wwPDB X-ray Structure Validation Summary Report (i)

Dec 12, 2023 – 10:31 AM EST

PDB ID	:	1V55
Title	:	Bovine heart cytochrome c oxidase at the fully reduced state
Authors	:	Tsukihara, T.; Shimokata, K.; Katayama, Y.; Shimada, H.; Muramoto, K.; Aoyama, H.; Mochizuki, M.; Shinzawa-Itoh, K.; Yamashita, E.; Yao, M.; Ishimura, Y.; Yoshikawa, S.
Deposited on	:	2003-11-21
Resolution	:	1.90 Å(reported)

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

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

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

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

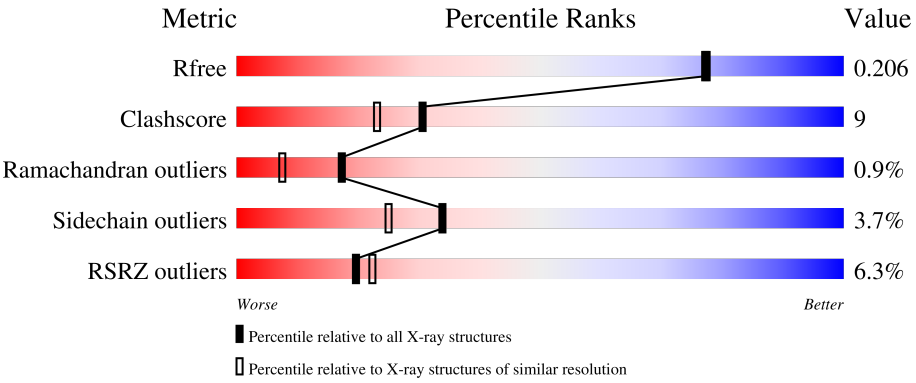
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

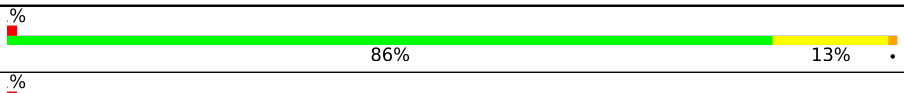
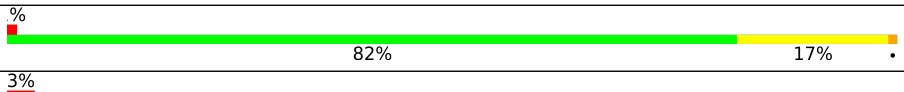
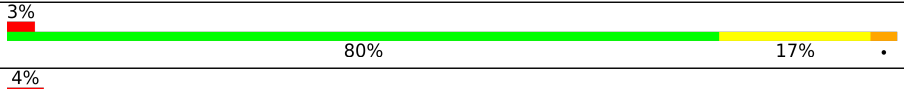
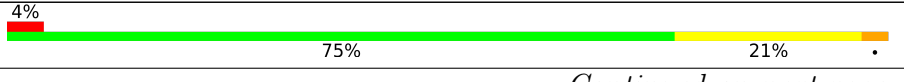
The reported resolution of this entry is 1.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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

Mol	Chain	Length	Quality of chain
1	A	514	
1	N	514	
2	B	227	
2	O	227	

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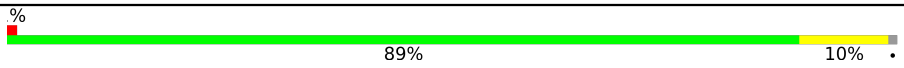
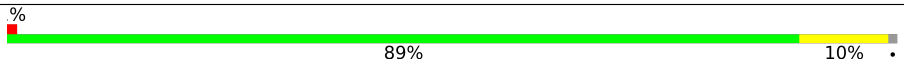
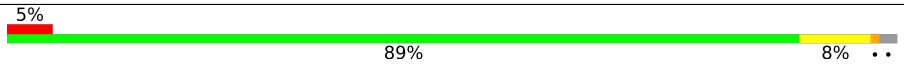
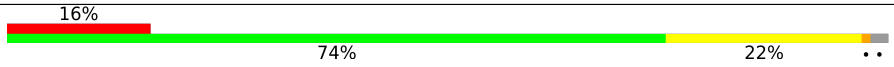
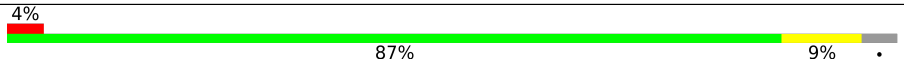
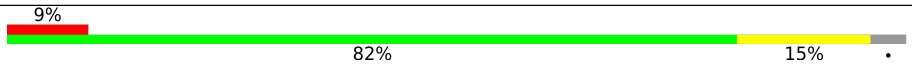
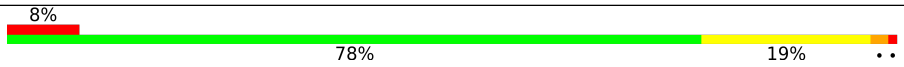
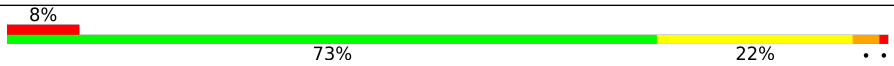
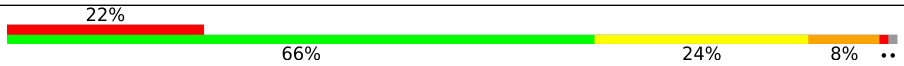
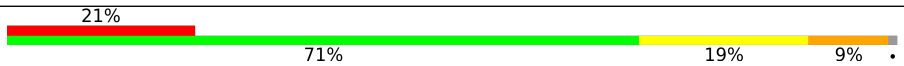
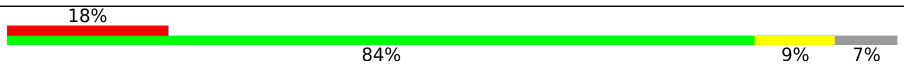
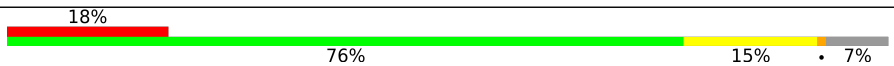
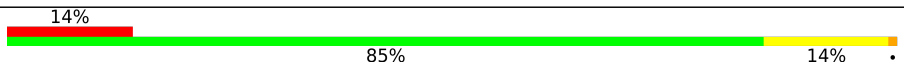
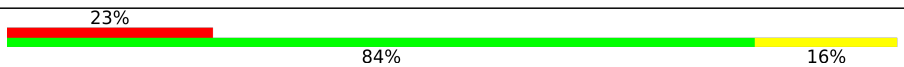
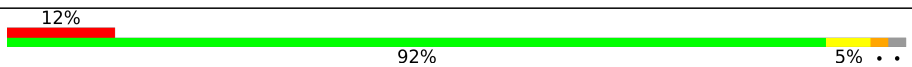
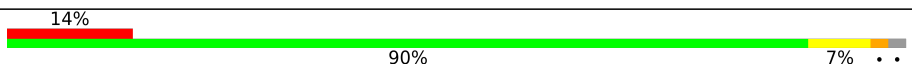
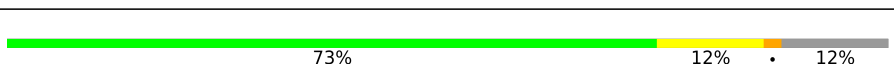
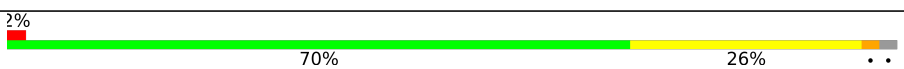
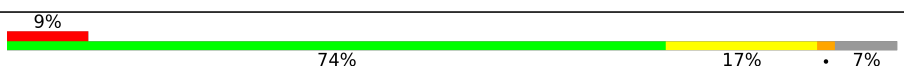
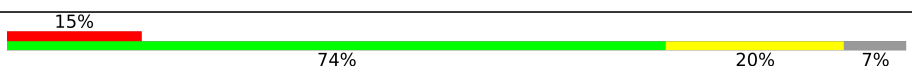
Mol	Chain	Length	Quality of chain
3	C	261	
3	P	261	
4	D	147	
4	Q	147	
5	E	109	
5	R	109	
6	F	98	
6	S	98	
7	G	85	
7	T	85	
8	H	85	
8	U	85	
9	I	73	
9	V	73	
10	J	59	
10	W	59	
11	K	56	
11	X	56	
12	L	47	
12	Y	47	
13	M	46	
13	Z	46	

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
18	TGL	A	3522	-	-	X	-
18	TGL	N	4521	-	-	X	-
21	CHD	C	3271	X	-	-	-
21	CHD	J	3060	X	-	-	X
21	CHD	P	4271	X	-	-	-
21	CHD	W	4060	X	-	-	X
22	CDL	C	3270	-	-	X	-
23	PEK	T	3263	-	-	-	X
27	DMU	M	3526	X	-	-	-
27	DMU	Z	4526	X	-	-	-
9	SAC	I	1	-	X	-	-
9	SAC	V	1	-	X	-	X

2 Entry composition (i)

There are 28 unique types of molecules in this entry. The entry contains 32609 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 polypeptide I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	514	Total	C	N	O	S	0	0	0
			4027	2691	623	678	35			
1	N	514	Total	C	N	O	S	0	0	0
			4027	2691	623	678	35			

- Molecule 2 is a protein called Cytochrome c oxidase polypeptide II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	227	Total	C	N	O	S	0	0	0
			1824	1185	281	340	18			
2	O	227	Total	C	N	O	S	0	0	0
			1824	1185	281	340	18			

- Molecule 3 is a protein called Cytochrome c oxidase polypeptide III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	259	Total	C	N	O	S	0	0	0
			2110	1412	336	350	12			
3	P	259	Total	C	N	O	S	0	0	0
			2110	1412	336	350	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	144	Total	C	N	O	S	0	0	0
			1195	777	196	218	4			
4	Q	144	Total	C	N	O	S	0	0	0
			1195	777	196	218	4			

- Molecule 5 is a protein called Cytochrome c oxidase polypeptide Va.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	105	Total	C	N	O	S	0	0	0
			852	544	144	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 polypeptide Vb.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	98	Total	C	N	O	S	0	0	0
			748	464	134	145	5			
6	S	98	Total	C	N	O	S	0	0	0
			748	464	134	145	5			

- Molecule 7 is a protein called Cytochrome c oxidase polypeptide VIa-heart.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
7	G	84	Total	C	N	O	P	S	0	0	0
			675	431	129	113	1	1			
7	T	84	Total	C	N	O	P	S	0	0	0
			675	431	129	113	1	1			

- Molecule 8 is a protein called Cytochrome c oxidase polypeptide VIb.

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 polypeptide VIc.

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	0	0
			601	390	107	100	4			

- Molecule 10 is a protein called Cytochrome c oxidase polypeptide VIIa-heart.

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 polypeptide VIIb.

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

- Molecule 12 is a protein called Cytochrome c oxidase polypeptide VIIc.

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 polypeptide VIII-heart.

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 COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

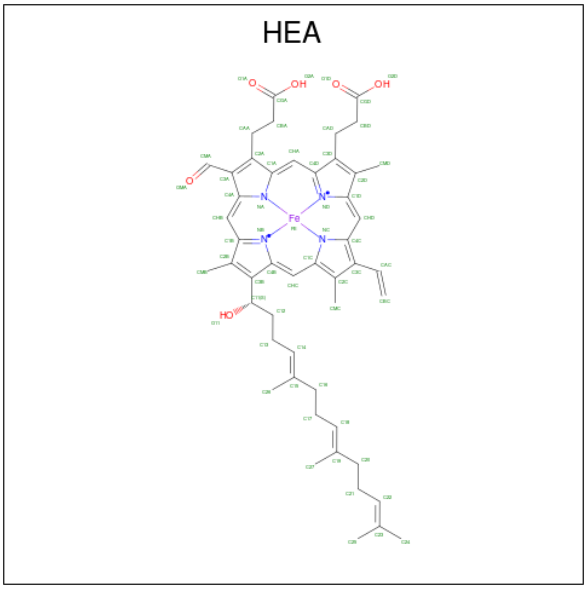
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 16 is SODIUM ION (three-letter code: NA) (formula: Na).

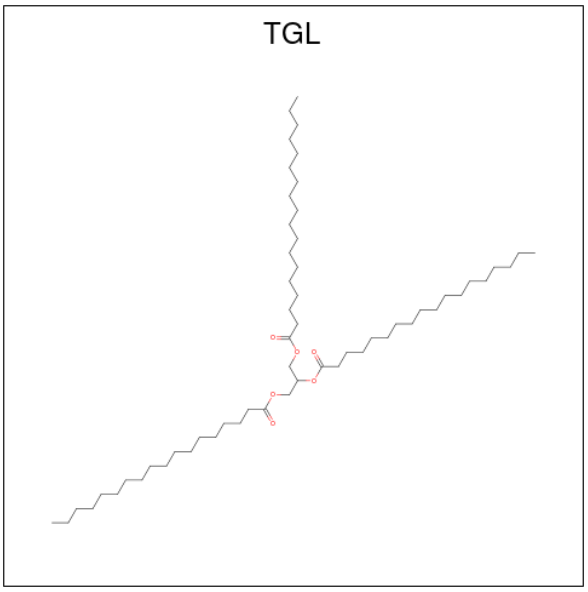
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	A	1	Total Na 1 1	0	0
16	N	1	Total Na 1 1	0	0

- Molecule 17 is HEME-A (three-letter code: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



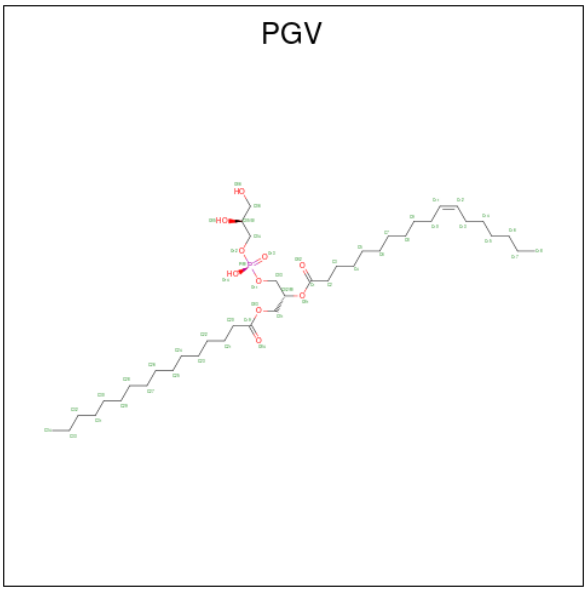
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total C Fe N O 60 49 1 4 6	0	0
17	A	1	Total C Fe N O 60 49 1 4 6	0	0
17	N	1	Total C Fe N O 60 49 1 4 6	0	0
17	N	1	Total C Fe N O 60 49 1 4 6	0	0

- Molecule 18 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: $C_{57}H_{110}O_6$).



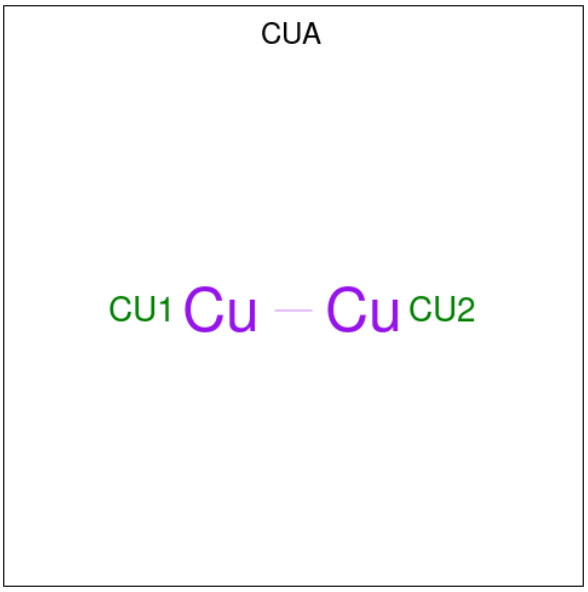
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total C O 63 57 6	0	0
18	A	1	Total C O 63 57 6	0	0
18	A	1	Total C O 63 57 6	0	0
18	N	1	Total C O 63 57 6	0	0
18	N	1	Total C O 63 57 6	0	0
18	Q	1	Total C O 63 57 6	0	0

- Molecule 19 is (1R)-2-{[{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: $C_{40}H_{77}O_{10}P$).



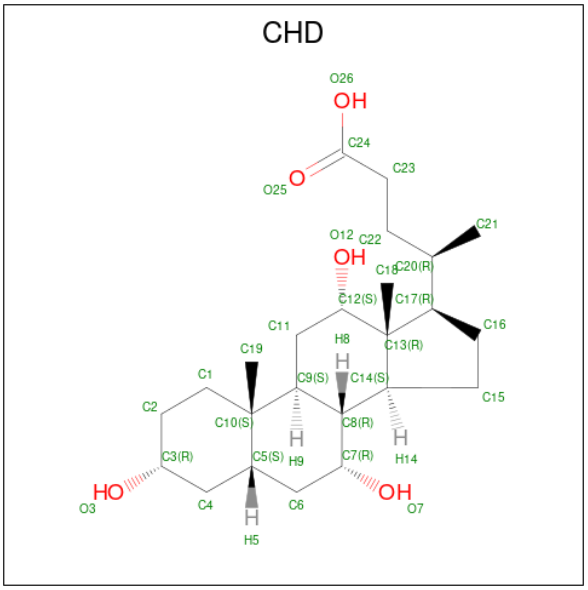
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	P	1	Total	C	O	P	0	0
			51	40	10	1		
19	P	1	Total	C	O	P	0	0
			51	40	10	1		

- Molecule 20 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu_2).



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

- Molecule 21 is CHOLIC ACID (three-letter code: CHD) (formula: $C_{24}H_{40}O_5$).



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

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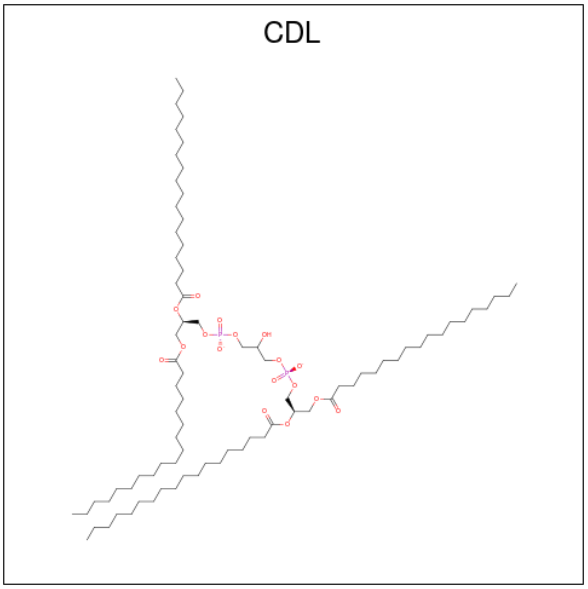
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	C	1	Total C O 29 24 5	0	0
21	J	1	Total C O 29 24 5	0	0
21	O	1	Total C O 29 24 5	0	0
21	P	1	Total C O 29 24 5	0	0
21	P	1	Total C O 29 24 5	0	0
21	W	1	Total C O 29 24 5	0	0

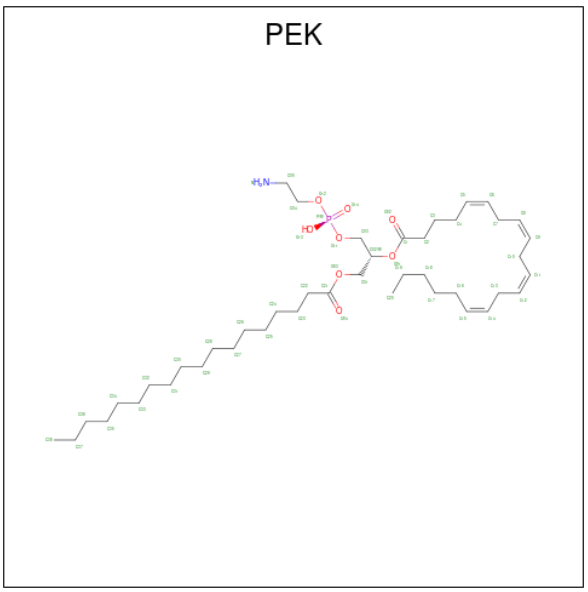
- Molecule 22 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	C	1	Total C O P 100 81 17 2	0	0
22	G	1	Total C O P 100 81 17 2	0	0
22	P	1	Total C O P 100 81 17 2	0	0
22	T	1	Total C O P 100 81 17 2	0	0

- Molecule 23 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: $C_{43}H_{78}NO_8P$).

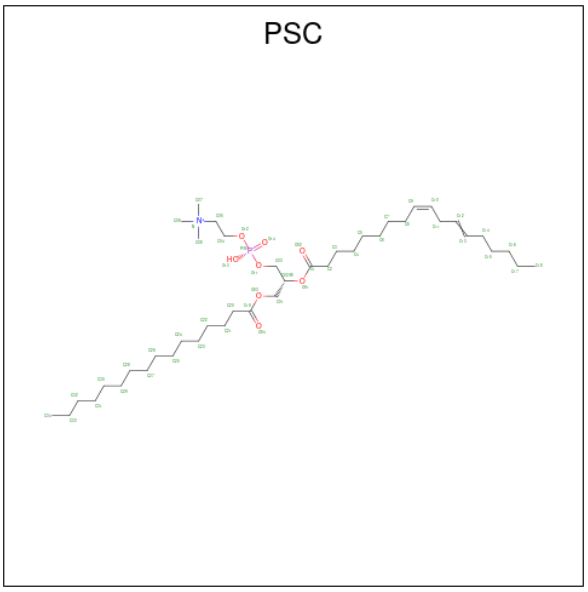


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
23	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
23	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
23	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
23	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
23	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

- Molecule 24 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

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

- Molecule 25 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: $C_{42}H_{81}NO_8P$).

