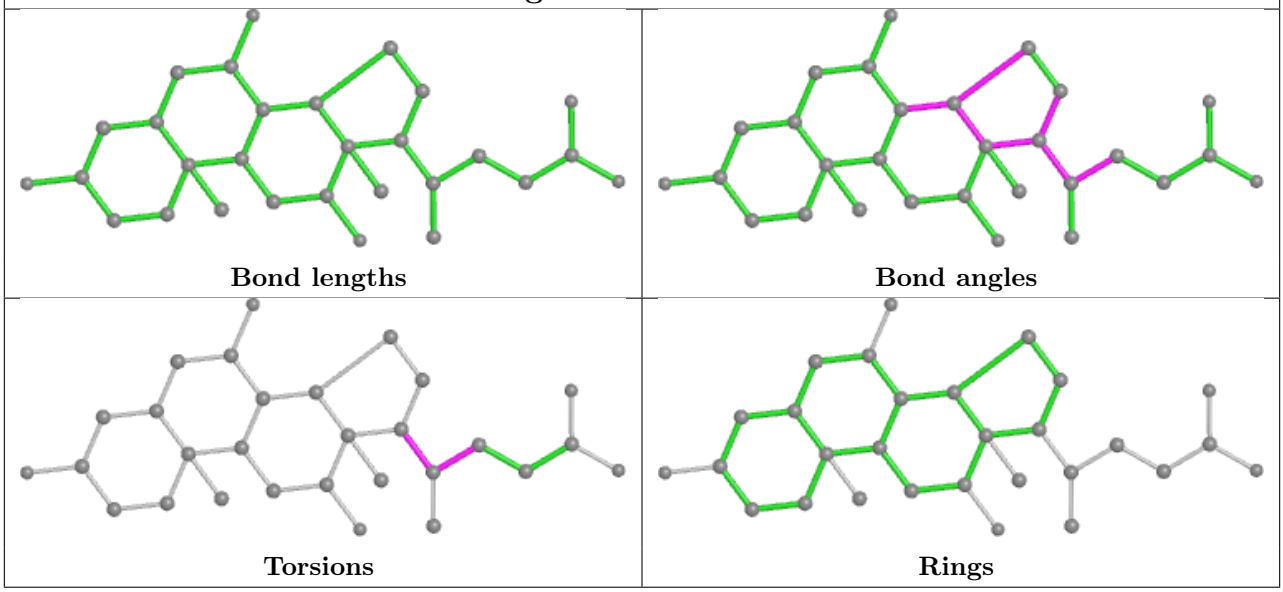


Rings

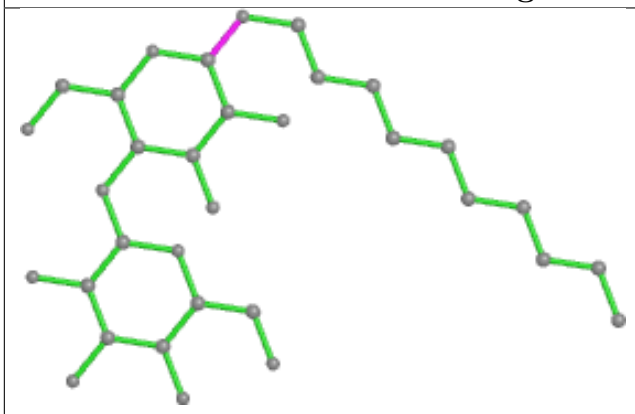
Ligand PEK P 308



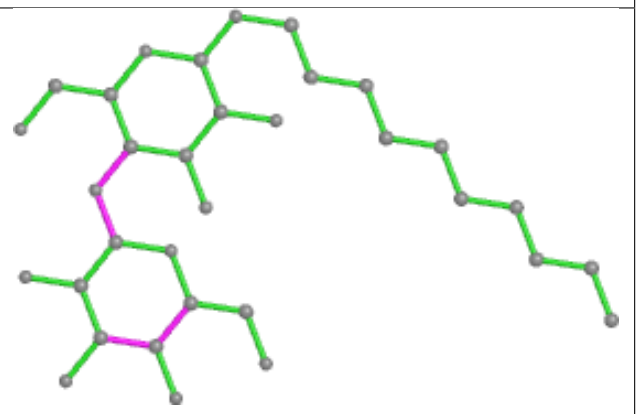
Ligand CHD J 101



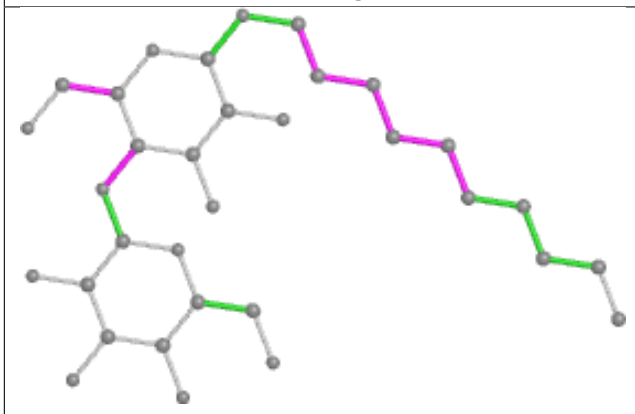
Ligand DMU K 103



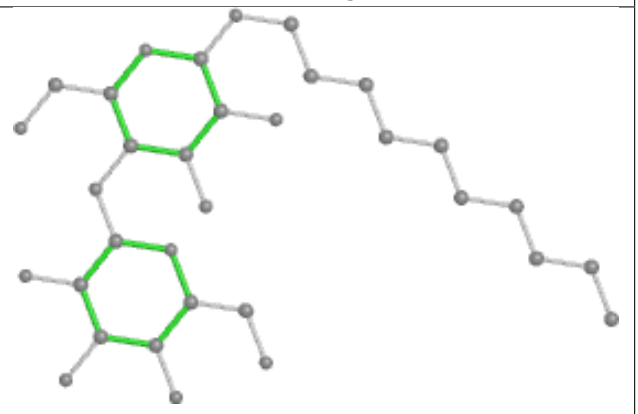
Bond lengths



Bond angles

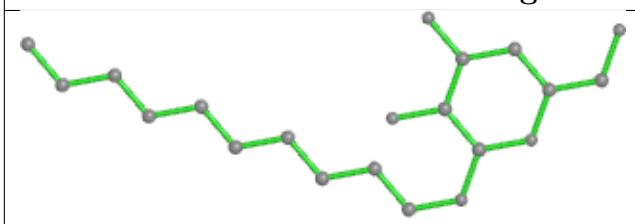


Torsions

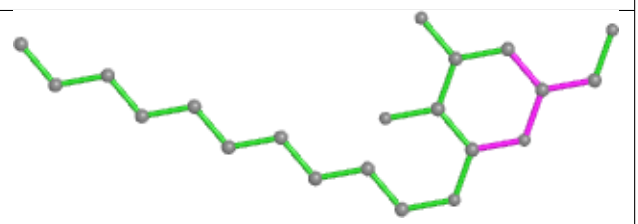


Rings

Ligand DMU L 102

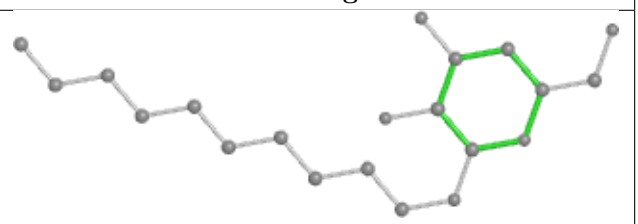


Bond lengths



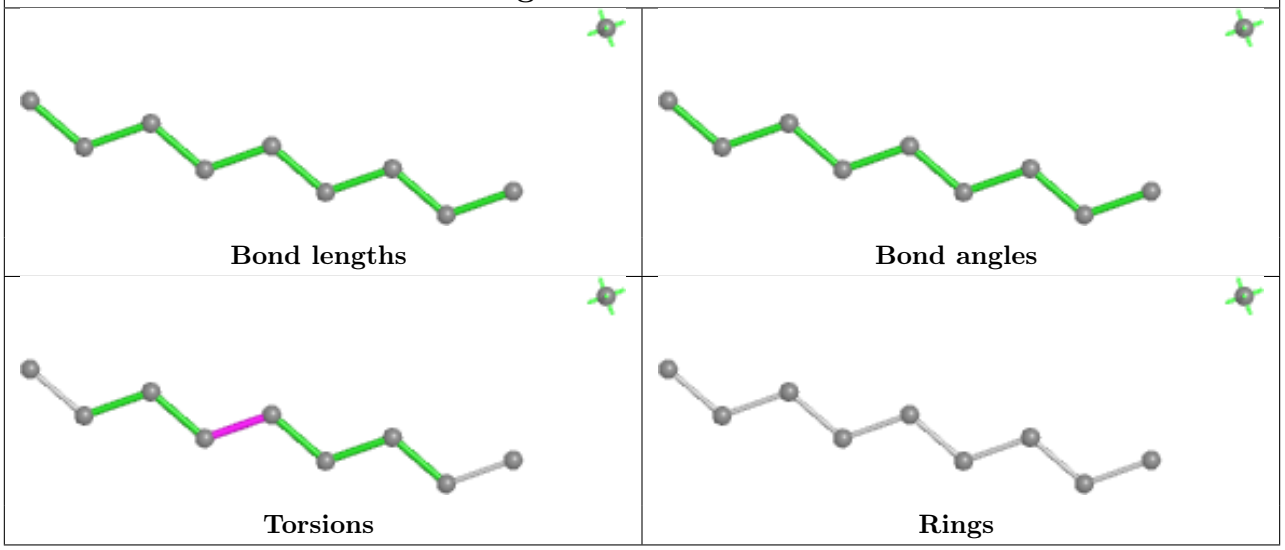
Bond angles

Torsions

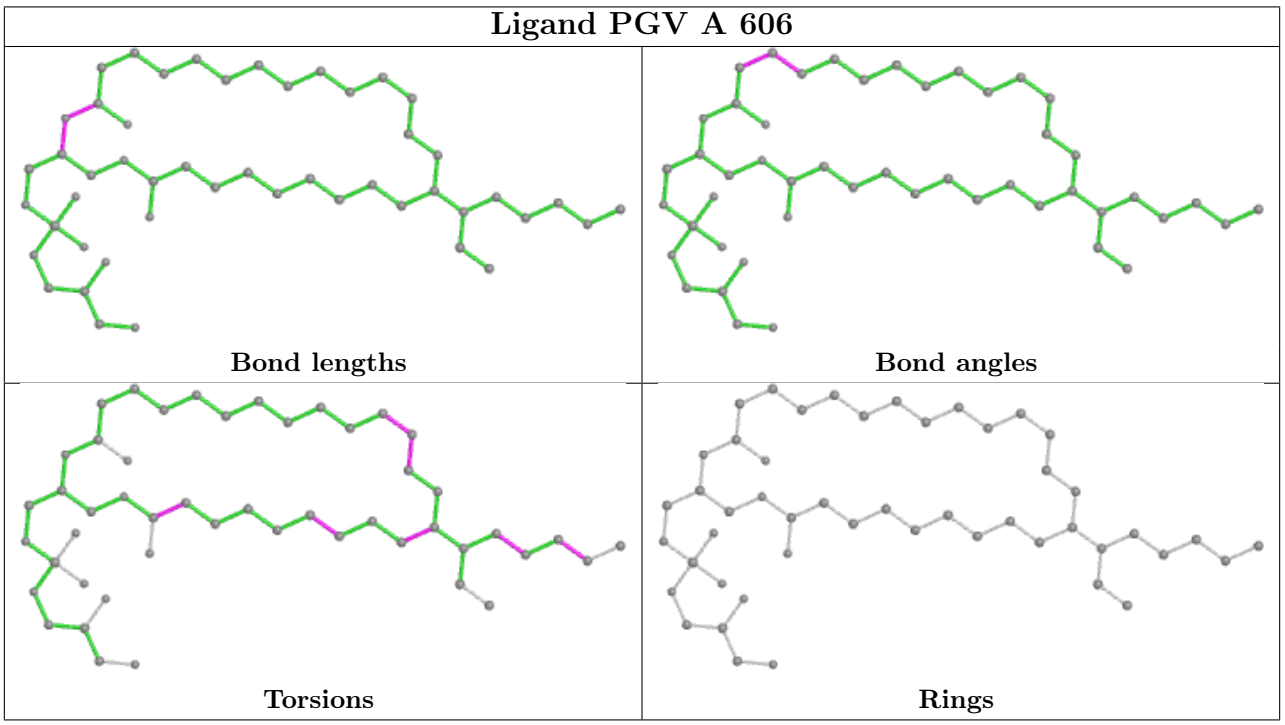


Rings

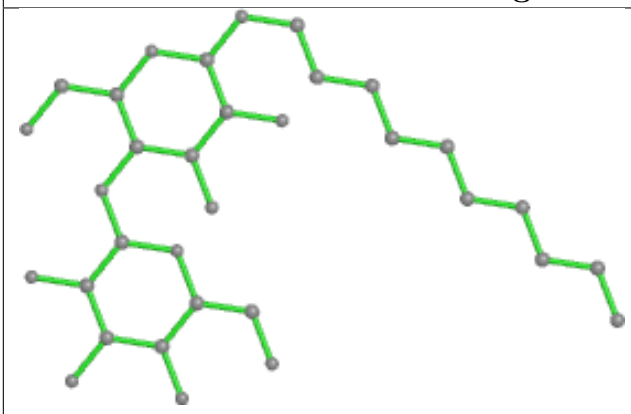
Ligand DMU K 104



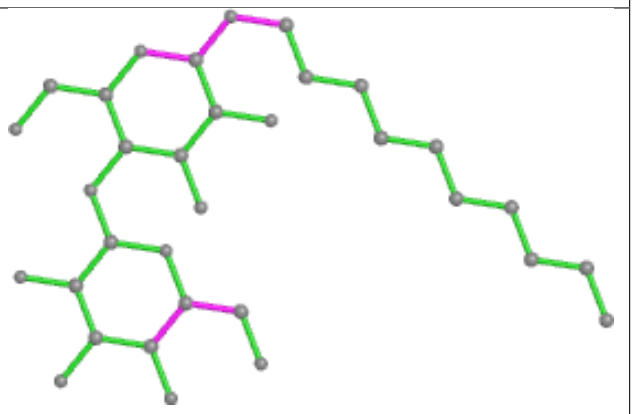
Ligand PGV A 606



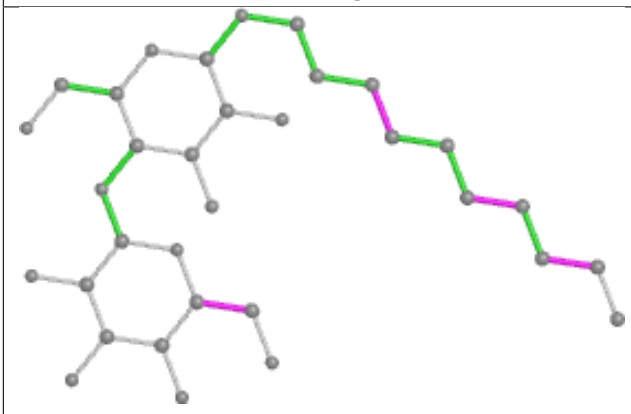
Ligand DMU M 101



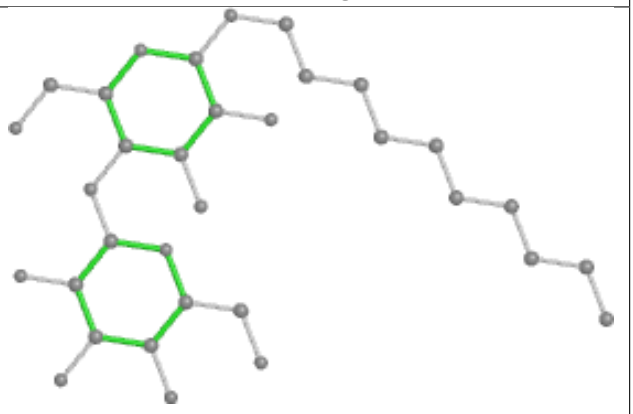
Bond lengths



Bond angles

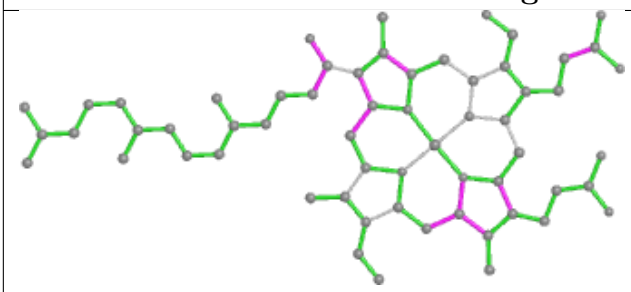


Torsions

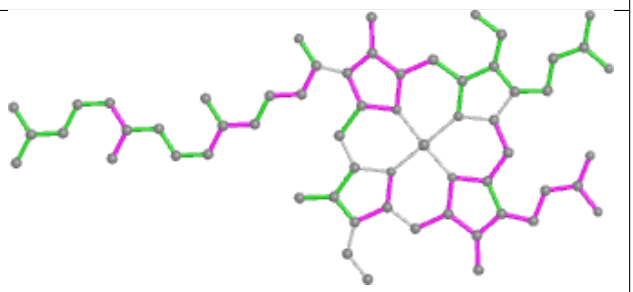


Rings

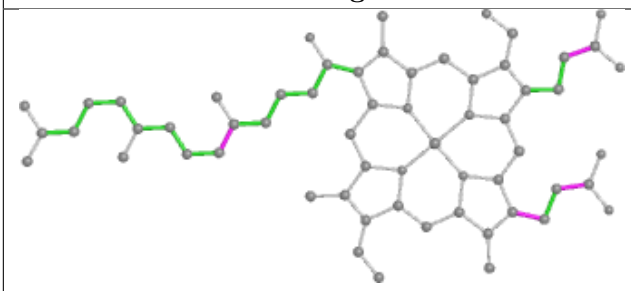
Ligand HEA N 602



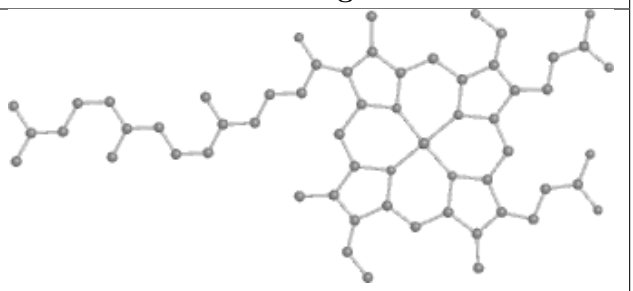
Bond lengths



Bond angles

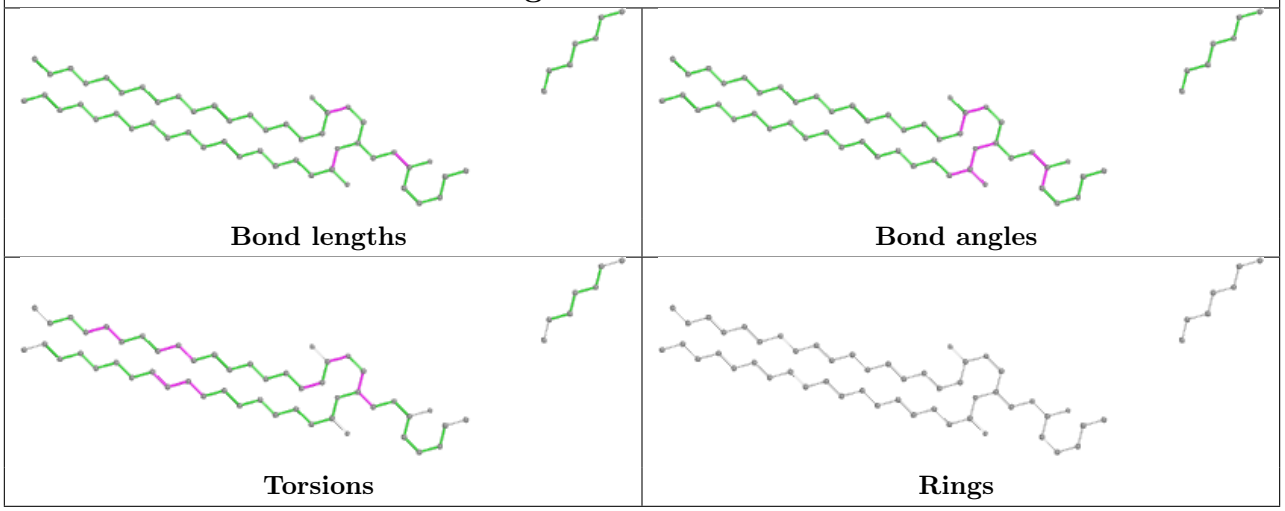


Torsions

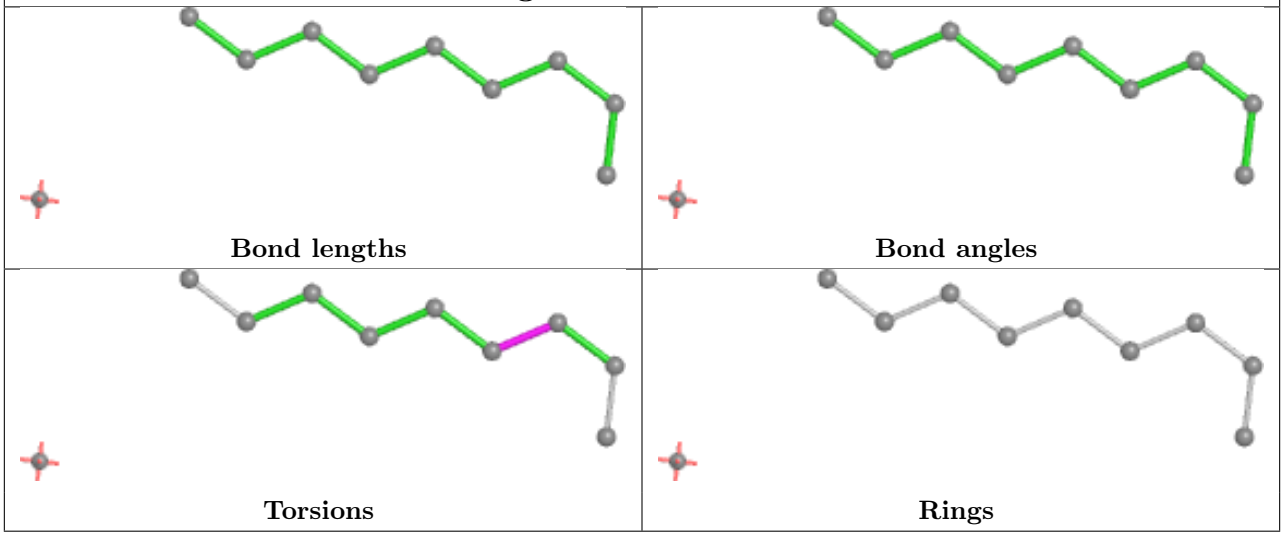


Rings

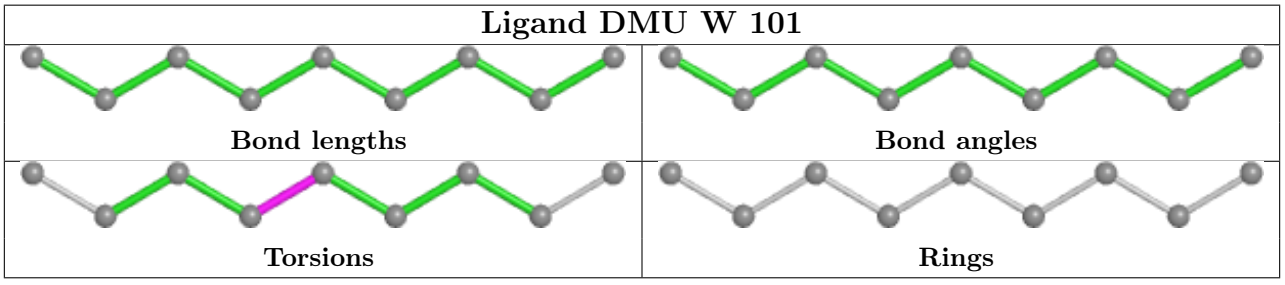
Ligand TGL O 301



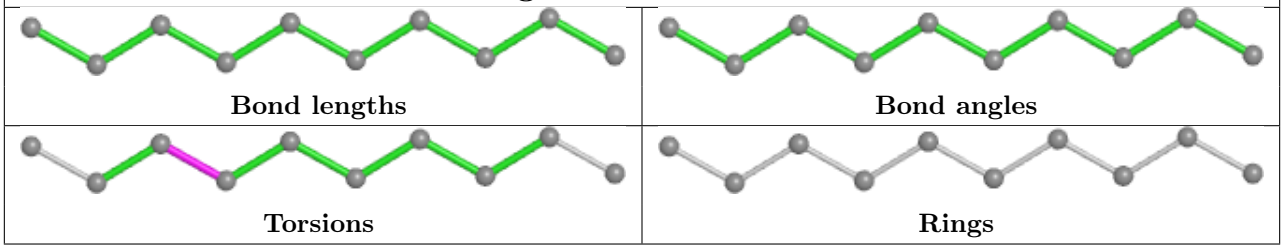
Ligand DMU K 101



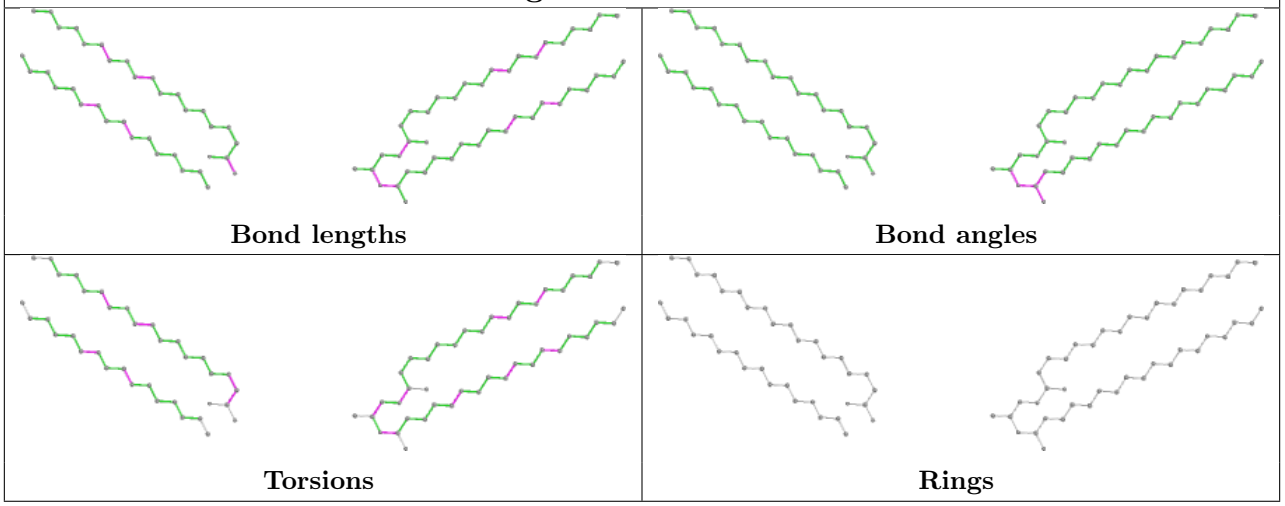
Ligand DMU W 101



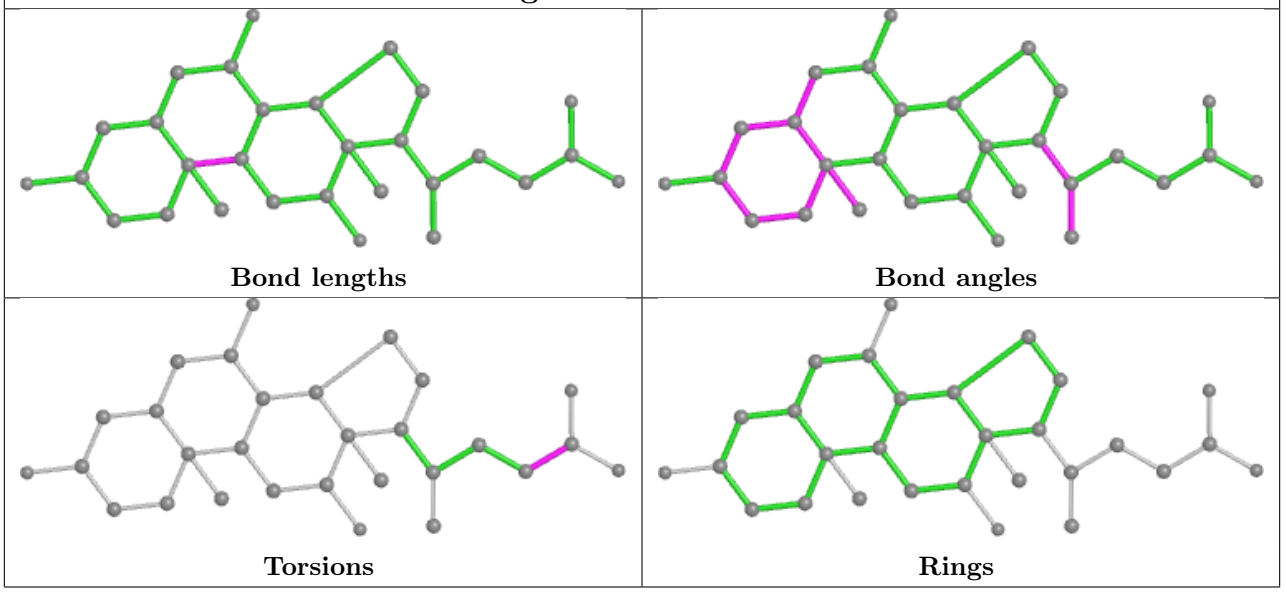
Ligand DMU X 104



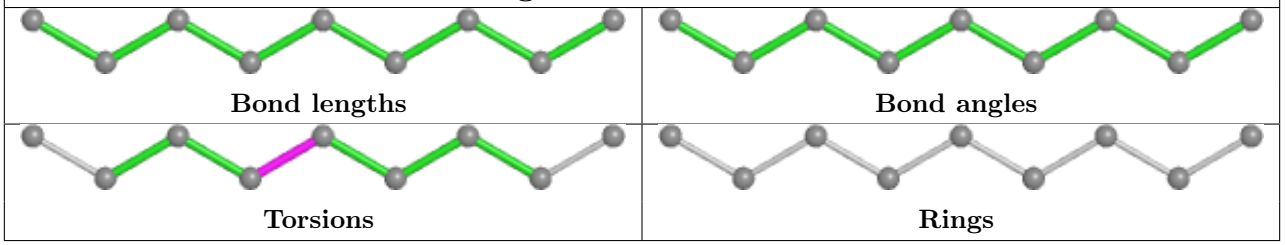
Ligand CDL T 101



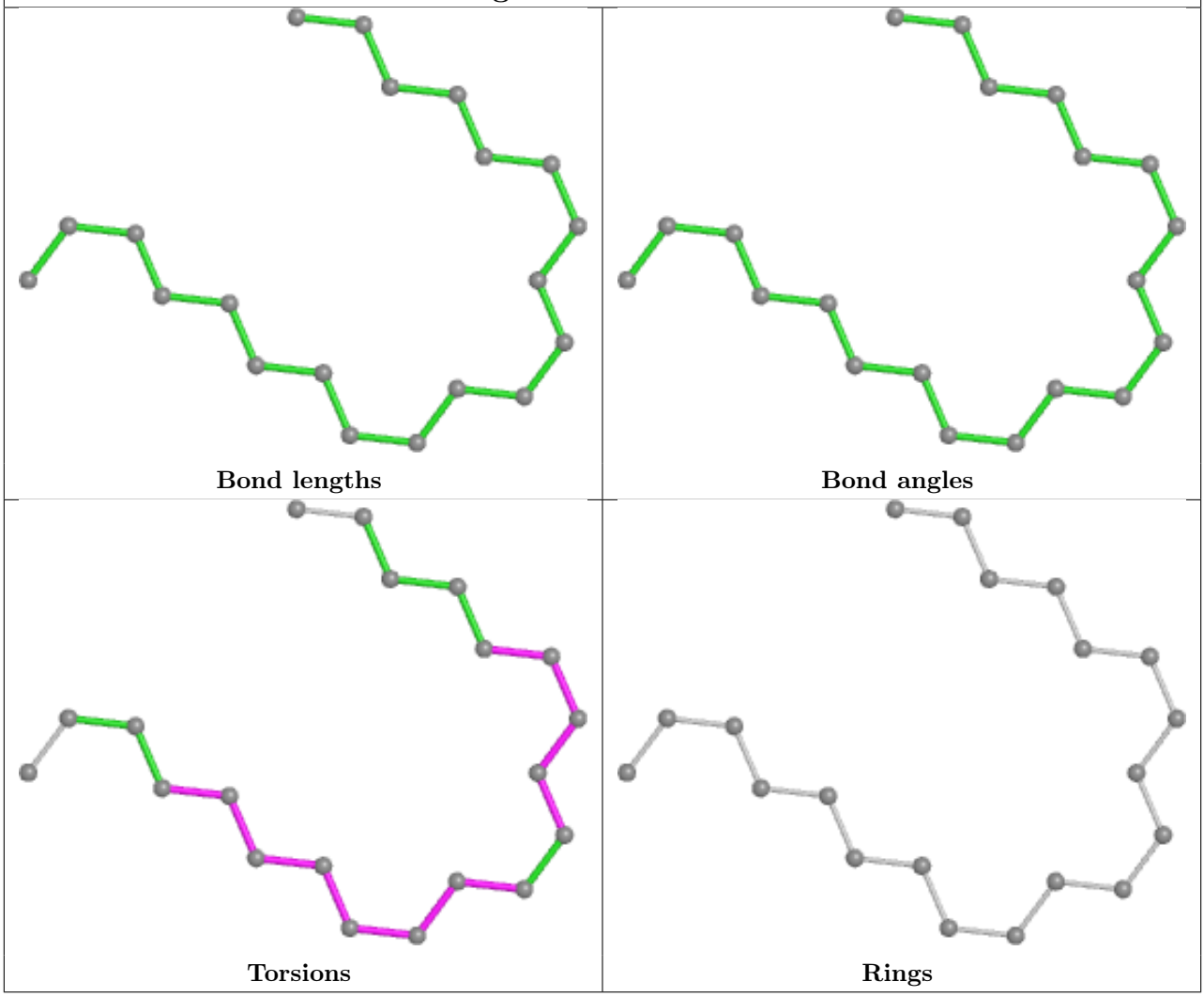
Ligand CHD G 103



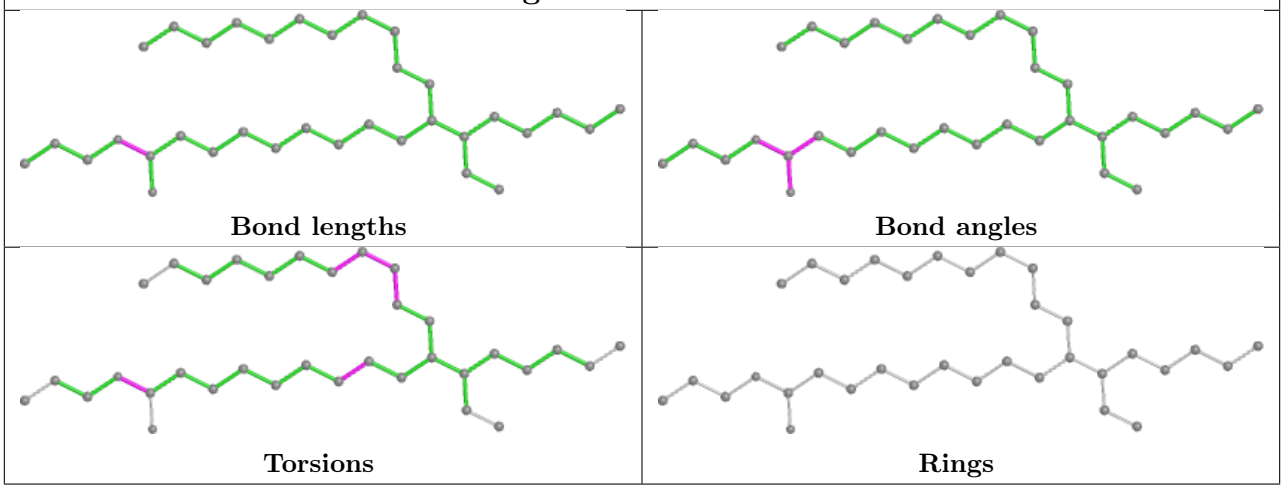
Ligand DMU K 106



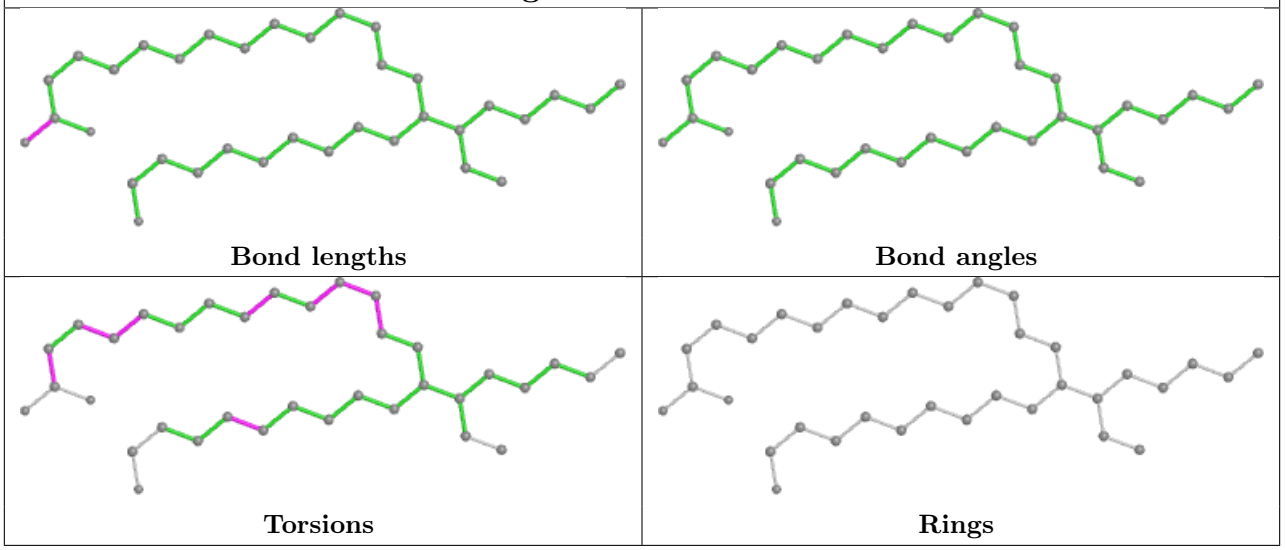
Ligand PEK P 301



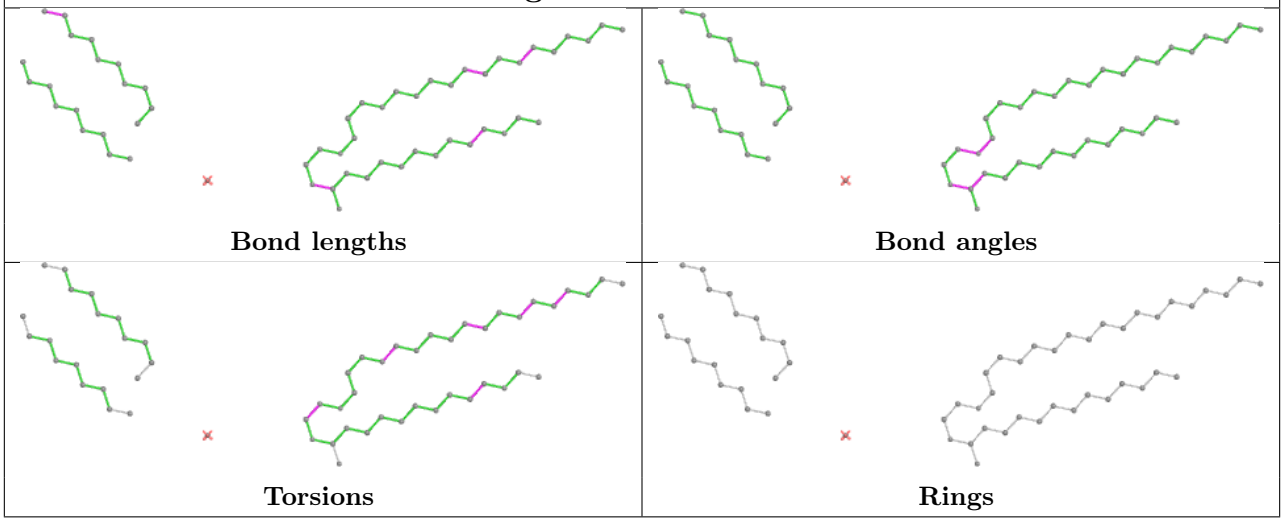
Ligand PGV C 306



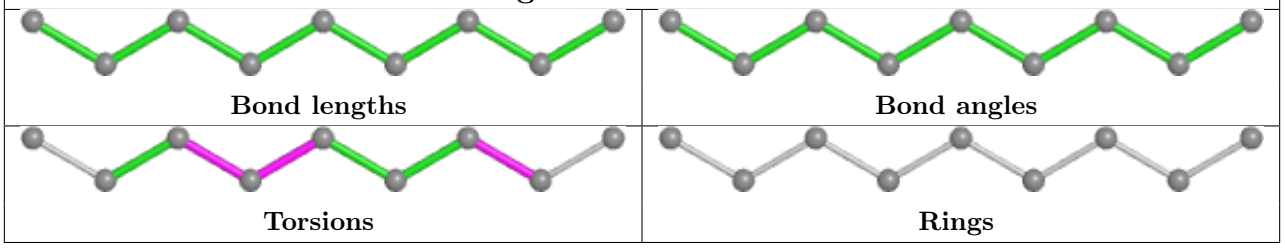
Ligand PGV A 607



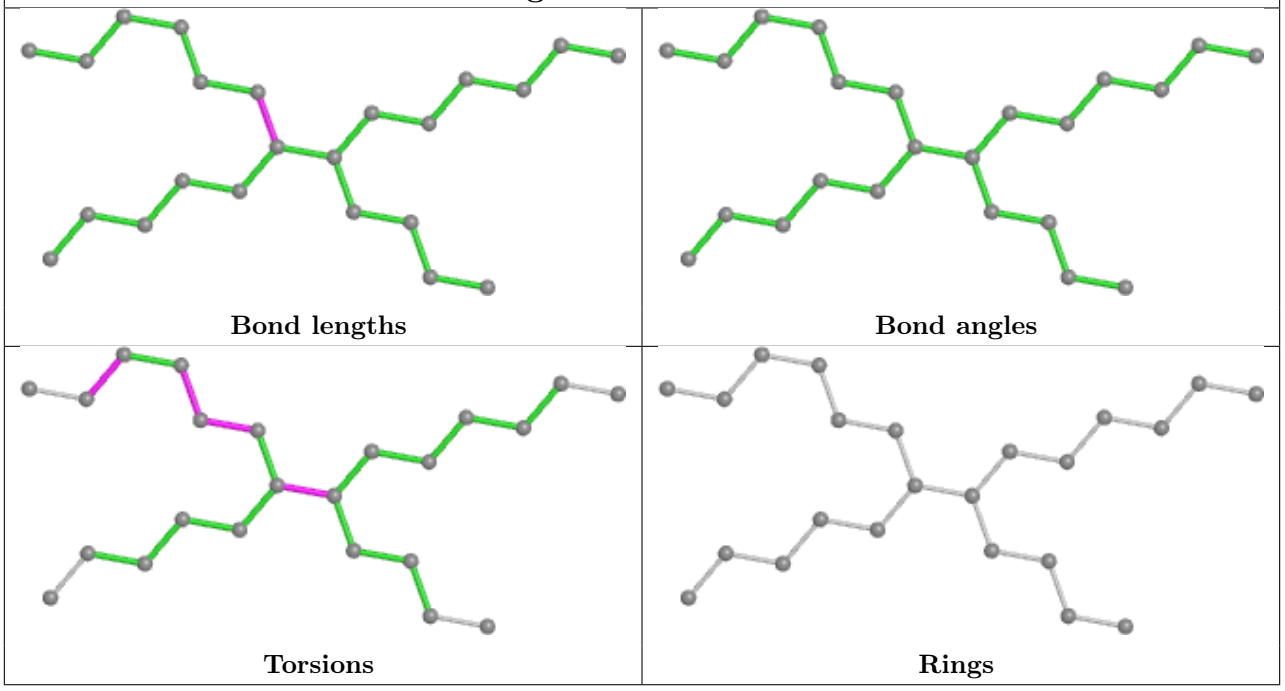
Ligand CDL C 303



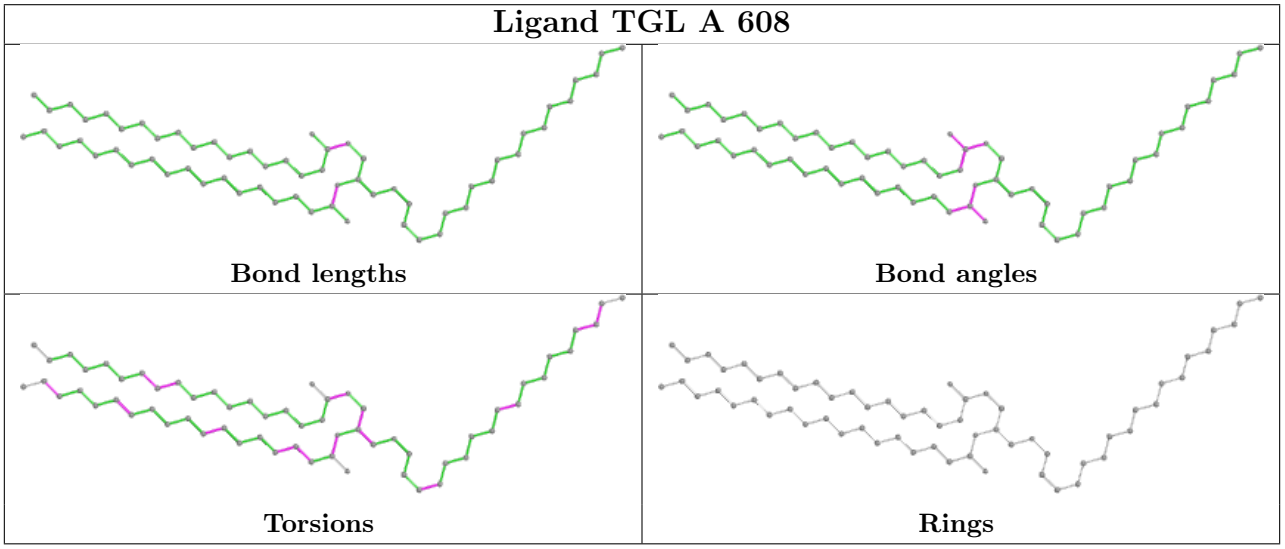
Ligand DMU K 102



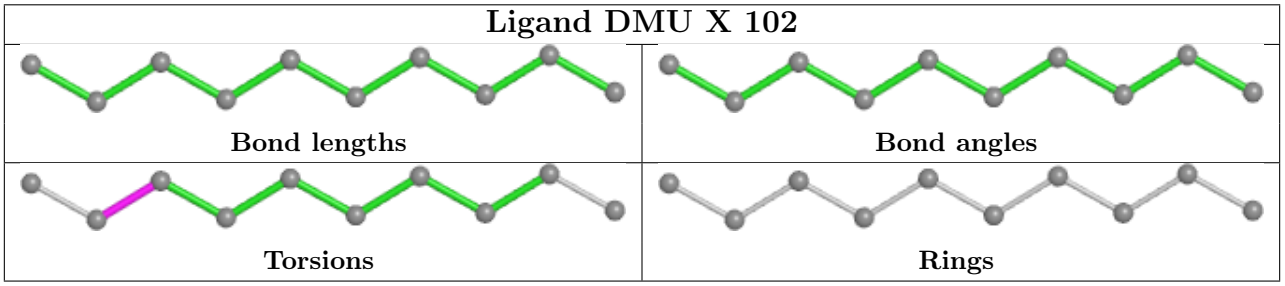
Ligand PSC A 609

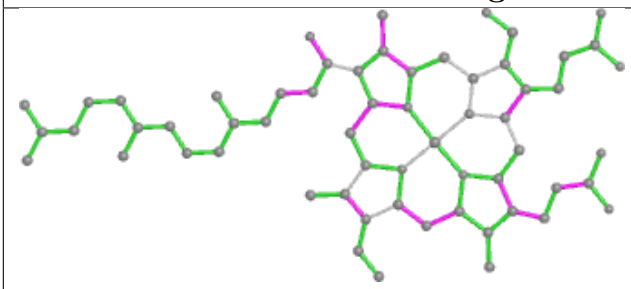
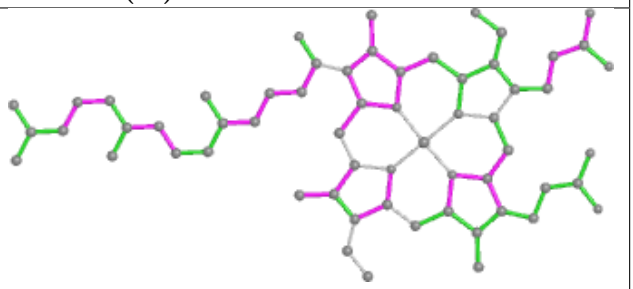
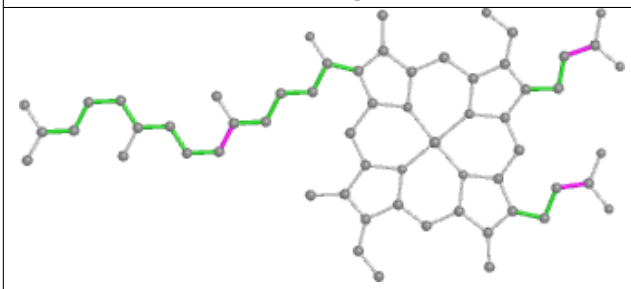
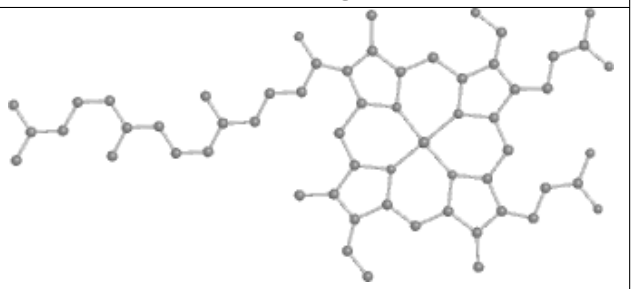


Ligand TGL A 608



Ligand DMU X 102



Ligand HEA A 601 (A)	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	513/514 (99%)	-0.62	0 100 100	16, 20, 29, 79	0
1	N	513/514 (99%)	-0.55	2 (0%) 92 92	18, 23, 33, 82	0
2	B	226/227 (99%)	-0.54	2 (0%) 84 84	19, 28, 57, 115	0
2	O	226/227 (99%)	-0.47	4 (1%) 68 67	24, 33, 77, 129	0
3	C	259/259 (100%)	-0.85	0 100 100	18, 24, 41, 82	0