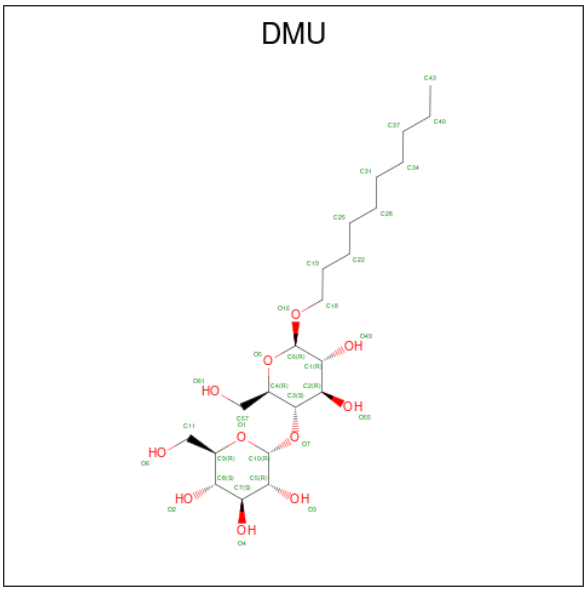


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	E	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
25	O	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

- Molecule 26 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 27 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: $C_{22}H_{42}O_{11}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	M	1	Total C O 33 22 11	0	0
27	Z	1	Total C O 33 22 11	0	0

- Molecule 28 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	229	Total O 229 229	0	0
28	B	167	Total O 167 167	0	0
28	C	107	Total O 107 107	0	0
28	D	112	Total O 112 112	0	0
28	E	90	Total O 90 90	0	0
28	F	109	Total O 109 109	0	0
28	G	54	Total O 54 54	0	0
28	H	61	Total O 61 61	0	0
28	I	50	Total O 50 50	0	0
28	J	34	Total O 34 34	0	0

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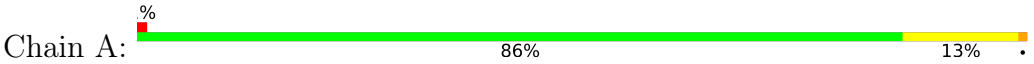
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	K	28	Total O 28 28	0	0
28	L	21	Total O 21 21	0	0
28	M	33	Total O 33 33	0	0
28	N	214	Total O 214 214	0	0
28	O	116	Total O 116 116	0	0
28	P	112	Total O 112 112	0	0
28	Q	72	Total O 72 72	0	0
28	R	48	Total O 48 48	0	0
28	S	77	Total O 77 77	0	0
28	T	48	Total O 48 48	0	0
28	U	54	Total O 54 54	0	0
28	V	32	Total O 32 32	0	0
28	W	20	Total O 20 20	0	0
28	X	20	Total O 20 20	0	0
28	Y	22	Total O 22 22	0	0
28	Z	13	Total O 13 13	0	0

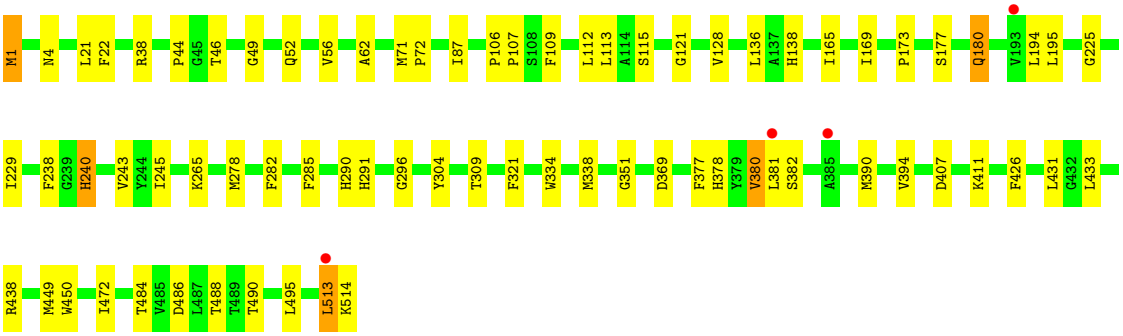
3 Residue-property plots (i)

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 polypeptide I

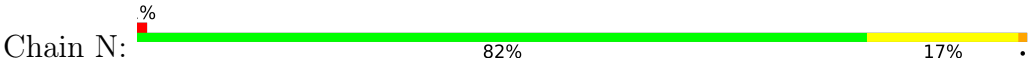
Chain A:

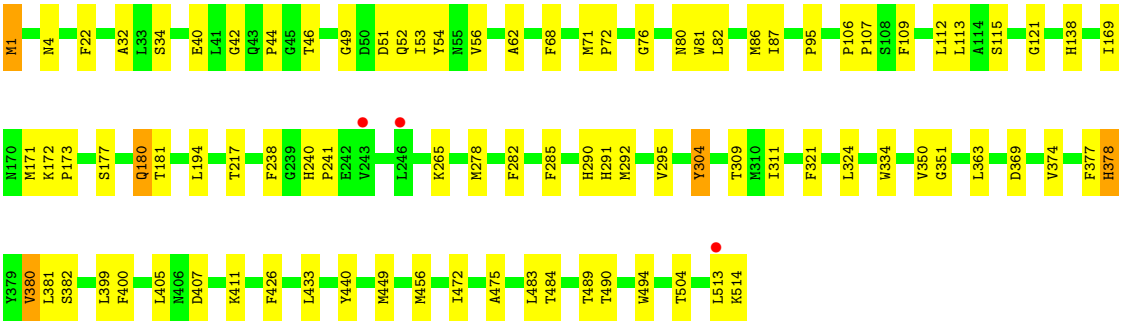




• Molecule 1: Cytochrome c oxidase polypeptide I

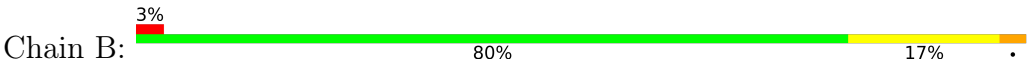
Chain N:

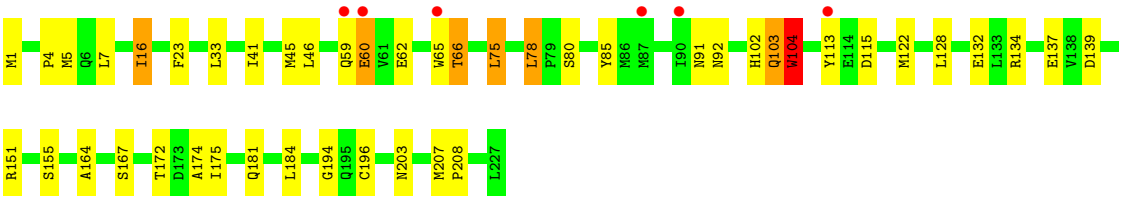




• Molecule 2: Cytochrome c oxidase polypeptide II

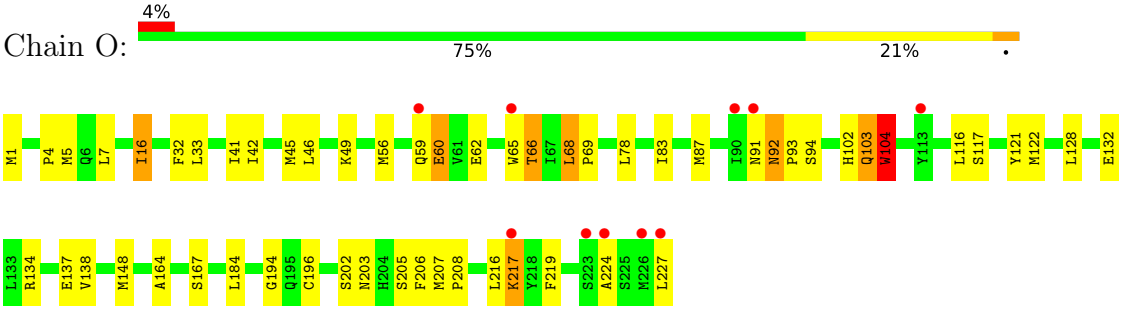
Chain B:





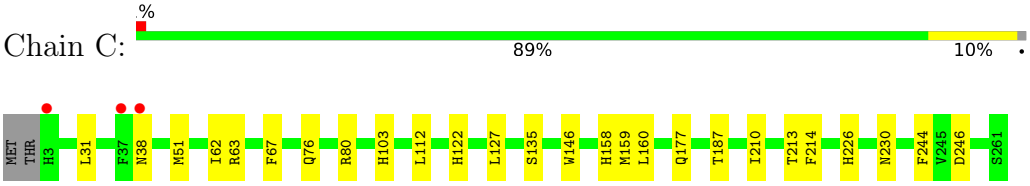
• Molecule 2: Cytochrome c oxidase polypeptide II

Chain O:



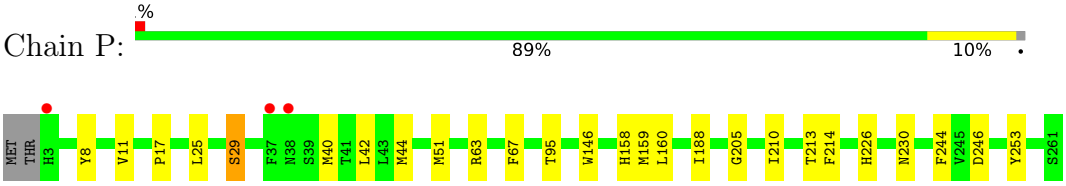
• Molecule 3: Cytochrome c oxidase polypeptide III

Chain C:



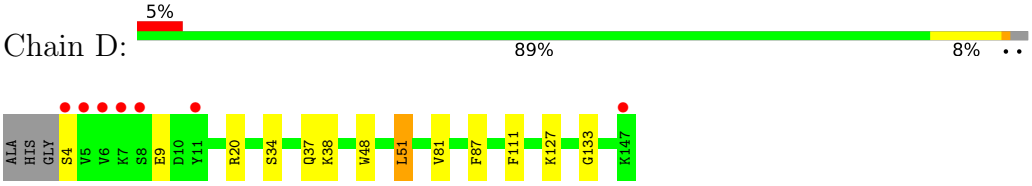
• Molecule 3: Cytochrome c oxidase polypeptide III

Chain P:



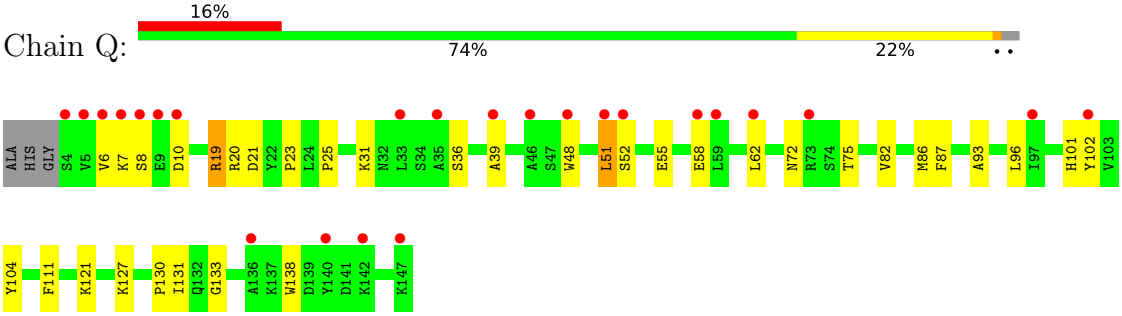
• Molecule 4: Cytochrome c oxidase subunit IV isoform 1

Chain D:



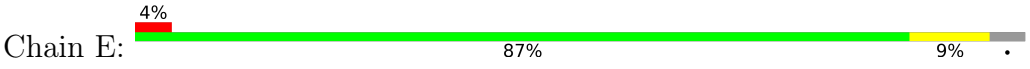
• Molecule 4: Cytochrome c oxidase subunit IV isoform 1

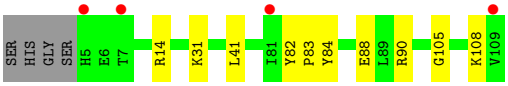
Chain Q:



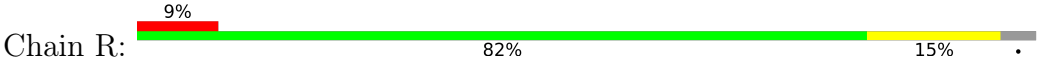
• Molecule 5: Cytochrome c oxidase polypeptide Va

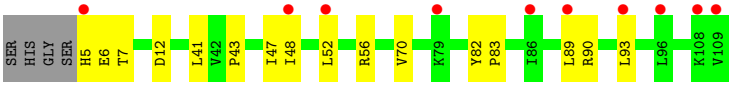
Chain E:



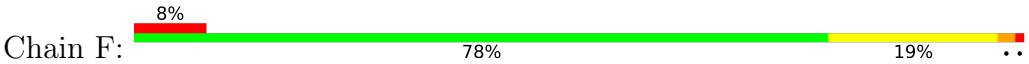


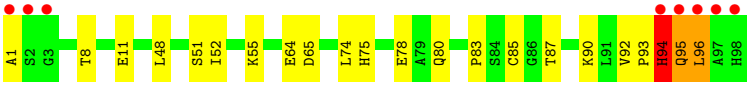
• Molecule 5: Cytochrome c oxidase polypeptide Va



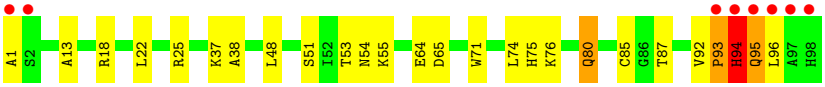


• Molecule 6: Cytochrome c oxidase polypeptide Vb

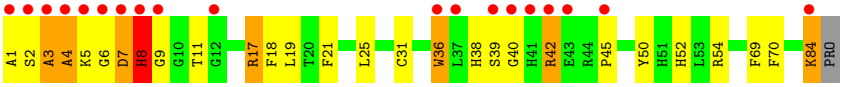




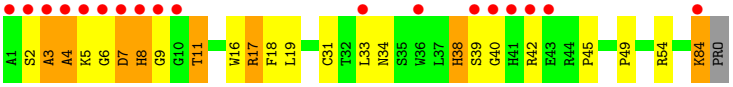
• Molecule 6: Cytochrome c oxidase polypeptide Vb



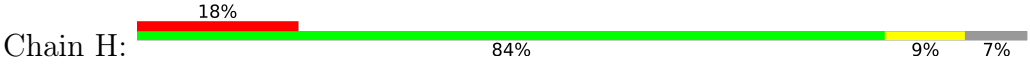
• Molecule 7: Cytochrome c oxidase polypeptide VIa-heart

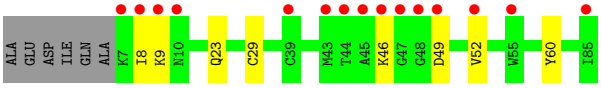


• Molecule 7: Cytochrome c oxidase polypeptide VIa-heart



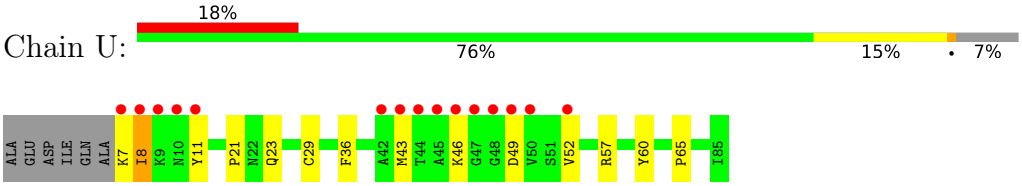
• Molecule 8: Cytochrome c oxidase polypeptide VIb





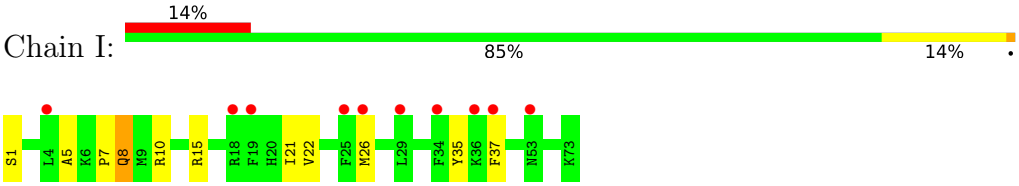
• Molecule 8: Cytochrome c oxidase polypeptide VIb

Chain U:



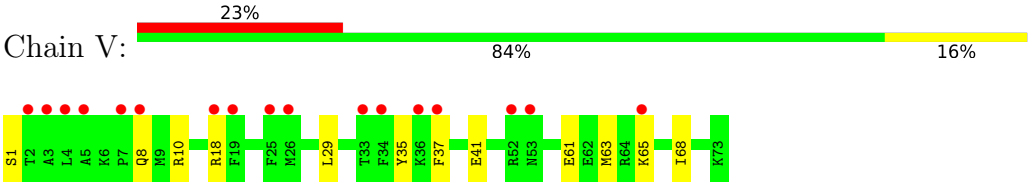
• Molecule 9: Cytochrome c oxidase polypeptide VIc

Chain I:



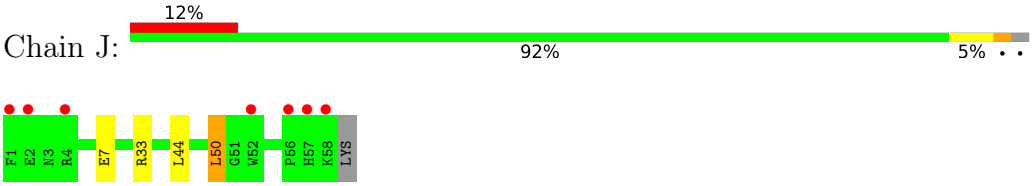
• Molecule 9: Cytochrome c oxidase polypeptide VIc

Chain V:



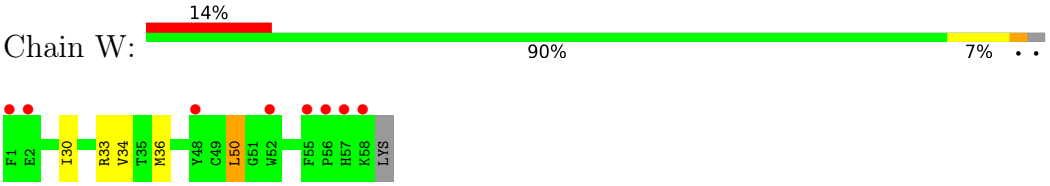
• Molecule 10: Cytochrome c oxidase polypeptide VIIa-heart

Chain J:



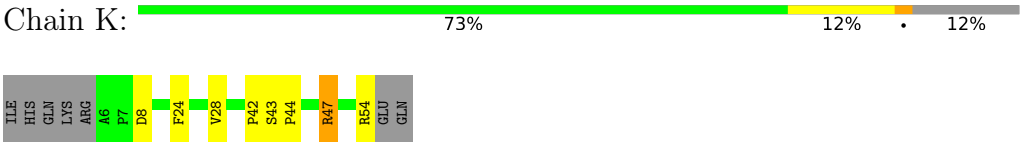
• Molecule 10: Cytochrome c oxidase polypeptide VIIa-heart

Chain W:



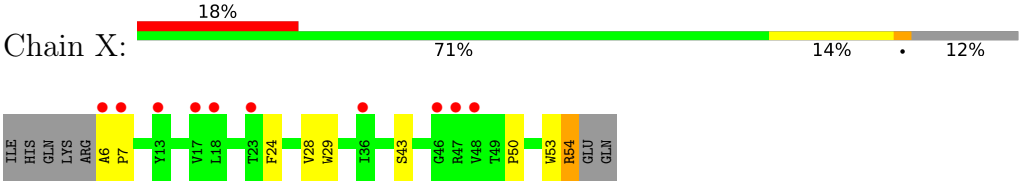
• Molecule 11: Cytochrome c oxidase polypeptide VIIb

Chain K:



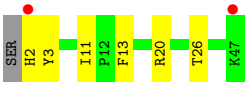
• Molecule 11: Cytochrome c oxidase polypeptide VIIb

Chain X:



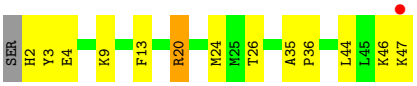
• Molecule 12: Cytochrome c oxidase polypeptide VIIc

Chain L:



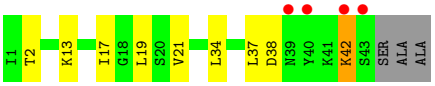
• Molecule 12: Cytochrome c oxidase polypeptide VIIc

Chain Y:



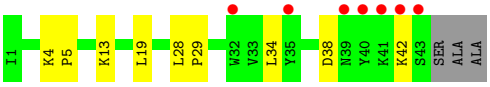
• Molecule 13: Cytochrome c oxidase polypeptide VIII-heart

Chain M:



• Molecule 13: Cytochrome c oxidase polypeptide VIII-heart

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	183.06Å 206.58Å 178.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.90 64.24 – 1.89	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-1.90) 98.1 (64.24-1.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.95 (at 1.90Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.203 , 0.230 0.205 , 0.206	Depositor DCC
R_{free} test set	26086 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	25.3	Xtriage
Anisotropy	0.539	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 65.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.007 for l,-k,h	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	32609	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.28% 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: TPO, PSC, PEK, MG, PGV, ZN, DMU, TGL, NA, HEA, CDL, CHD, CUA, SAC, UNX, CU, FME

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.53	0/4156	0.69	1/5678 (0.0%)
1	N	0.53	0/4156	0.68	1/5678 (0.0%)
2	B	0.52	0/1860	0.82	4/2534 (0.2%)
2	O	0.52	0/1860	0.82	3/2534 (0.1%)
3	C	0.53	0/2197	0.61	0/3005
3	P	0.52	0/2197	0.63	0/3005
4	D	0.50	0/1229	0.67	1/1658 (0.1%)
4	Q	0.51	0/1229	0.65	1/1658 (0.1%)
5	E	0.51	0/871	0.66	0/1182
5	R	0.51	0/871	0.67	0/1182
6	F	0.50	0/765	0.81	2/1038 (0.2%)
6	S	0.47	0/765	0.82	2/1038 (0.2%)
7	G	0.53	0/690	0.71	0/937
7	T	0.54	0/690	0.72	1/937 (0.1%)
8	H	0.48	0/682	0.67	0/921
8	U	0.51	0/682	0.69	0/921
9	I	0.52	0/605	0.64	0/802
9	V	0.53	0/605	0.61	0/802
10	J	0.47	0/471	0.63	0/636
10	W	0.49	0/471	0.66	0/636
11	K	0.54	0/398	0.68	0/546
11	X	0.56	0/398	0.68	0/546
12	L	0.54	0/393	0.55	0/526
12	Y	0.55	0/393	0.58	0/526
13	M	0.47	0/345	0.62	0/470
13	Z	0.45	0/345	0.62	0/470
All	All	0.52	0/29324	0.69	16/39866 (0.0%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	N	0	2
2	B	0	2
2	O	0	1
8	U	0	1
All	All	0	7

There are no bond length outliers.

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	103	GLN	CA-C-N	-6.93	101.94	117.20
6	S	94	HIS	N-CA-C	6.19	127.71	111.00
4	D	133	GLY	N-CA-C	6.09	128.33	113.10
2	O	103	GLN	CA-C-N	-6.04	103.91	117.20
6	F	94	HIS	N-CA-C	5.98	127.14	111.00

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
2	B	103	GLN	Mainchain
2	B	85	TYR	Sidechain
1	N	240	HIS	Sidechain
1	N	304	TYR	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4027	0	4001	60	0
1	N	4027	0	4001	80	0
2	B	1824	0	1833	27	0
2	O	1824	0	1833	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	2110	0	2027	27	0
3	P	2110	0	2027	26	0
4	D	1195	0	1183	13	0
4	Q	1195	0	1183	28	0
5	E	852	0	845	6	0
5	R	852	0	845	8	0
6	F	748	0	728	13	0
6	S	748	0	728	19	0
7	G	675	0	643	26	0
7	T	675	0	643	25	0
8	H	662	0	623	3	0
8	U	662	0	623	6	0
9	I	601	0	613	7	0
9	V	601	0	613	6	0
10	J	460	0	459	4	0
10	W	460	0	459	4	0
11	K	384	0	366	5	0
11	X	384	0	366	10	0
12	L	380	0	380	13	0
12	Y	380	0	380	11	0
13	M	335	0	352	6	0
13	Z	335	0	352	3	0
14	A	1	0	0	0	0
14	N	1	0	0	0	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	120	0	108	5	0
17	N	120	0	108	6	0
18	A	189	0	330	47	0
18	N	126	0	220	41	0
18	Q	63	0	110	6	0
19	A	102	0	152	7	0
19	C	102	0	152	9	0
19	N	102	0	152	6	0
19	P	102	0	152	6	0
20	B	2	0	0	0	0
20	O	2	0	0	0	0
21	B	29	0	39	1	0
21	C	58	0	78	4	0
21	J	29	0	39	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	O	29	0	39	0	0
21	P	58	0	78	2	0
21	W	29	0	39	3	0
22	C	100	0	156	23	0
22	G	100	0	156	17	0
22	P	100	0	156	20	0
22	T	100	0	156	20	0
23	C	106	0	154	13	0
23	G	53	0	77	6	0
23	P	106	0	154	8	0
23	T	53	0	77	8	0
24	C	1	0	0	0	0
24	P	1	0	0	0	0
25	E	52	0	80	12	0
25	O	52	0	80	11	0
26	F	1	0	0	0	0
26	S	1	0	0	0	0
27	M	33	0	37	0	0
27	Z	33	0	37	0	0
28	A	229	0	0	6	0
28	B	167	0	0	2	0
28	C	107	0	0	4	0
28	D	112	0	0	3	0
28	E	90	0	0	1	0
28	F	109	0	0	1	0
28	G	54	0	0	3	0
28	H	61	0	0	2	0
28	I	50	0	0	3	0
28	J	34	0	0	2	0
28	K	28	0	0	0	0
28	L	21	0	0	1	0
28	M	33	0	0	1	0
28	N	214	0	0	3	0
28	O	116	0	0	1	0
28	P	112	0	0	4	0
28	Q	72	0	0	3	0
28	R	48	0	0	0	0
28	S	77	0	0	3	0
28	T	48	0	0	2	0
28	U	54	0	0	1	0
28	V	32	0	0	2	0
28	W	20	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	X	20	0	0	1	0
28	Y	22	0	0	0	0
28	Z	13	0	0	1	0
All	All	32609	0	31222	568	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 9.

The worst 5 of 568 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)
7:T:84:LYS:HD2	7:T:84:LYS:H	1.21	1.03
7:G:84:LYS:H	7:G:84:LYS:HD2	1.21	1.03
10:W:33:ARG:HG2	21:W:4060:CHD:H152	1.42	0.99
18:A:3522:TGL:HC32	12:L:20:ARG:HH22	1.29	0.98
4:D:34:SER:H	4:D:37:GLN:HE21	1.14	0.92

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	512/514 (100%)	500 (98%)	12 (2%)	0	100 100
1	N	512/514 (100%)	500 (98%)	12 (2%)	0	100 100
2	B	225/227 (99%)	210 (93%)	12 (5%)	3 (1%)	12 4
2	O	225/227 (99%)	208 (92%)	14 (6%)	3 (1%)	12 4
3	C	257/261 (98%)	251 (98%)	5 (2%)	1 (0%)	34 24
3	P	257/261 (98%)	251 (98%)	6 (2%)	0	100 100
4	D	142/147 (97%)	139 (98%)	3 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	Q	142/147 (97%)	139 (98%)	3 (2%)	0	100	100
5	E	103/109 (94%)	103 (100%)	0	0	100	100
5	R	103/109 (94%)	102 (99%)	1 (1%)	0	100	100
6	F	96/98 (98%)	89 (93%)	4 (4%)	3 (3%)	4	0
6	S	96/98 (98%)	91 (95%)	2 (2%)	3 (3%)	4	0
7	G	81/85 (95%)	66 (82%)	8 (10%)	7 (9%)	1	0
7	T	81/85 (95%)	65 (80%)	9 (11%)	7 (9%)	1	0
8	H	77/85 (91%)	70 (91%)	4 (5%)	3 (4%)	3	0
8	U	77/85 (91%)	70 (91%)	5 (6%)	2 (3%)	5	1
9	I	71/73 (97%)	68 (96%)	3 (4%)	0	100	100
9	V	71/73 (97%)	68 (96%)	3 (4%)	0	100	100
10	J	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
10	W	56/59 (95%)	56 (100%)	0	0	100	100
11	K	47/56 (84%)	47 (100%)	0	0	100	100
11	X	47/56 (84%)	47 (100%)	0	0	100	100
12	L	44/47 (94%)	42 (96%)	2 (4%)	0	100	100
12	Y	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
13	M	41/46 (89%)	40 (98%)	1 (2%)	0	100	100
13	Z	41/46 (89%)	40 (98%)	1 (2%)	0	100	100
All	All	3504/3614 (97%)	3360 (96%)	112 (3%)	32 (1%)	17	7

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	95	GLN
7	G	4	ALA
7	G	7	ASP
7	G	8	HIS
7	G	39	SER

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	426/426 (100%)	415 (97%)	11 (3%)	46	39
1	N	426/426 (100%)	416 (98%)	10 (2%)	50	45
2	B	210/210 (100%)	198 (94%)	12 (6%)	20	11
2	O	210/210 (100%)	198 (94%)	12 (6%)	20	11
3	C	224/226 (99%)	220 (98%)	4 (2%)	59	55
3	P	224/226 (99%)	219 (98%)	5 (2%)	52	47
4	D	128/129 (99%)	127 (99%)	1 (1%)	81	82
4	Q	128/129 (99%)	125 (98%)	3 (2%)	50	45
5	E	92/95 (97%)	91 (99%)	1 (1%)	73	73
5	R	92/95 (97%)	89 (97%)	3 (3%)	38	29
6	F	81/81 (100%)	77 (95%)	4 (5%)	25	15
6	S	81/81 (100%)	76 (94%)	5 (6%)	18	9
7	G	67/68 (98%)	59 (88%)	8 (12%)	5	1
7	T	67/68 (98%)	60 (90%)	7 (10%)	7	2
8	H	71/75 (95%)	69 (97%)	2 (3%)	43	36
8	U	71/75 (95%)	67 (94%)	4 (6%)	21	11
9	I	57/57 (100%)	55 (96%)	2 (4%)	36	27
9	V	57/57 (100%)	54 (95%)	3 (5%)	22	13
10	J	49/50 (98%)	48 (98%)	1 (2%)	55	51
10	W	49/50 (98%)	48 (98%)	1 (2%)	55	51
11	K	39/46 (85%)	37 (95%)	2 (5%)	24	14
11	X	39/46 (85%)	38 (97%)	1 (3%)	46	39
12	L	39/40 (98%)	38 (97%)	1 (3%)	46	39
12	Y	39/40 (98%)	37 (95%)	2 (5%)	24	14
13	M	37/38 (97%)	33 (89%)	4 (11%)	6	2
13	Z	37/38 (97%)	33 (89%)	4 (11%)	6	2
All	All	3040/3082 (99%)	2927 (96%)	113 (4%)	34	25

5 of 113 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	241	PRO
13	Z	34	LEU
2	O	94	SER
13	Z	13	LYS
8	U	29	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
3	P	68	GLN
7	T	71	HIS
4	Q	37	GLN
6	S	54	ASN
4	D	143	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)

8 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	2.78	2 (28%)	8,9,11	3.15	5 (62%)
2	FME	O	1	2	8,9,10	0.72	0	7,9,11	2.27	2 (28%)
2	FME	B	1	2	8,9,10	0.85	0	7,9,11	1.71	2 (28%)
7	TPO	T	11	7	8,10,11	1.40	1 (12%)	10,14,16	1.00	0
1	FME	N	1	1	8,9,10	0.77	0	7,9,11	1.83	2 (28%)
7	TPO	G	11	7	8,10,11	1.31	1 (12%)	10,14,16	1.02	0
1	FME	A	1	1	8,9,10	0.68	0	7,9,11	1.26	1 (14%)
9	SAC	I	1	9	7,8,9	2.46	2 (28%)	8,9,11	2.99	5 (62%)

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	-
2	FME	O	1	2	-	1/7/9/11	-
2	FME	B	1	2	-	1/7/9/11	-
7	TPO	T	11	7	-	5/9/11/13	-
1	FME	N	1	1	-	3/7/9/11	-
7	TPO	G	11	7	-	4/9/11/13	-
1	FME	A	1	1	-	3/7/9/11	-
9	SAC	I	1	9	-	3/7/8/10	-

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	V	1	SAC	OAC-C1A	5.17	1.34	1.23
9	I	1	SAC	OAC-C1A	4.97	1.34	1.23
9	V	1	SAC	CA-N	4.80	1.53	1.46
9	I	1	SAC	CA-N	3.93	1.51	1.46
7	T	11	TPO	CB-CA	2.65	1.59	1.53

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	V	1	SAC	CA-N-C1A	-6.58	111.00	123.15
9	I	1	SAC	CA-N-C1A	-6.27	111.58	123.15
2	O	1	FME	C-CA-N	4.38	117.64	109.73
1	N	1	FME	CA-N-CN	-4.22	116.33	122.82
2	O	1	FME	CA-N-CN	-3.93	116.77	122.82

There are no chirality outliers.

5 of 23 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
2	B	1	FME	O1-CN-N-CA
7	G	11	TPO	N-CA-CB-CG2
7	G	11	TPO	N-CA-CB-OG1

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	T	11	TPO	1	0
1	N	1	FME	1	0
1	A	1	FME	5	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 52 ligands modelled in this entry, 8 are monoatomic and 2 are unknown - leaving 42 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	$\#\|Z\| > 2$
18	TGL	A	3522	-	62,62,62	1.39	6 (9%)	65,65,65	1.20	5 (7%)
23	PEK	P	4265	-	52,52,52	1.64	11 (21%)	55,57,57	0.95	4 (7%)
20	CUA	O	228	2	0,1,1	-	-	-		
23	PEK	T	3263	-	52,52,52	1.64	10 (19%)	55,57,57	0.97	3 (5%)
23	PEK	P	4264	-	52,52,52	1.42	6 (11%)	55,57,57	1.23	7 (12%)
17	HEA	N	515	1	57,67,67	1.16	5 (8%)	61,103,103	1.16	5 (8%)
18	TGL	A	3523	-	62,62,62	1.07	3 (4%)	65,65,65	1.06	4 (6%)
19	PGV	N	4266	-	50,50,50	0.90	2 (4%)	53,56,56	0.79	3 (5%)
27	DMU	M	3526	-	34,34,34	3.26	8 (23%)	45,45,45	4.08	20 (44%)
21	CHD	W	4060	-	32,32,32	1.16	3 (9%)	51,51,51	3.30	26 (50%)
19	PGV	A	3524	-	50,50,50	1.08	3 (6%)	53,56,56	1.05	6 (11%)
22	CDL	G	3269	-	99,99,99	0.97	7 (7%)	105,111,111	0.88	6 (5%)
22	CDL	P	4270	-	99,99,99	0.75	1 (1%)	105,111,111	0.86	5 (4%)
23	PEK	G	4263	-	52,52,52	1.60	9 (17%)	55,57,57	0.99	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
18	TGL	N	4521	-	62,62,62	1.12	4 (6%)	65,65,65	1.09	5 (7%)
19	PGV	P	4268	-	50,50,50	1.07	3 (6%)	53,56,56	0.69	0
17	HEA	A	515	1	57,67,67	1.12	4 (7%)	61,103,103	1.30	6 (9%)
25	PSC	E	3230	-	51,51,51	1.20	3 (5%)	57,59,59	1.05	4 (7%)
19	PGV	N	4524	-	50,50,50	1.11	4 (8%)	53,56,56	1.02	3 (5%)
23	PEK	C	3264	-	52,52,52	1.42	5 (9%)	55,57,57	1.19	7 (12%)
17	HEA	N	516	1	57,67,67	1.11	5 (8%)	61,103,103	1.33	9 (14%)
21	CHD	P	4271	-	32,32,32	0.82	0	51,51,51	3.57	24 (47%)
19	PGV	A	3266	-	50,50,50	0.86	1 (2%)	53,56,56	0.72	0
19	PGV	C	3267	-	50,50,50	0.80	1 (2%)	53,56,56	0.86	2 (3%)
22	CDL	C	3270	-	99,99,99	0.74	1 (1%)	105,111,111	0.86	5 (4%)
23	PEK	C	3265	-	52,52,52	1.61	8 (15%)	55,57,57	0.96	4 (7%)
18	TGL	A	3521	-	62,62,62	1.09	4 (6%)	65,65,65	1.12	5 (7%)
21	CHD	B	4085	-	32,32,32	0.80	1 (3%)	51,51,51	1.83	15 (29%)
21	CHD	P	4525	-	32,32,32	0.82	1 (3%)	51,51,51	1.62	9 (17%)
18	TGL	Q	4523	-	62,62,62	1.10	3 (4%)	65,65,65	1.04	5 (7%)
21	CHD	J	3060	-	32,32,32	1.12	2 (6%)	51,51,51	3.26	26 (50%)
21	CHD	C	3271	-	32,32,32	0.87	0	51,51,51	3.59	24 (47%)
22	CDL	T	4269	-	99,99,99	0.96	5 (5%)	105,111,111	0.90	6 (5%)
25	PSC	O	4230	-	51,51,51	1.20	3 (5%)	57,59,59	1.04	4 (7%)
21	CHD	O	3085	-	32,32,32	0.84	1 (3%)	51,51,51	1.88	16 (31%)
19	PGV	C	3268	-	50,50,50	1.07	3 (6%)	53,56,56	0.69	1 (1%)
19	PGV	P	4267	-	50,50,50	0.83	1 (2%)	53,56,56	0.86	1 (1%)
27	DMU	Z	4526	-	34,34,34	3.22	9 (26%)	45,45,45	4.06	20 (44%)
18	TGL	N	4522	-	62,62,62	1.44	8 (12%)	65,65,65	1.18	4 (6%)
20	CUA	B	228	2	0,1,1	-	-	-		
21	CHD	C	3525	-	32,32,32	0.89	0	51,51,51	1.66	11 (21%)
17	HEA	A	516	1	57,67,67	1.15	5 (8%)	61,103,103	1.35	9 (14%)

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
18	TGL	A	3522	-	-	32/65/65/65	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	PEK	P	4265	-	-	20/56/56/56	-
23	PEK	T	3263	-	-	25/56/56/56	-
23	PEK	P	4264	-	-	21/56/56/56	-
17	HEA	N	515	1	-	2/32/76/76	-
18	TGL	A	3523	-	-	25/65/65/65	-
27	DMU	M	3526	-	5/5/10/10	10/19/59/59	0/2/2/2
19	PGV	N	4266	-	-	13/55/55/55	-
21	CHD	W	4060	-	5/5/12/12	8/9/74/74	0/4/4/4
19	PGV	A	3524	-	-	30/55/55/55	-
22	CDL	G	3269	-	-	66/110/110/110	-
22	CDL	P	4270	-	-	77/110/110/110	-
23	PEK	G	4263	-	-	25/56/56/56	-
18	TGL	N	4521	-	-	31/65/65/65	-
19	PGV	P	4268	-	-	29/55/55/55	-
17	HEA	A	515	1	-	3/32/76/76	-
25	PSC	E	3230	-	-	34/55/55/55	-
19	PGV	N	4524	-	-	31/55/55/55	-
23	PEK	C	3264	-	-	21/56/56/56	-
17	HEA	N	516	1	-	7/32/76/76	-
21	CHD	P	4271	-	5/5/12/12	8/9/74/74	0/4/4/4
19	PGV	A	3266	-	-	13/55/55/55	-
19	PGV	C	3267	-	-	16/55/55/55	-
22	CDL	C	3270	-	-	77/110/110/110	-
23	PEK	C	3265	-	-	20/56/56/56	-
18	TGL	A	3521	-	-	31/65/65/65	-
21	CHD	B	4085	-	-	2/9/74/74	0/4/4/4
21	CHD	P	4525	-	-	2/9/74/74	0/4/4/4
18	TGL	Q	4523	-	-	25/65/65/65	-
21	CHD	J	3060	-	5/5/12/12	8/9/74/74	0/4/4/4
21	CHD	C	3271	-	5/5/12/12	8/9/74/74	0/4/4/4
22	CDL	T	4269	-	-	67/110/110/110	-
25	PSC	O	4230	-	-	33/55/55/55	-
21	CHD	O	3085	-	-	2/9/74/74	0/4/4/4
19	PGV	C	3268	-	-	29/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	PGV	P	4267	-	-	16/55/55/55	-
27	DMU	Z	4526	-	5/5/10/10	10/19/59/59	0/2/2/2
18	TGL	N	4522	-	-	32/65/65/65	-
21	CHD	C	3525	-	-	2/9/74/74	0/4/4/4
17	HEA	A	516	1	-	7/32/76/76	-

The worst 5 of 159 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	M	3526	DMU	O7-C3	-8.12	1.22	1.43
27	Z	4526	DMU	O16-C6	-7.94	1.26	1.40
27	M	3526	DMU	O16-C6	-7.77	1.26	1.40
27	Z	4526	DMU	O7-C3	-7.61	1.24	1.43
27	M	3526	DMU	O5-C4	-7.12	1.27	1.44

The worst 5 of 322 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	M	3526	DMU	C10-C5-C7	10.25	131.34	110.00
27	Z	4526	DMU	C10-C5-C7	10.20	131.24	110.00
21	P	4271	CHD	C17-C13-C14	9.90	110.08	100.09
21	C	3271	CHD	C17-C13-C14	9.71	109.88	100.09
21	P	4271	CHD	C10-C9-C8	8.91	121.38	111.82

5 of 30 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
21	C	3271	CHD	C8
21	C	3271	CHD	C3
21	C	3271	CHD	C14
21	C	3271	CHD	C9
21	C	3271	CHD	C12

5 of 918 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	A	3521	TGL	CB2-CB1-OG2-CG2
18	A	3521	TGL	OB1-CB1-OG2-CG2
18	A	3523	TGL	OB1-CB1-OG2-CG2
18	N	4521	TGL	CB2-CB1-OG2-CG2
18	N	4521	TGL	OB1-CB1-OG2-CG2

There are no ring outliers.

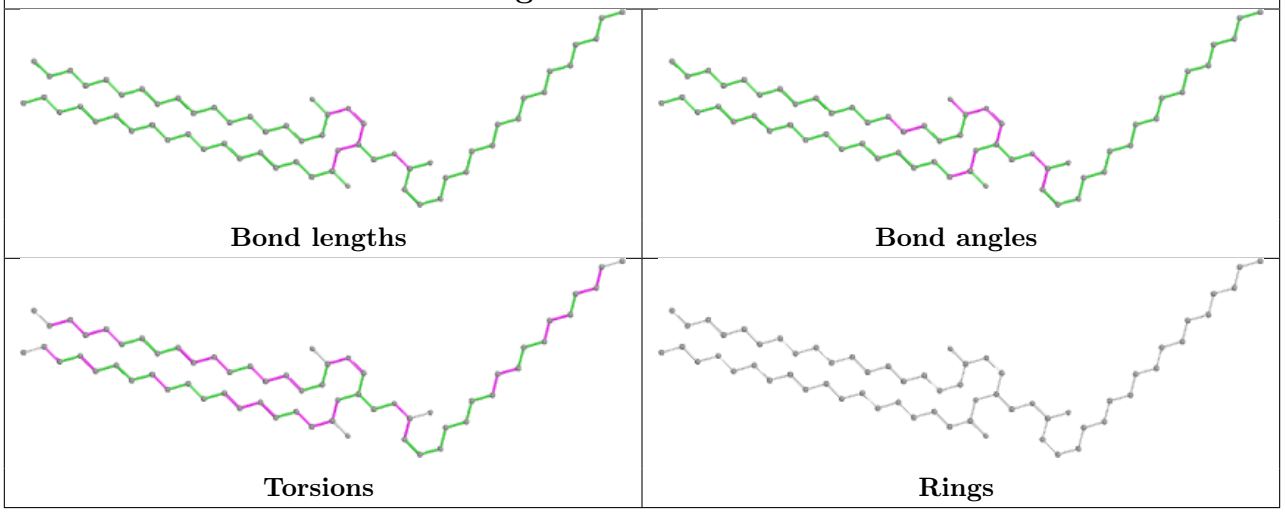
33 monomers are involved in 278 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A	3522	TGL	25	0
23	P	4265	PEK	4	0
23	T	3263	PEK	8	0
23	P	4264	PEK	4	0
17	N	515	HEA	3	0
18	A	3523	TGL	6	0
21	W	4060	CHD	3	0
19	A	3524	PGV	7	0
22	G	3269	CDL	17	0
22	P	4270	CDL	20	0
23	G	4263	PEK	6	0
18	N	4521	TGL	24	0
19	P	4268	PGV	3	0
17	A	515	HEA	2	0
25	E	3230	PSC	12	0
19	N	4524	PGV	6	0
23	C	3264	PEK	4	0
17	N	516	HEA	3	0
21	P	4271	CHD	2	0
19	C	3267	PGV	6	0
22	C	3270	CDL	23	0
23	C	3265	PEK	9	0
18	A	3521	TGL	16	0
21	B	4085	CHD	1	0
18	Q	4523	TGL	6	0
21	J	3060	CHD	3	0
21	C	3271	CHD	4	0
22	T	4269	CDL	20	0
25	O	4230	PSC	11	0
19	C	3268	PGV	3	0
19	P	4267	PGV	3	0
18	N	4522	TGL	17	0
17	A	516	HEA	3	0

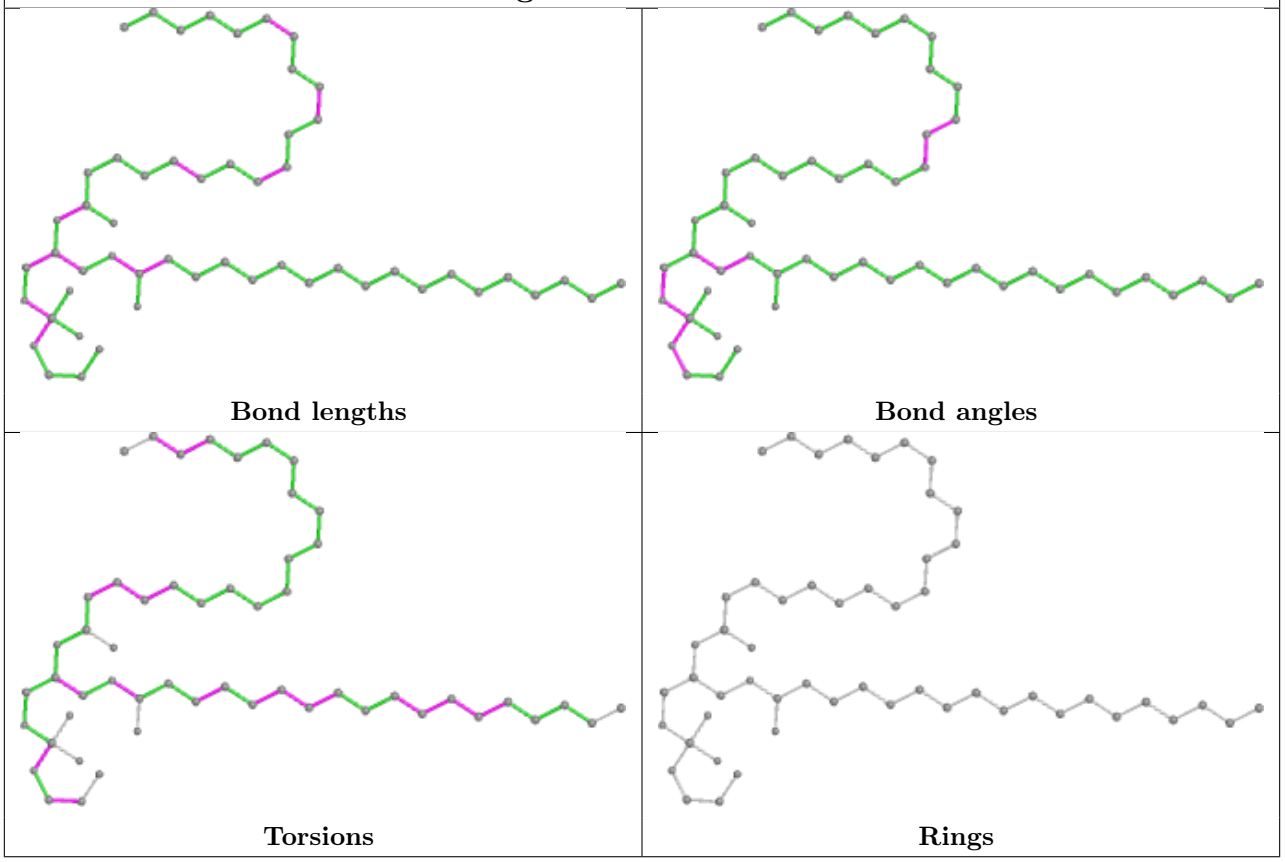
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