3	P	259/259 (100%)	-0.80	1 (0%) 92 92	19, 25, 40, 87	0
4	D	144/144 (100%)	-0.74	1 (0%) 87 87	22, 30, 53, 94	0
4	Q	144/144 (100%)	0.65	11 (7%) 13 12	28, 44, 92, 221	0
5	E	105/105 (100%)	-0.65	3 (2%) 51 49	23, 30, 62, 164	0
5	R	105/105 (100%)	-0.25	2 (1%) 66 65	26, 36, 79, 178	0
6	F	98/98 (100%)	-0.06	7 (7%) 16 14	20, 30, 118, 222	0
6	S	98/98 (100%)	0.01	8 (8%) 11 10	20, 29, 143, 247	0
7	G	84/84 (100%)	1.06	19 (22%) 0 0	23, 32, 149, 231	0
7	T	84/84 (100%)	0.88	15 (17%) 1 1	21, 34, 132, 230	0
8	H	79/79 (100%)	0.12	7 (8%) 9 8	24, 34, 153, 180	0
8	U	79/79 (100%)	0.19	8 (10%) 7 5	29, 39, 141, 209	0
9	I	72/73 (98%)	0.16	6 (8%) 11 10	26, 41, 76, 101	0
9	V	72/73 (98%)	0.25	4 (5%) 24 22	27, 50, 95, 229	0
10	J	58/58 (100%)	0.37	4 (6%) 16 15	25, 34, 92, 143	0
10	W	58/58 (100%)	-0.14	3 (5%) 27 24	25, 36, 99, 164	0
11	K	49/49 (100%)	-0.36	1 (2%) 65 64	26, 34, 60, 64	0
11	X	49/49 (100%)	0.68	3 (6%) 21 19	34, 44, 91, 111	0
12	L	46/46 (100%)	-0.82	1 (2%) 62 60	21, 25, 53, 114	0
12	Y	46/46 (100%)	-0.59	1 (2%) 62 60	25, 32, 73, 145	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	M	43/43 (100%)	-0.40	4 (9%)	8	7	22, 26, 75, 150	0
13	Z	43/43 (100%)	-0.09	4 (9%)	8	7	30, 35, 128, 256	0
All	All	3552/3558 (99%)	-0.34	121 (3%)	45	42	16, 28, 76, 256	0

All (121) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	4	SER	40.0
4	Q	6	VAL	32.2
6	S	97	ALA	29.3
7	G	2	SER	21.5
4	Q	5	VAL	18.3
7	T	2	SER	17.2
10	J	1	PHE	16.9
4	Q	7	LYS	16.4
7	T	1	ALA	15.2
8	H	8	ILE	13.6
7	G	1	ALA	12.1
8	U	7	LYS	11.6
6	F	95	GLN	11.1
8	U	9	LYS	11.0
5	R	5	HIS	10.1
6	F	98	HIS	9.9
6	S	96	LEU	9.6
6	S	95	GLN	9.5
6	F	96	LEU	9.5
7	T	9	GLY	8.7
6	S	98	HIS	8.6
7	G	11	THR	8.5
7	T	3	ALA	8.5
7	T	11	THR	8.4
7	G	3	ALA	8.2
8	U	8	ILE	8.1
6	S	1	ALA	8.0
8	H	46	LYS	7.9
8	H	45	ALA	7.9
7	G	9	GLY	7.6
9	V	2	THR	7.4
10	J	58	LYS	7.4
9	V	37	PHE	7.3
12	Y	47	LYS	7.0

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Mol	Chain	Res	Type	RSRZ
7	T	6	GLY	6.8
8	U	45	ALA	6.8
7	G	6	GLY	6.6
10	W	1	PHE	6.5
6	F	97	ALA	6.4
5	R	109	VAL	6.4
8	H	47	GLY	6.2
9	I	37	PHE	6.1
8	U	46	LYS	6.1
11	X	6	ALA	6.0
7	T	36[A]	TRP	6.0
2	O	90	ILE	6.0
5	E	5	HIS	5.9
4	Q	8	SER	5.8
6	S	94	HIS	5.8
7	T	8	HIS	5.6
4	Q	51	LEU	5.4
7	G	7	ASP	5.3
7	T	10	GLY	5.2
10	W	58	LYS	5.1
8	U	10	ASN	5.1
9	I	29	LEU	4.9
7	G	10	GLY	4.8
7	G	36	TRP	4.8
8	H	48	GLY	4.8
2	O	91	ASN	4.5
7	G	5	LYS	4.5
7	T	5	LYS	4.4
7	G	8	HIS	4.4
8	H	7	LYS	4.3
13	Z	43	SER	4.3
7	G	84	LYS	4.2
6	F	2	SER	4.1
8	U	48	GLY	3.9
7	G	42	ARG	3.9
13	M	40	TYR	3.9
7	T	84	LYS	3.8
13	Z	42	LYS	3.8
6	S	2	SER	3.7
6	F	1	ALA	3.6
8	H	44	THR	3.5
7	G	41	HIS	3.5

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Mol	Chain	Res	Type	RSRZ
7	T	42	ARG	3.5
13	Z	40	TYR	3.4
11	X	7	PRO	3.4
13	M	43	SER	3.4
9	I	25	PHE	3.3
7	T	7	ASP	3.2
7	G	40	GLY	3.2
12	L	2	HIS	3.1
4	Q	147	LYS	3.1
6	S	93	PRO	3.1
10	J	2	GLU	3.1
4	Q	9	GLU	3.0
2	B	90	ILE	3.0
4	D	4	SER	2.9
10	J	4	ARG	2.8
13	M	42	LYS	2.8
6	F	94	HIS	2.8
5	E	6	GLU	2.6
8	U	47	GLY	2.6
9	V	25	PHE	2.6
1	N	113[A]	LEU	2.5
9	I	21	ILE	2.4
9	I	41	GLU	2.4
7	T	4	ALA	2.4
4	Q	73	ARG	2.3
2	B	59	GLN	2.3
1	N	297[A]	MET	2.3
3	P	3	HIS	2.2
7	G	39	SER	2.2
4	Q	39	ALA	2.2
7	G	37	LEU	2.2
4	Q	43	LYS	2.2
7	T	40	GLY	2.2
11	K	6	ALA	2.2
13	M	39	ASN	2.1
5	E	7	THR	2.1
13	Z	39	ASN	2.1
10	W	2	GLU	2.1
9	V	34	PHE	2.1
11	X	13	TYR	2.1
9	I	34	PHE	2.1
7	G	43	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
2	O	113	TYR	2.0
7	G	4	ALA	2.0
2	O	87	MET	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
9	SAC	V	1	9/10	0.26	0.64	178,202,219,230	0
9	SAC	I	1	9/10	0.73	0.21	102,127,159,160	0
1	FME	N	1	10/11	0.95	0.11	31,37,74,75	0
2	FME	B	1	10/11	0.95	0.10	17,27,59,100	0
1	FME	A	1	10/11	0.96	0.07	31,42,90,117	0
2	FME	O	1	10/11	0.98	0.05	30,34,37,88	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	DMU	D	203	9/33	0.24	0.62	67,73,89,108	0
24	DMU	X	103	9/33	0.30	0.25	71,75,93,95	0
24	DMU	K	103	33/33	0.48	0.50	53,116,180,196	0
24	DMU	X	101	33/33	0.48	0.49	56,111,187,198	0
23	CHD	J	101	29/29	0.48	0.64	59,123,157,161	0
24	DMU	X	104	10/33	0.56	0.33	60,65,106,130	0
25	CDL	G	102	64/100	0.57	0.37	50,77,106,116	0
26	PEK	C	305	37/53	0.62	0.27	41,67,97,107	0
24	DMU	J	102	12/33	0.63	0.21	51,62,91,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
25	CDL	T	101	79/100	0.65	0.32	49,80,113,135	0
21	EDO	W	103	4/4	0.66	0.16	55,62,82,96	0
26	PEK	P	309	39/53	0.66	0.32	36,74,102,104	0
21	EDO	C	309	4/4	0.67	0.30	44,49,70,77	0
21	EDO	N	621	4/4	0.67	0.14	40,55,66,68	0
23	CHD	P	306	29/29	0.68	0.34	59,87,115,124	0
26	PEK	P	301	20/53	0.70	0.23	41,52,86,90	0
25	CDL	P	305	69/100	0.72	0.42	41,76,134,145	0
18	PGV	P	302	41/51	0.73	0.31	46,78,111,124	0
24	DMU	W	101	9/33	0.74	0.22	61,64,72,87	0
24	DMU	K	104	10/33	0.74	0.30	46,68,94,156	0
21	EDO	N	612	4/4	0.75	0.17	44,59,71,81	0
21	EDO	C	311	4/4	0.76	0.31	31,70,77,85	0
21	EDO	C	312	4/4	0.76	0.24	38,70,75,119	0
24	DMU	P	303	33/33	0.76	0.18	46,92,140,148	0
25	CDL	C	303	56/100	0.76	0.34	37,62,94,99	0
19	TGL	D	201	63/63	0.76	0.25	30,73,104,130	0
18	PGV	C	306	36/51	0.77	0.33	35,74,108,121	0
24	DMU	L	102	21/33	0.78	0.21	46,81,117,144	0
26	PEK	C	307	26/53	0.78	0.25	40,56,95,102	0
19	TGL	L	101	59/63	0.79	0.22	26,59,112,149	0
19	TGL	N	608	57/63	0.79	0.25	37,67,99,118	0
19	TGL	O	301	58/63	0.79	0.28	46,69,105,116	0
21	EDO	Y	101	4/4	0.79	0.16	43,48,52,89	0
20	PSC	A	609	25/52	0.80	0.23	44,68,88,93	0
19	TGL	Q	201	63/63	0.80	0.23	41,73,102,123	0
24	DMU	C	308	12/33	0.81	0.15	55,59,89,91	0
24	DMU	X	105	11/33	0.81	0.46	49,80,93,110	0
24	DMU	K	102	9/33	0.82	0.41	59,68,90,92	0
21	EDO	Q	203	4/4	0.82	0.14	33,38,60,65	0
20	PSC	O	303	24/52	0.83	0.22	35,62,98,102	0
21	EDO	R	201	4/4	0.83	0.07	43,47,48,52	0
24	DMU	K	105	9/33	0.83	0.58	59,82,91,107	0
21	EDO	N	617	4/4	0.84	0.14	40,72,73,74	0
24	DMU	X	102	10/33	0.84	0.20	48,60,96,115	0
21	EDO	S	102	4/4	0.84	0.11	40,42,47,64	0
21	EDO	J	103	4/4	0.84	0.18	60,61,61,99	0
24	DMU	P	310	11/33	0.84	0.18	47,64,82,98	0
24	DMU	Z	101	33/33	0.84	0.17	35,46,65,75	0
19	TGL	A	608	62/63	0.84	0.20	36,70,100,112	0
18	PGV	N	606	40/51	0.85	0.27	37,69,127,133	0
18	PGV	A	607	37/51	0.86	0.21	33,60,113,122	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	DMU	K	101	10/33	0.86	0.25	43,70,82,180	0
21	EDO	B	304	4/4	0.86	0.20	50,51,53,97	0
21	EDO	A	617	4/4	0.87	0.10	35,40,42,43	0
21	EDO	T	102	4/4	0.87	0.17	36,52,64,76	0
21	EDO	W	102	4/4	0.87	0.10	39,55,67,102	0
28	PO4	U	101	5/5	0.87	0.52	72,73,93,94	5
21	EDO	A	613	4/4	0.88	0.11	32,34,37,41	0
24	DMU	M	101	33/33	0.88	0.11	31,36,67,74	0
24	DMU	D	202	12/33	0.89	0.17	43,67,98,130	0
24	DMU	O	304	10/33	0.89	0.12	41,49,79,82	0
24	DMU	C	301	9/33	0.89	0.13	25,44,63,71	0
21	EDO	B	306	4/4	0.89	0.13	27,39,40,47	0
21	EDO	S	103	4/4	0.90	0.16	28,55,84,92	0
21	EDO	O	307	4/4	0.90	0.17	31,64,82,96	0
24	DMU	K	106	9/33	0.90	0.12	36,50,95,95	0
28	PO4	H	101	5/5	0.90	0.44	57,64,83,100	5
21	EDO	F	105	4/4	0.90	0.16	29,42,54,61	0
21	EDO	N	609	4/4	0.91	0.13	36,36,41,47	0
21	EDO	A	615	4/4	0.91	0.23	36,37,51,110	0
21	EDO	F	102	4/4	0.91	0.13	42,45,57,87	0
21	EDO	A	619	4/4	0.92	0.16	25,30,35,41	0
21	EDO	B	305	4/4	0.92	0.13	32,43,44,54	0
21	EDO	S	106	4/4	0.92	0.14	29,57,60,67	0
21	EDO	N	619	4/4	0.93	0.12	29,40,56,95	0
21	EDO	T	103	4/4	0.93	0.16	52,69,83,104	0
21	EDO	F	104	4/4	0.93	0.09	30,33,35,44	0
21	EDO	N	613	4/4	0.93	0.07	33,38,40,69	0
21	EDO	F	103	4/4	0.93	0.09	33,39,61,104	0
21	EDO	P	313	4/4	0.94	0.07	31,34,37,39	0
23	CHD	P	307	29/29	0.94	0.08	22,27,31,36	0
21	EDO	J	104	4/4	0.94	0.22	39,44,62,104	0
21	EDO	P	311	4/4	0.94	0.09	26,28,38,61	0
21	EDO	P	312	4/4	0.94	0.10	47,57,60,67	0
21	EDO	N	610	4/4	0.95	0.06	30,32,32,33	0
21	EDO	G	104	4/4	0.95	0.06	27,29,33,35	0
26	PEK	G	101	53/53	0.95	0.15	23,42,90,126	0
21	EDO	Q	204	4/4	0.95	0.13	49,51,59,60	0
21	EDO	A	612	4/4	0.95	0.10	30,34,72,79	0
23	CHD	B	302	29/29	0.95	0.07	20,24,28,37	0
23	CHD	C	304	29/29	0.95	0.08	22,26,31,32	0
21	EDO	N	611	4/4	0.96	0.09	27,36,42,77	0
21	EDO	C	313	4/4	0.96	0.10	27,28,38,68	0

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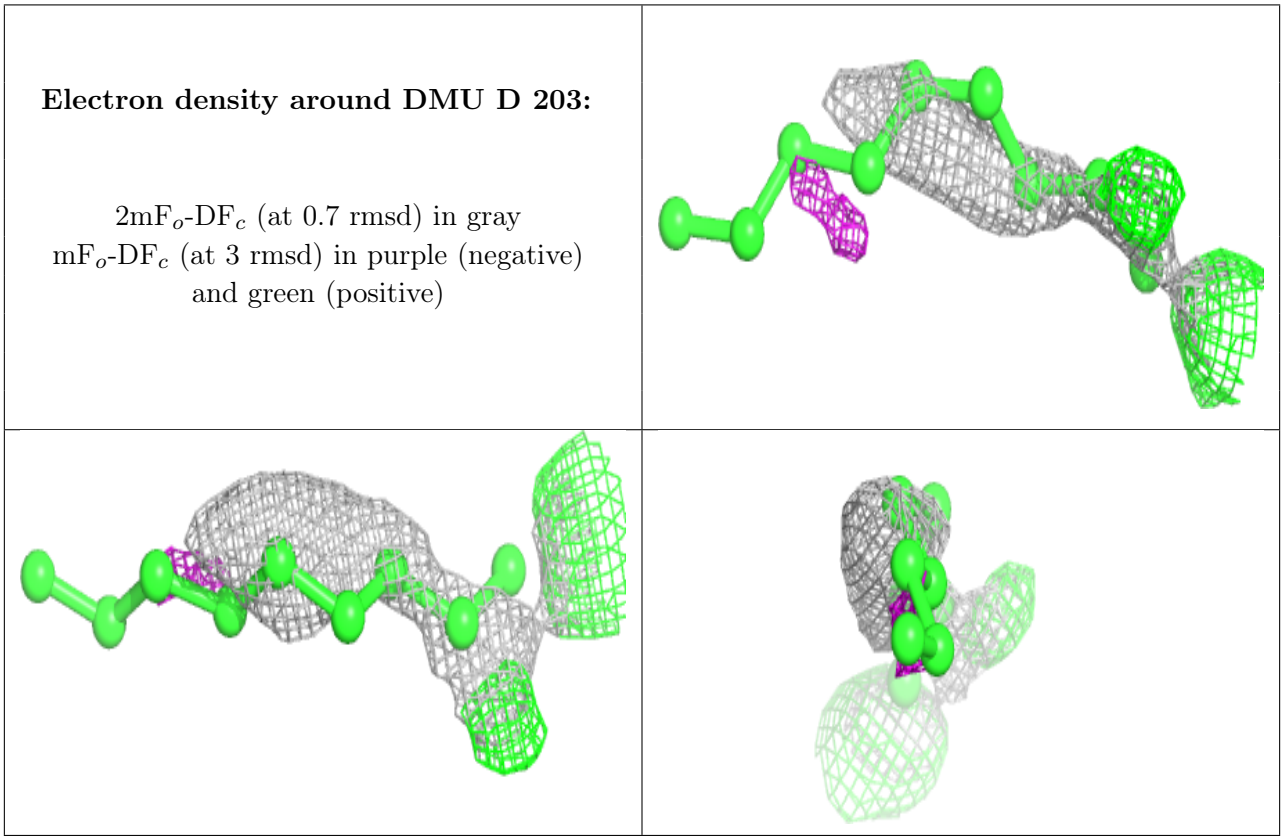
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
21	EDO	E	201	4/4	0.96	0.07	33,35,35,36	0
21	EDO	N	614	4/4	0.96	0.08	28,30,58,80	0
21	EDO	N	615	4/4	0.96	0.10	25,34,70,102	0
21	EDO	E	202	4/4	0.96	0.09	33,36,38,41	0
23	CHD	G	103	29/29	0.96	0.06	20,23,27,34	0
17	NA	N	605	1/1	0.96	0.05	27,27,27,27	0
26	PEK	P	308	53/53	0.96	0.11	26,43,95,124	0
21	EDO	A	610	4/4	0.96	0.08	28,28,35,77	0
21	EDO	O	306	4/4	0.96	0.09	37,37,40,43	0
21	EDO	A	614	4/4	0.96	0.06	22,23,25,26	0
21	EDO	S	105	4/4	0.97	0.05	30,32,35,35	0
21	EDO	Q	202	4/4	0.97	0.07	26,33,55,56	0
21	EDO	N	616	4/4	0.97	0.07	22,23,24,26	0
21	EDO	A	616	4/4	0.97	0.08	26,33,34,42	0
21	EDO	C	310	4/4	0.97	0.06	28,30,31,34	0
18	PGV	P	304	50/51	0.97	0.08	19,30,70,100	0
21	EDO	O	305	4/4	0.97	0.06	28,28,29,32	0
21	EDO	S	104	4/4	0.97	0.06	20,21,21,22	0
21	EDO	B	303	4/4	0.98	0.04	21,23,23,26	0
21	EDO	A	611	4/4	0.98	0.12	19,20,20,25	0
14	HEA	N	602	60/60	0.98	0.07	16,20,28,30	0
17	NA	A	605	1/1	0.98	0.04	22,22,22,22	0
18	PGV	N	607	51/51	0.98	0.08	20,25,70,93	0
14	HEA	N	601[A]	60/60	0.98	0.07	19,22,34,44	10
18	PGV	A	606	51/51	0.98	0.08	18,24,66,83	0
21	EDO	N	618	4/4	0.98	0.06	29,37,44,45	0
14	HEA	N	601[B]	60/60	0.98	0.07	12,22,35,46	10
21	EDO	N	620	4/4	0.98	0.10	21,24,24,28	0
21	EDO	A	618	4/4	0.98	0.10	28,35,67,106	0
18	PGV	C	302	51/51	0.98	0.08	19,26,75,97	0
21	EDO	F	106	4/4	0.99	0.04	19,20,20,22	0
16	MG	A	604	1/1	0.99	0.04	17,17,17,17	0
16	MG	N	604	1/1	0.99	0.04	20,20,20,20	0
14	HEA	A	601[A]	60/60	0.99	0.07	15,18,28,40	10
27	ZN	S	101	1/1	0.99	0.03	24,24,24,24	0
14	HEA	A	601[B]	60/60	0.99	0.07	10,18,32,53	10
14	HEA	A	602	60/60	0.99	0.06	15,18,26,31	0
22	CUA	B	301	2/2	1.00	0.05	20,20,20,20	0
27	ZN	F	101	1/1	1.00	0.02	23,23,23,23	0
22	CUA	O	302	2/2	1.00	0.05	24,24,24,25	0
15	CU	A	603	1/1	1.00	0.06	17,17,17,17	0
15	CU	N	603	1/1	1.00	0.06	20,20,20,20	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.

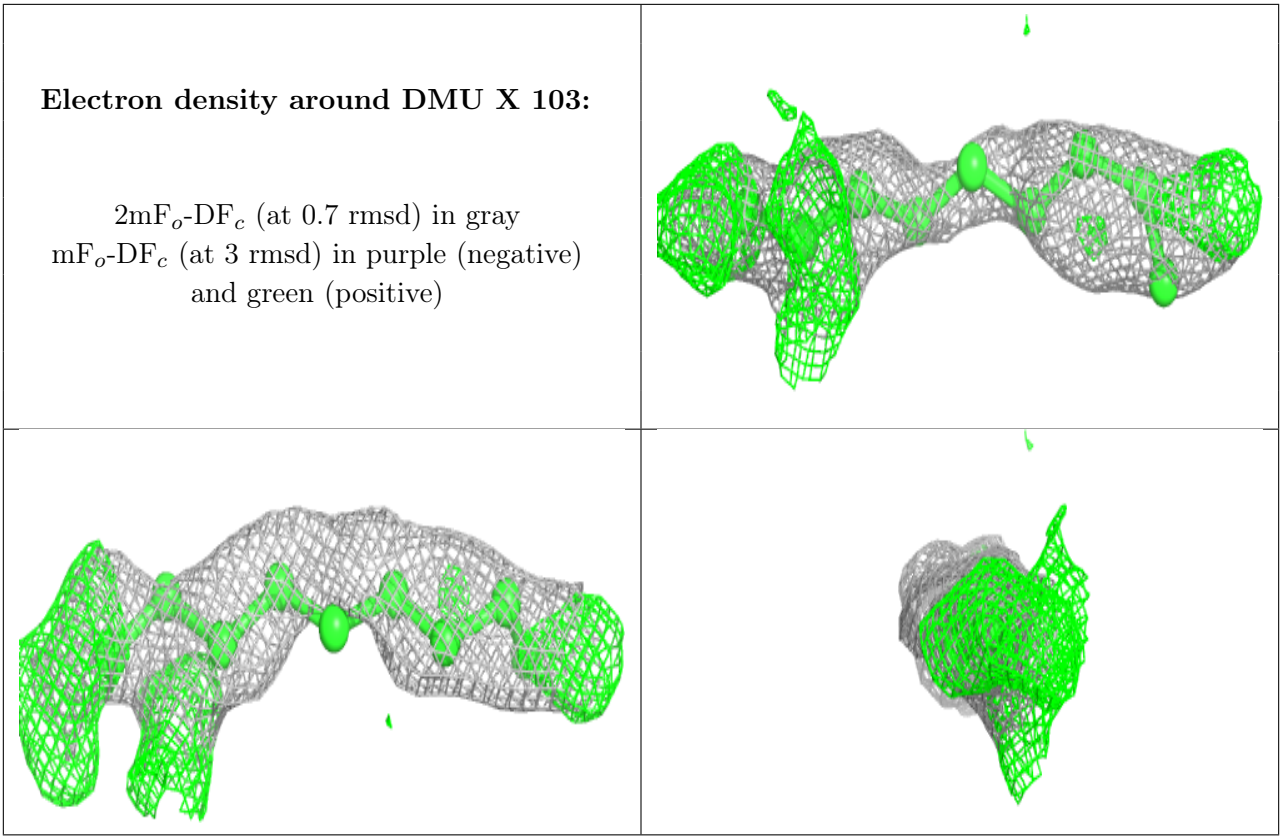
Electron density around DMU D 203:

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



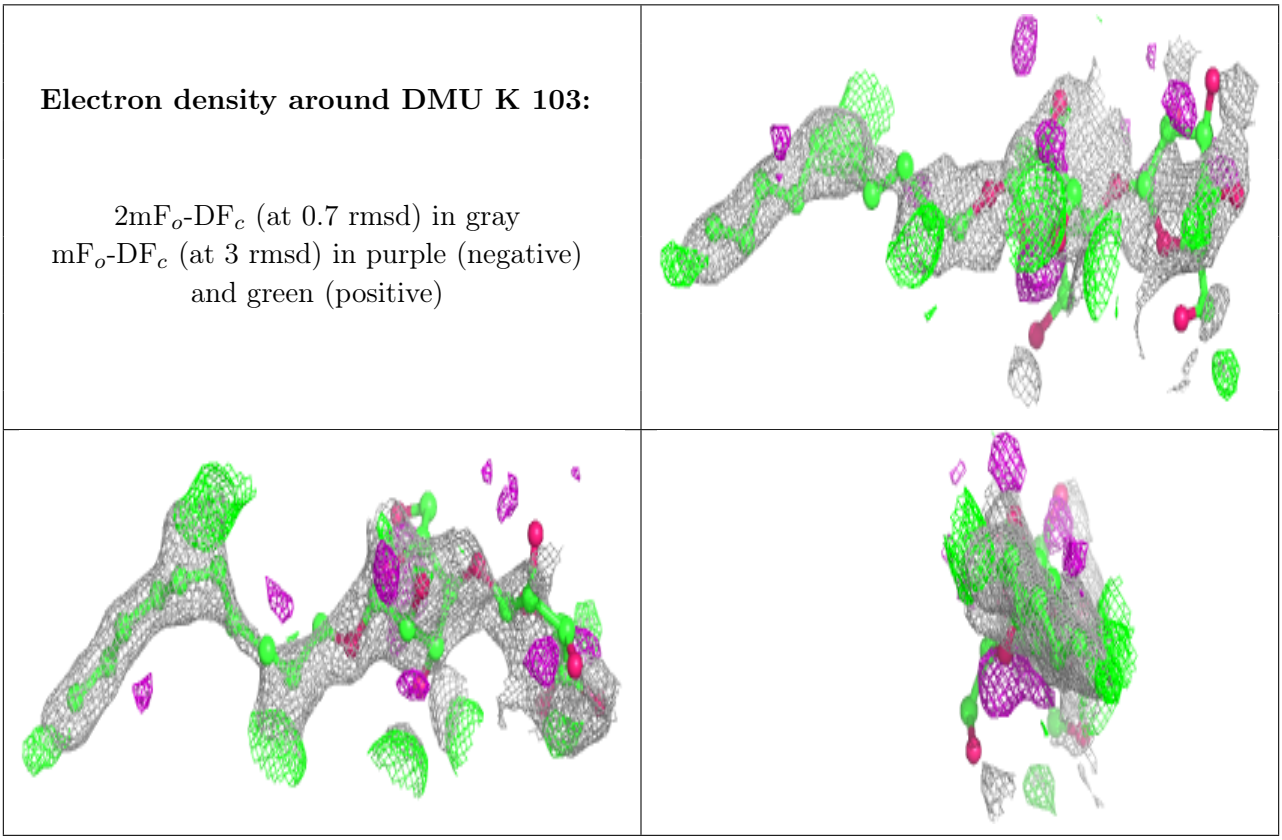
Electron density around DMU X 103:

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



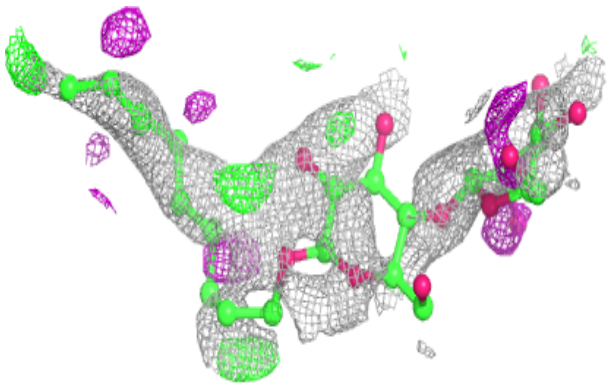
Electron density around DMU K 103:

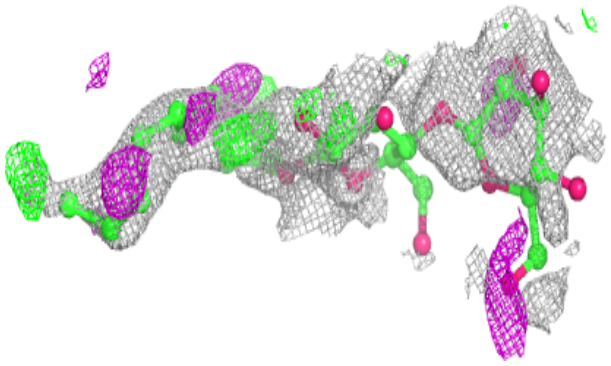
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

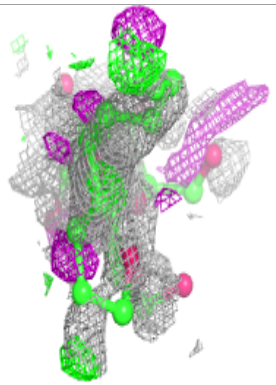


Electron density around DMU X 101:

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

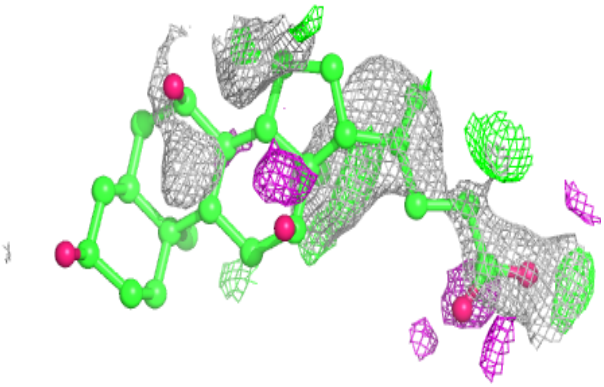


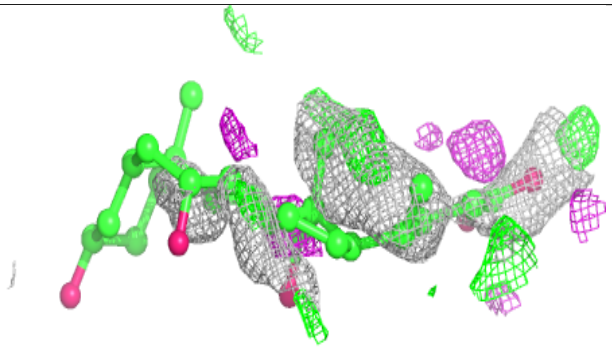


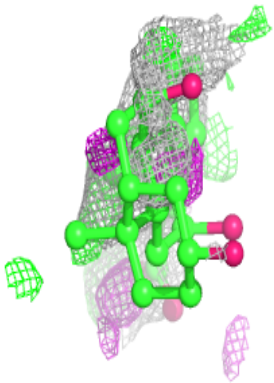


Electron density around CHD J 101:

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

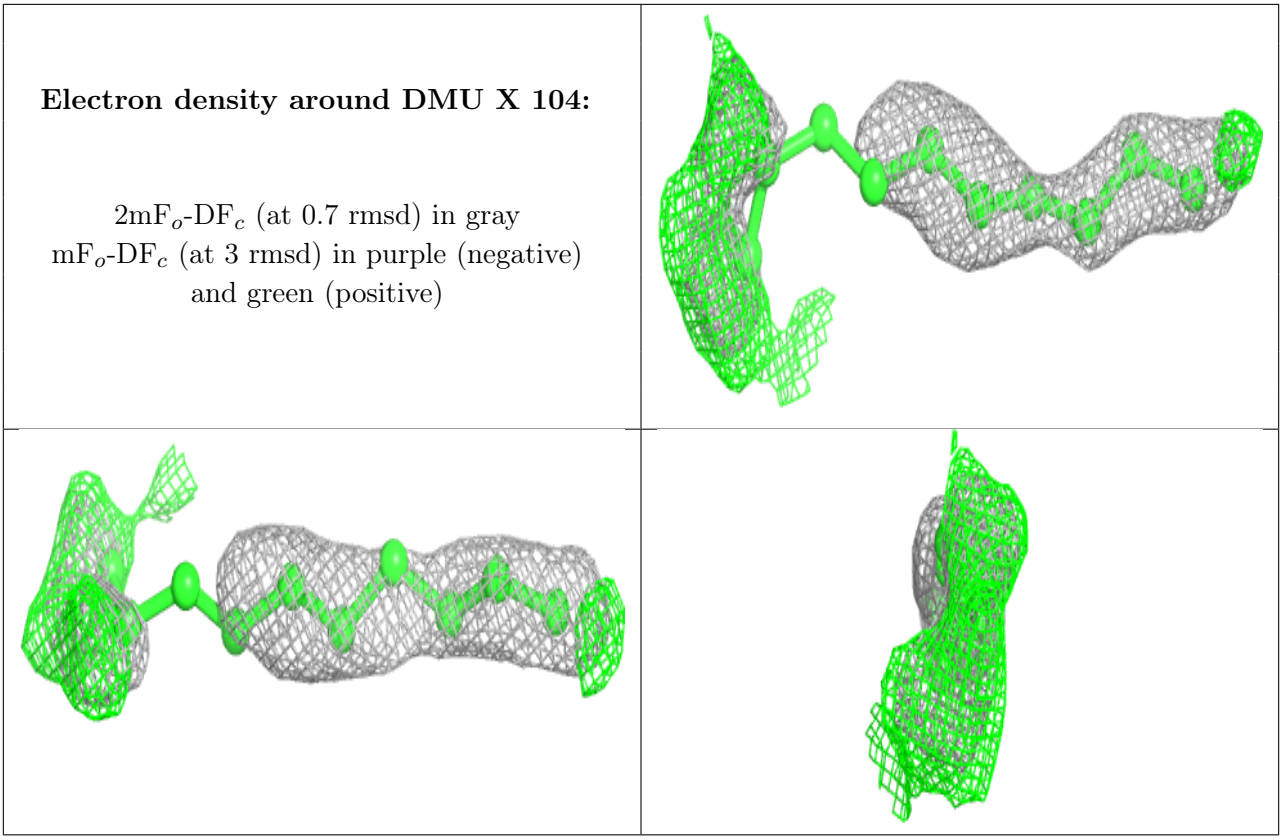






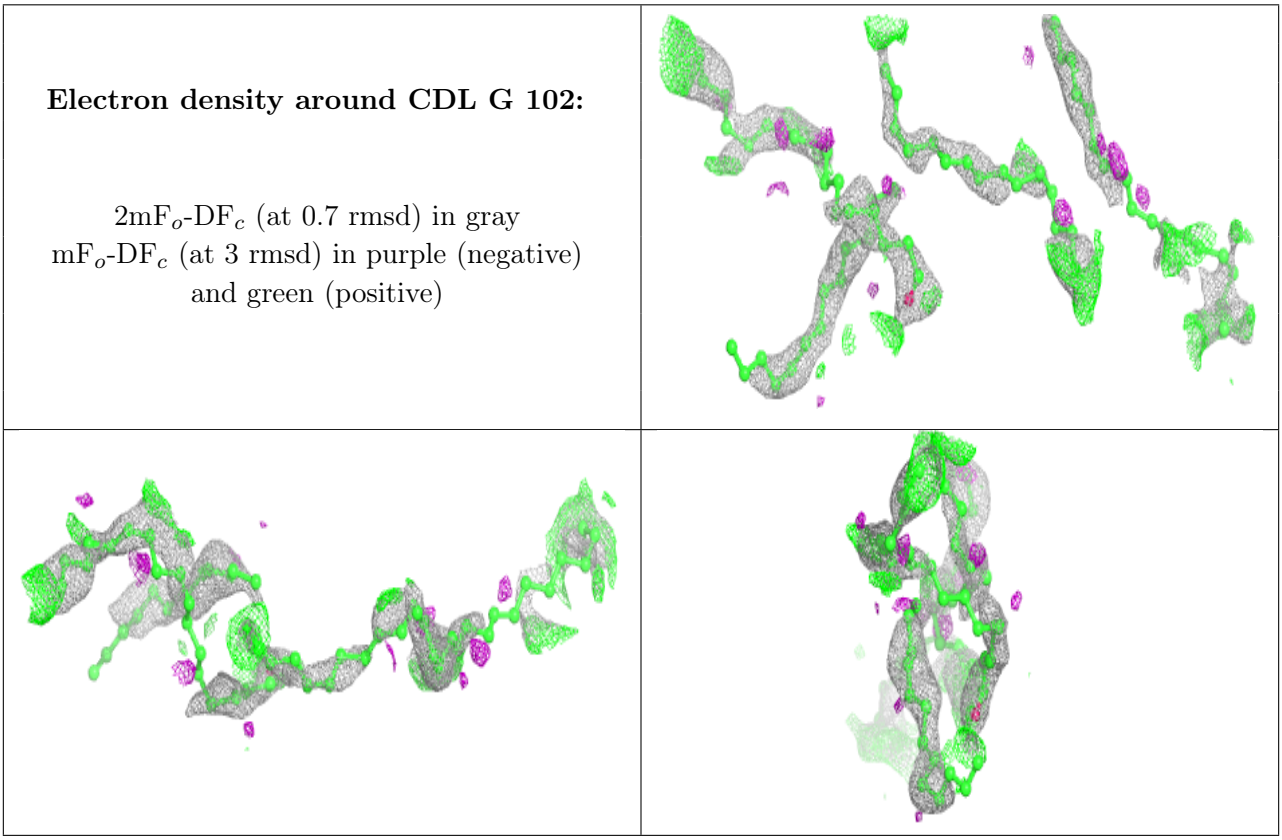
Electron density around DMU X 104:

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



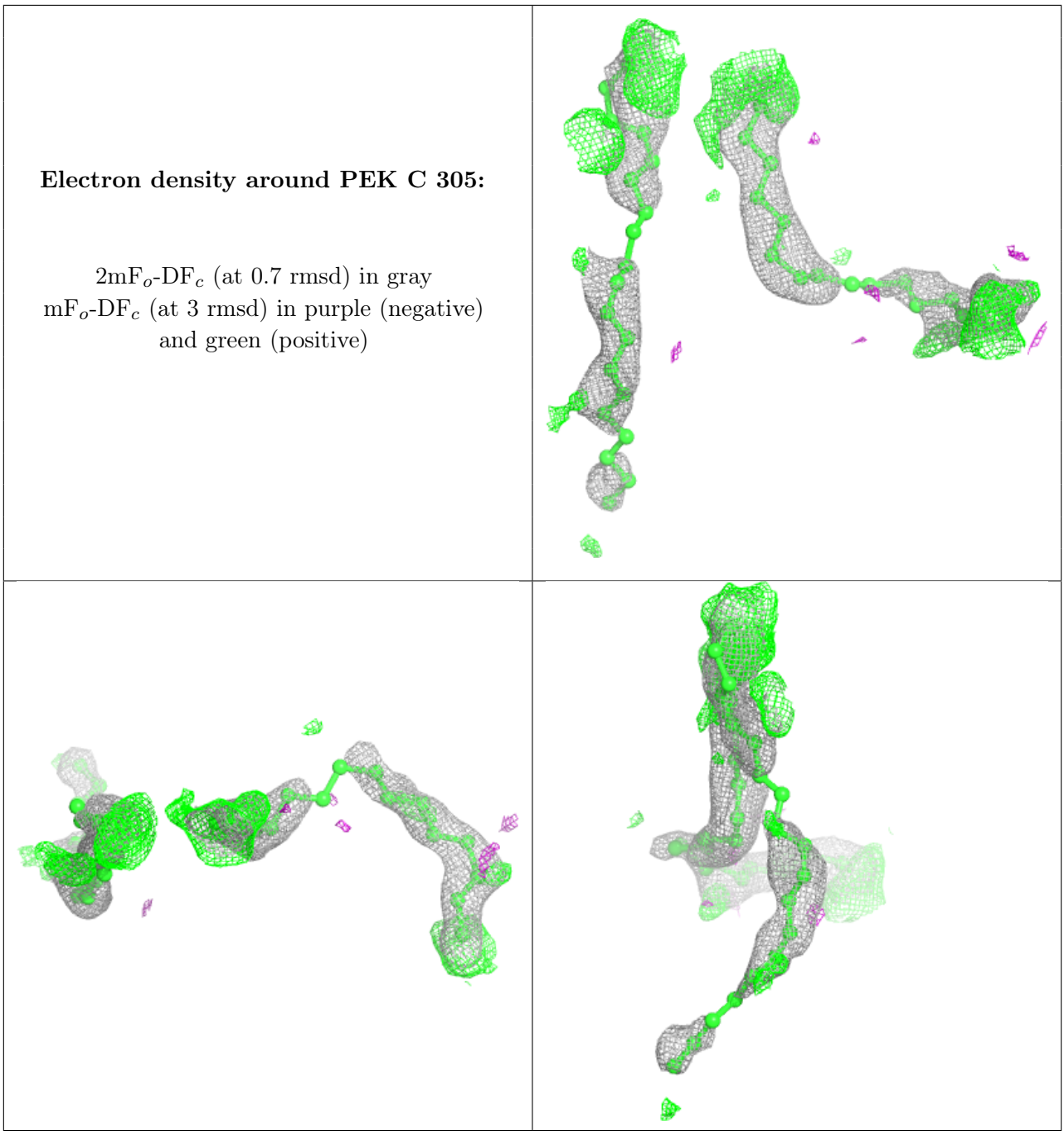
Electron density around CDL G 102:

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



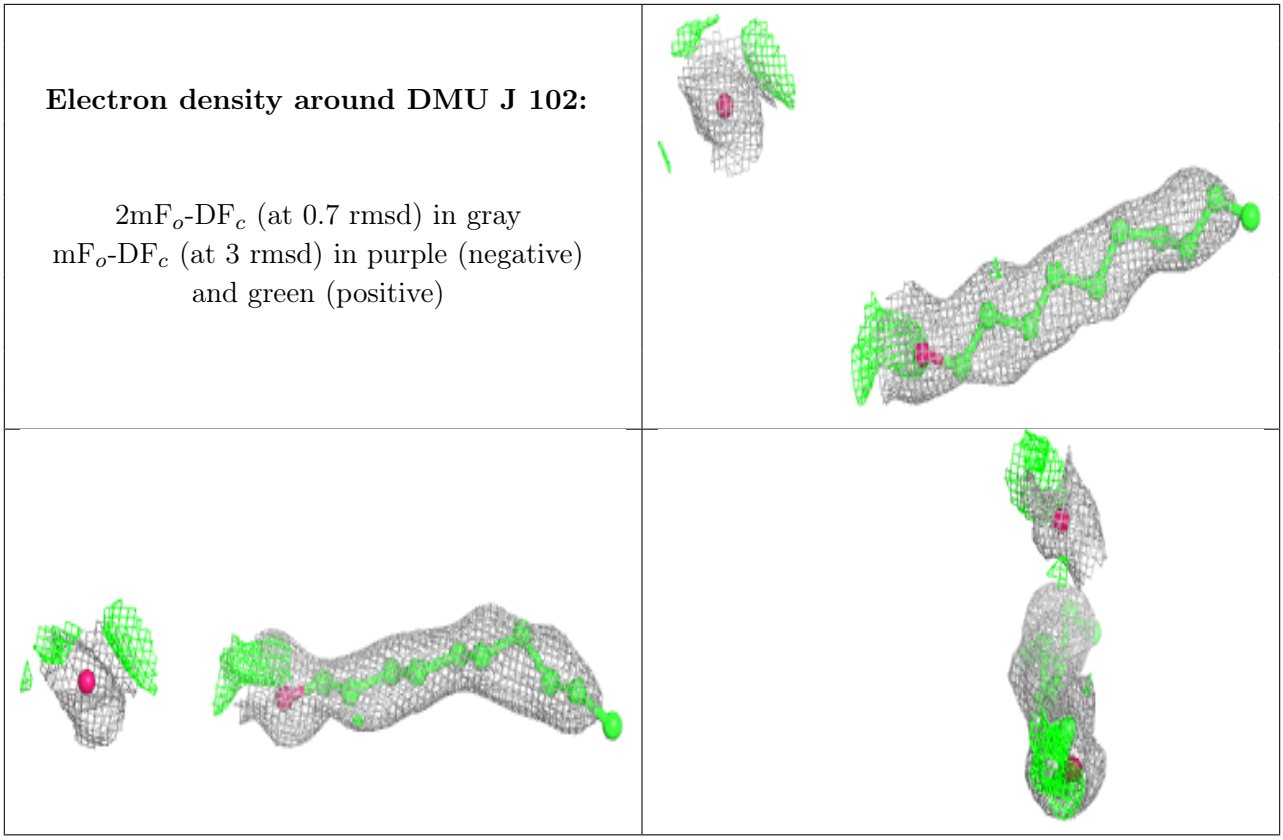
Electron density around PEK C 305:

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



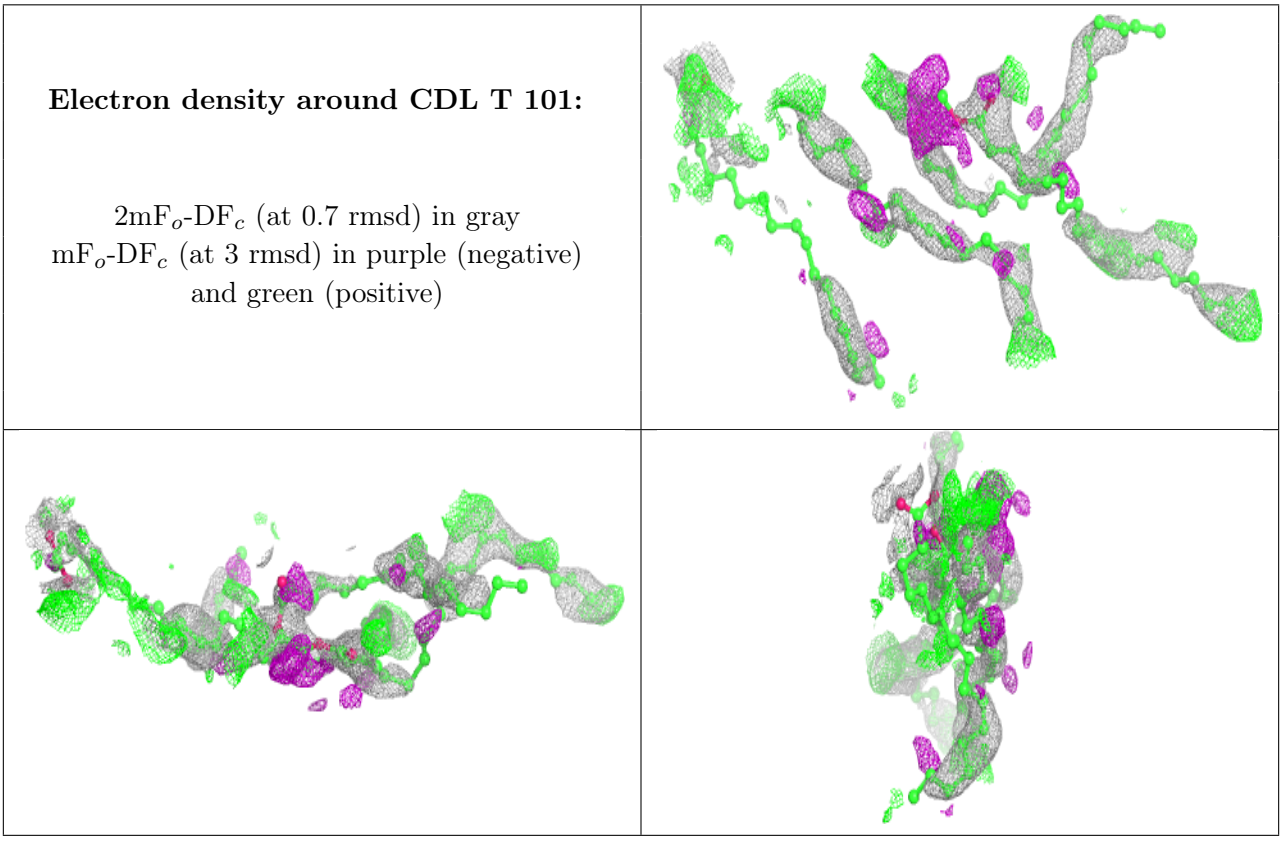
Electron density around DMU J 102:

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



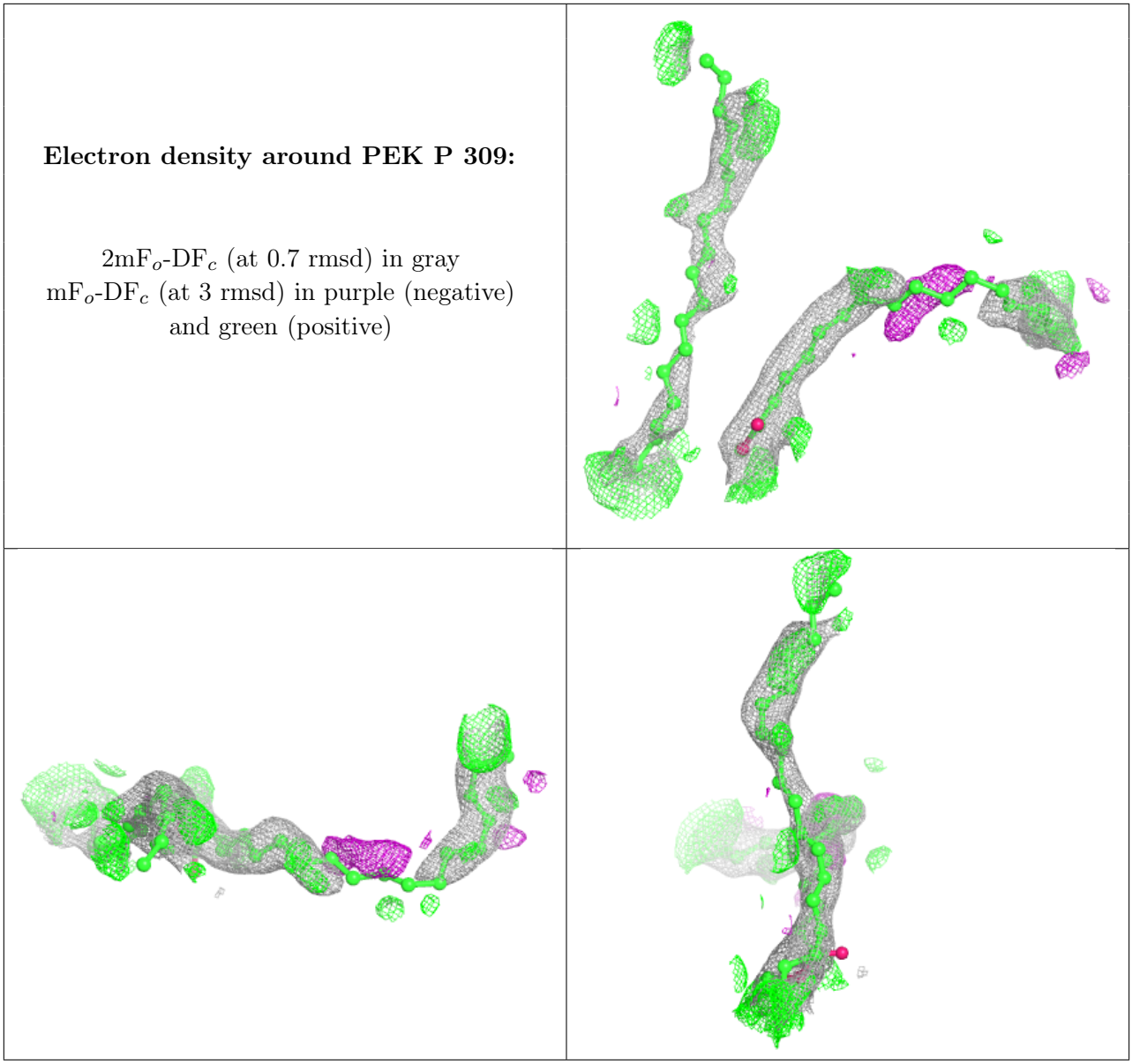
Electron density around CDL T 101:

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



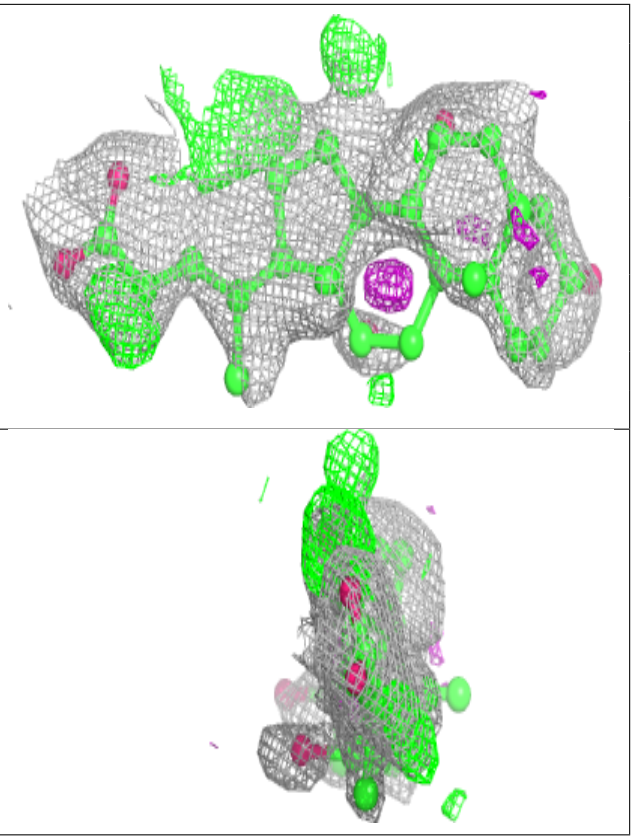
Electron density around PEK P 309:

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



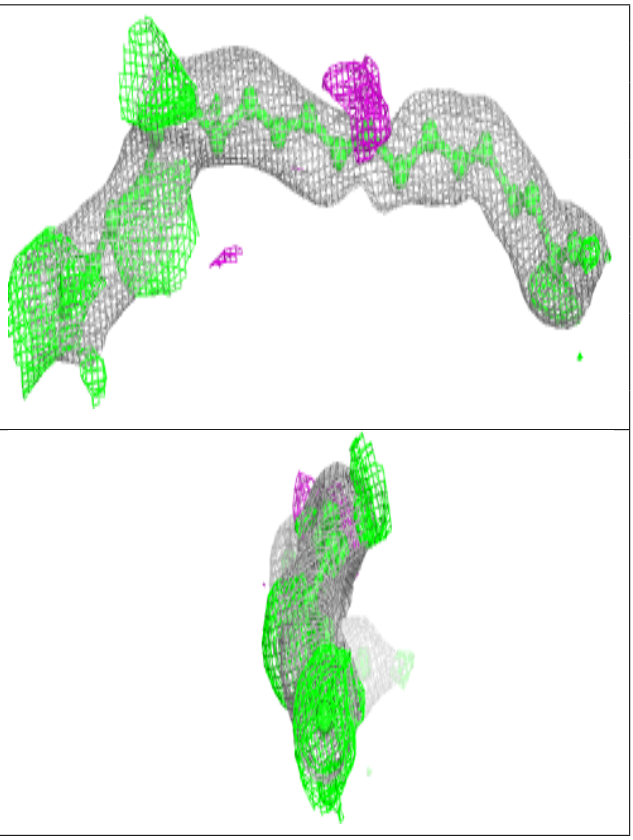
Electron density around CHD P 306:

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



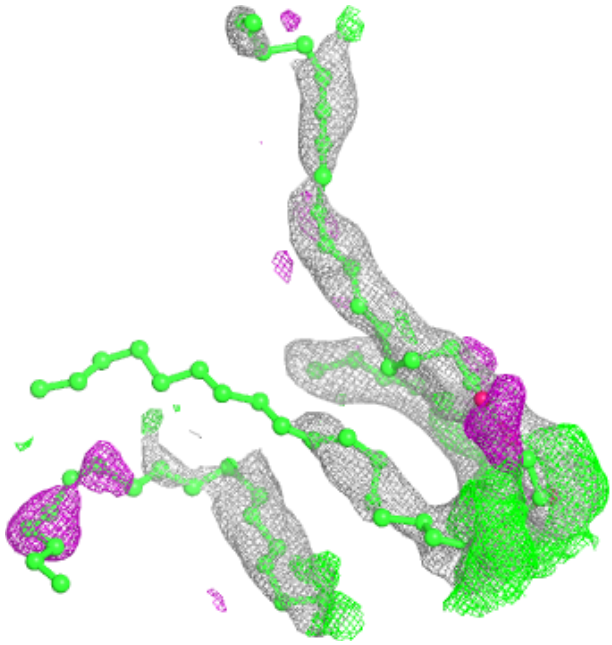
Electron density around PEK P 301:

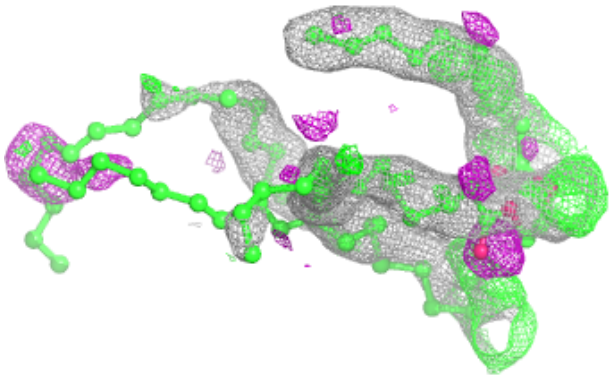
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

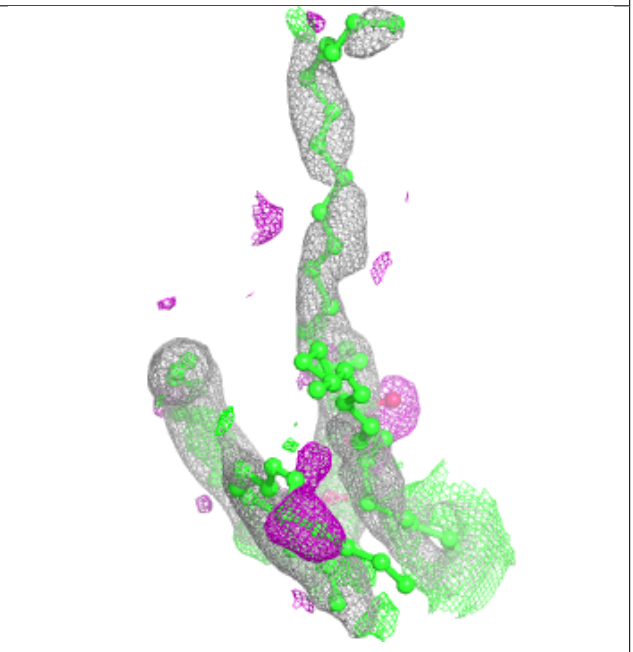


Electron density around CDL P 305:

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

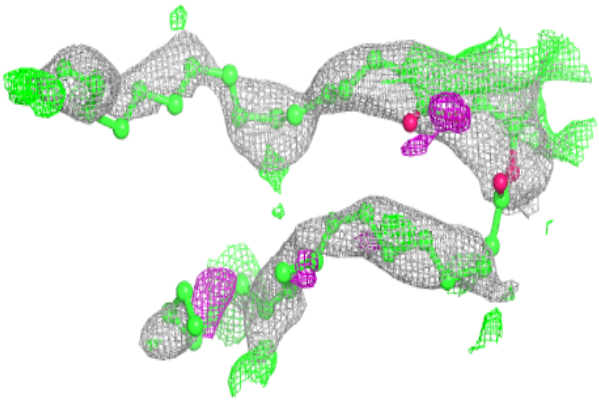


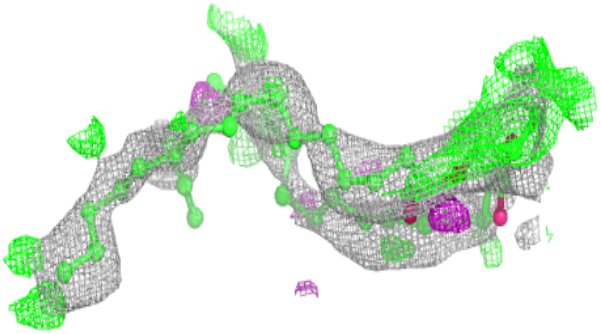


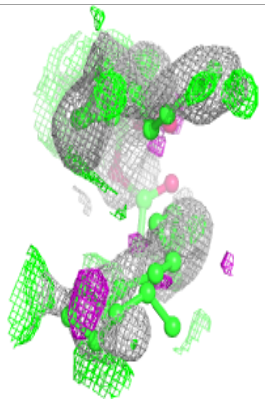


Electron density around PGV P 302:

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

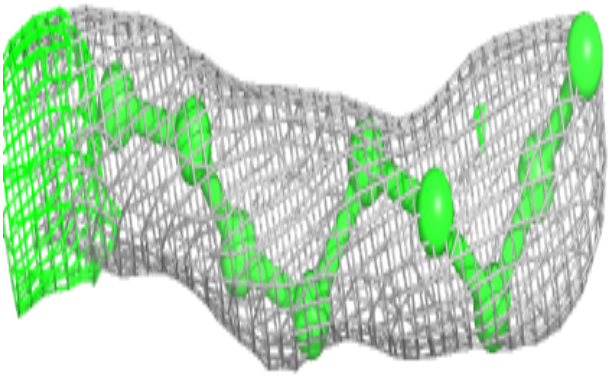


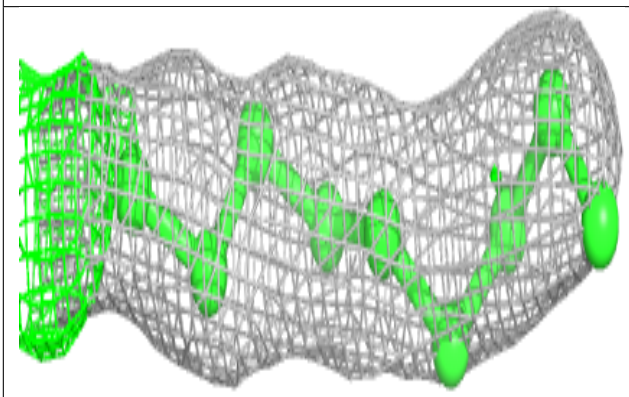


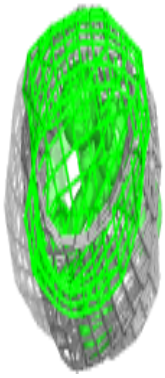


Electron density around DMU W 101:

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

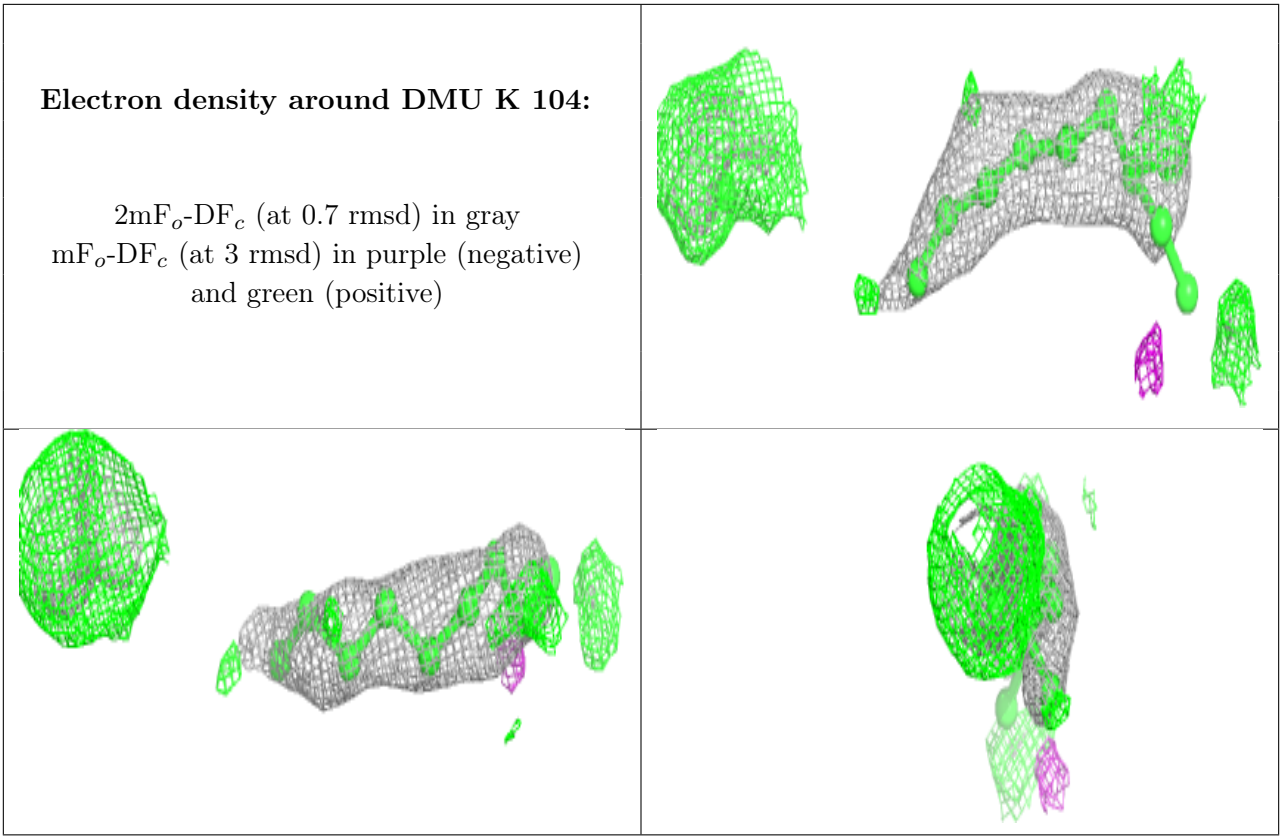






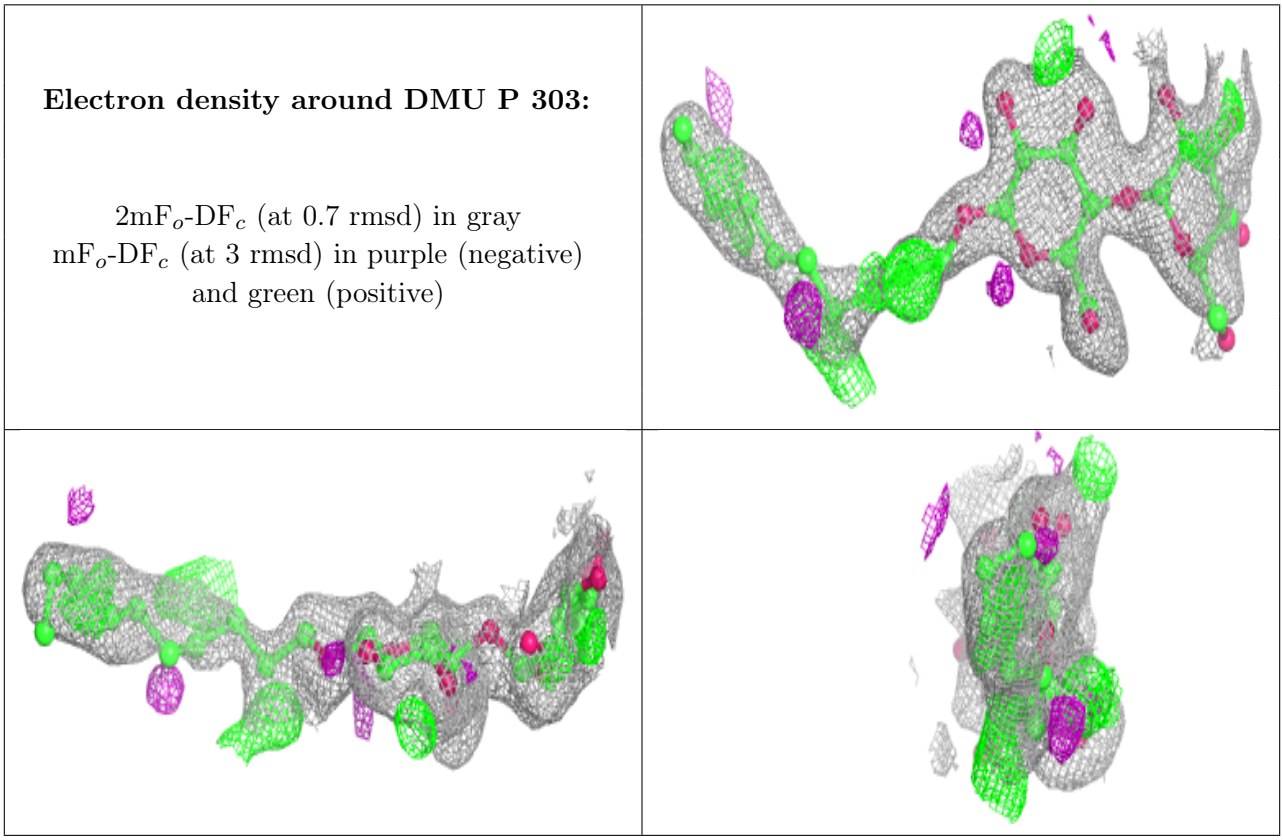
Electron density around DMU K 104:

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



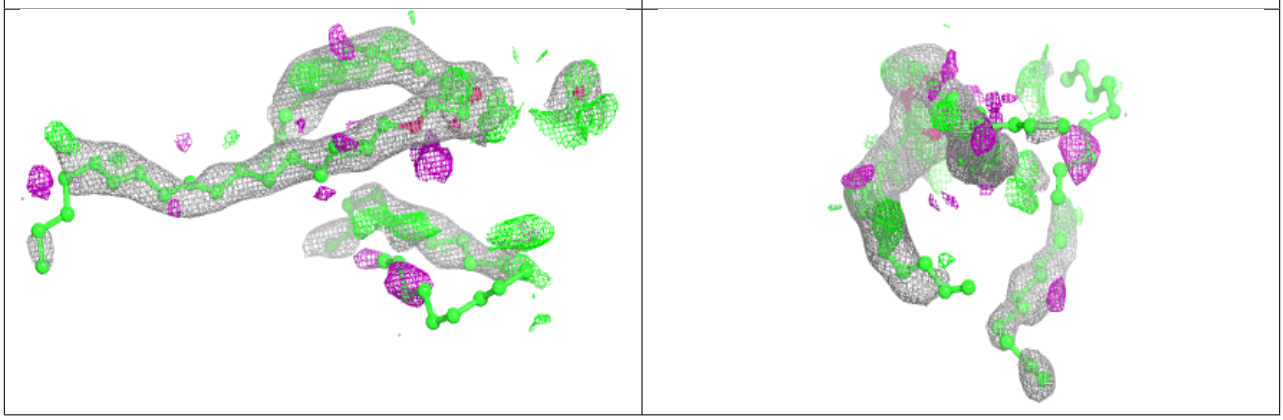
Electron density around DMU P 303:

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



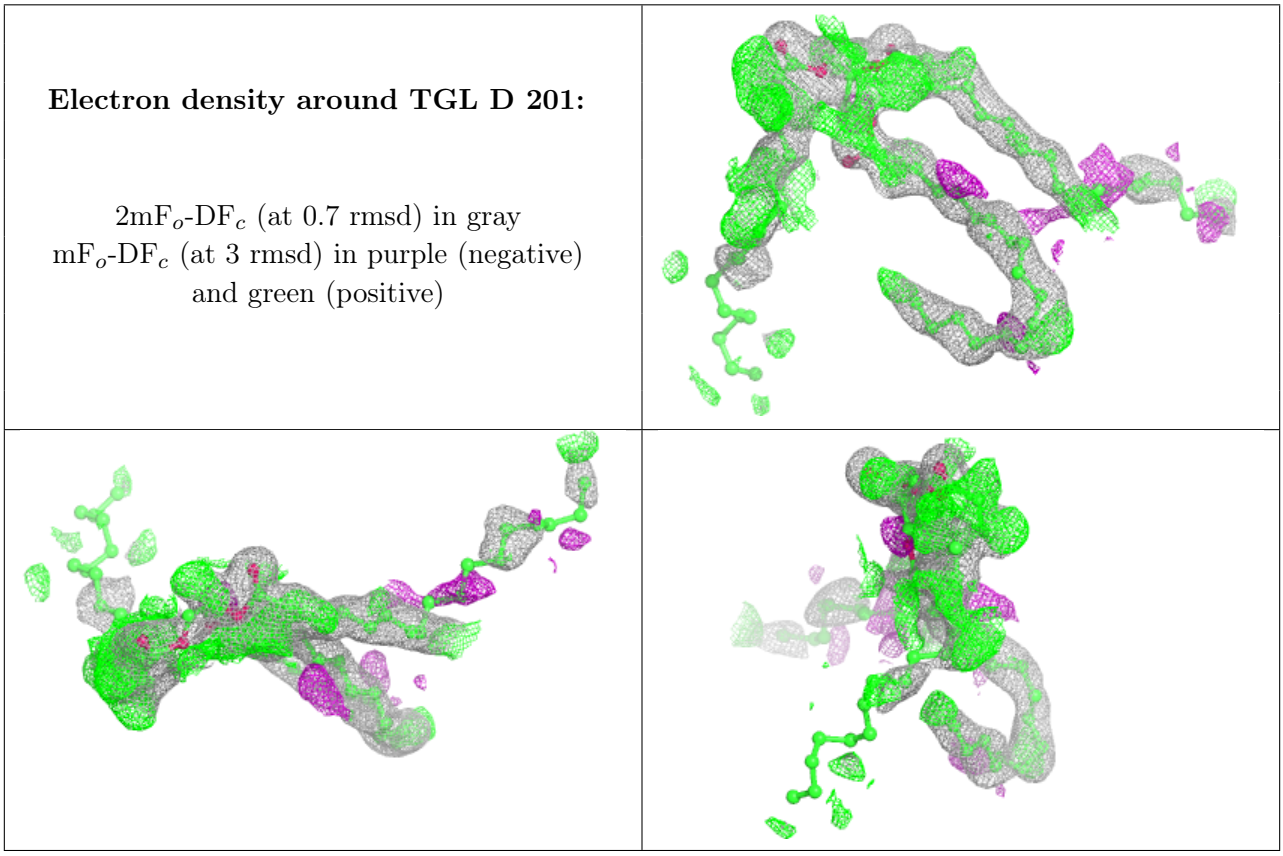
Electron density around CDL C 303:

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



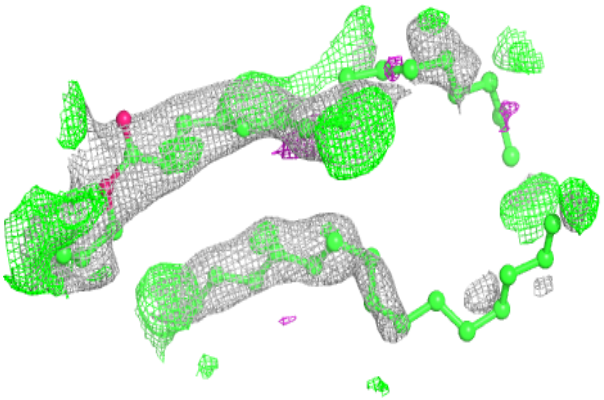
Electron density around TGL D 201:

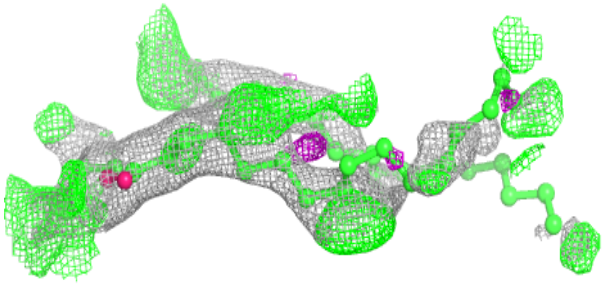
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around PGV C 306:

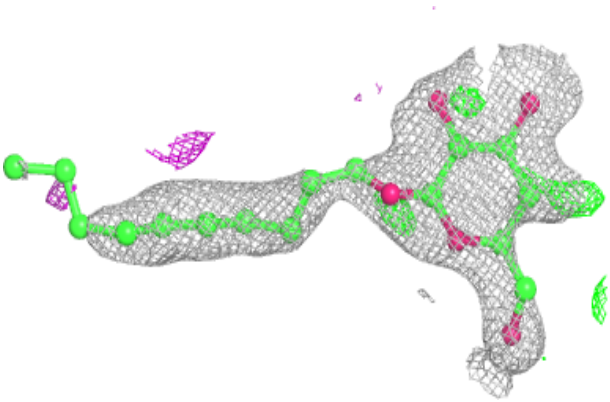
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

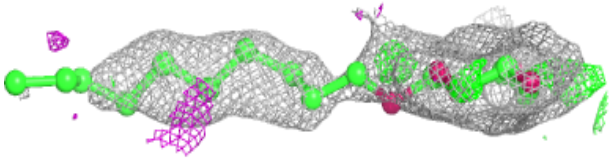


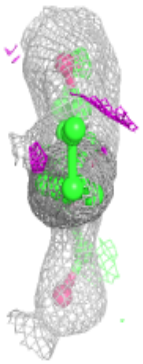


Electron density around DMU L 102:

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

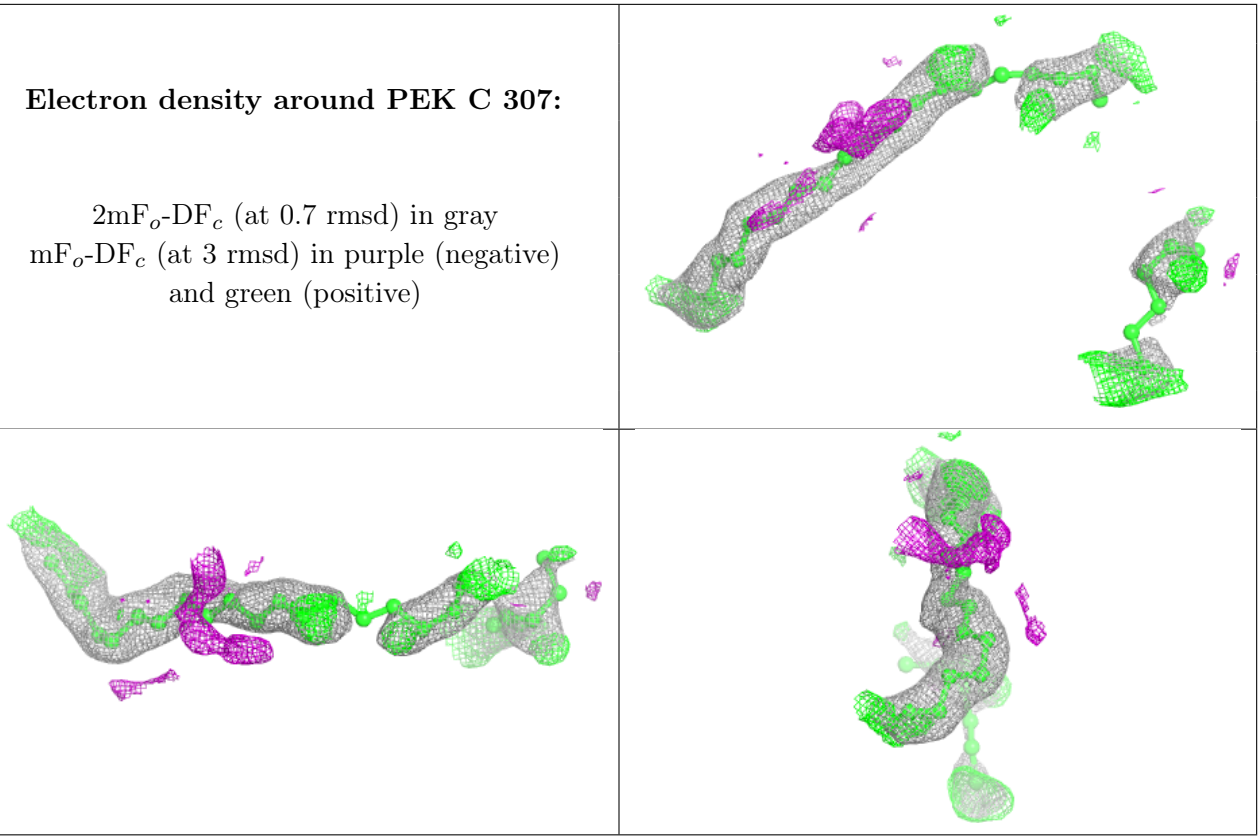






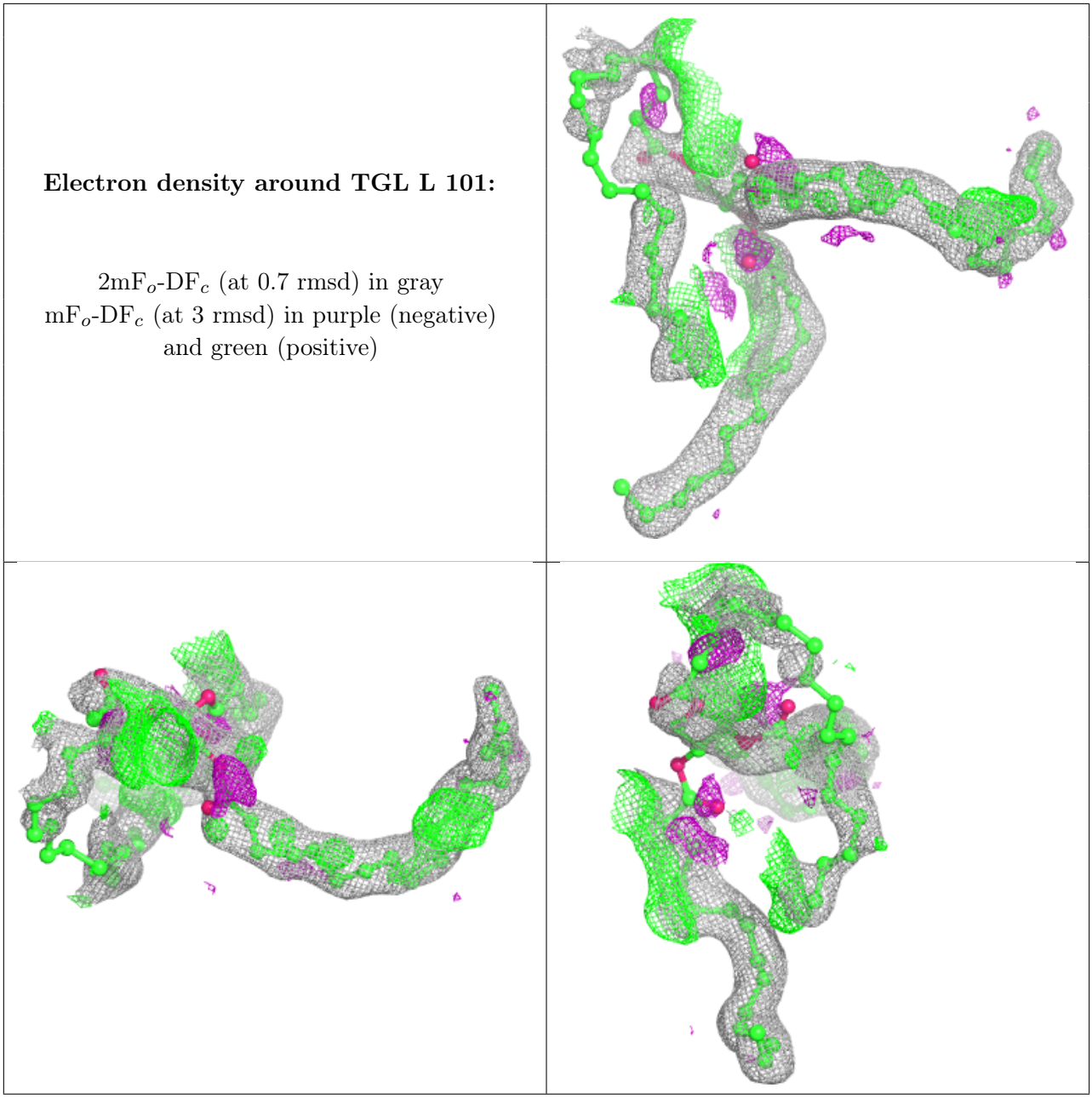
Electron density around PEK C 307:

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



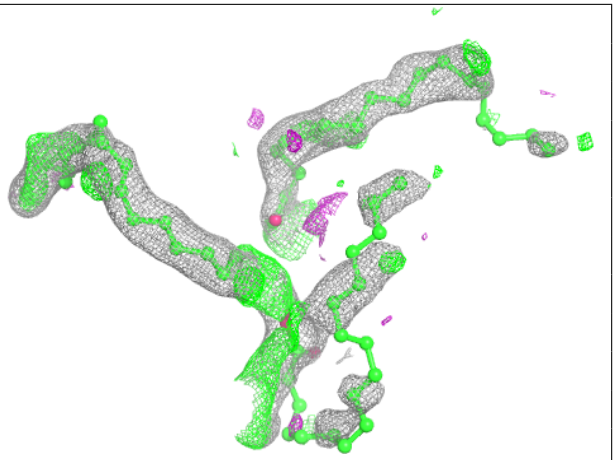
Electron density around TGL L 101:

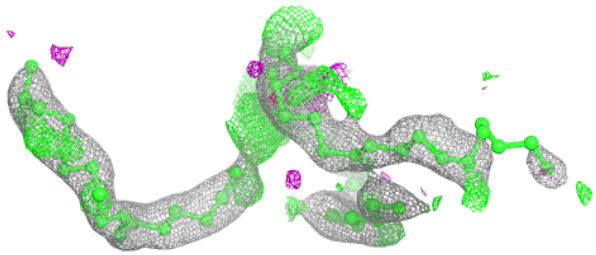
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

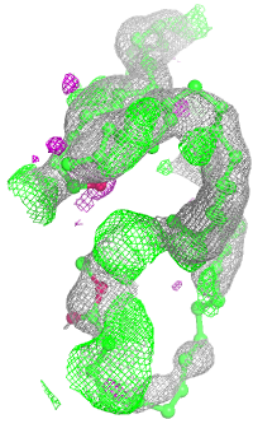


Electron density around TGL N 608:

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

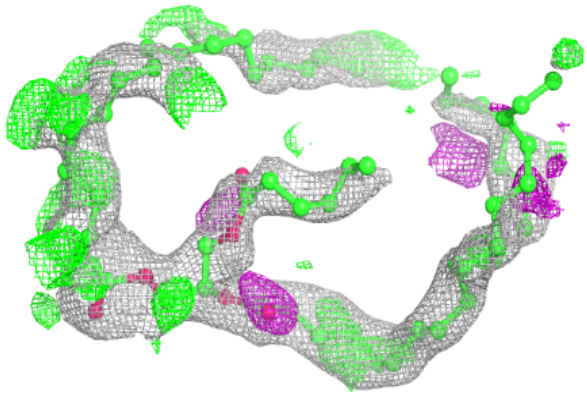


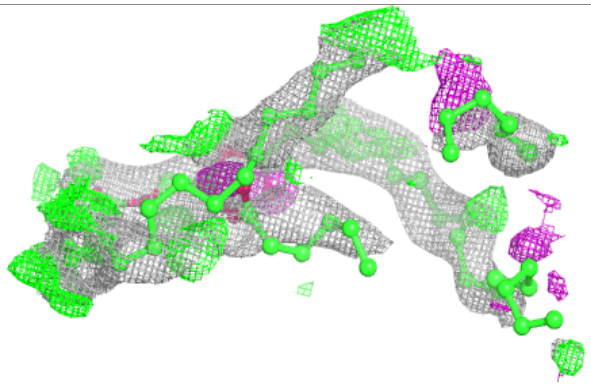


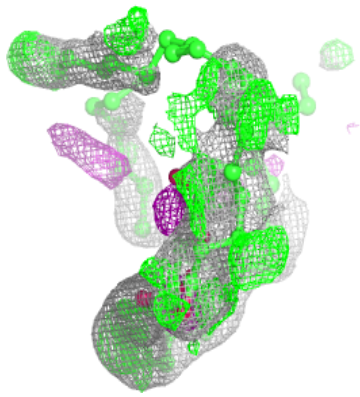


Electron density around TGL O 301:

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

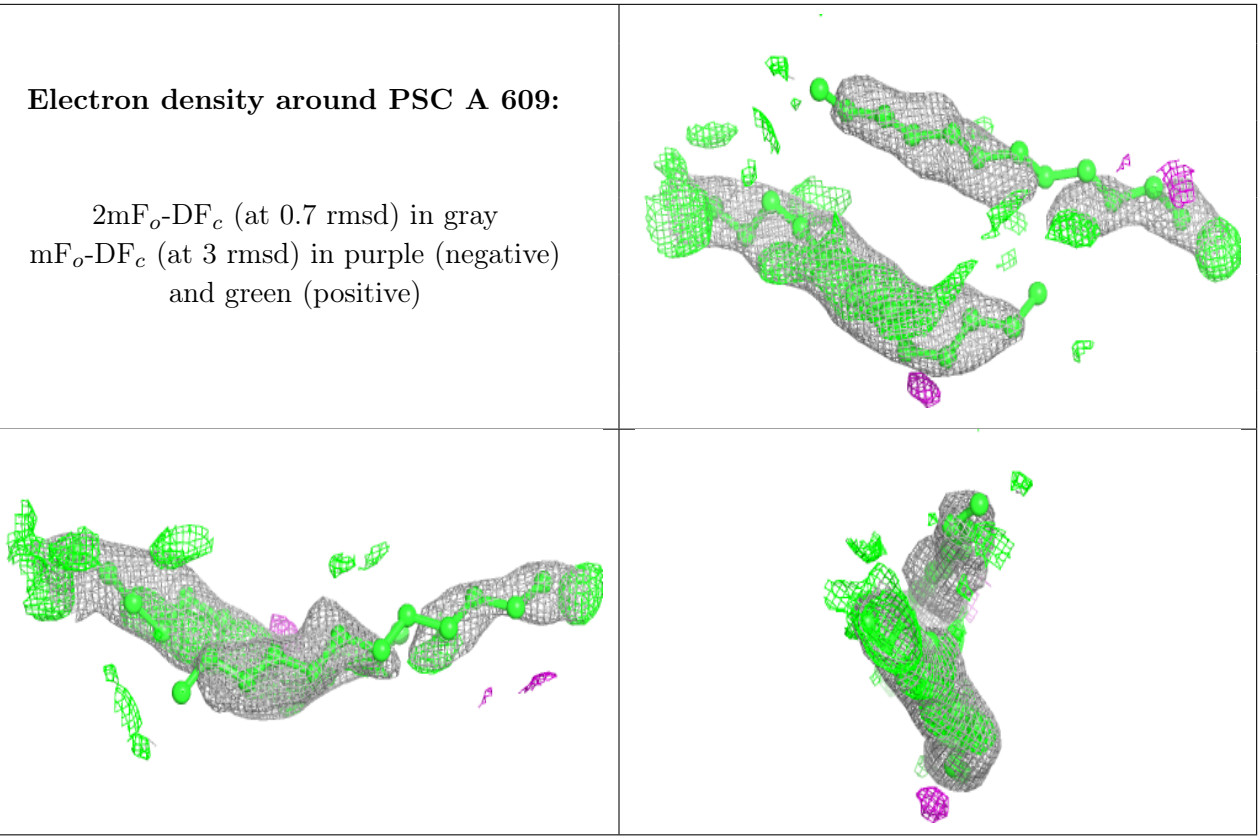






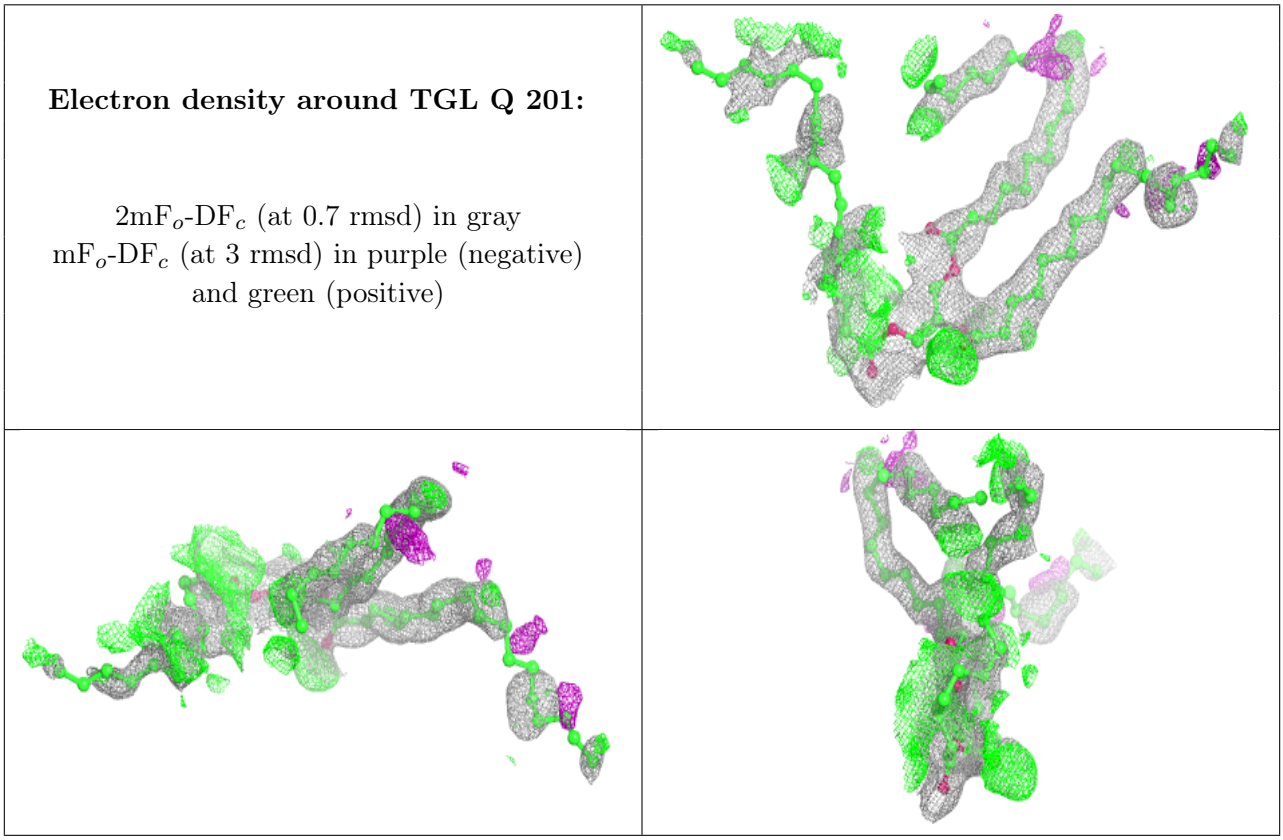
Electron density around PSC A 609:

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



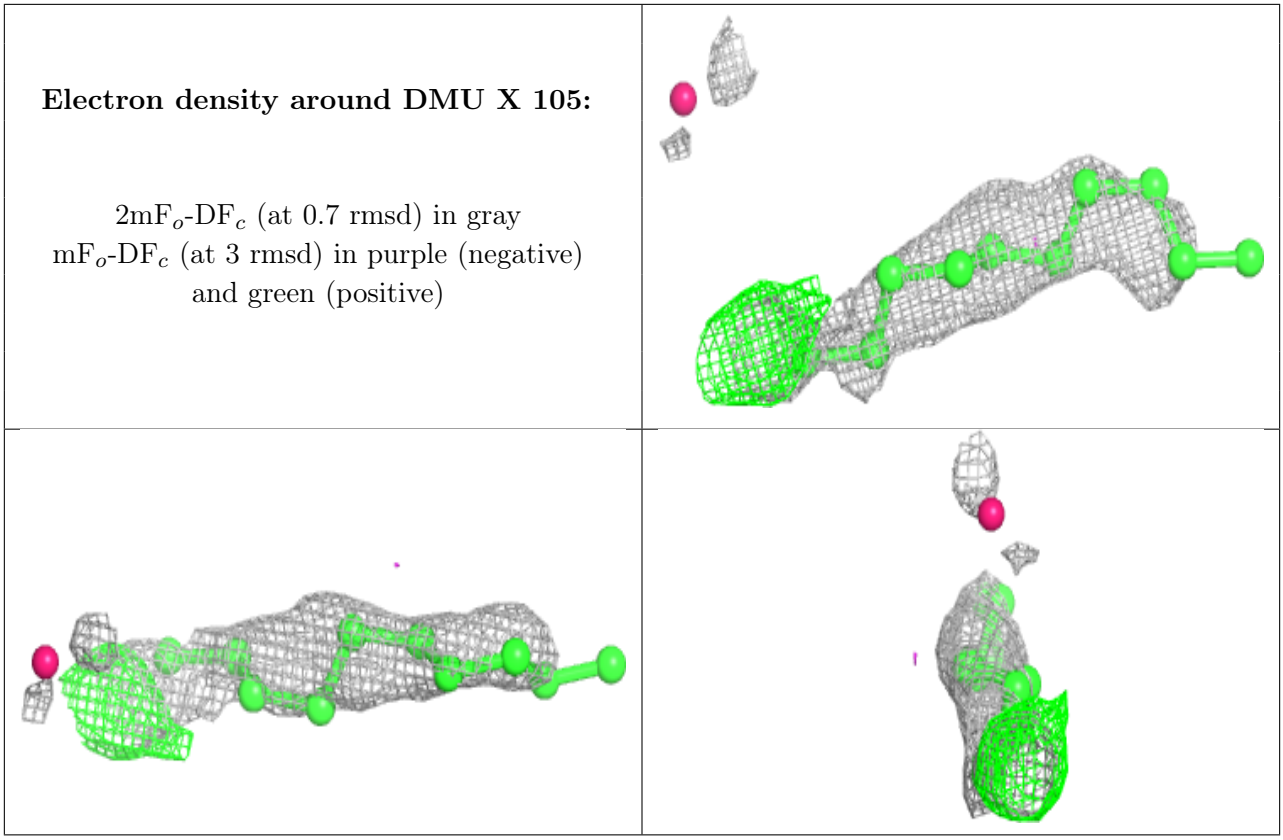
Electron density around TGL Q 201:

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



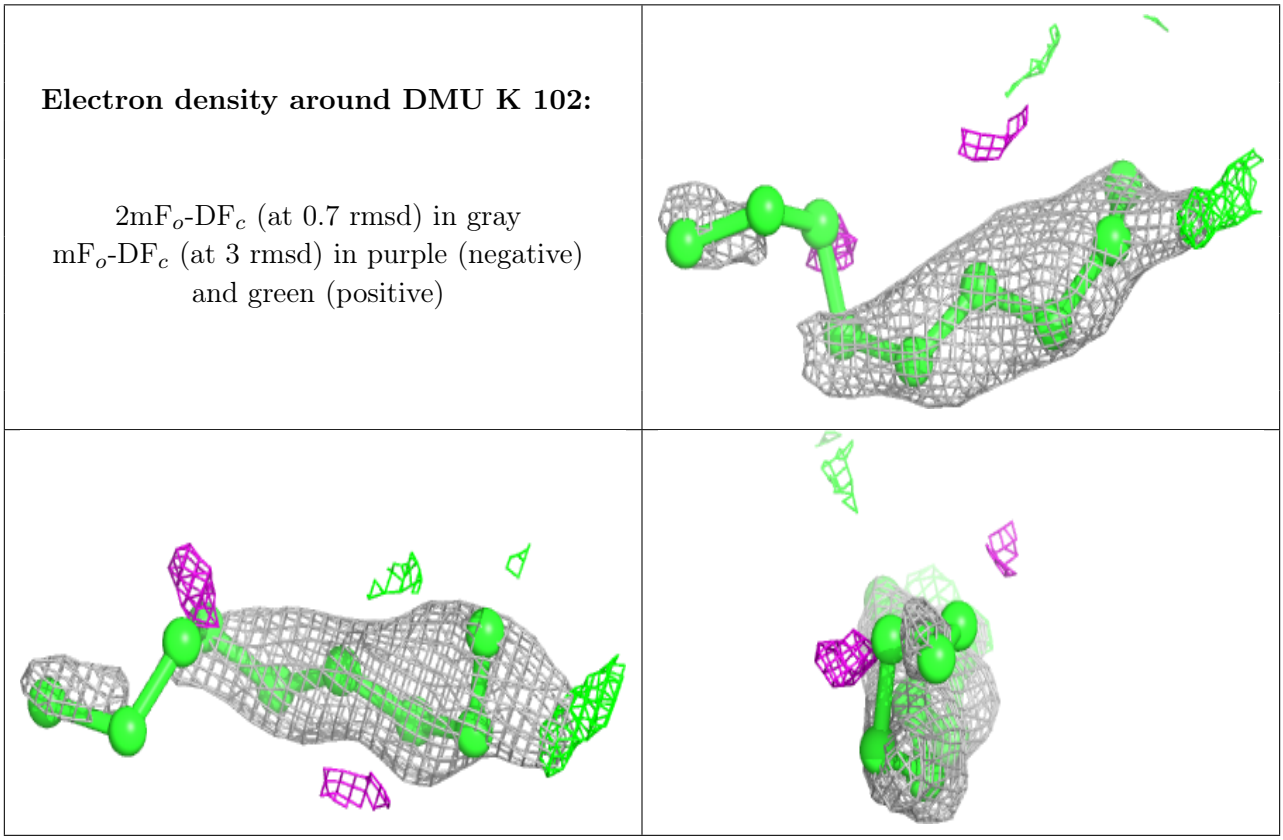
Electron density around DMU X 105:

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



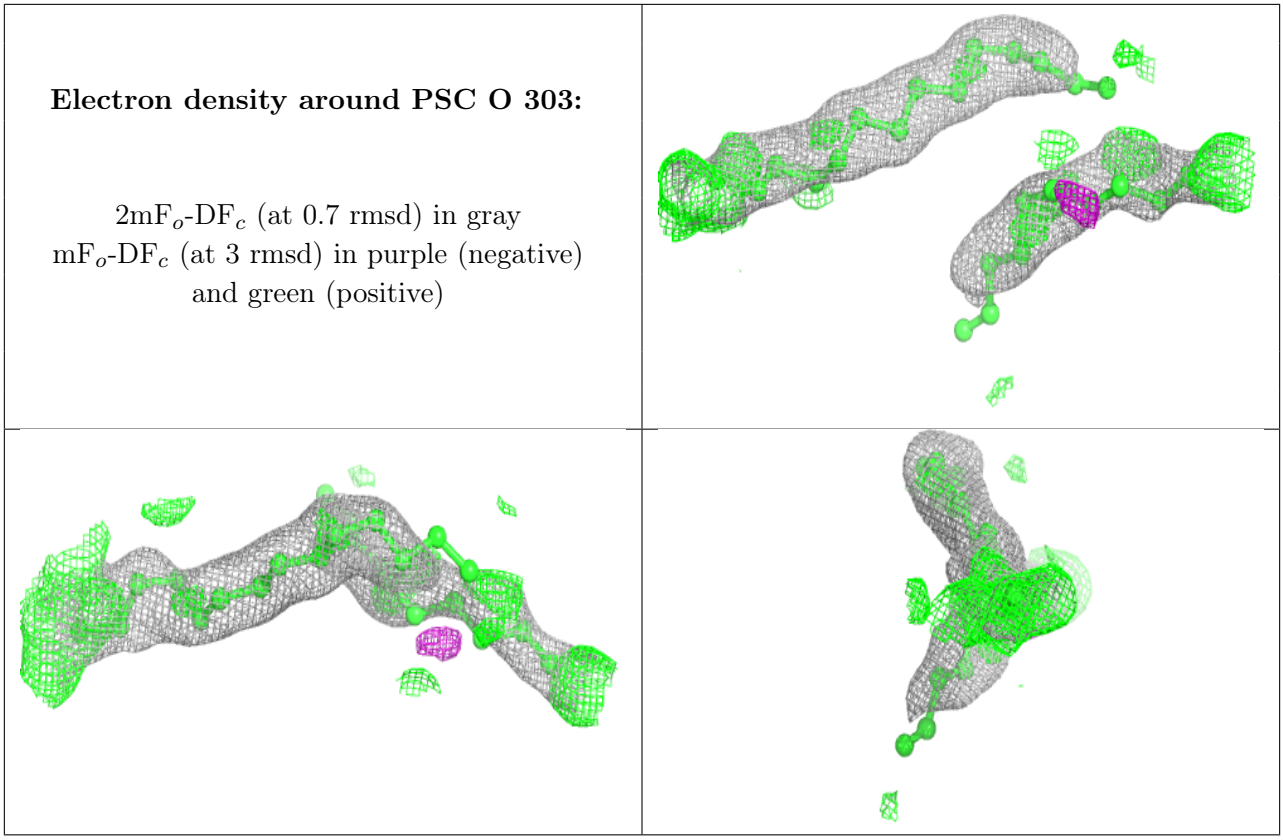
Electron density around DMU K 102:

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



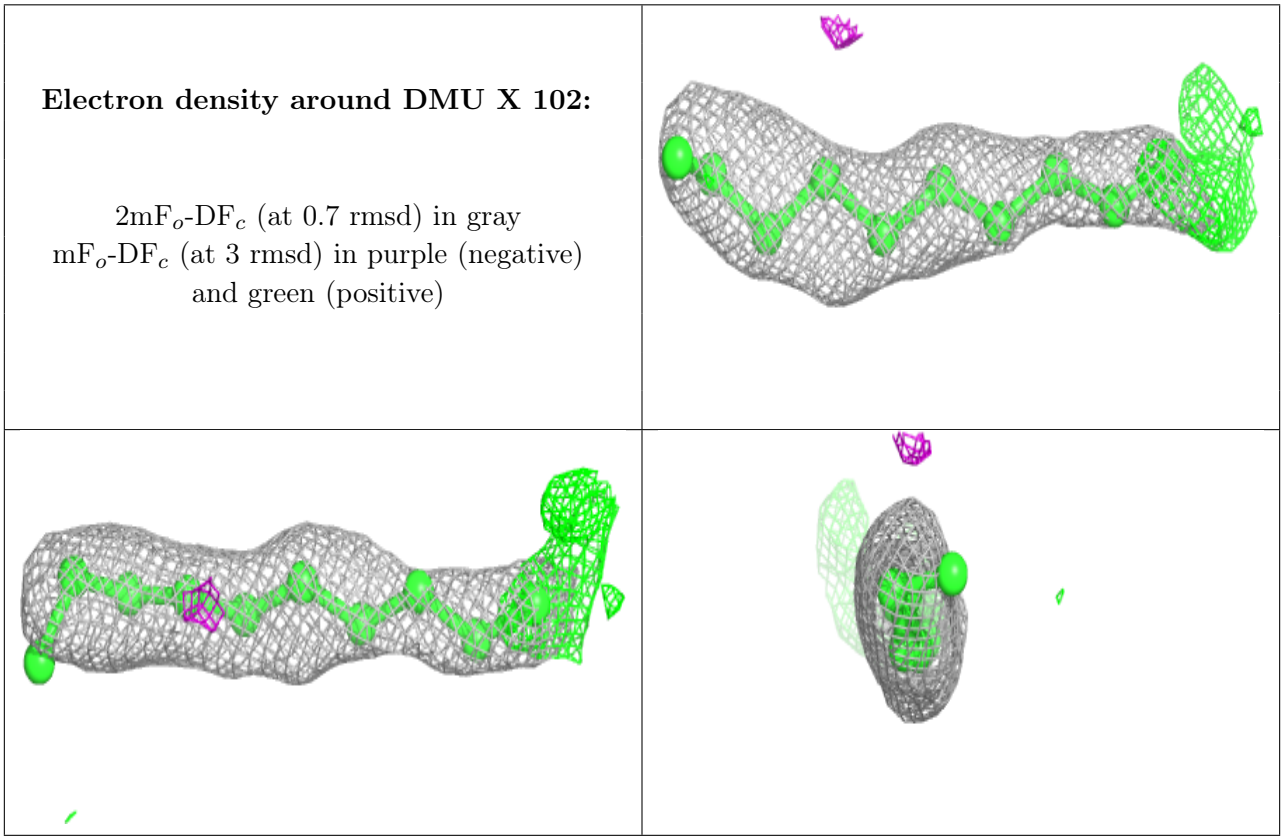
Electron density around PSC O 303:

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



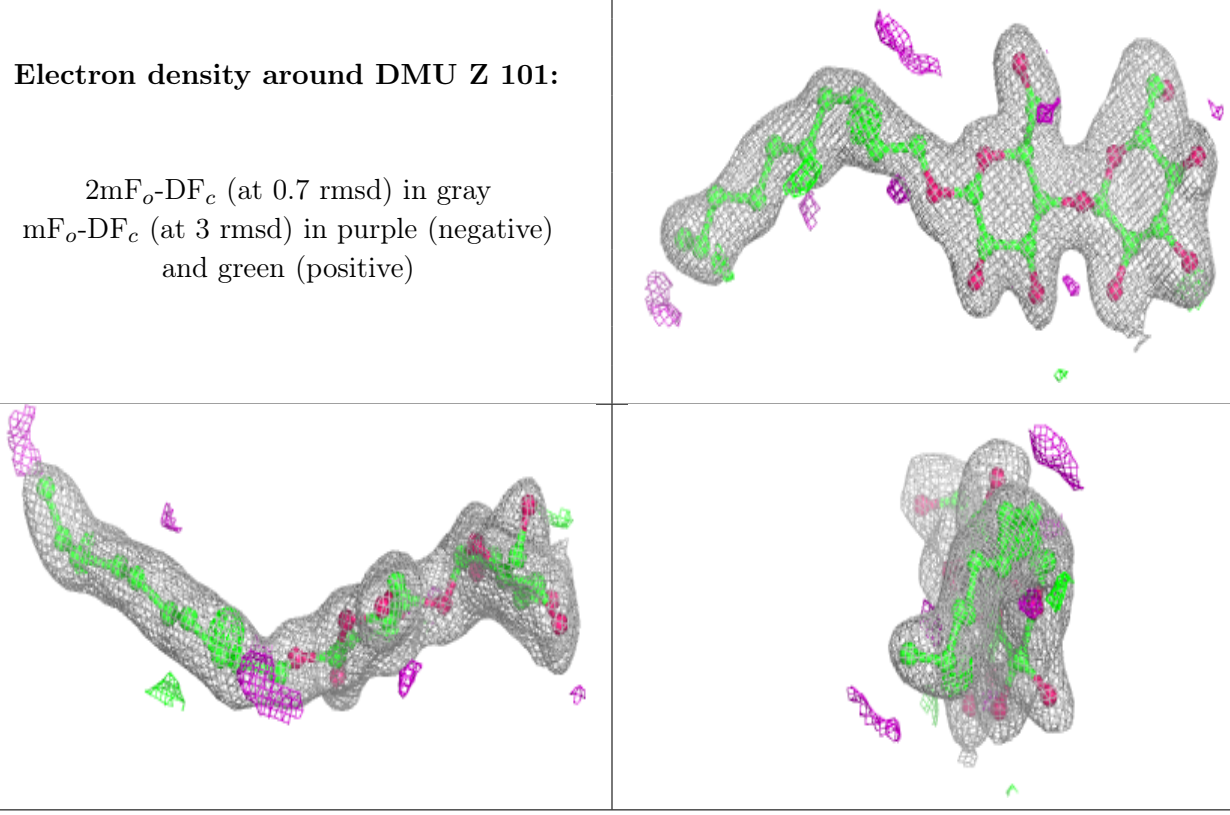
Electron density around DMU X 102:

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



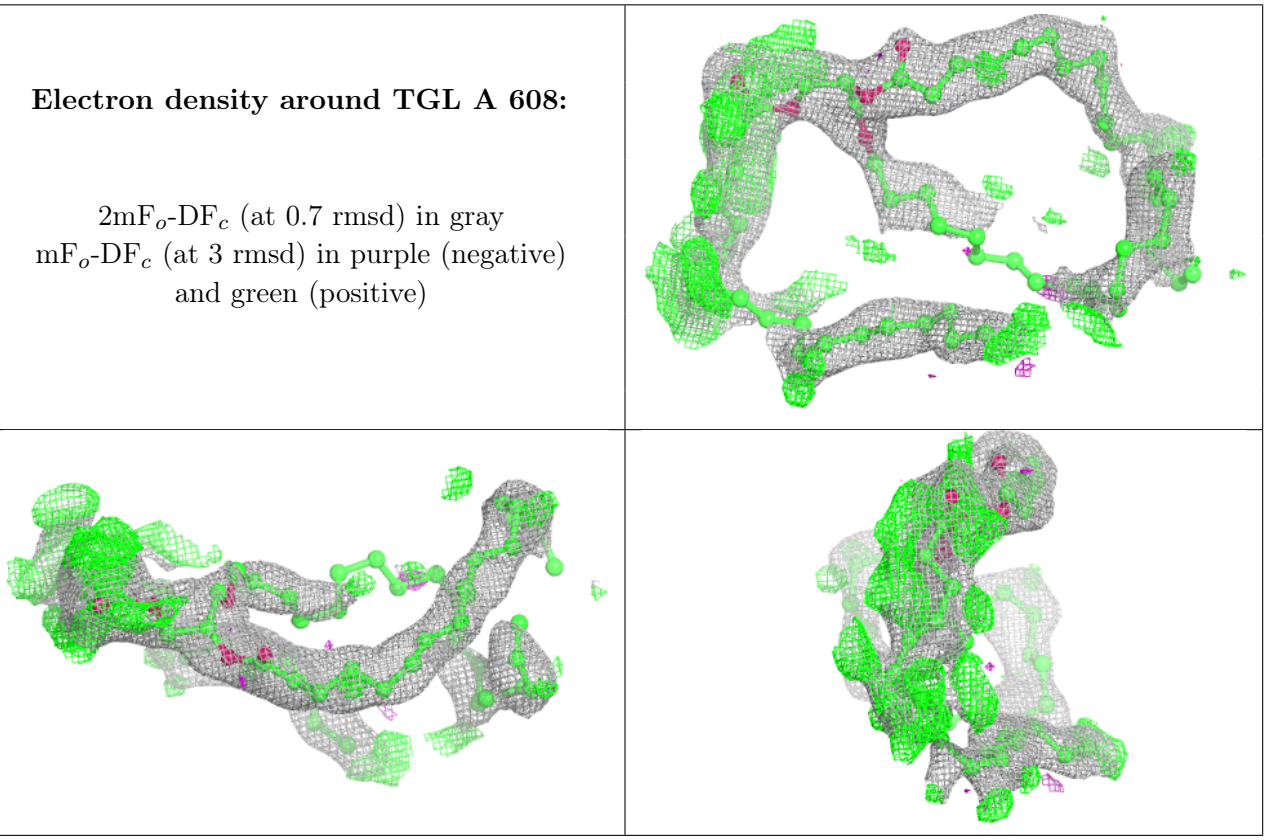
Electron density around DMU Z 101:

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



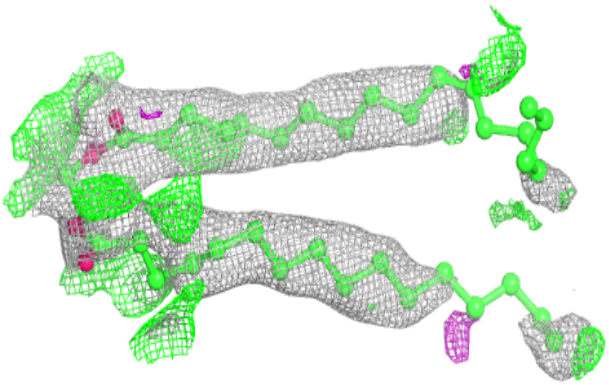
Electron density around TGL A 608:

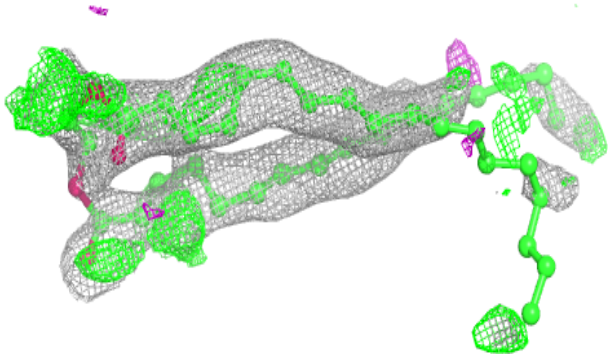
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

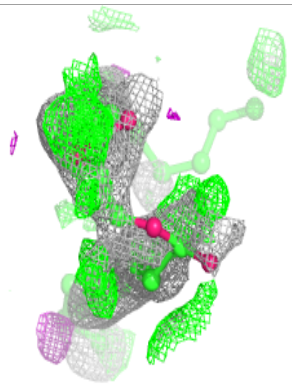


Electron density around PGV N 606:

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

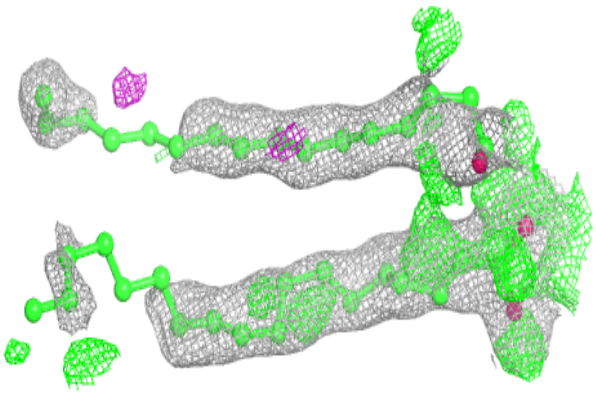


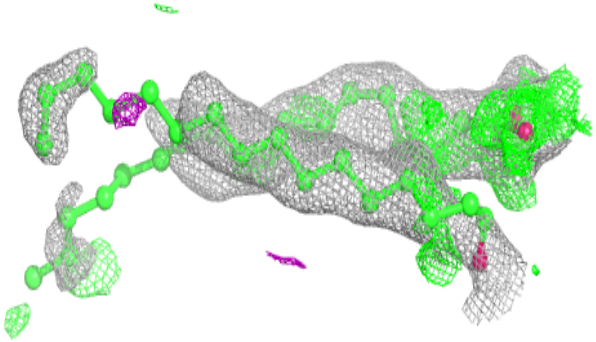


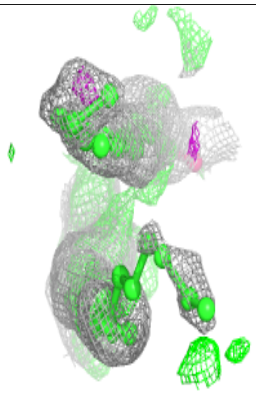


Electron density around PGV A 607:

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

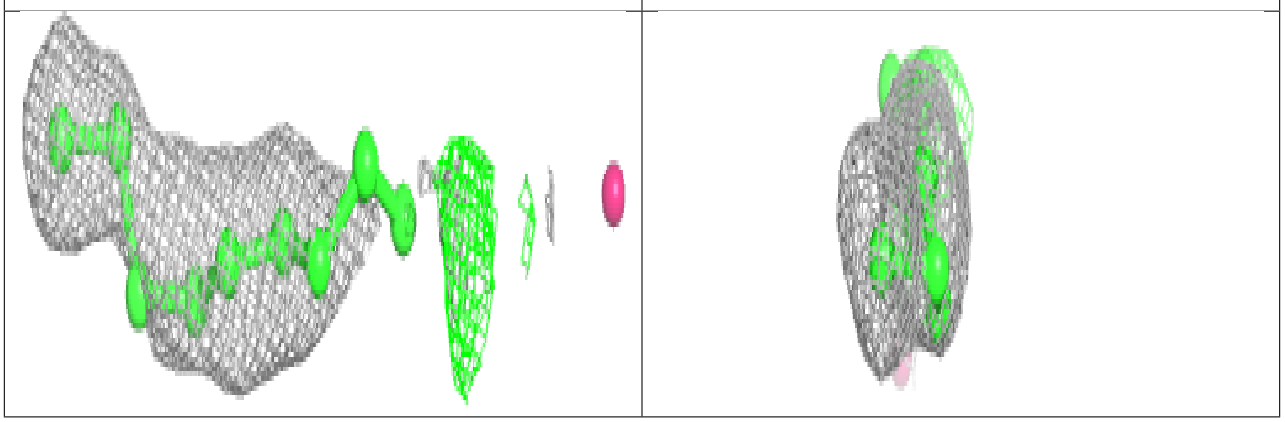






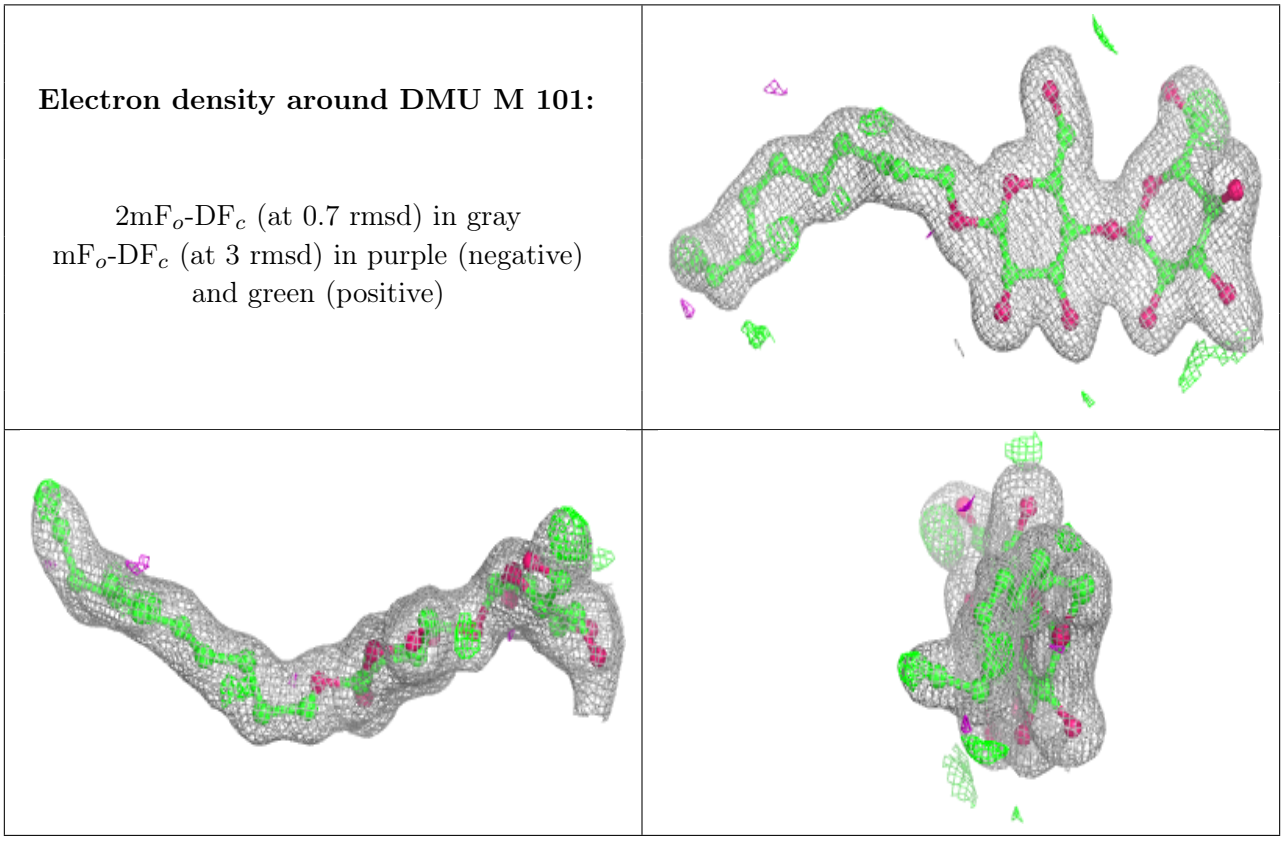
Electron density around DMU K 101:

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



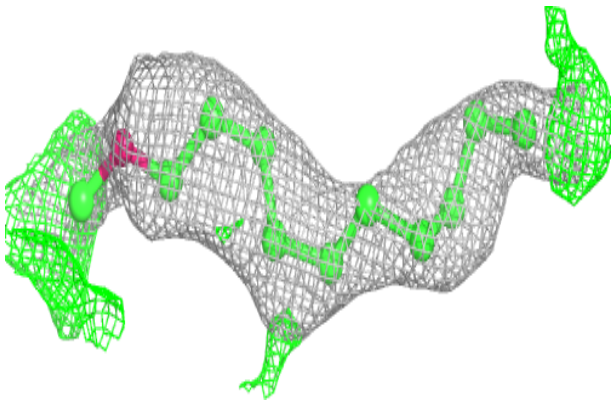
Electron density around DMU M 101:

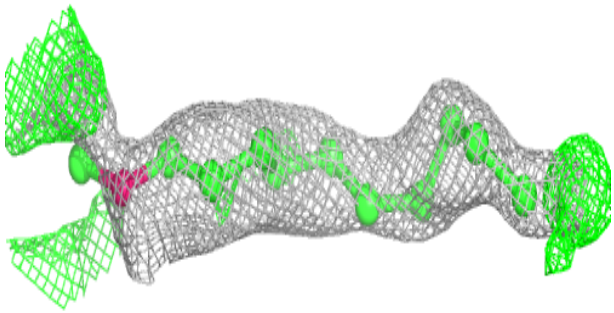
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

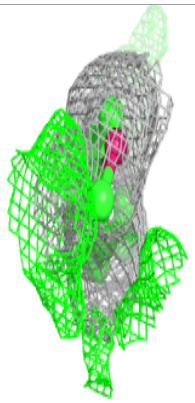


Electron density around DMU D 202:

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

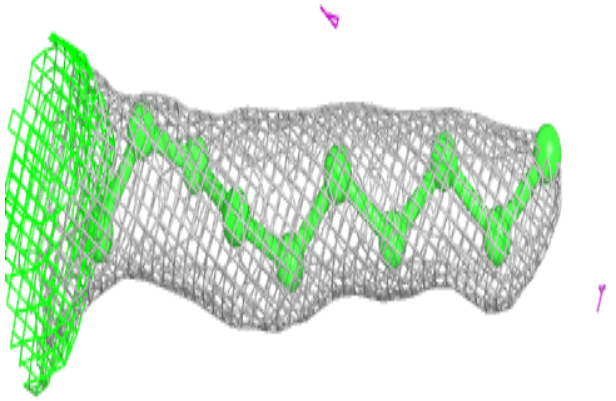


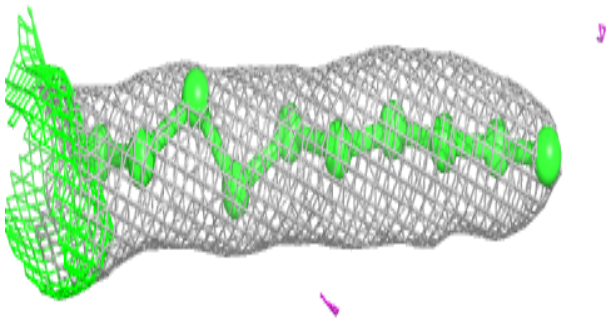


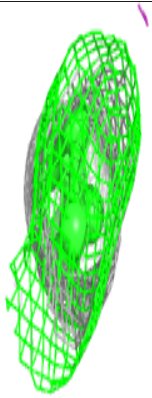


Electron density around DMU O 304:

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

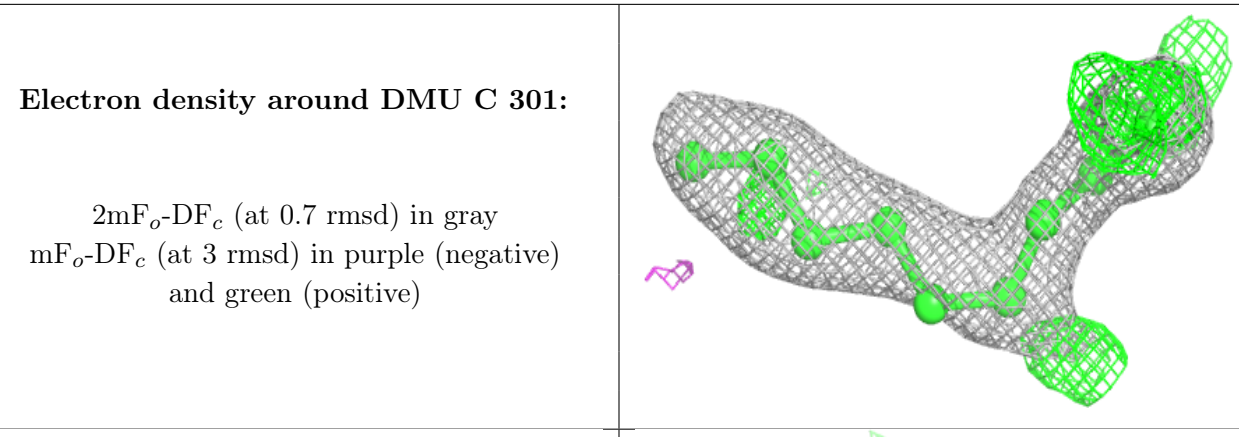






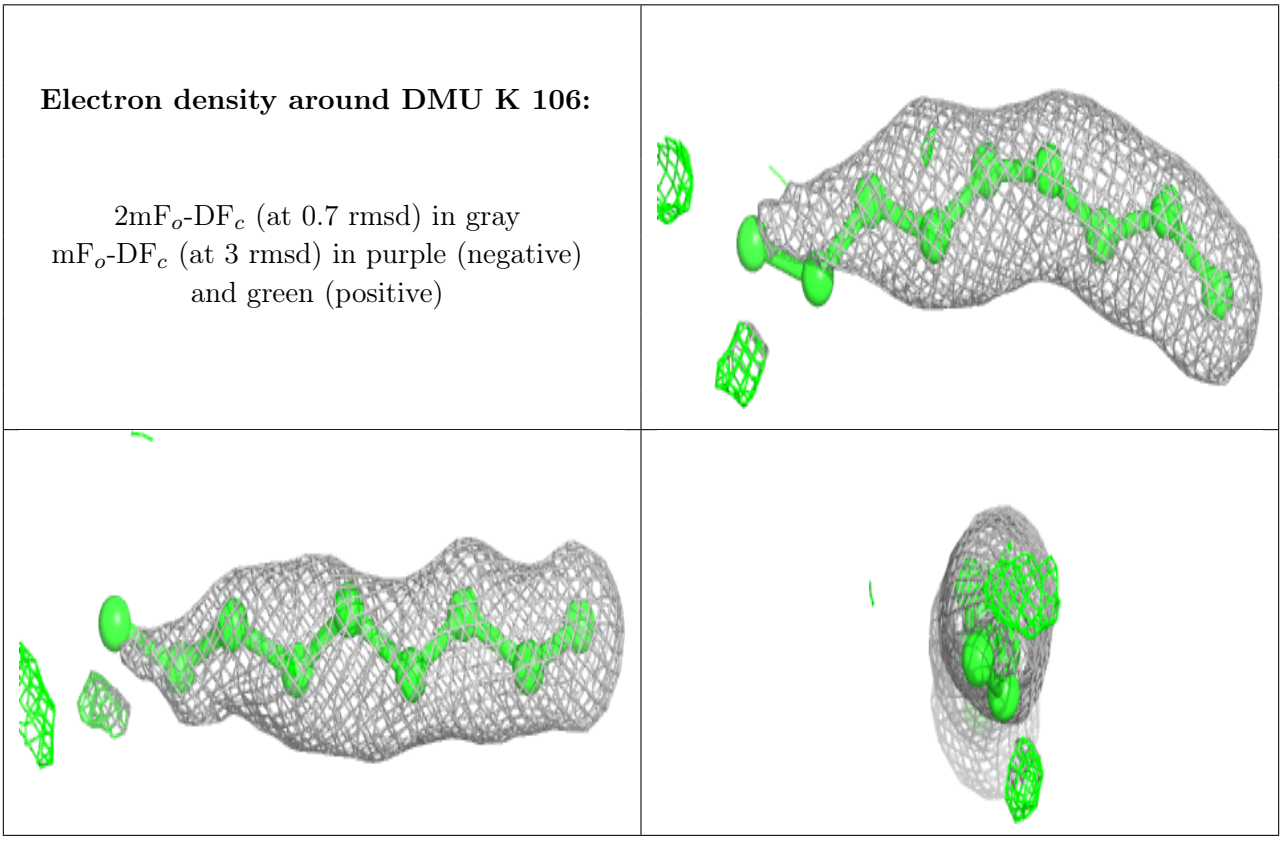
Electron density around DMU C 301:

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



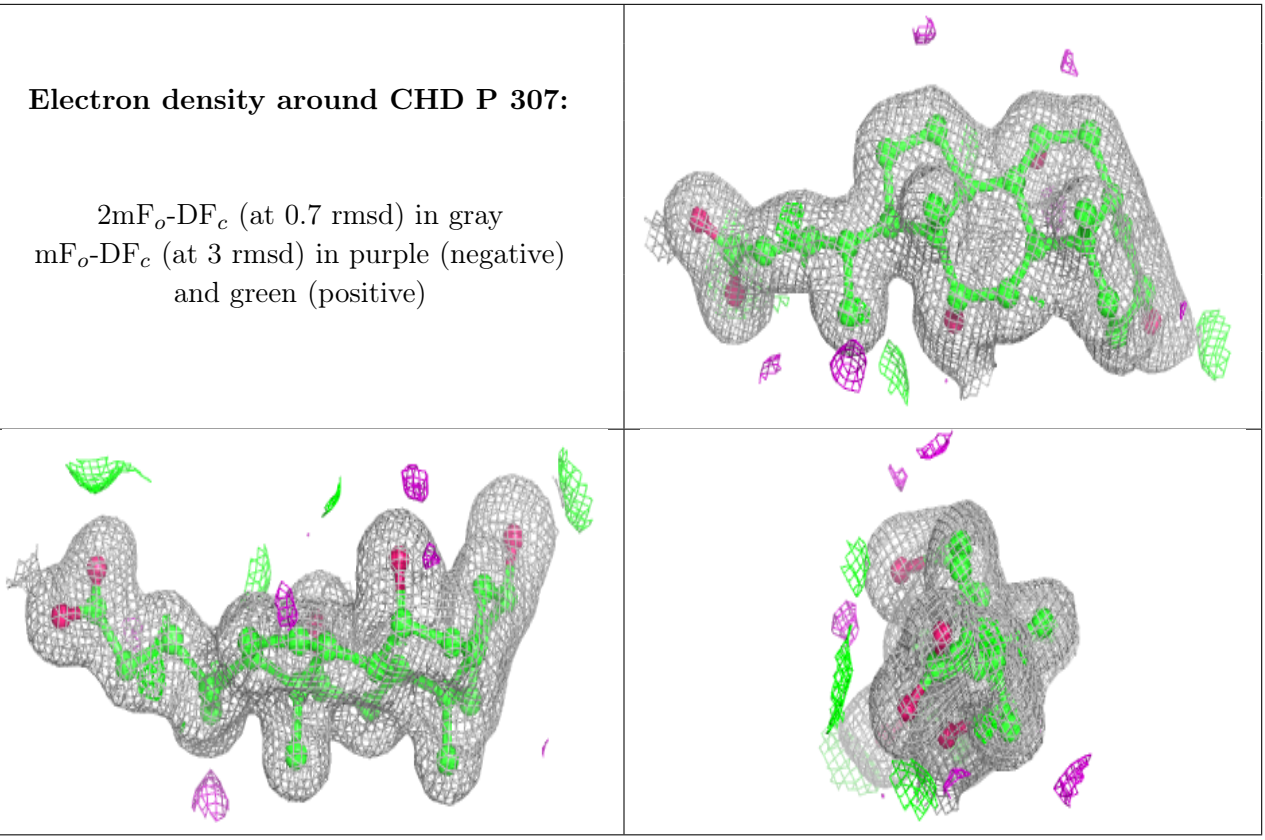
Electron density around DMU K 106:

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



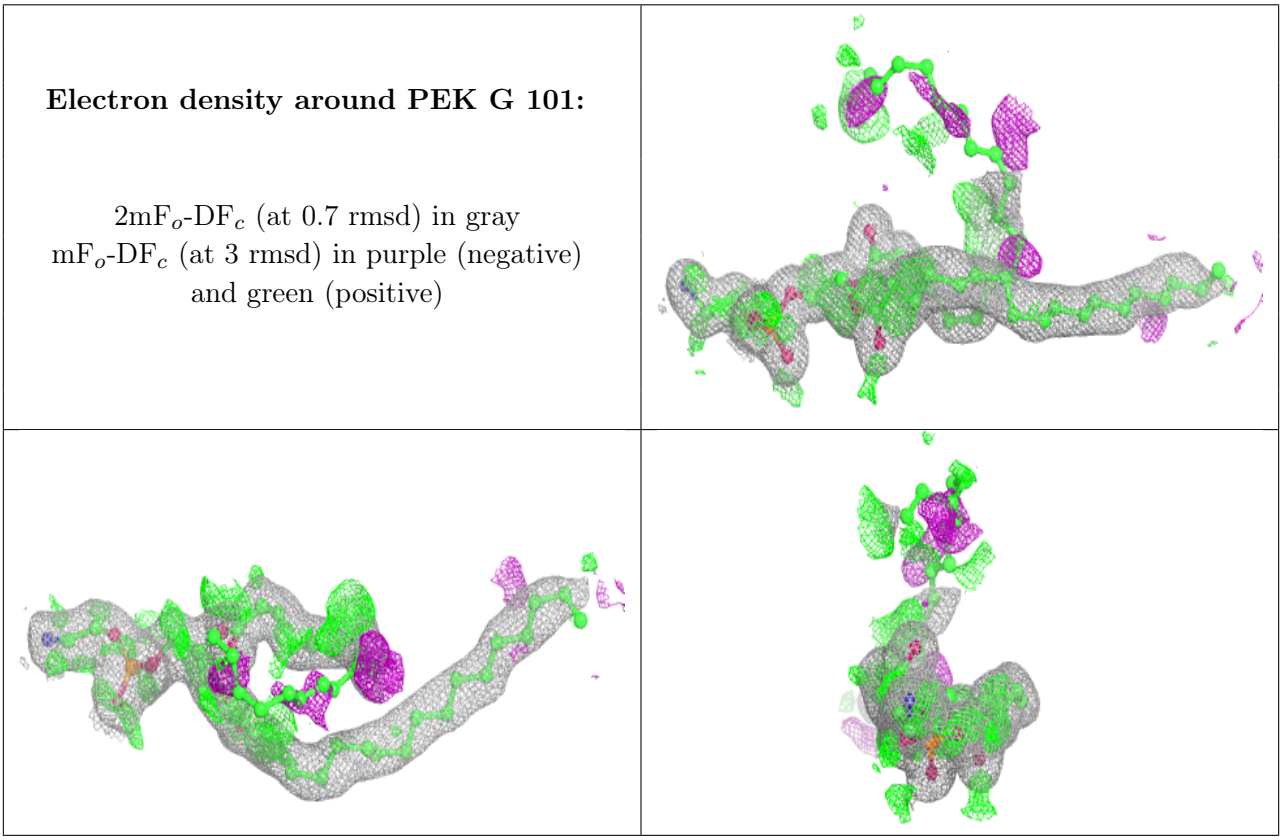
Electron density around CHD P 307:

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



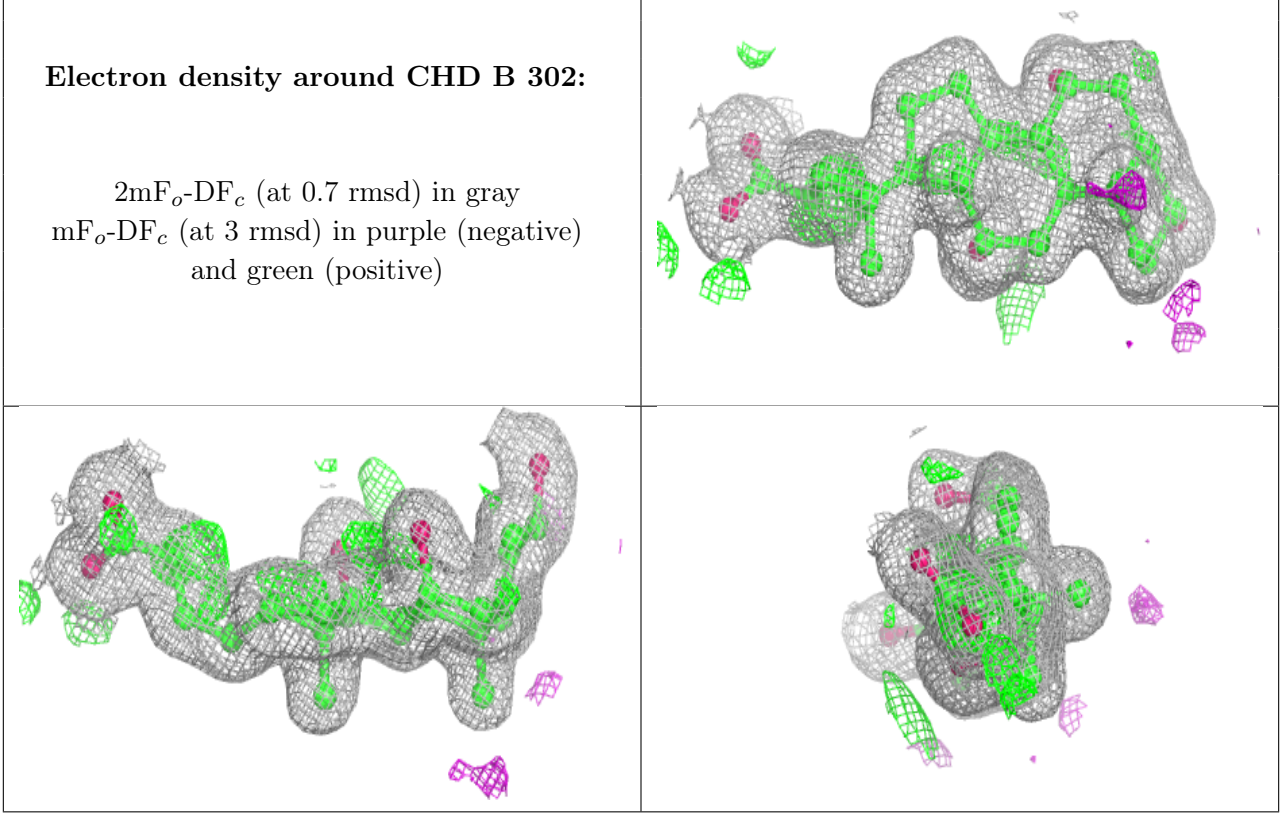
Electron density around PEK G 101:

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



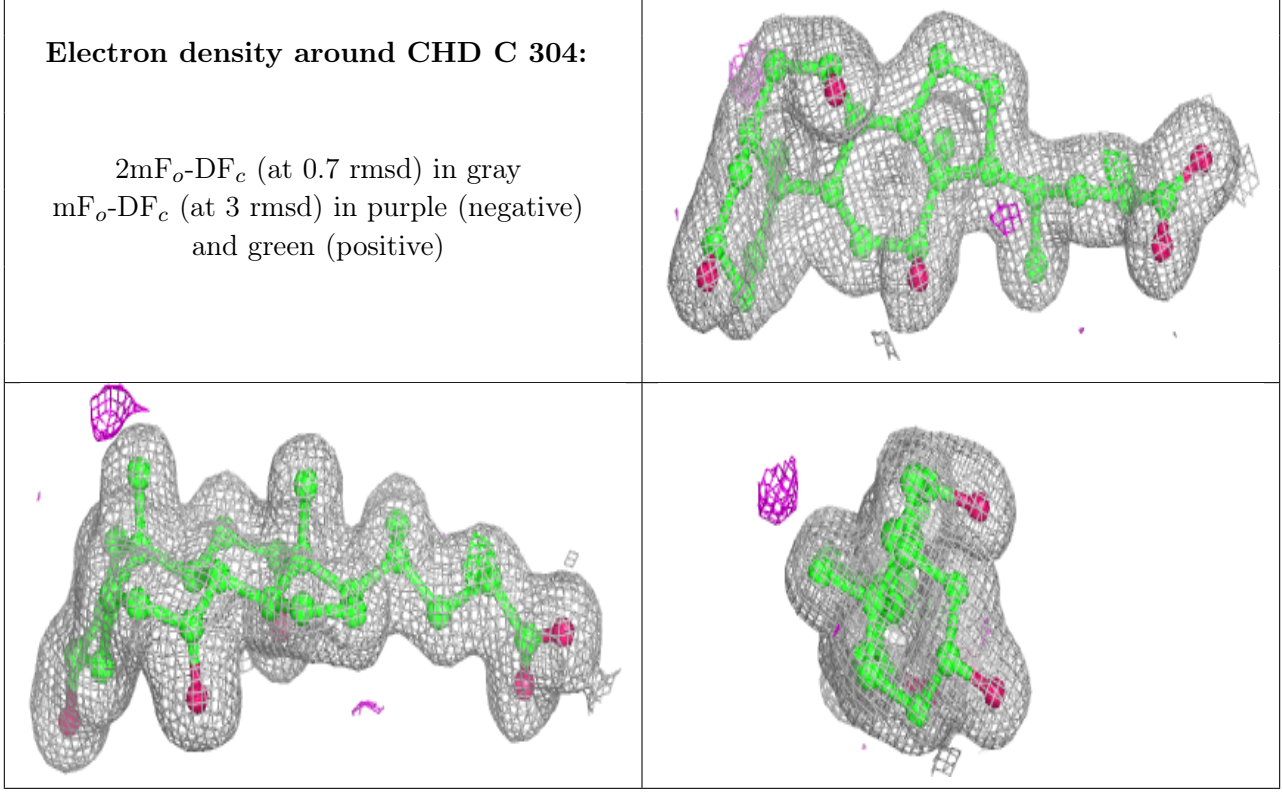
Electron density around CHD B 302:

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



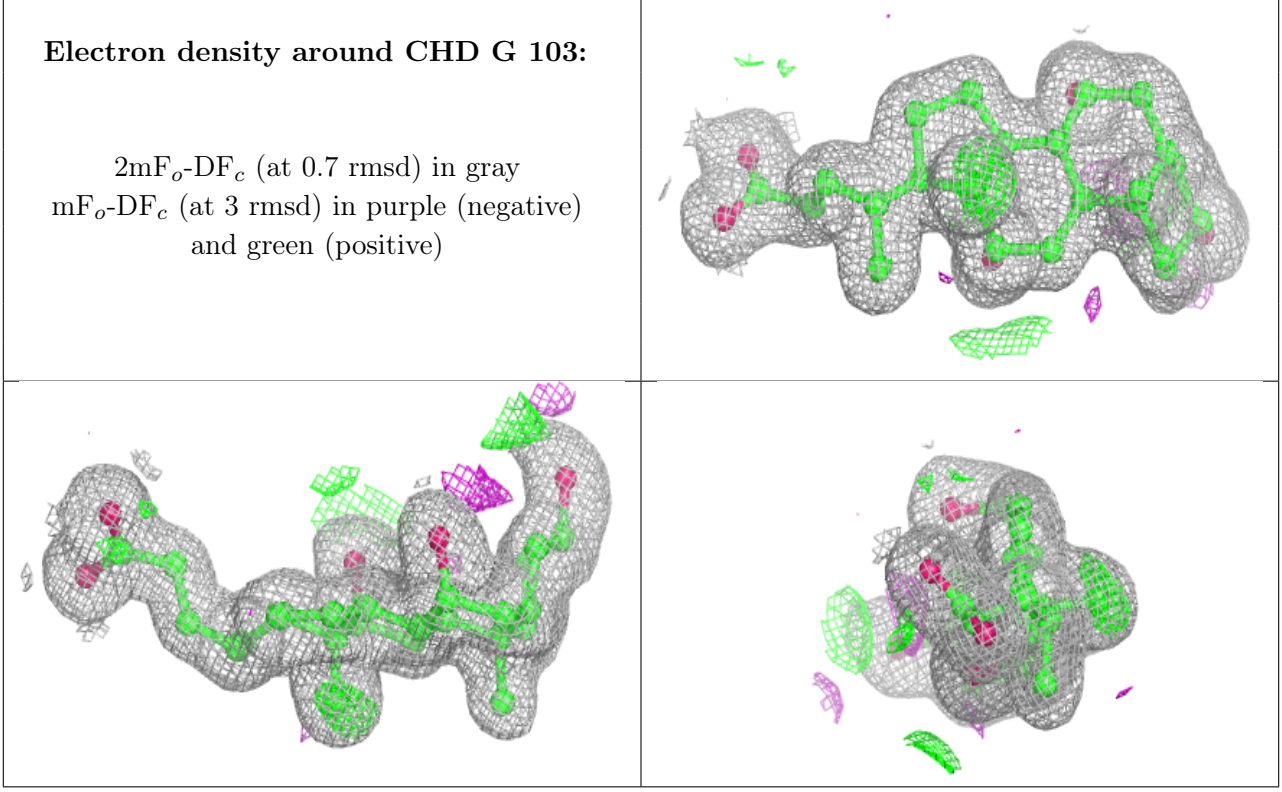
Electron density around CHD C 304:

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



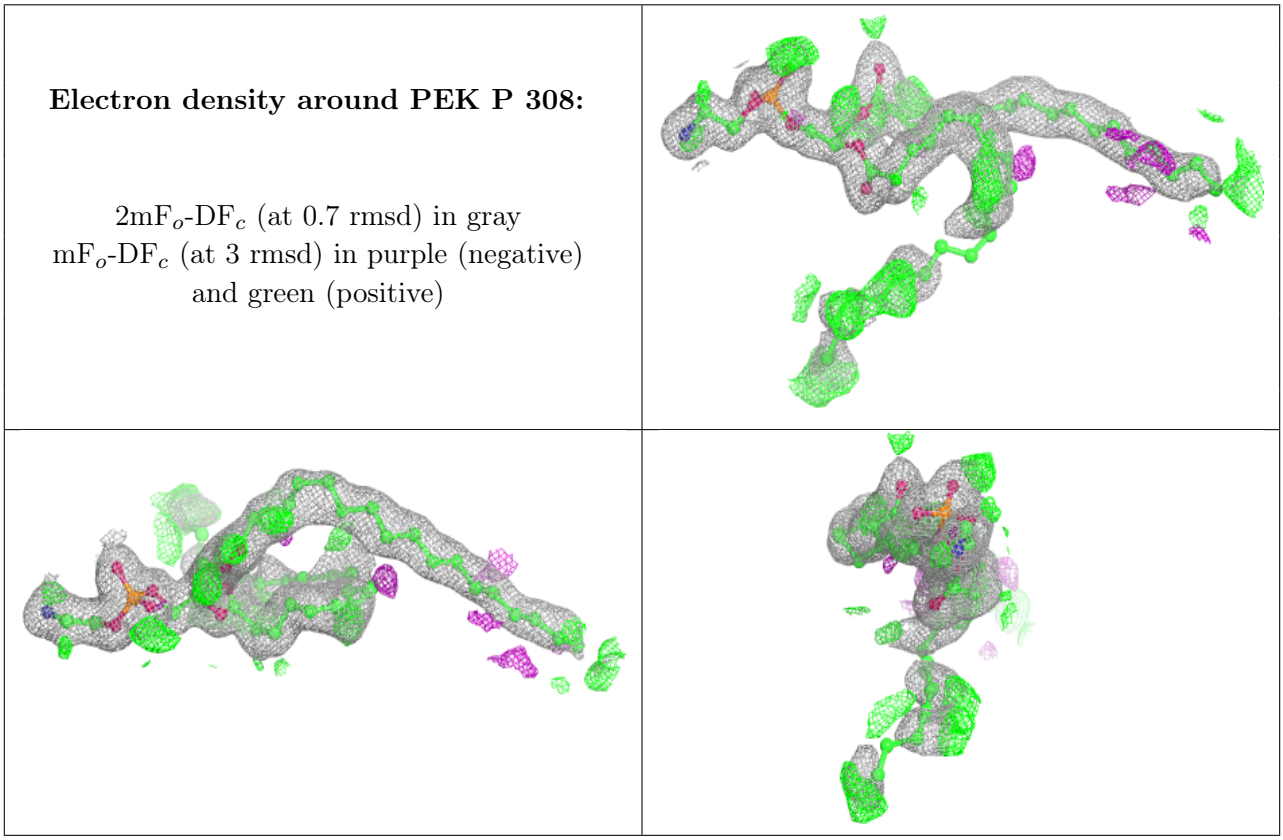
Electron density around CHD G 103:

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



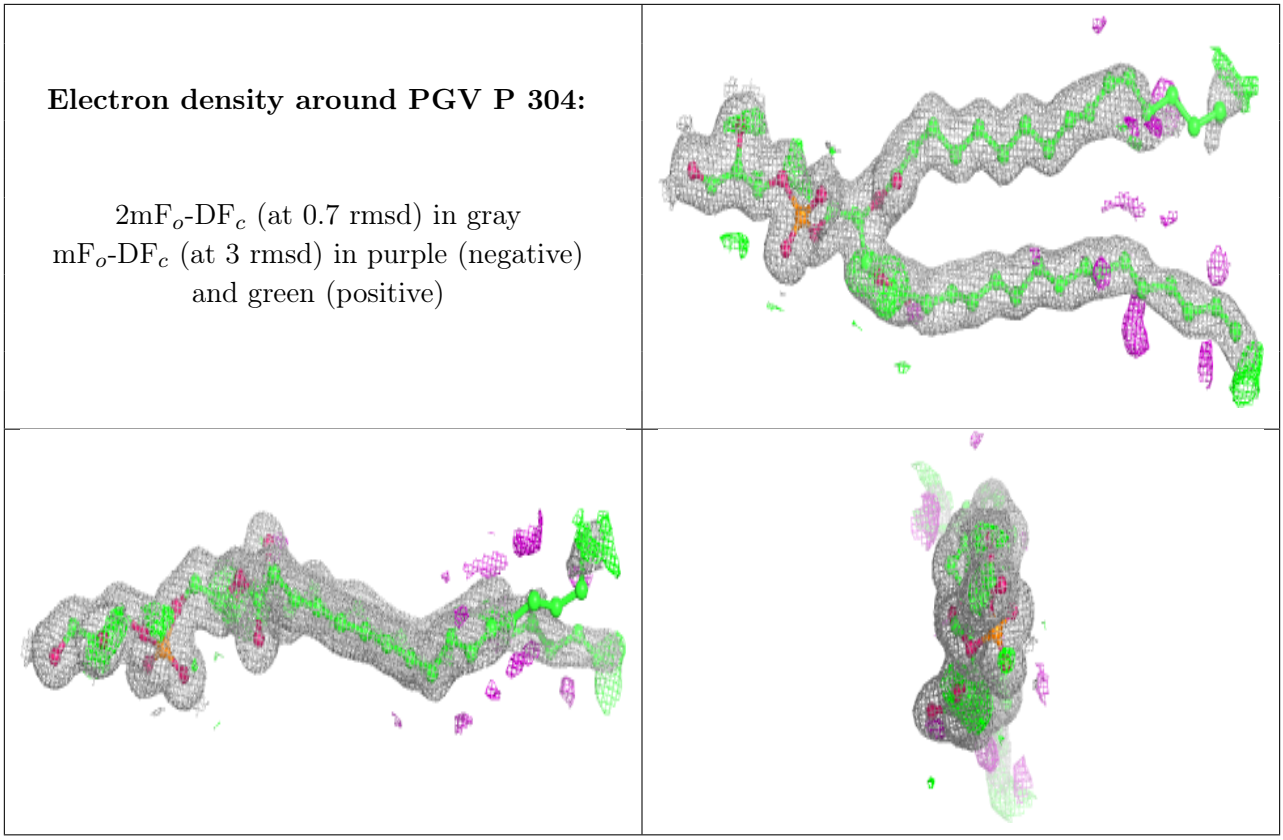
Electron density around PEK P 308:

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



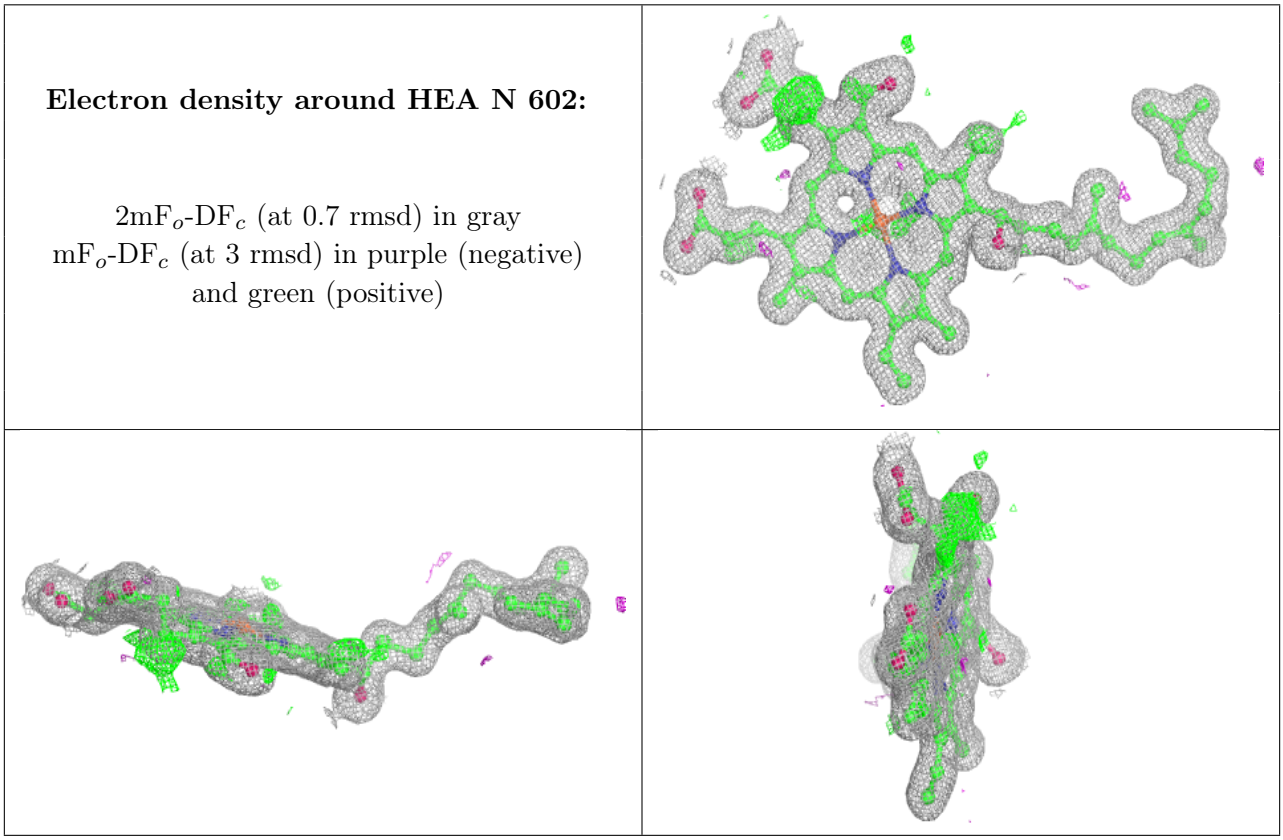
Electron density around PGV P 304:

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



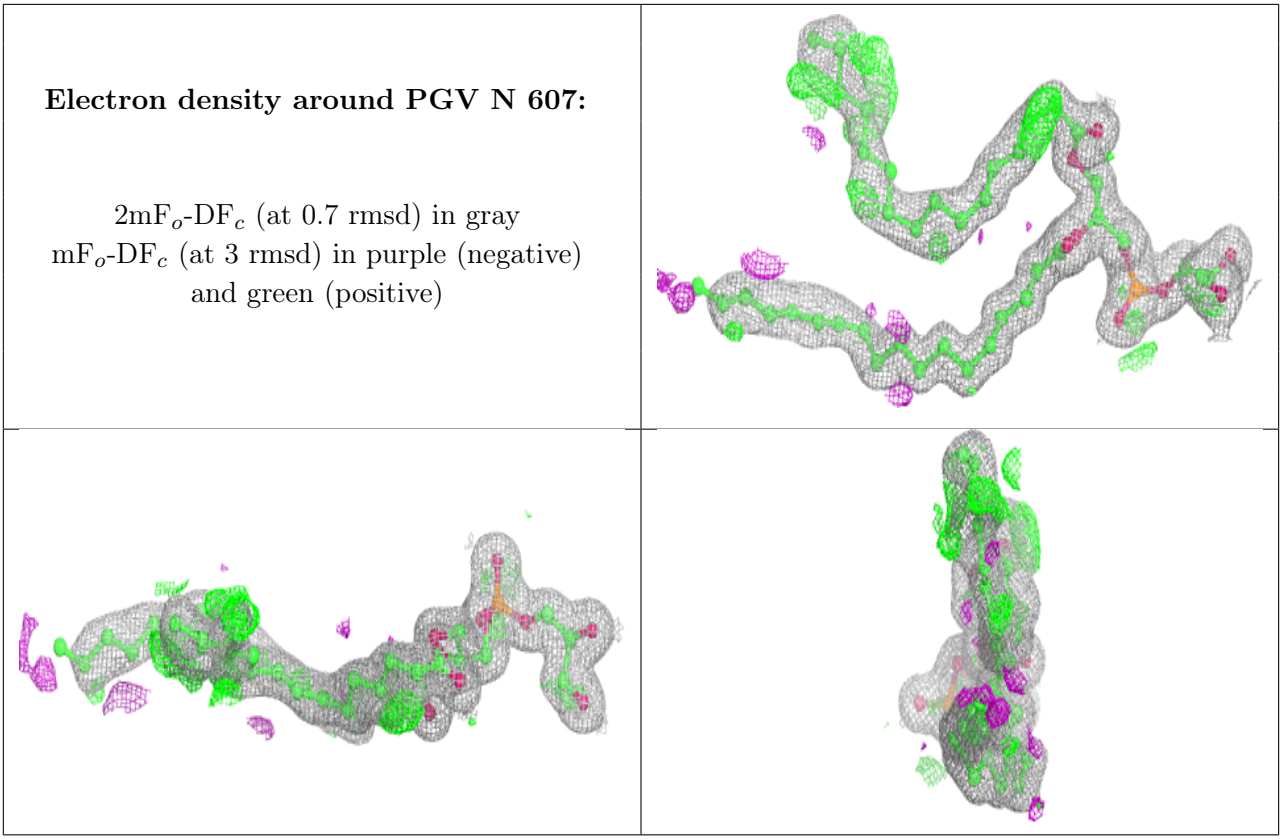
Electron density around HEA N 602:

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



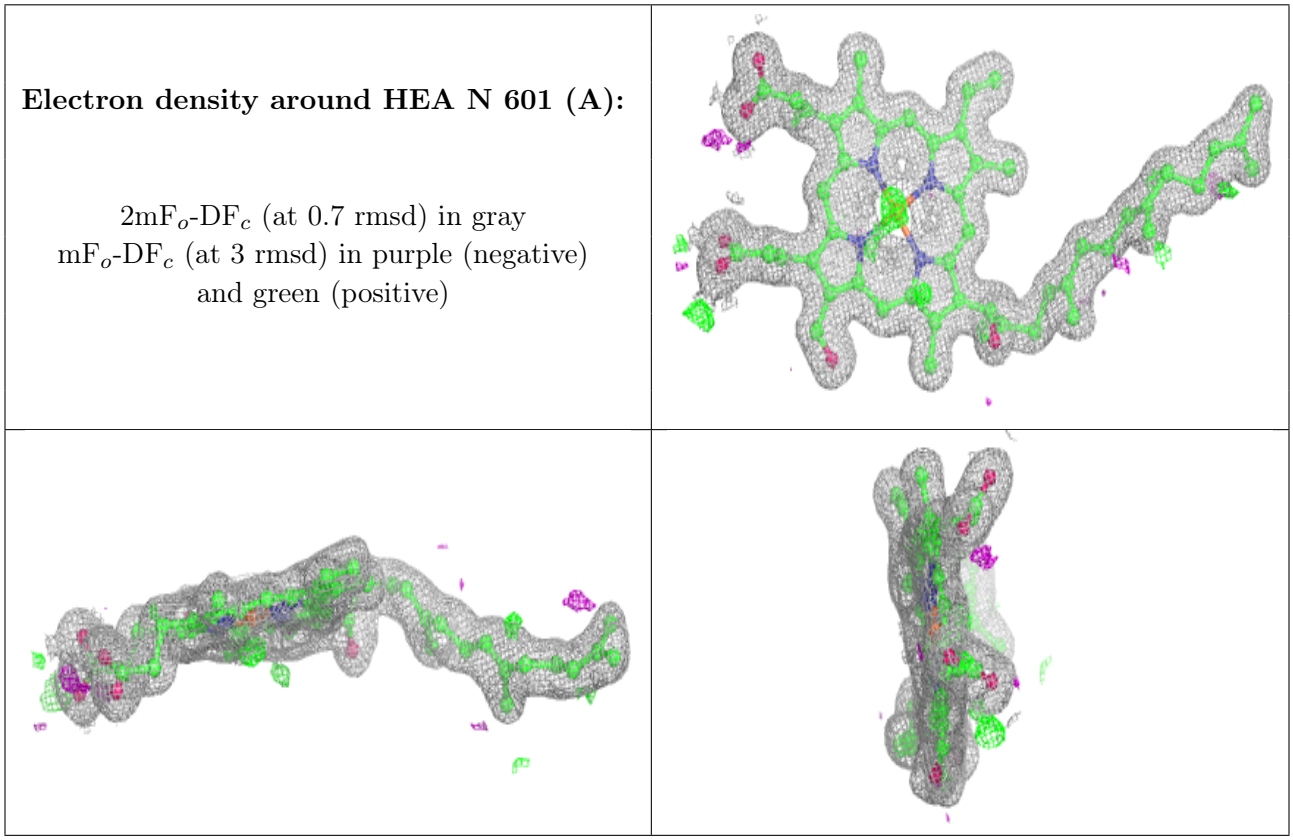
Electron density around PGV N 607:

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



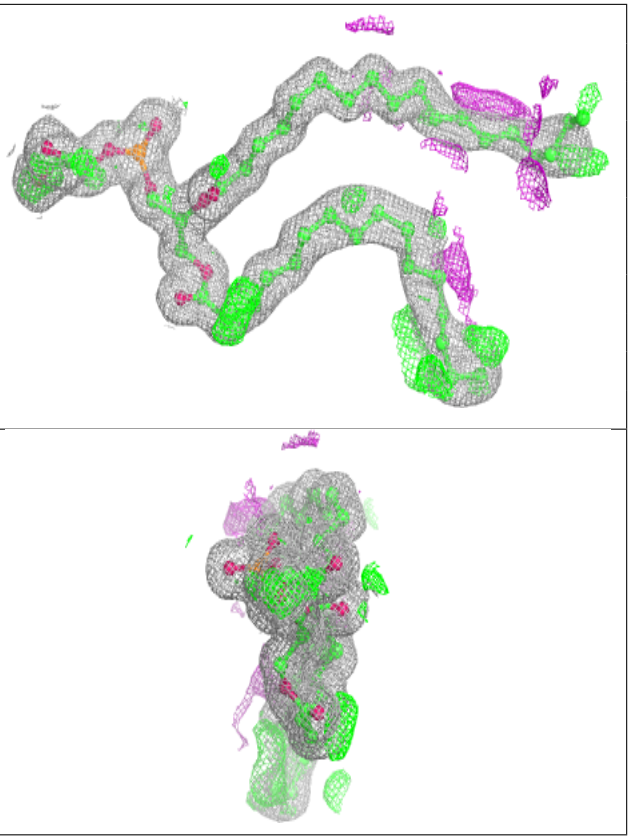
Electron density around HEA N 601 (A):

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



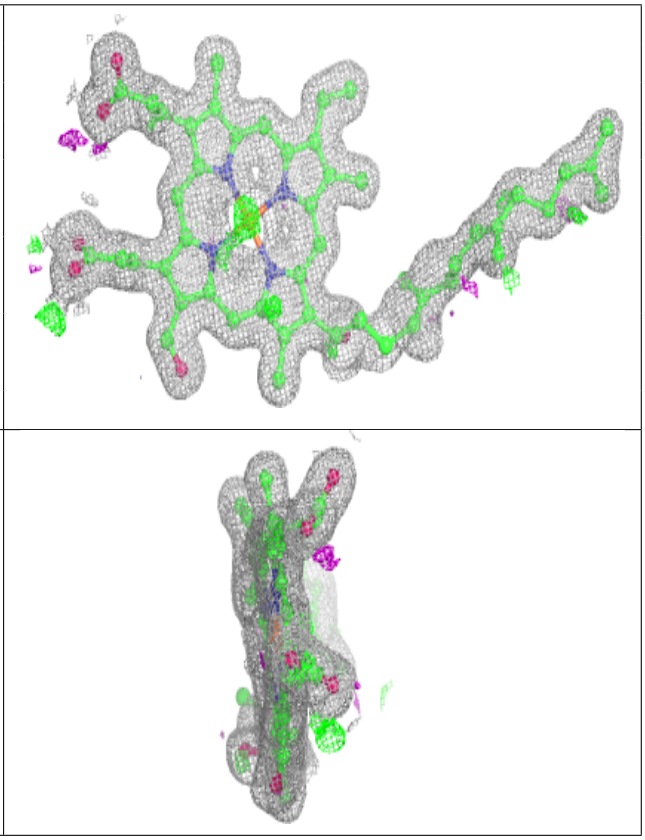
Electron density around PGV A 606:

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



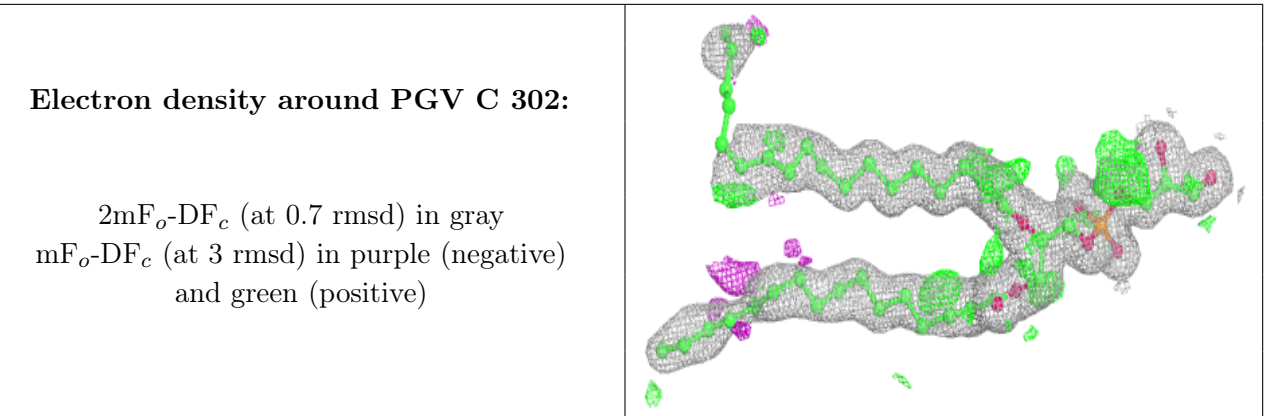
Electron density around HEA N 601 (B):

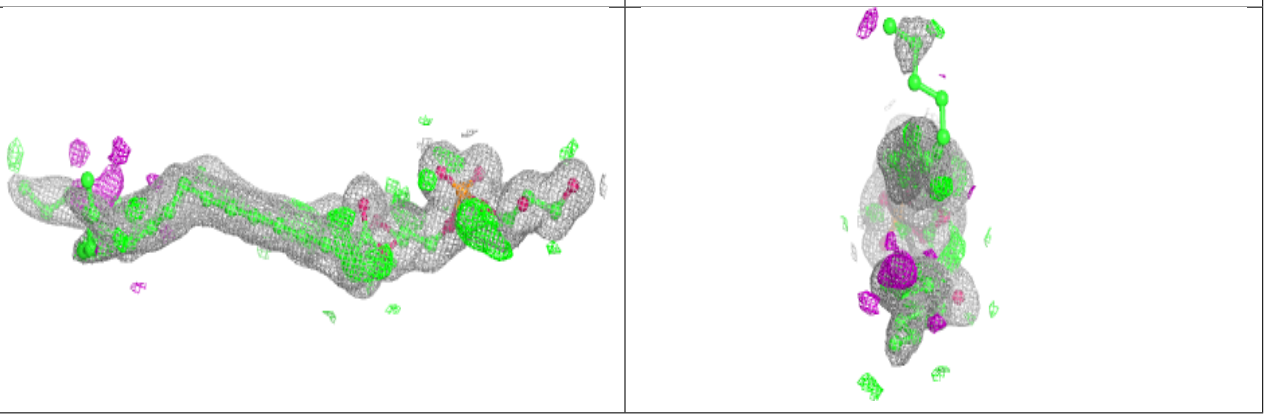
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around PGV C 302:

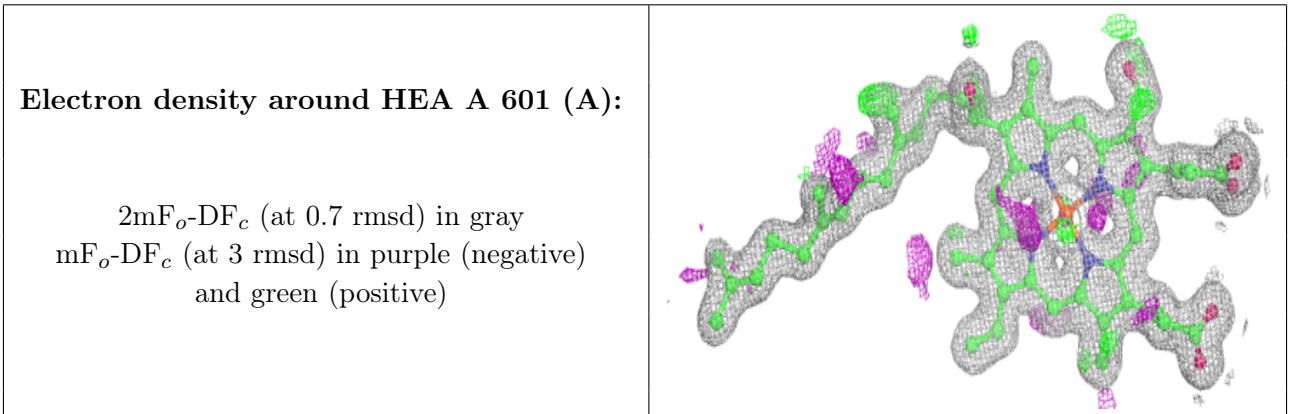
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

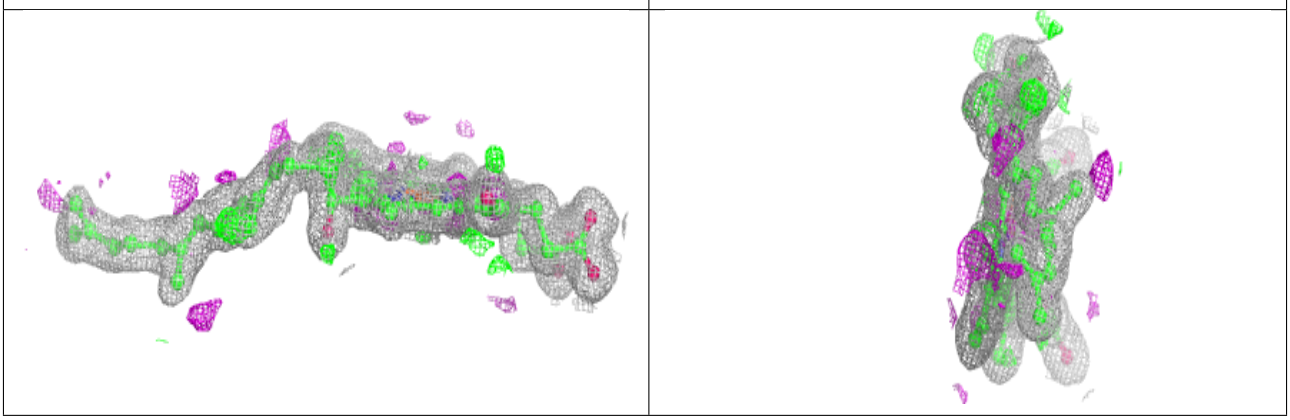




Electron density around HEA A 601 (A):

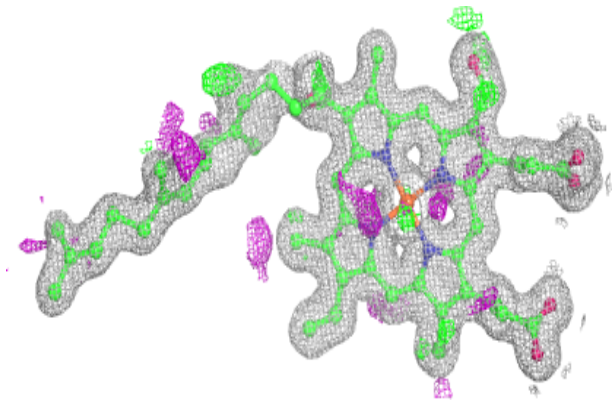
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

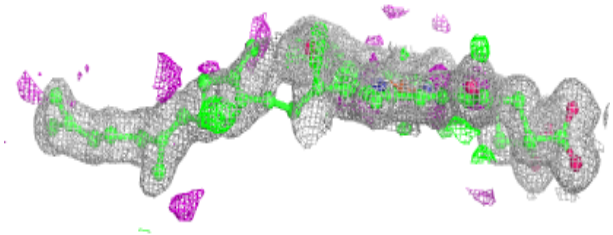


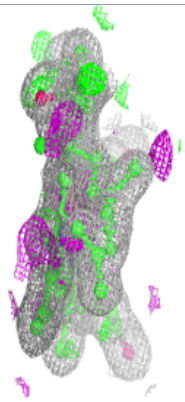


Electron density around HEA A 601 (B):

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

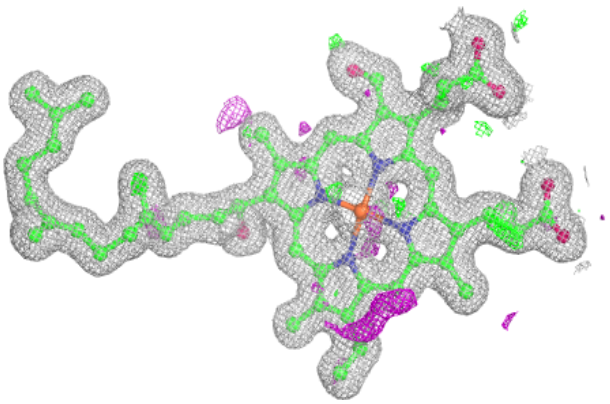


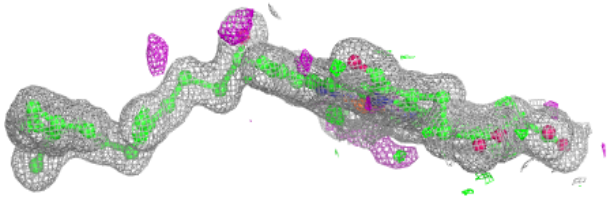


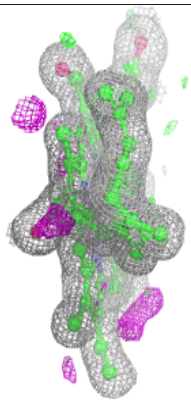


Electron density around HEA A 602:

$2mF_o$-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.