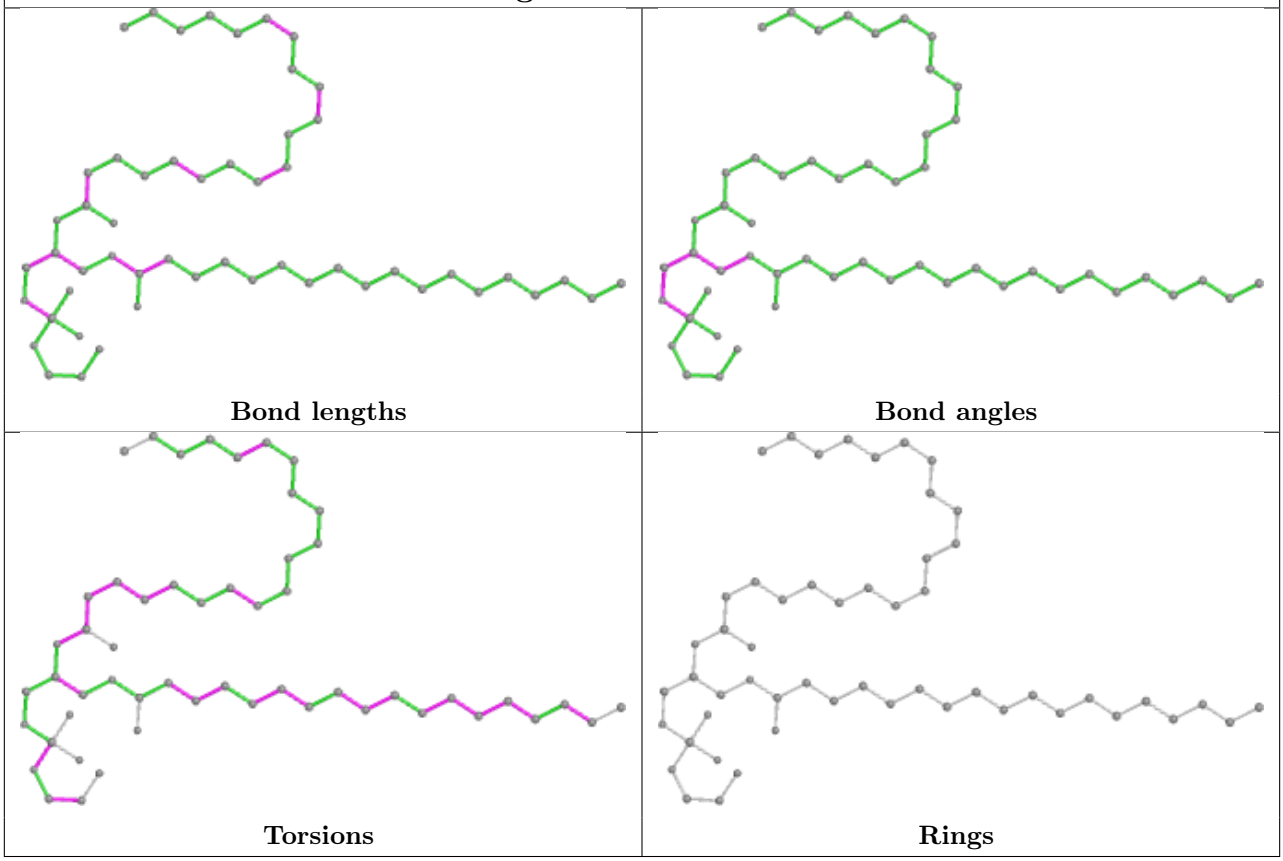
Ligand TGL A 3522



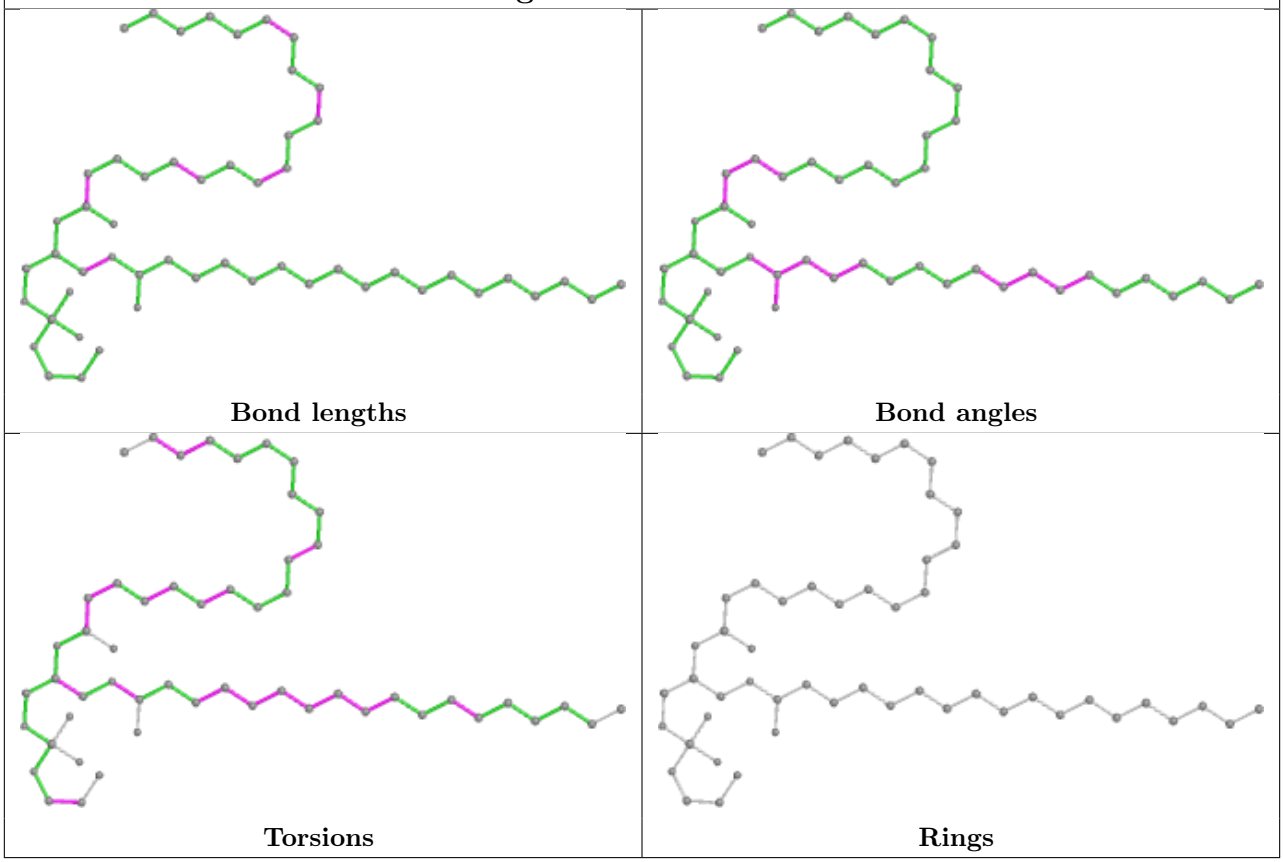
Ligand PEK P 4265



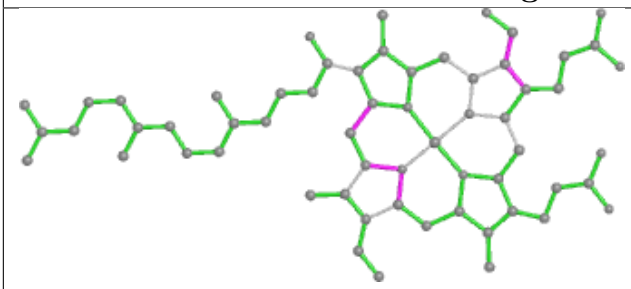
Ligand PEK T 3263



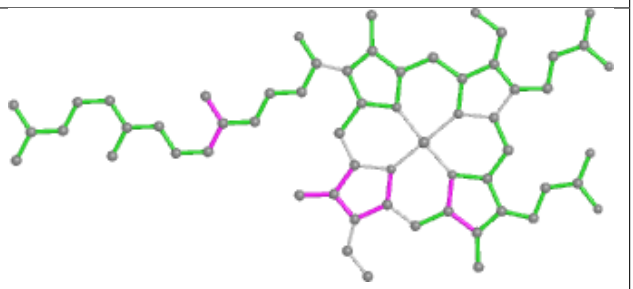
Ligand PEK P 4264



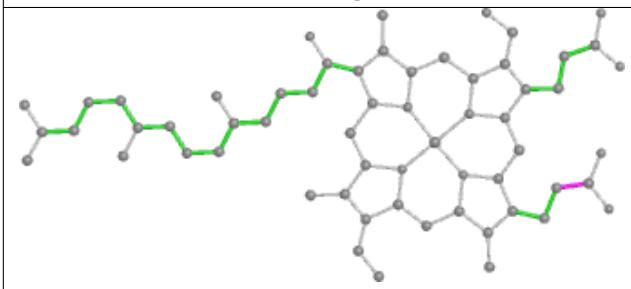
Ligand HEA N 515



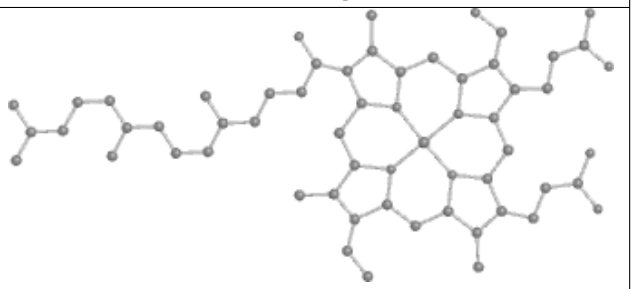
Bond lengths



Bond angles

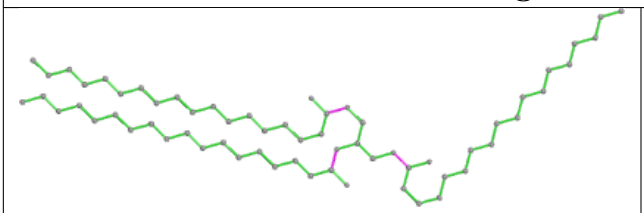


Torsions

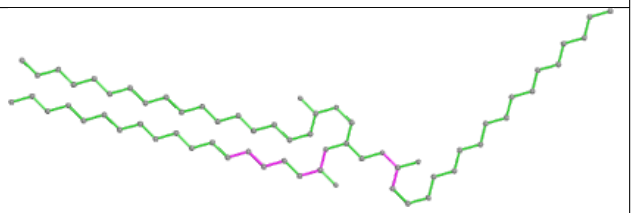


Rings

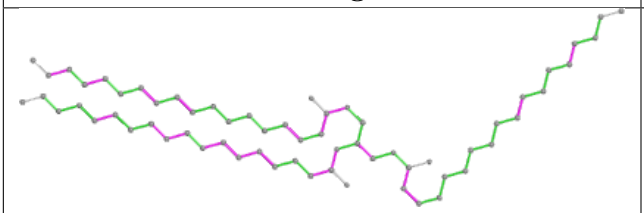
Ligand TGL A 3523



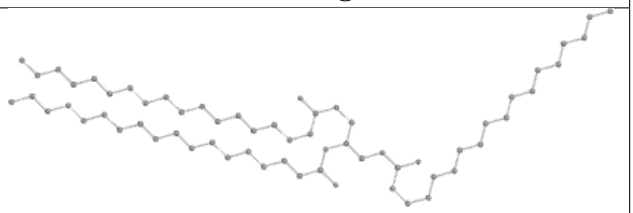
Bond lengths



Bond angles

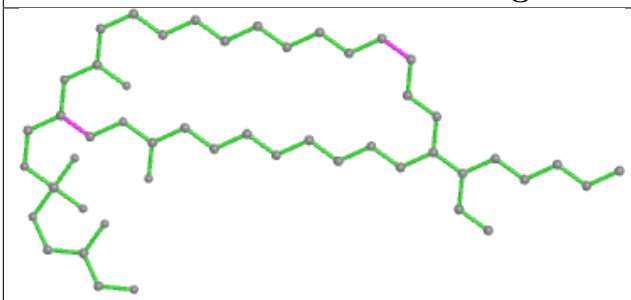


Torsions

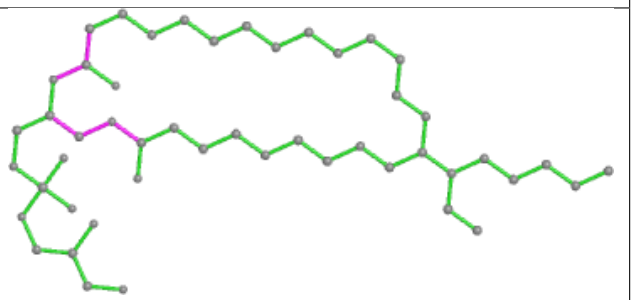


Rings

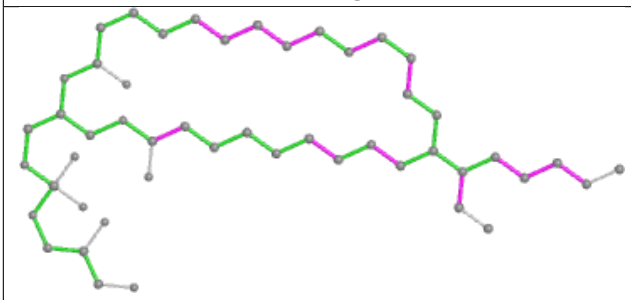
Ligand PGV N 4266



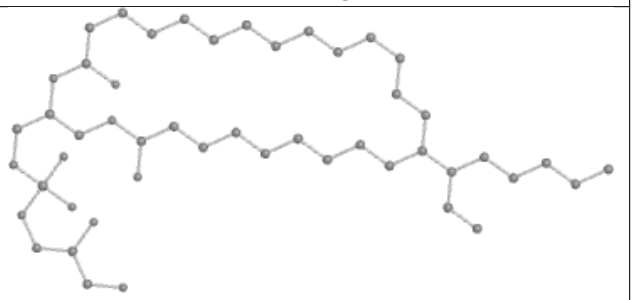
Bond lengths



Bond angles

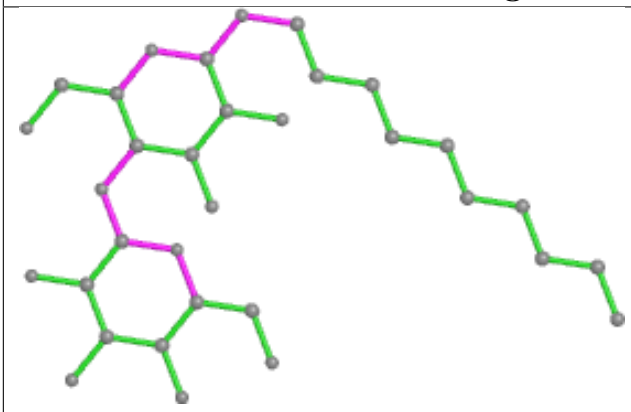


Torsions

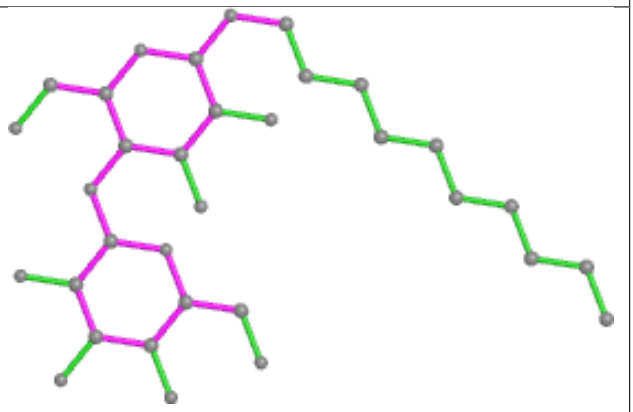


Rings

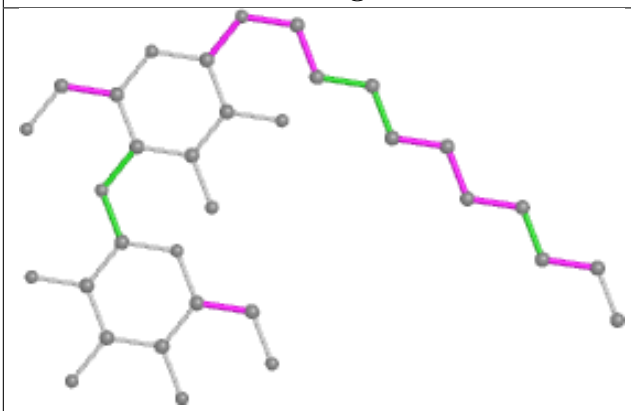
Ligand DMU M 3526



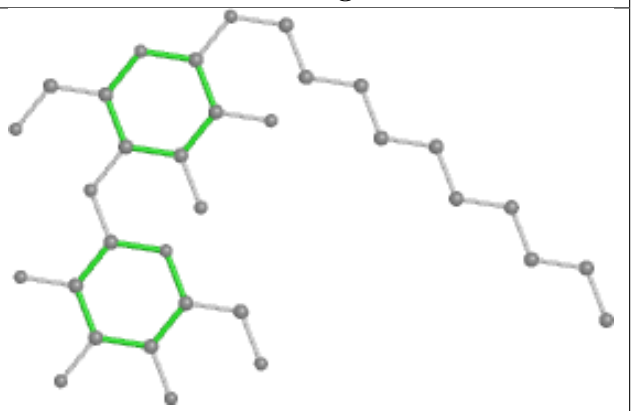
Bond lengths



Bond angles

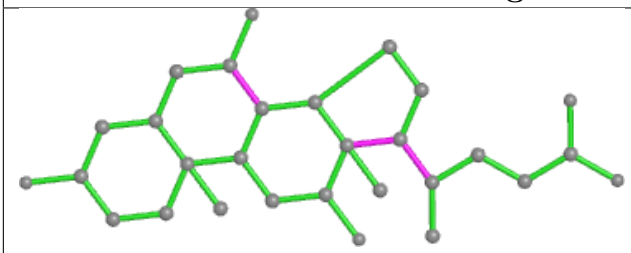


Torsions

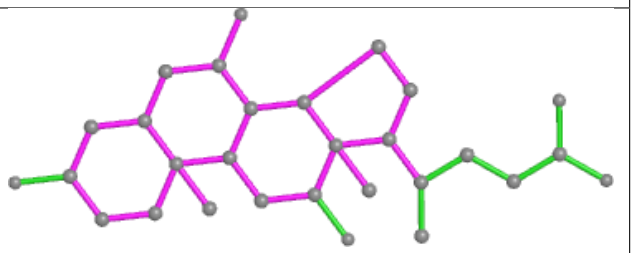


Rings

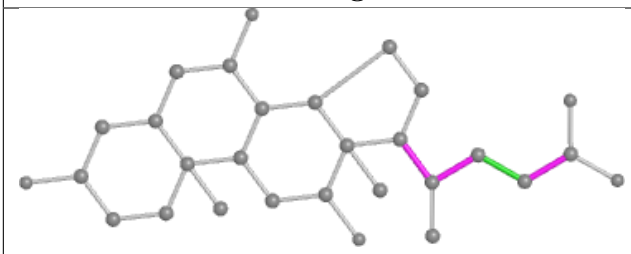
Ligand CHD W 4060



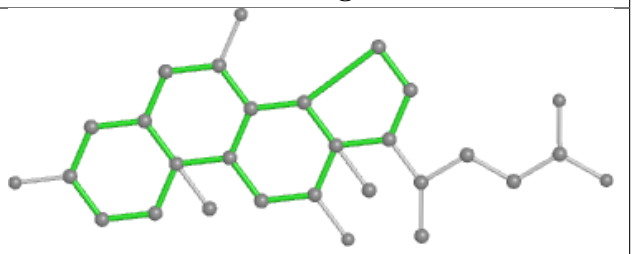
Bond lengths



Bond angles

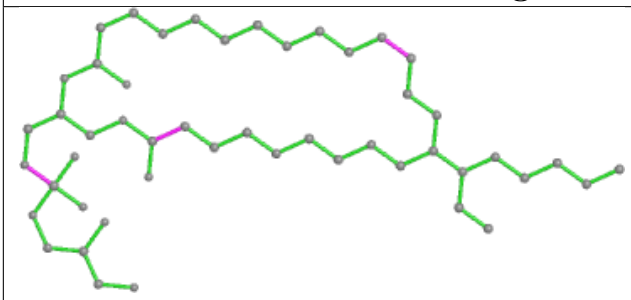


Torsions

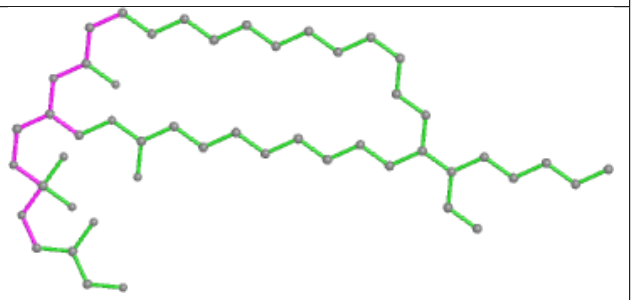


Rings

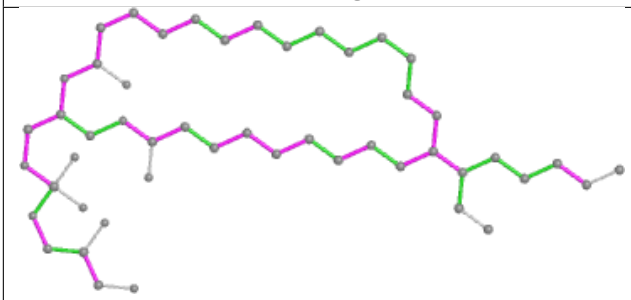
Ligand PGV A 3524



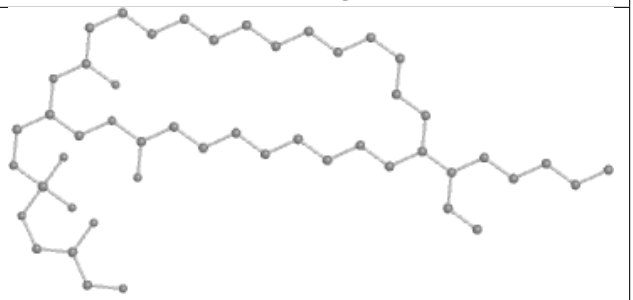
Bond lengths



Bond angles

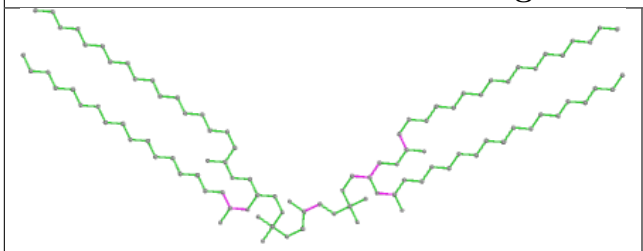


Torsions

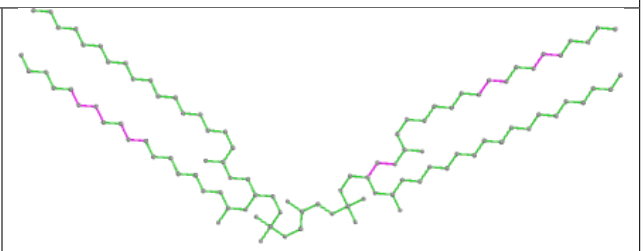


Rings

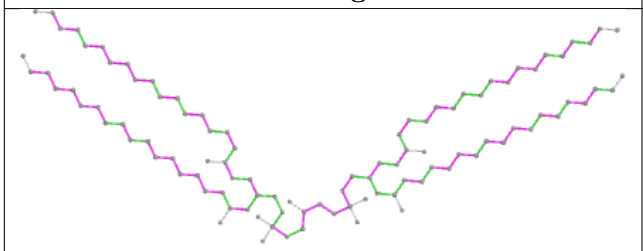
Ligand CDL G 3269



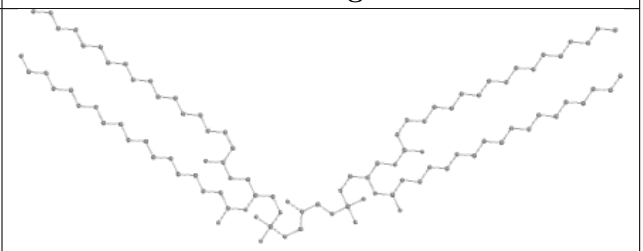
Bond lengths



Bond angles

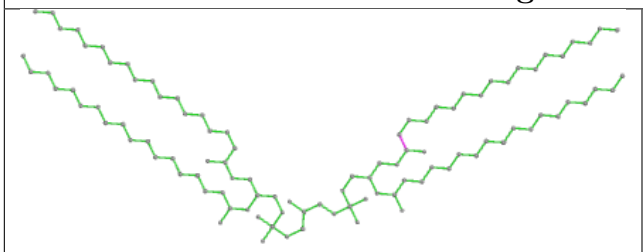


Torsions

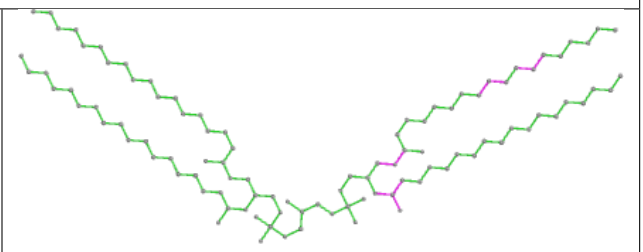


Rings

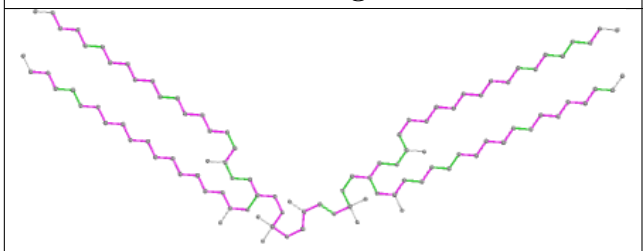
Ligand CDL P 4270



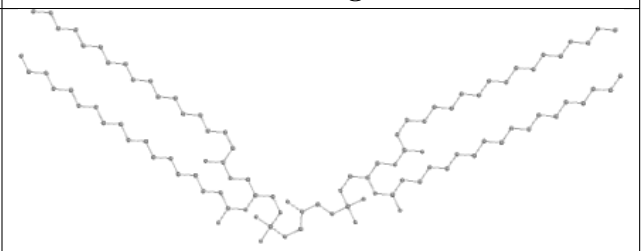
Bond lengths



Bond angles

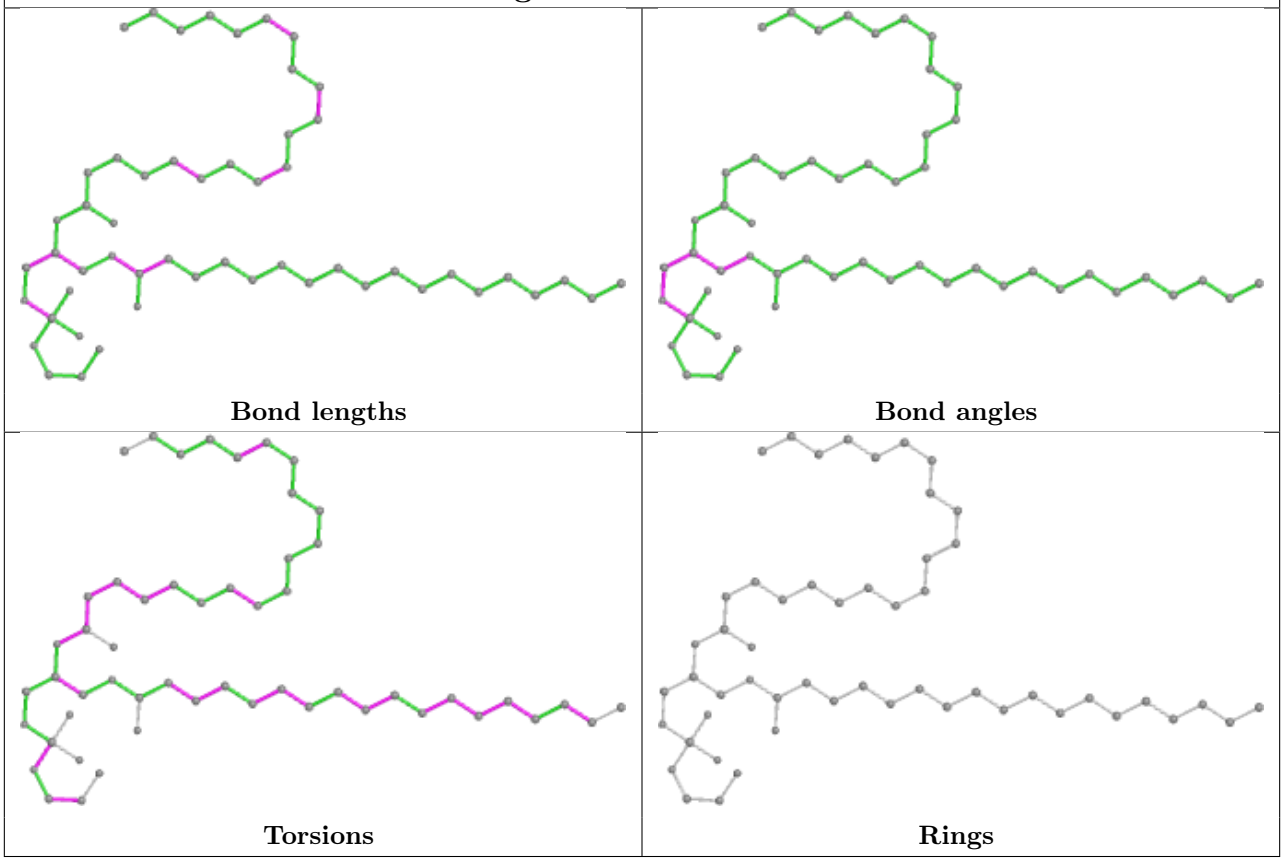


Torsions

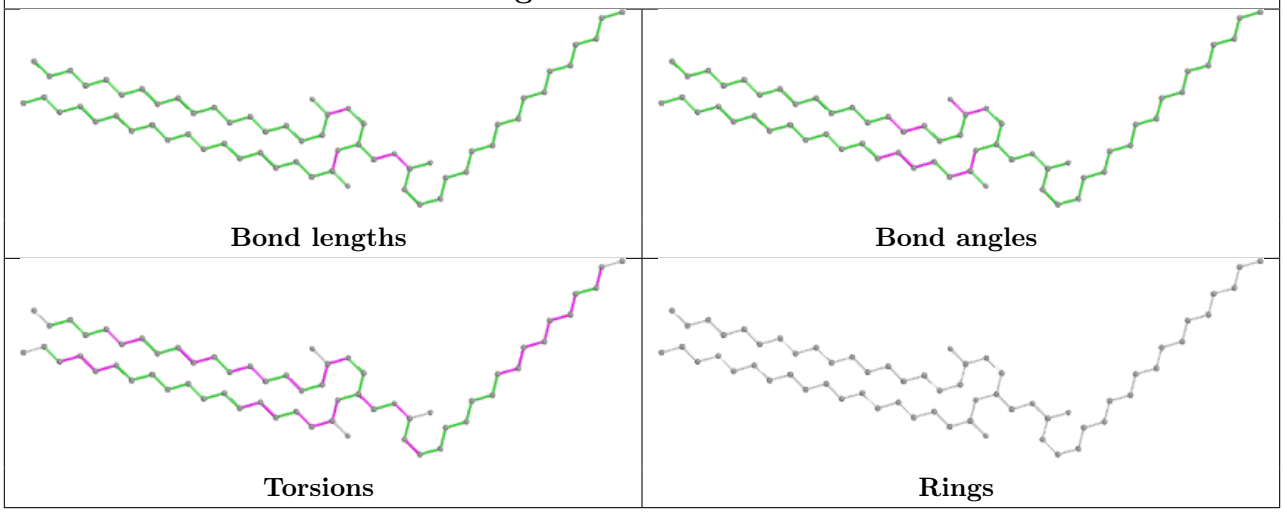


Rings

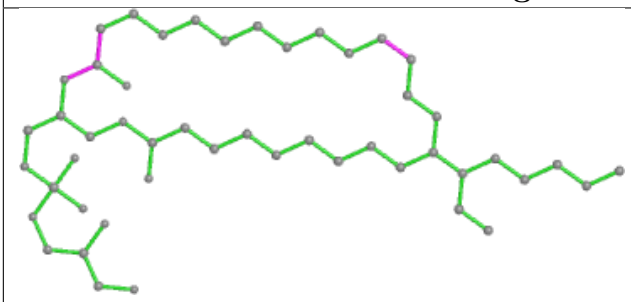
Ligand PEK G 4263



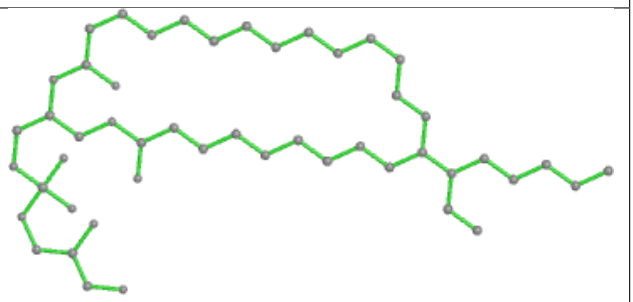
Ligand TGL N 4521



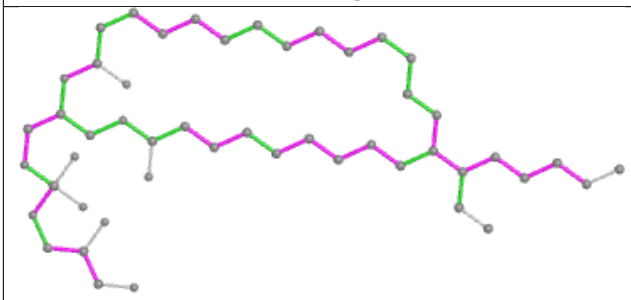
Ligand PGV P 4268



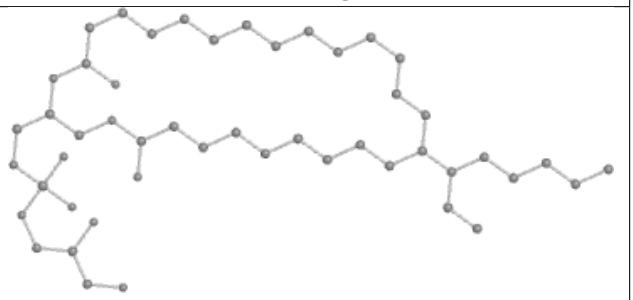
Bond lengths



Bond angles

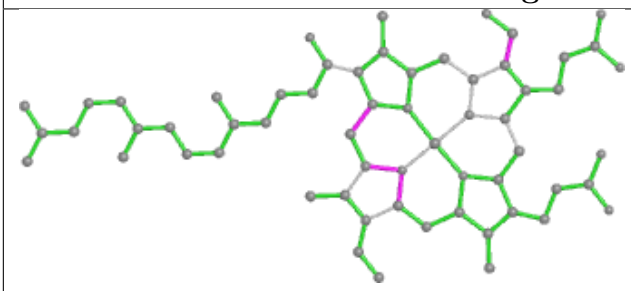


Torsions

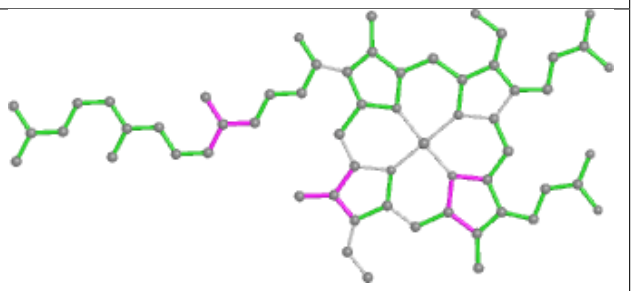


Rings

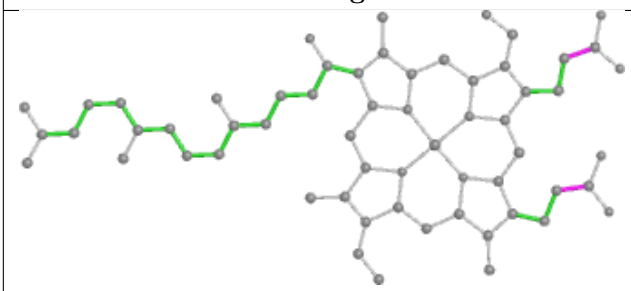
Ligand HEA A 515



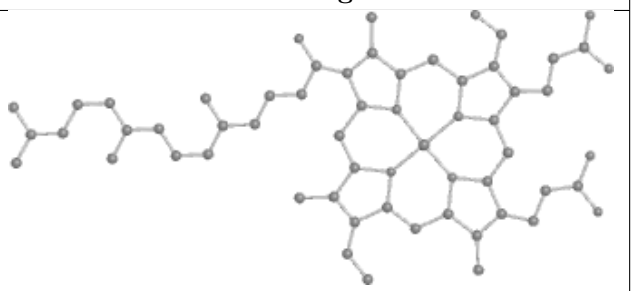
Bond lengths



Bond angles

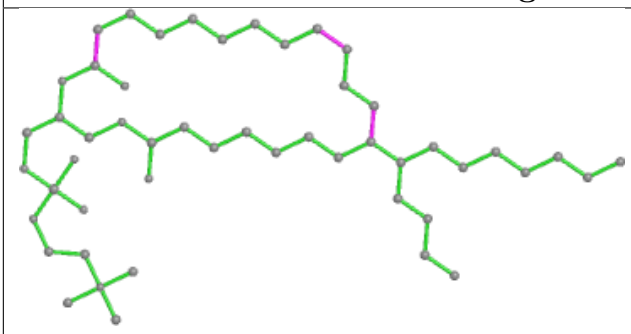


Torsions

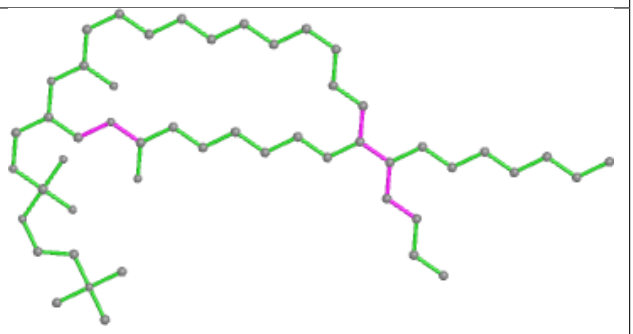


Rings

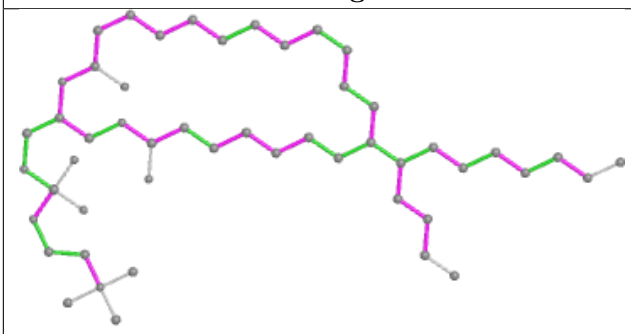
Ligand PSC E 3230



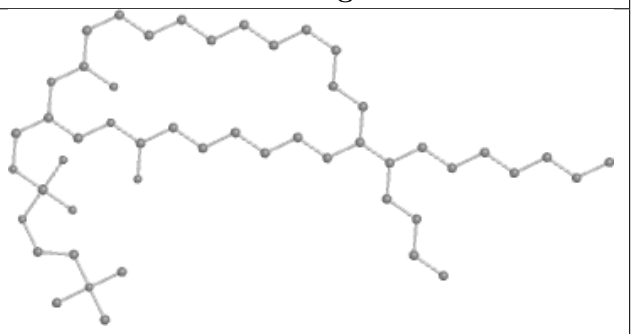
Bond lengths



Bond angles

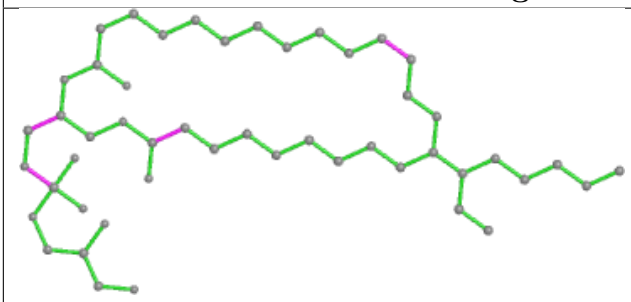


Torsions

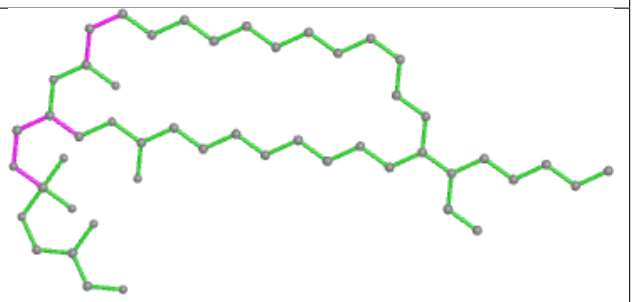


Rings

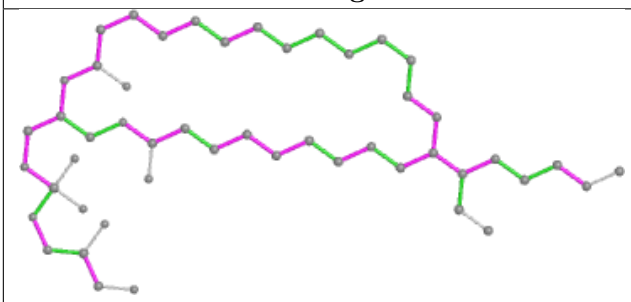
Ligand PGV N 4524



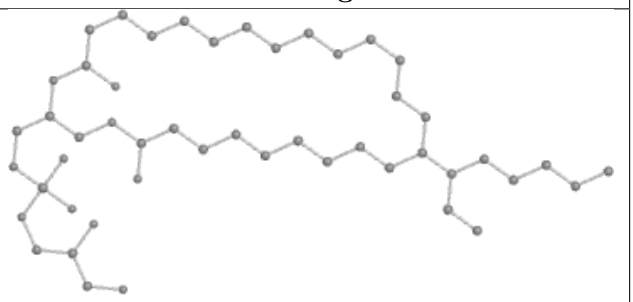
Bond lengths



Bond angles

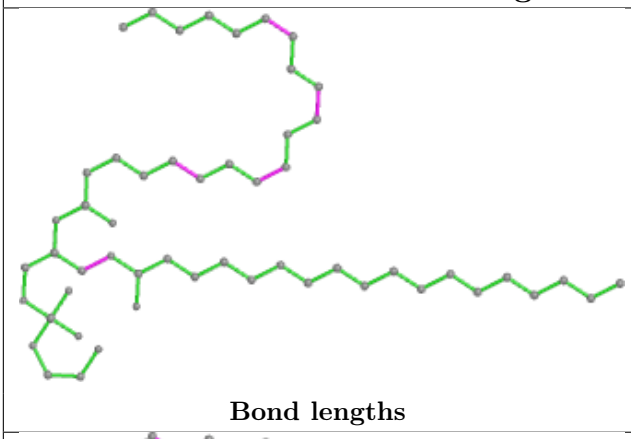


Torsions

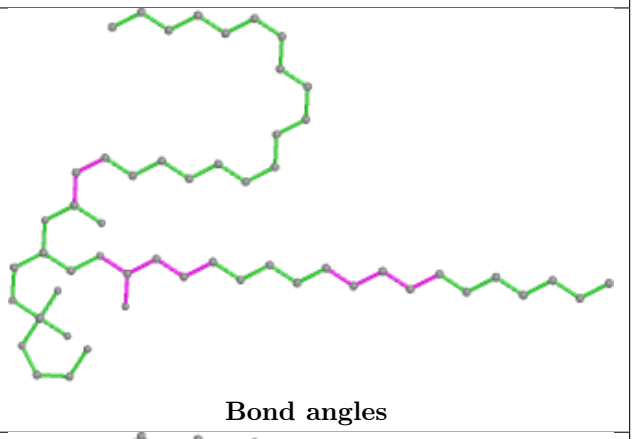


Rings

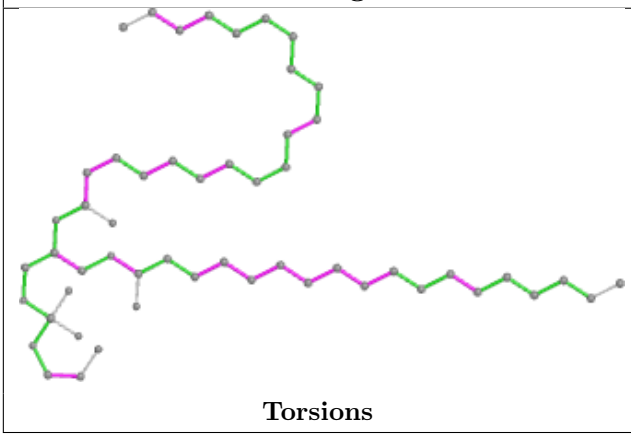
Ligand PEK C 3264



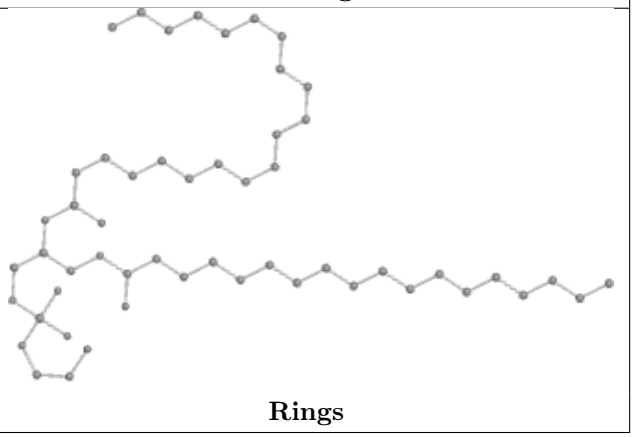
Bond lengths



Bond angles

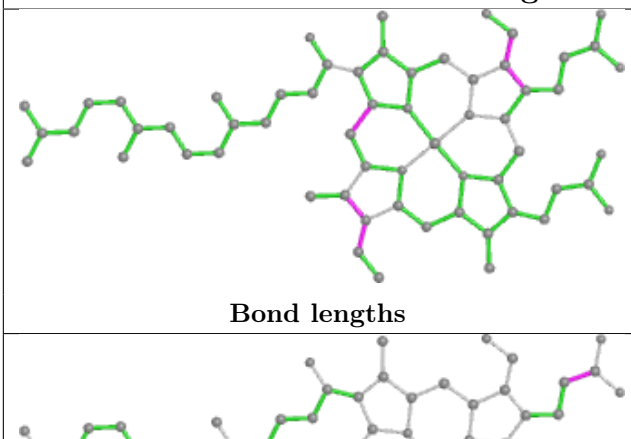


Torsions



Rings

Ligand HEA N 516



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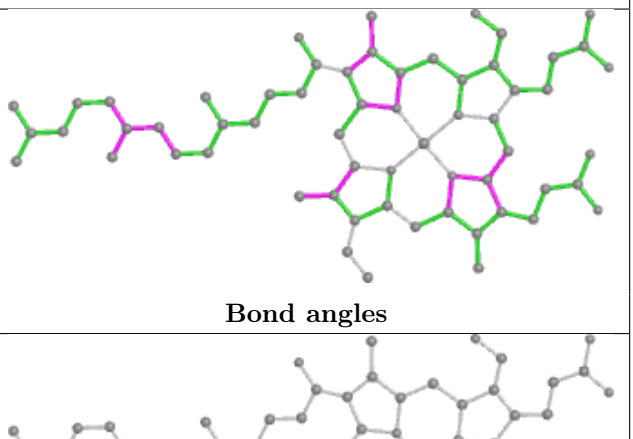
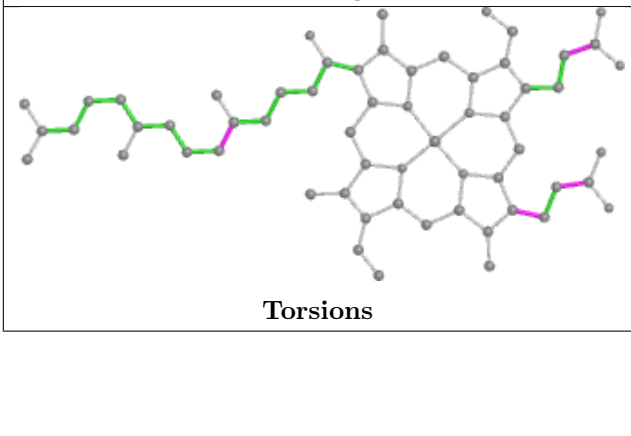
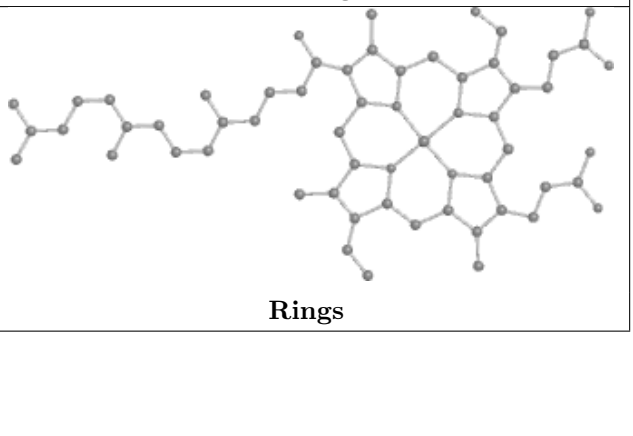


Bond angles

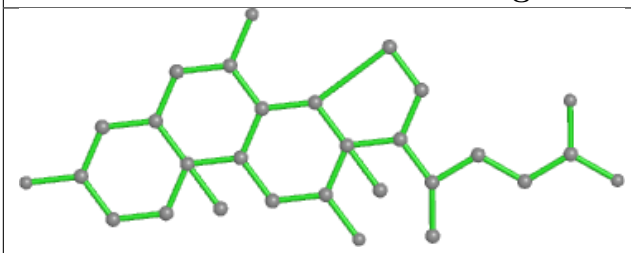


Torsions

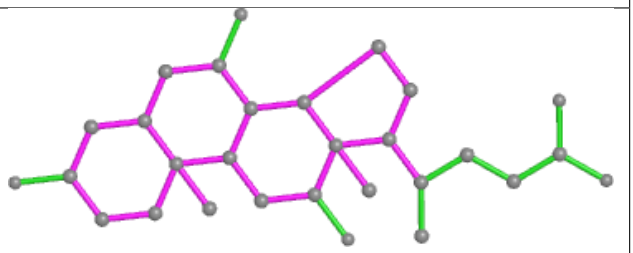


Rings

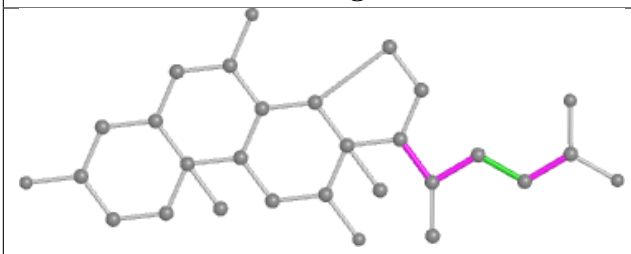
Ligand CHD P 4271



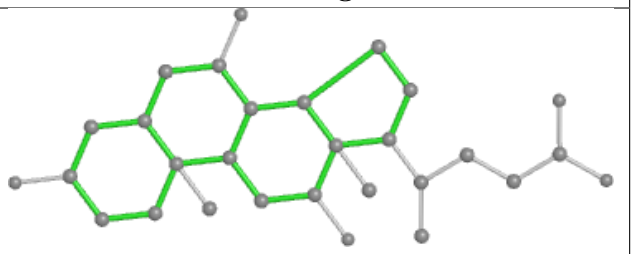
Bond lengths



Bond angles

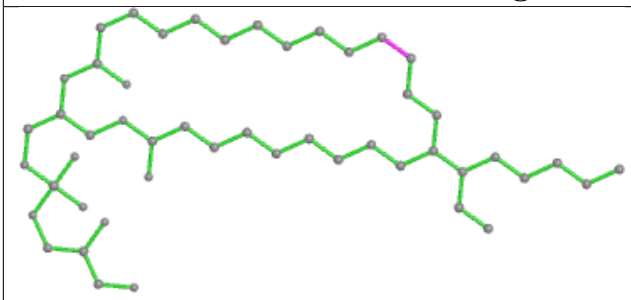


Torsions

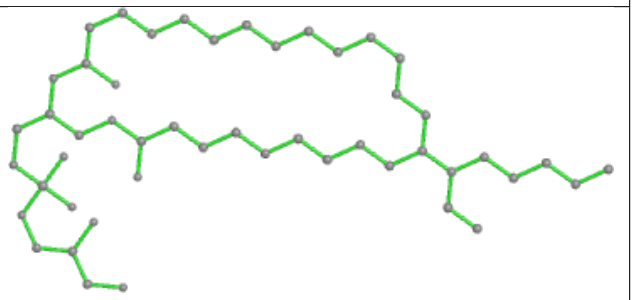


Rings

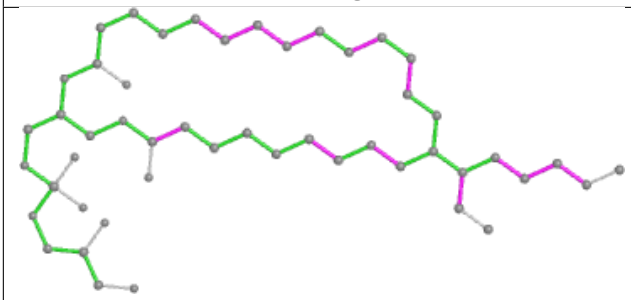
Ligand PGV A 3266



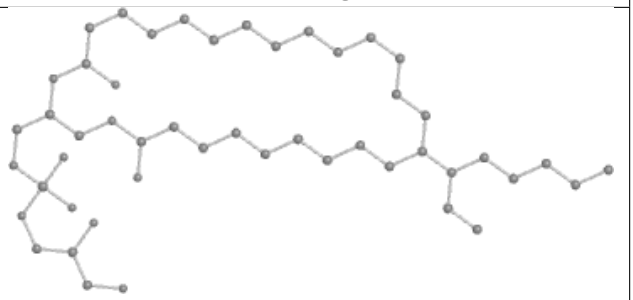
Bond lengths



Bond angles

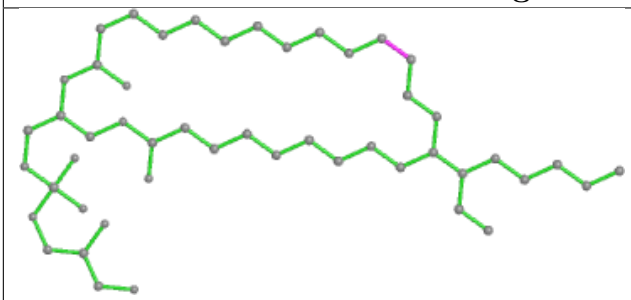


Torsions

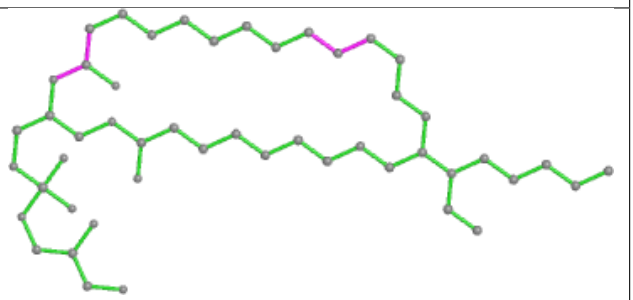


Rings

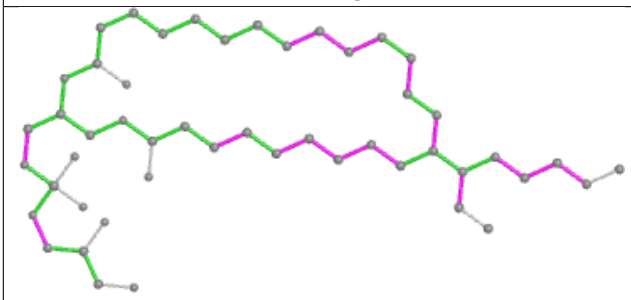
Ligand PGV C 3267



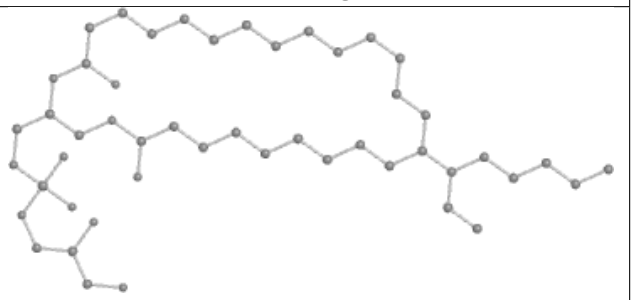
Bond lengths



Bond angles

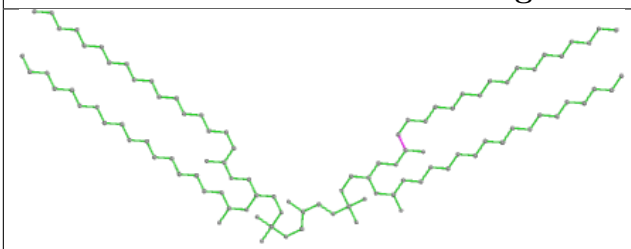


Torsions

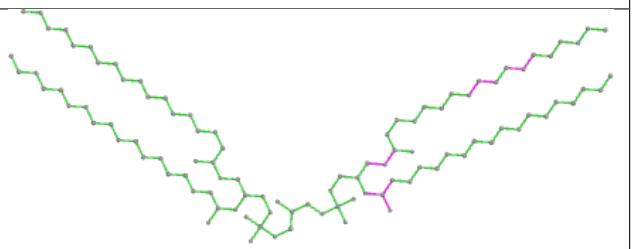


Rings

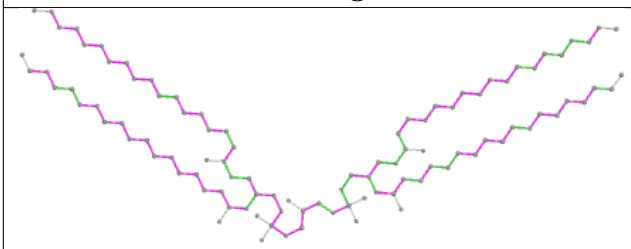
Ligand CDL C 3270



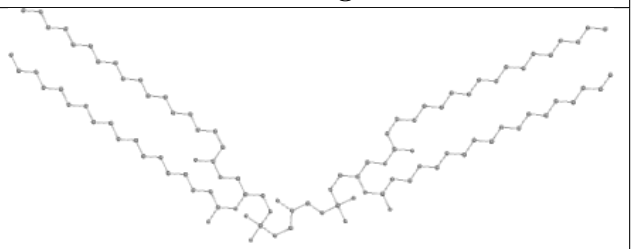
Bond lengths



Bond angles

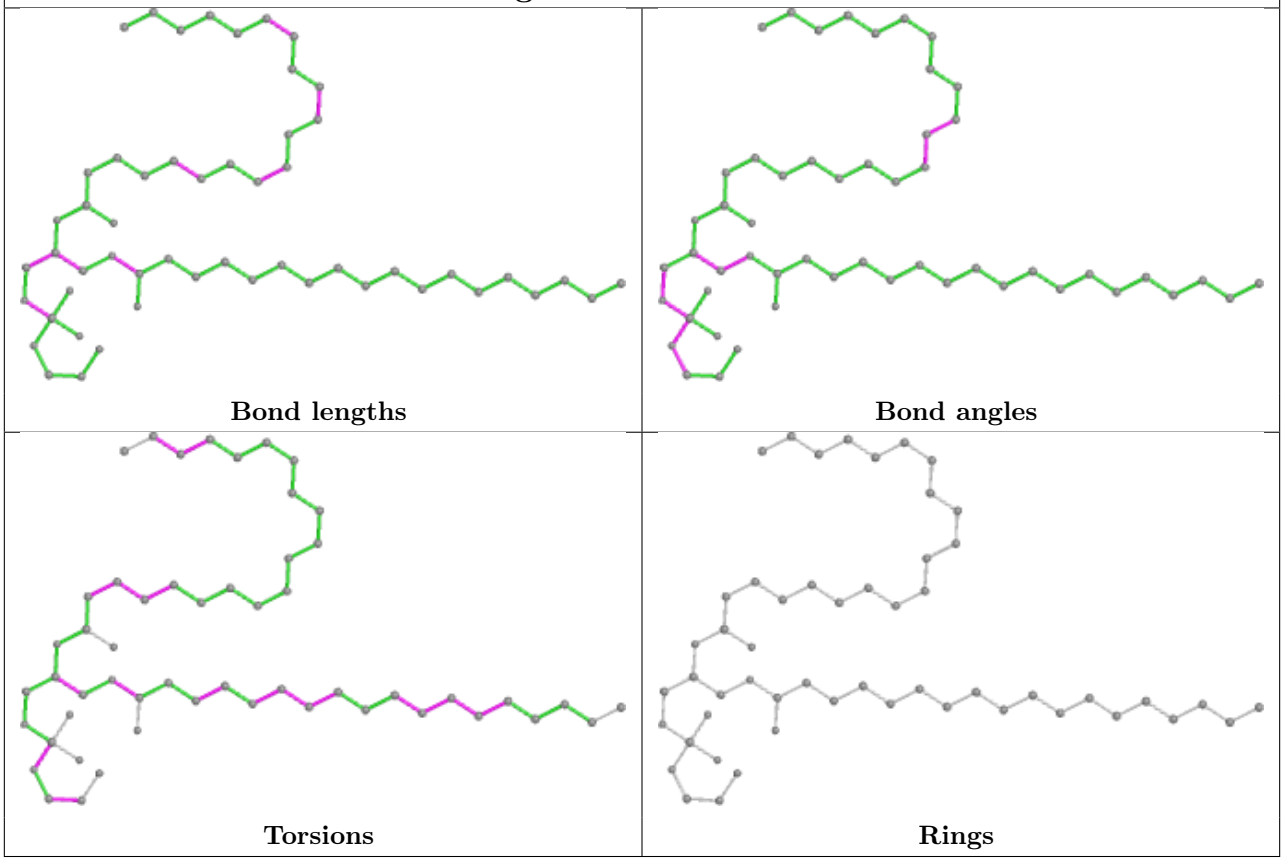


Torsions

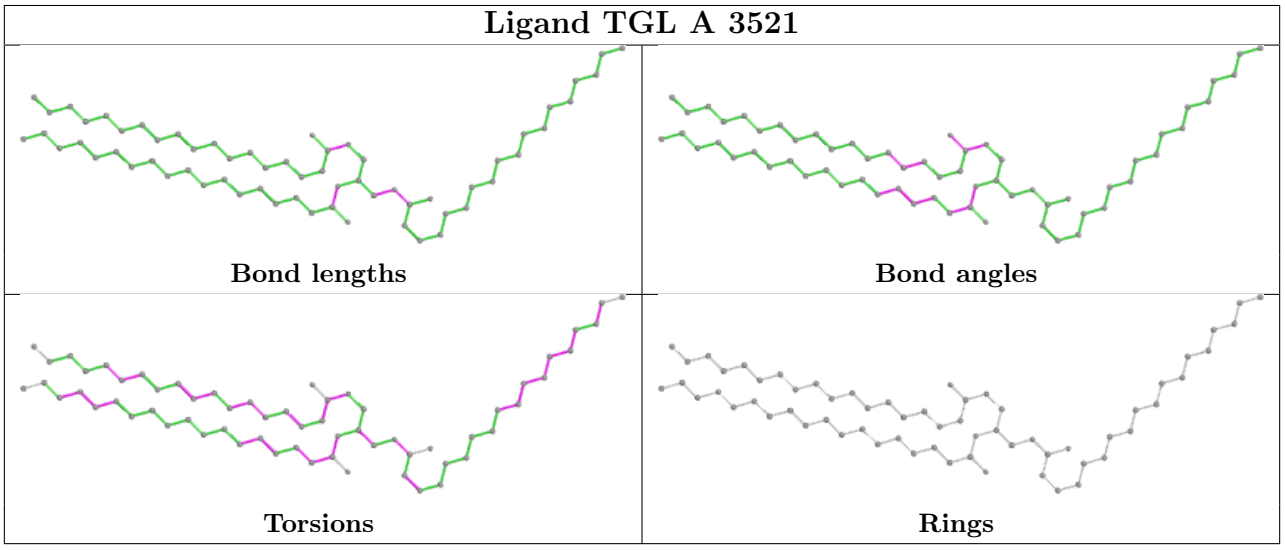


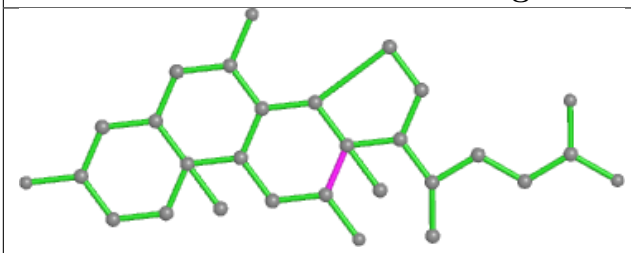
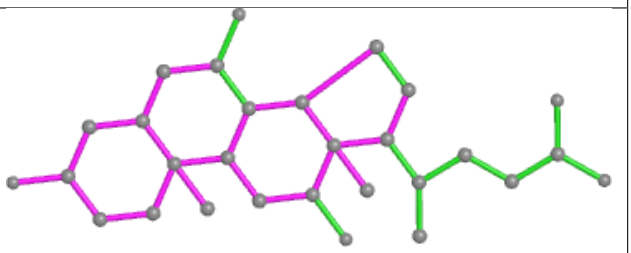
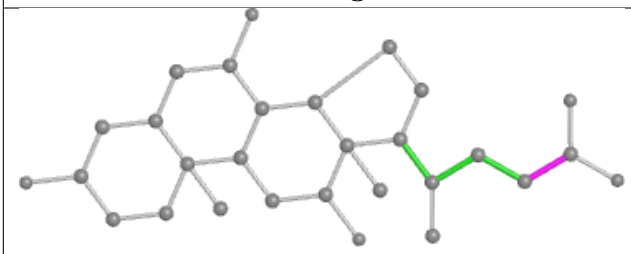
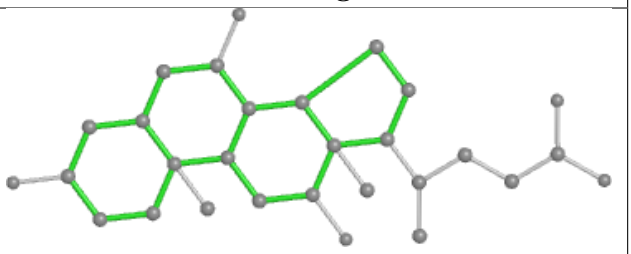
Rings

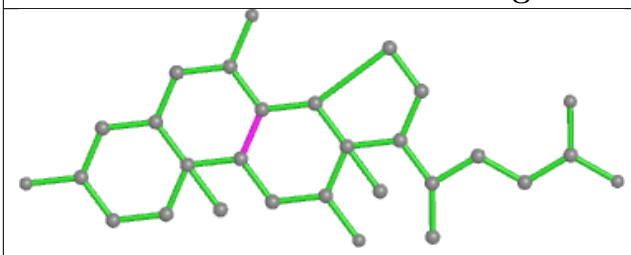
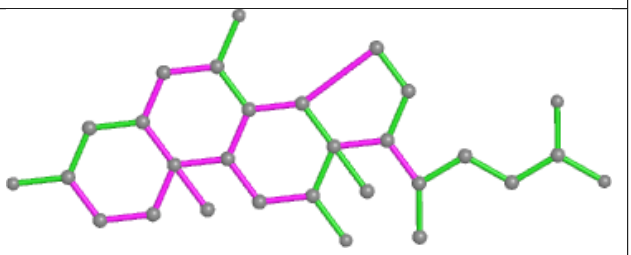
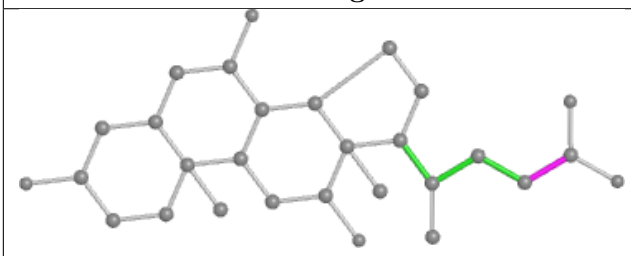
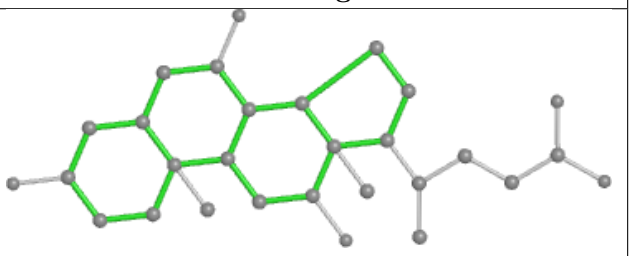
Ligand PEK C 3265



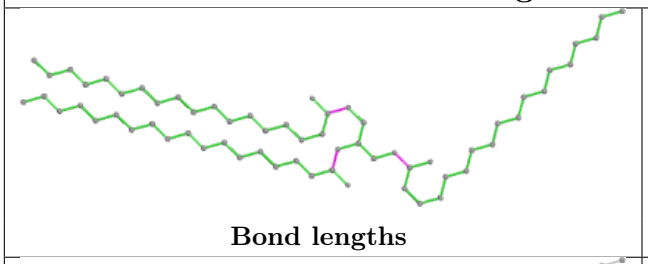
Ligand TGL A 3521



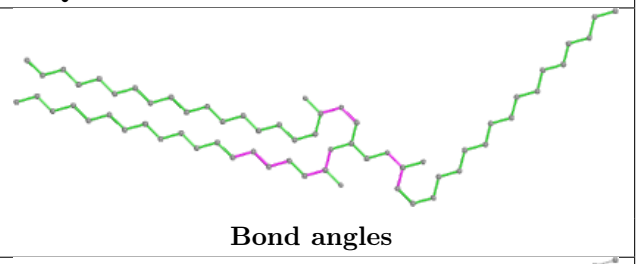
Ligand CHD B 4085	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CHD P 4525	
	
Bond lengths	Bond angles
	
Torsions	Rings

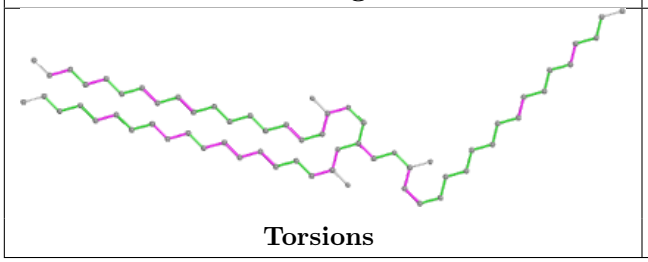
Ligand TGL Q 4523



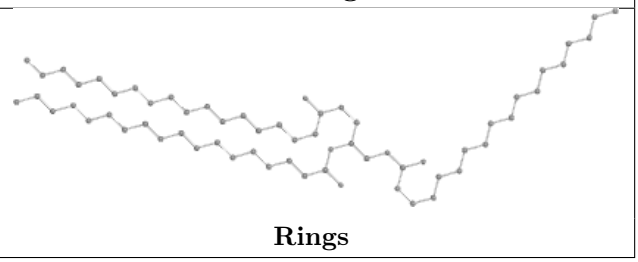
Bond lengths



Bond angles

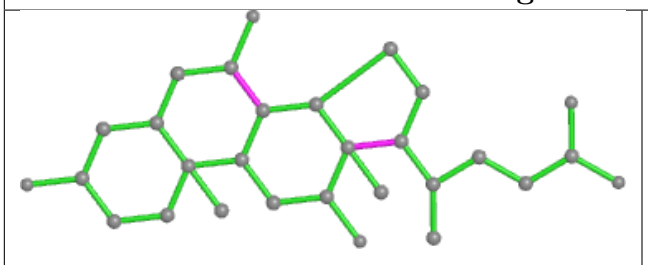


Torsions

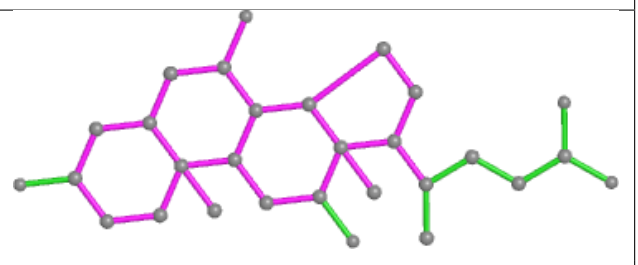


Rings

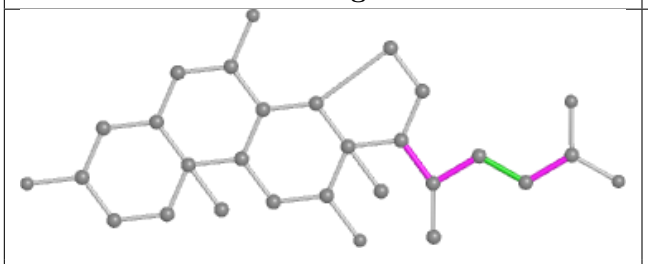
Ligand CHD J 3060



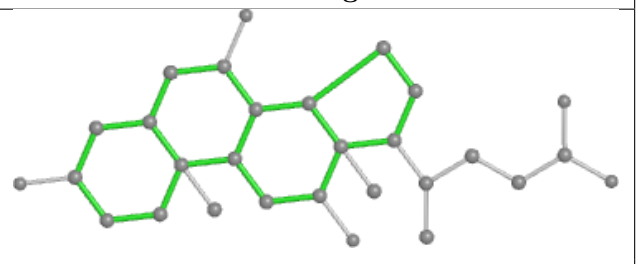
Bond lengths



Bond angles

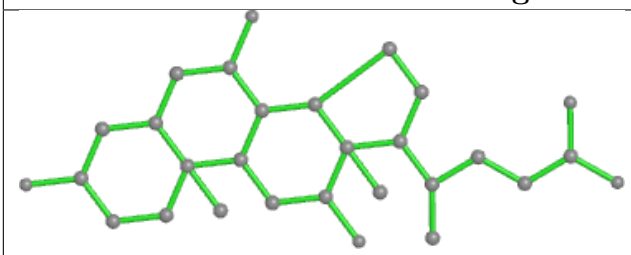


Torsions

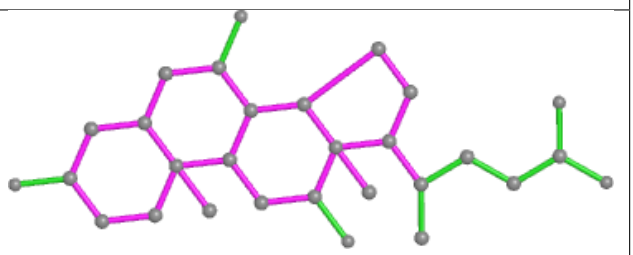


Rings

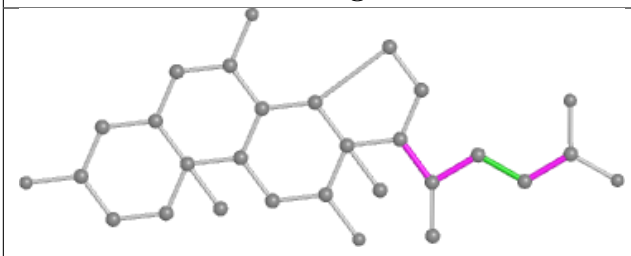
Ligand CHD C 3271



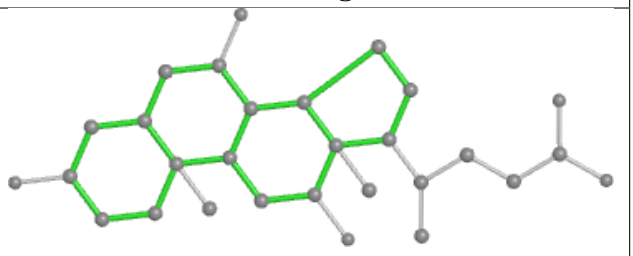
Bond lengths



Bond angles

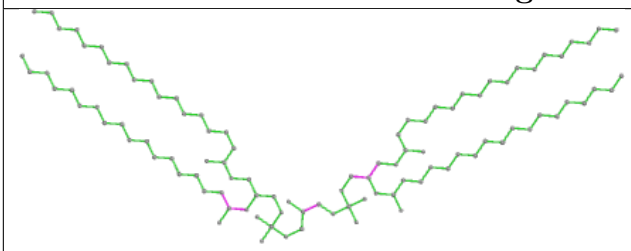


Torsions

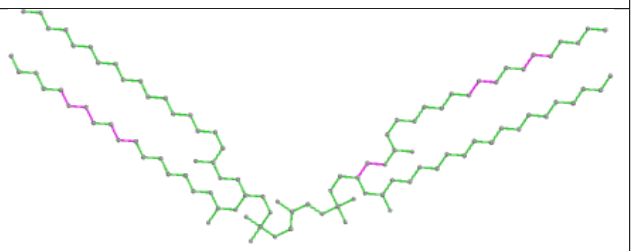


Rings

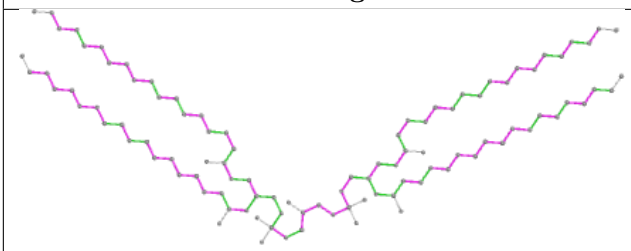
Ligand CDL T 4269



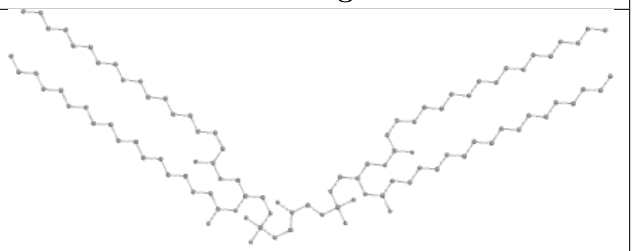
Bond lengths



Bond angles

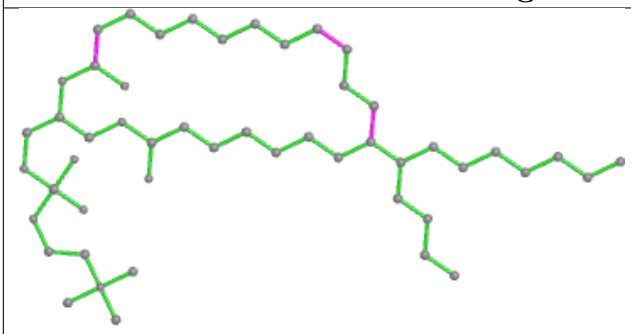


Torsions

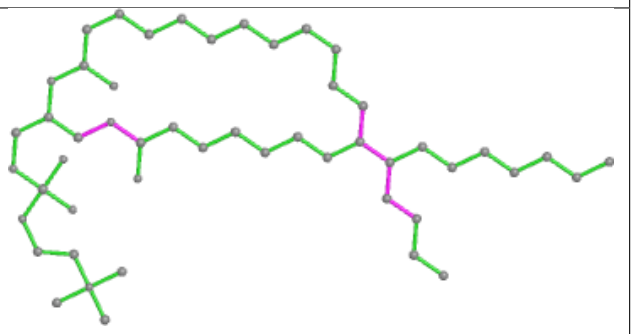


Rings

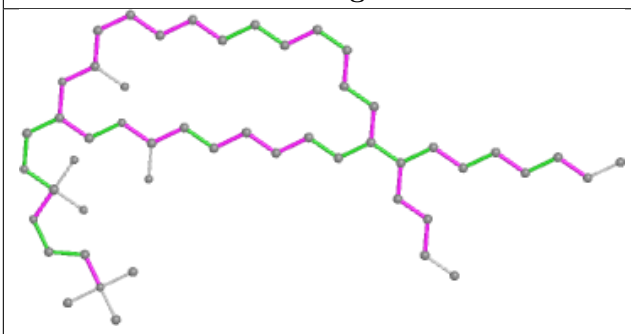
Ligand PSC O 4230



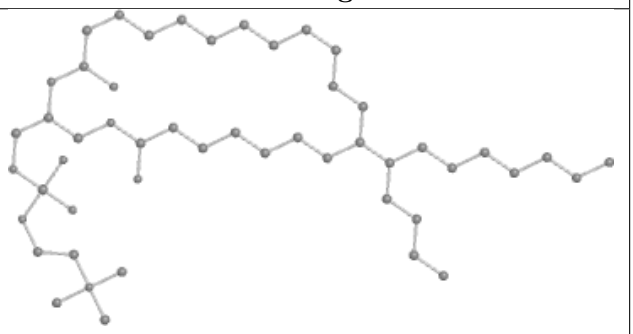
Bond lengths



Bond angles

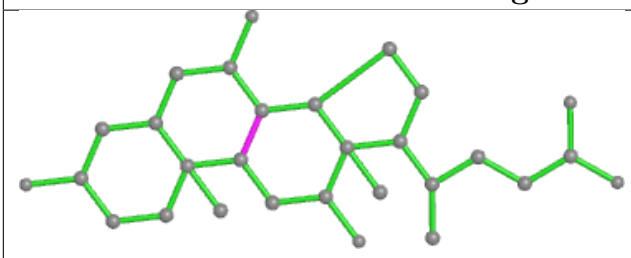


Torsions

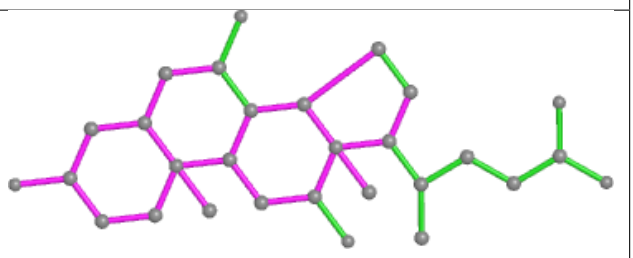


Rings

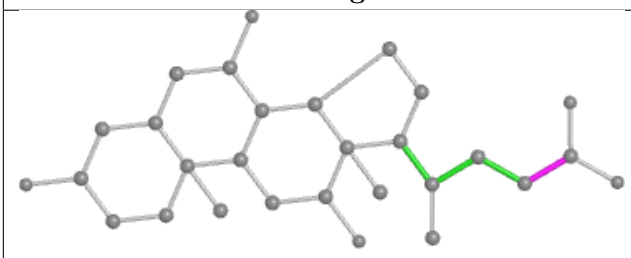
Ligand CHD O 3085



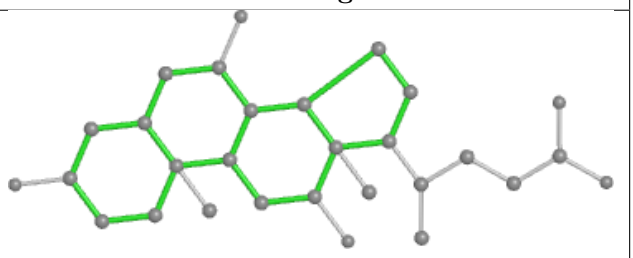
Bond lengths



Bond angles

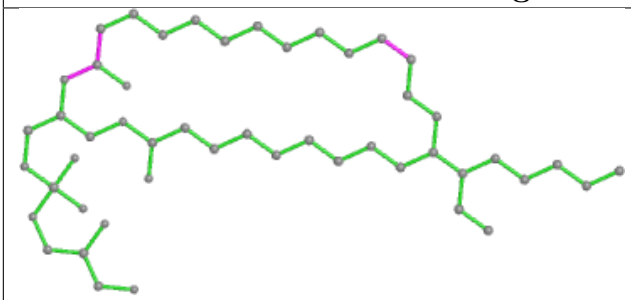


Torsions

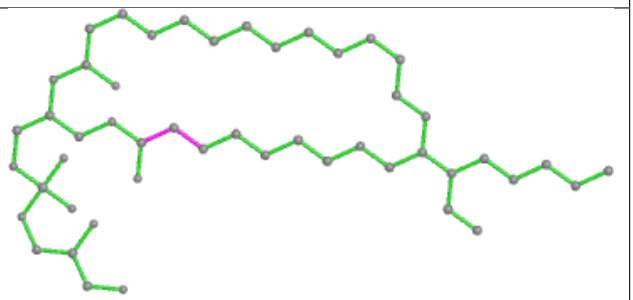


Rings

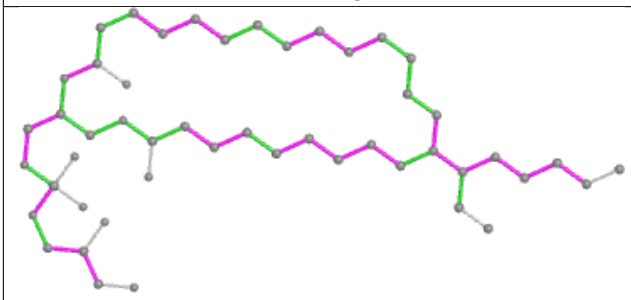
Ligand PGV C 3268



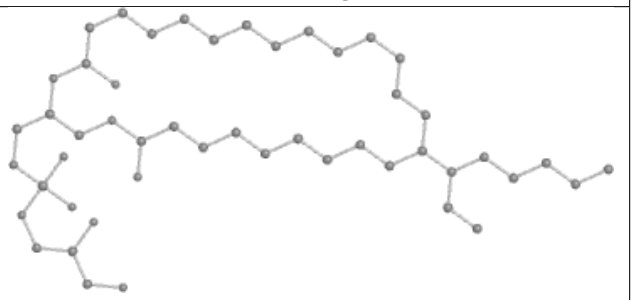
Bond lengths



Bond angles

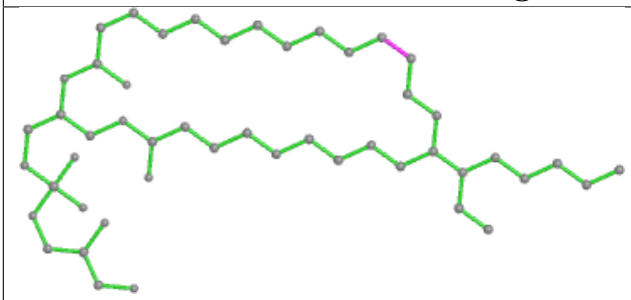


Torsions

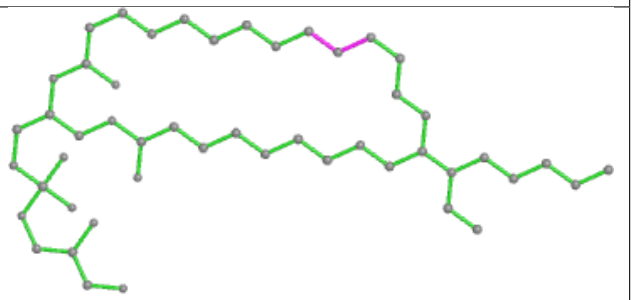


Rings

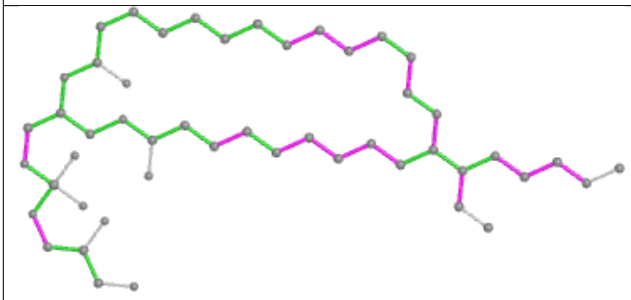
Ligand PGV P 4267



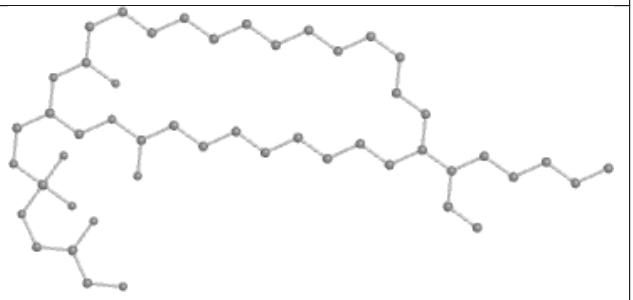
Bond lengths



Bond angles

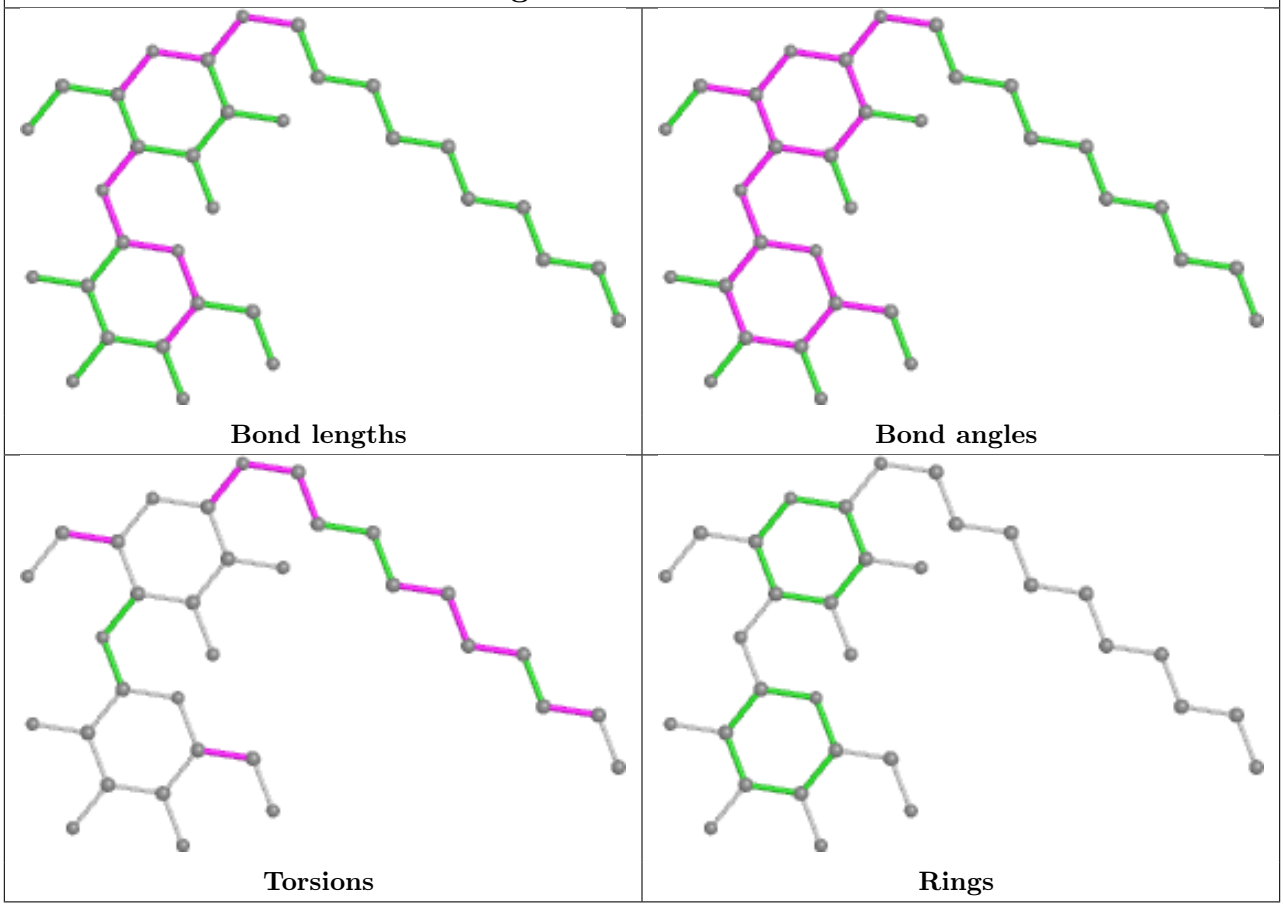


Torsions

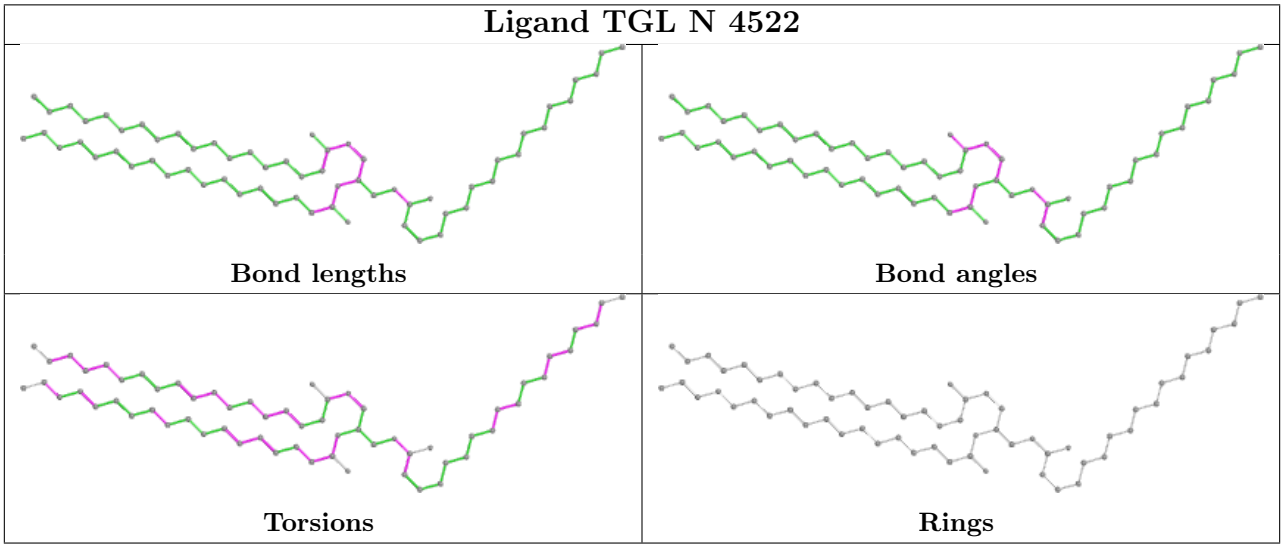


Rings

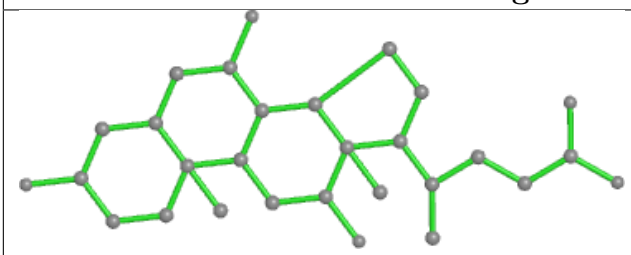
Ligand DMU Z 4526



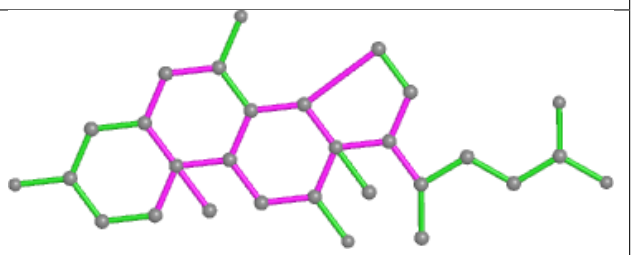
Ligand TGL N 4522



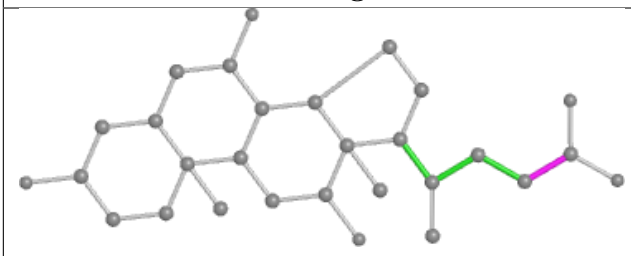
Ligand CHD C 3525



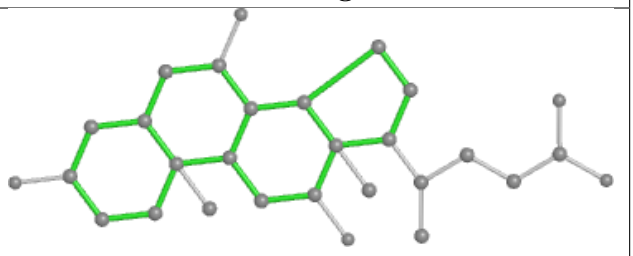
Bond lengths



Bond angles

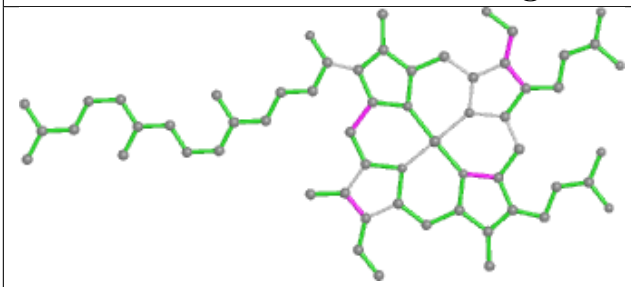


Torsions

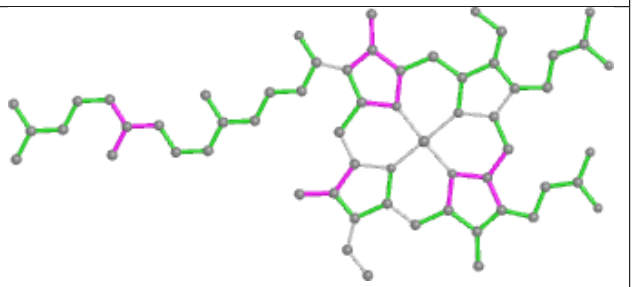


Rings

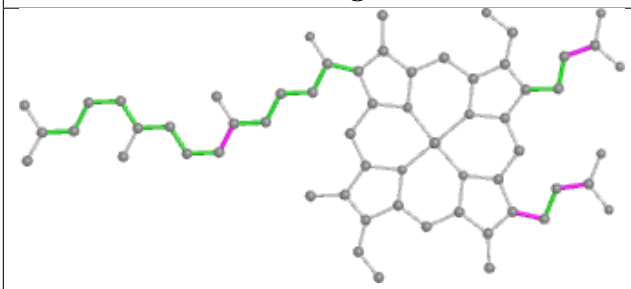
Ligand HEA A 516



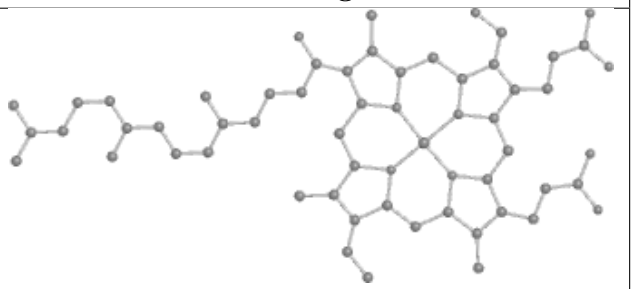
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	513/514 (99%)	0.20	4 (0%) 86 87	13, 19, 29, 66	0
1	N	513/514 (99%)	0.02	3 (0%) 89 90	17, 24, 34, 67	0
2	B	226/227 (99%)	-0.09	6 (2%) 54 57	14, 27, 52, 83	0
2	O	226/227 (99%)	0.14	10 (4%) 34 37	21, 33, 60, 87	0
3	C	259/261 (99%)	-0.40	3 (1%) 79 81	16, 23, 37, 65	0
3	P	259/261 (99%)	-0.34	3 (1%) 79 81	18, 25, 39, 65	0
4	D	144/147 (97%)	-0.04	7 (4%) 29 33	20, 30, 56, 81	0
4	Q	144/147 (97%)	1.41	24 (16%) 1 1	29, 41, 67, 98	0
5	E	105/109 (96%)	0.34	4 (3%) 40 43	23, 31, 57, 97	0
5	R	105/109 (96%)	0.87	10 (9%) 8 9	27, 37, 60, 97	0
6	F	98/98 (100%)	0.66	8 (8%) 11 13	20, 29, 85, 100	0
6	S	98/98 (100%)	0.65	8 (8%) 11 13	21, 31, 91, 100	0
7	G	83/85 (97%)	1.06	19 (22%) 0 0	21, 31, 97, 99	0
7	T	83/85 (97%)	1.06	18 (21%) 0 0	20, 35, 94, 98	0
8	H	79/85 (92%)	0.83	15 (18%) 1 1	21, 34, 89, 100	0
8	U	79/85 (92%)	1.04	15 (18%) 1 1	27, 38, 91, 100	0
9	I	72/73 (98%)	0.73	10 (13%) 2 3	24, 41, 64, 81	0
9	V	72/73 (98%)	1.19	17 (23%) 0 0	27, 47, 66, 91	0
10	J	58/59 (98%)	0.48	7 (12%) 4 4	23, 32, 73, 94	0
10	W	58/59 (98%)	0.87	8 (13%) 2 3	26, 38, 76, 100	0
11	K	49/56 (87%)	-0.08	0 100 100	24, 34, 46, 67	0
11	X	49/56 (87%)	1.31	10 (20%) 1 1	33, 41, 58, 75	0
12	L	46/47 (97%)	-0.18	2 (4%) 35 38	20, 25, 44, 92	0
12	Y	46/47 (97%)	-0.05	1 (2%) 62 64	26, 33, 58, 85	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	M	43/46 (93%)	0.17	4 (9%) 8 10	21, 26, 77, 99	0
13	Z	43/46 (93%)	0.66	7 (16%) 1 1	28, 35, 84, 100	0
All	All	3550/3614 (98%)	0.28	223 (6%) 20 22	13, 28, 62, 100	0

The worst 5 of 223 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	4	SER	21.0
4	Q	6	VAL	19.3
4	Q	5	VAL	19.0
6	S	97	ALA	15.5
6	F	97	ALA	14.5

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	SAC	V	1	9/10	0.30	0.58	98,99,100,100	0
7	TPO	T	11	11/12	0.45	0.38	71,81,100,100	0
7	TPO	G	11	11/12	0.56	0.34	71,79,100,100	0
9	SAC	I	1	9/10	0.73	0.31	91,93,94,96	0
1	FME	A	1	10/11	0.83	0.16	41,45,67,71	0
1	FME	N	1	10/11	0.86	0.18	44,49,68,69	0
2	FME	B	1	10/11	0.94	0.14	20,27,36,41	0
2	FME	O	1	10/11	0.96	0.14	32,33,40,42	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, 95th percentile and maximum values of B factors of atoms in the group. The column

labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	PEK	P	4265	53/53	0.48	0.34	44,70,100,100	0
23	PEK	T	3263	53/53	0.55	0.45	44,91,100,100	0
23	PEK	C	3265	53/53	0.56	0.29	43,72,100,100	0
21	CHD	W	4060	29/29	0.58	0.57	84,98,100,100	0
25	PSC	O	4230	52/52	0.58	0.37	46,79,100,100	0
22	CDL	G	3269	100/100	0.59	0.33	48,87,100,100	0
21	CHD	J	3060	29/29	0.62	0.41	83,96,100,100	0
22	CDL	T	4269	100/100	0.62	0.31	45,85,100,100	0
25	PSC	E	3230	52/52	0.63	0.37	49,83,100,100	0
18	TGL	N	4522	63/63	0.63	0.33	38,63,76,84	0
19	PGV	N	4524	51/51	0.64	0.33	35,68,100,100	0
23	PEK	G	4263	53/53	0.65	0.37	44,87,100,100	0
19	PGV	C	3268	51/51	0.66	0.35	56,84,99,100	0
18	TGL	Q	4523	63/63	0.67	0.24	50,69,84,87	0
18	TGL	A	3522	63/63	0.68	0.32	31,61,76,79	0
22	CDL	P	4270	100/100	0.68	0.39	36,88,99,100	0
19	PGV	A	3524	51/51	0.68	0.30	29,69,99,100	0
18	TGL	N	4521	63/63	0.70	0.30	42,72,80,83	0
18	TGL	A	3523	63/63	0.72	0.26	49,66,83,87	0
22	CDL	C	3270	100/100	0.73	0.40	37,87,99,100	0
21	CHD	P	4271	29/29	0.74	0.36	79,91,95,97	0
21	CHD	C	3271	29/29	0.74	0.33	80,93,96,98	0
19	PGV	P	4268	51/51	0.74	0.29	62,83,98,100	0
18	TGL	A	3521	63/63	0.75	0.31	45,70,80,84	0
27	DMU	Z	4526	33/33	0.85	0.24	36,54,68,70	0
24	UNX	P	4262	1/1	0.87	0.36	28,28,28,28	0
27	DMU	M	3526	33/33	0.88	0.14	28,45,64,67	0
24	UNX	C	3262	1/1	0.91	0.30	33,33,33,33	0
21	CHD	P	4525	29/29	0.94	0.12	21,27,30,31	0
15	MG	N	4518	1/1	0.94	0.12	27,27,27,27	0
16	NA	N	4519	1/1	0.94	0.06	30,30,30,30	0
23	PEK	P	4264	53/53	0.94	0.14	25,42,70,71	0
23	PEK	C	3264	53/53	0.95	0.12	21,41,70,72	0
19	PGV	P	4267	51/51	0.96	0.12	20,29,57,59	0
19	PGV	C	3267	51/51	0.96	0.12	20,30,54,59	0
21	CHD	C	3525	29/29	0.96	0.13	18,25,28,32	0
19	PGV	N	4266	51/51	0.97	0.11	19,30,48,53	0
20	CUA	O	228	2/2	0.97	0.08	24,24,24,27	0
21	CHD	B	4085	29/29	0.97	0.08	18,22,29,33	0
19	PGV	A	3266	51/51	0.97	0.11	17,27,49,51	0
16	NA	A	3519	1/1	0.97	0.09	25,25,25,25	0
17	HEA	N	515	60/60	0.98	0.15	17,23,33,35	0

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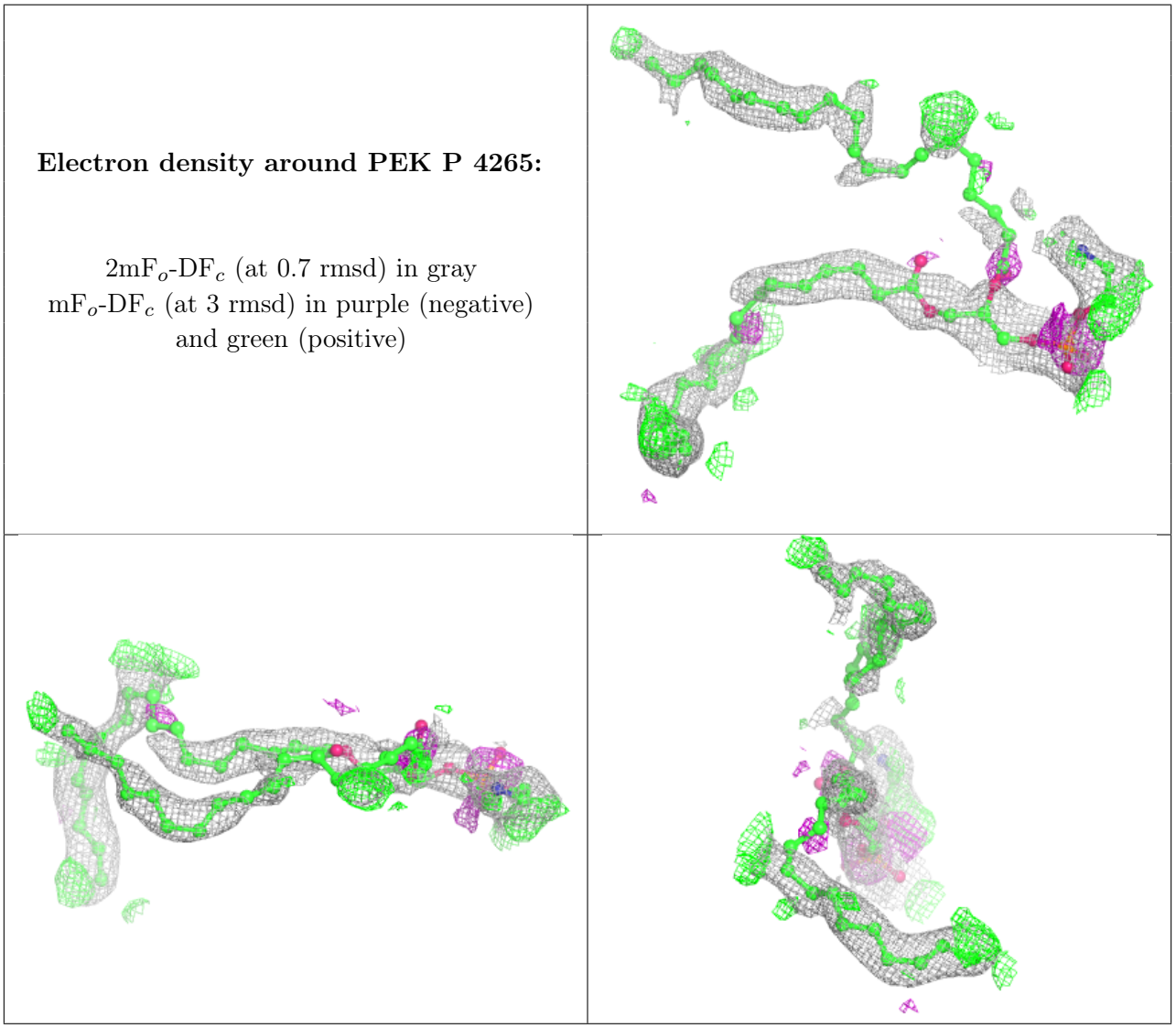
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
21	CHD	O	3085	29/29	0.98	0.08	18,22,26,30	0
17	HEA	N	516	60/60	0.98	0.13	15,19,29,30	0
15	MG	A	3518	1/1	0.99	0.12	17,17,17,17	0
14	CU	N	517	1/1	0.99	0.10	19,19,19,19	0
17	HEA	A	515	60/60	0.99	0.16	13,19,30,33	0
26	ZN	F	99	1/1	0.99	0.07	25,25,25,25	0
26	ZN	S	99	1/1	0.99	0.07	28,28,28,28	0
17	HEA	A	516	60/60	0.99	0.13	12,17,25,27	0
20	CUA	B	228	2/2	0.99	0.08	16,16,16,18	0
14	CU	A	517	1/1	1.00	0.09	16,16,16,16	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.

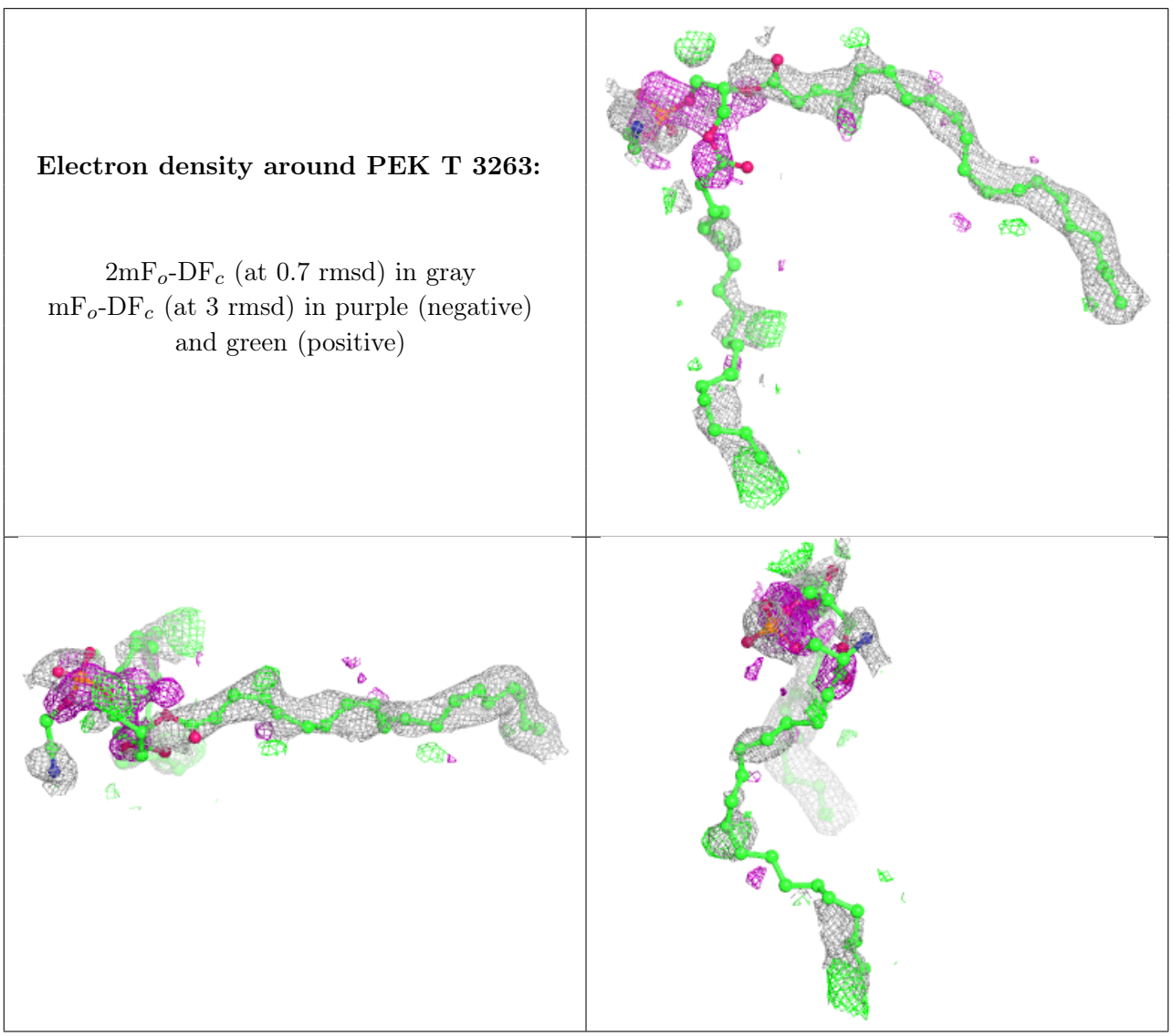
Electron density around PEK P 4265:

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



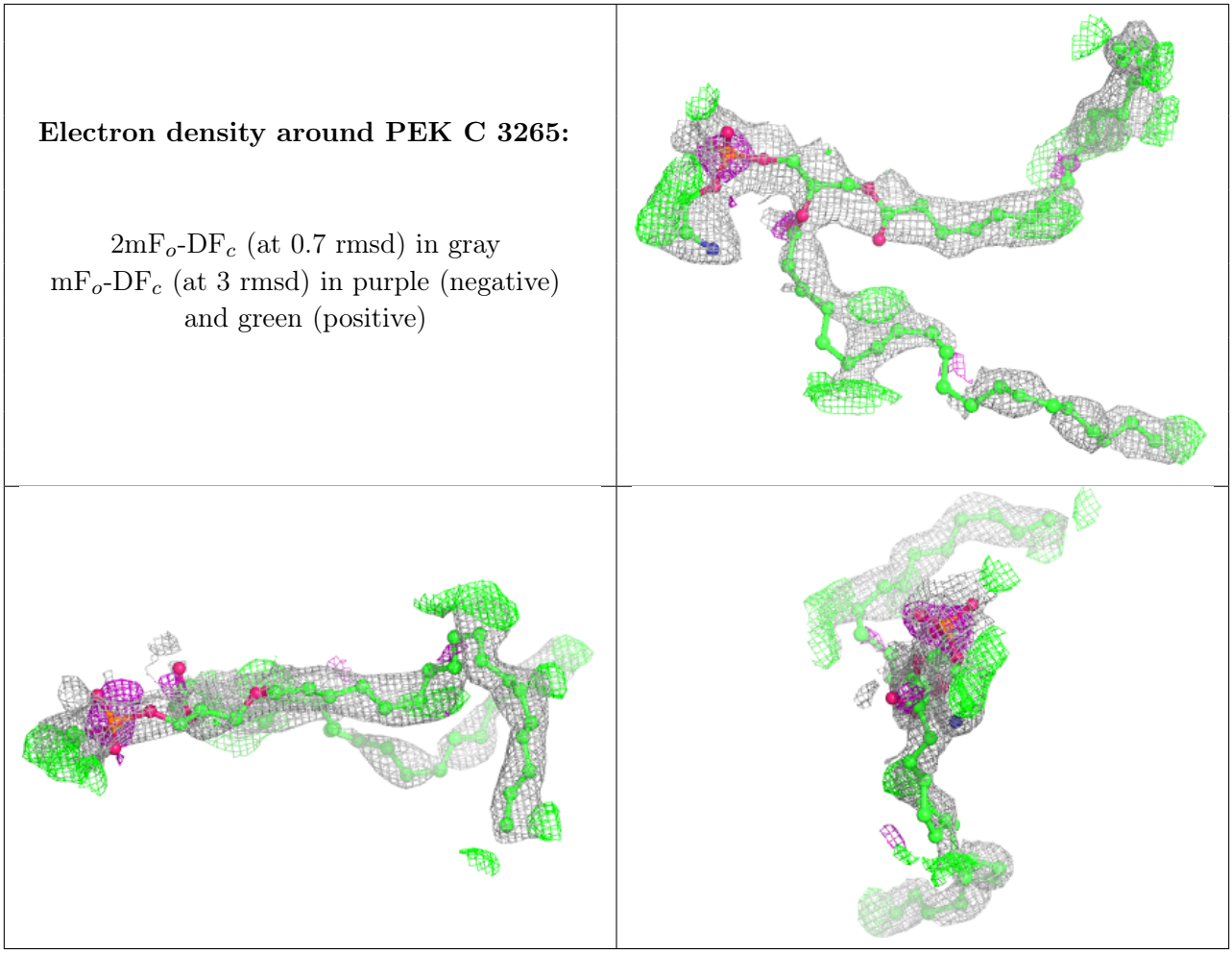
Electron density around PEK T 3263:

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



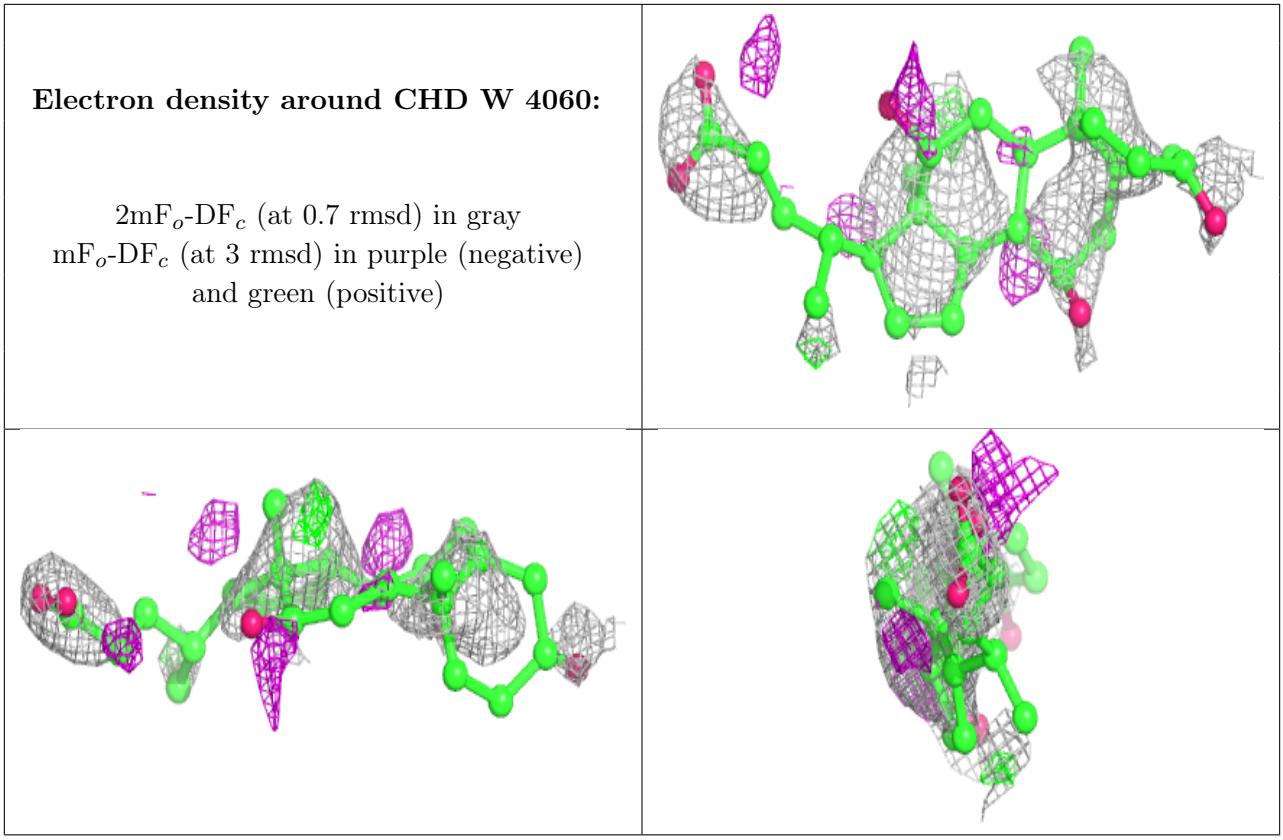
Electron density around PEK C 3265:

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



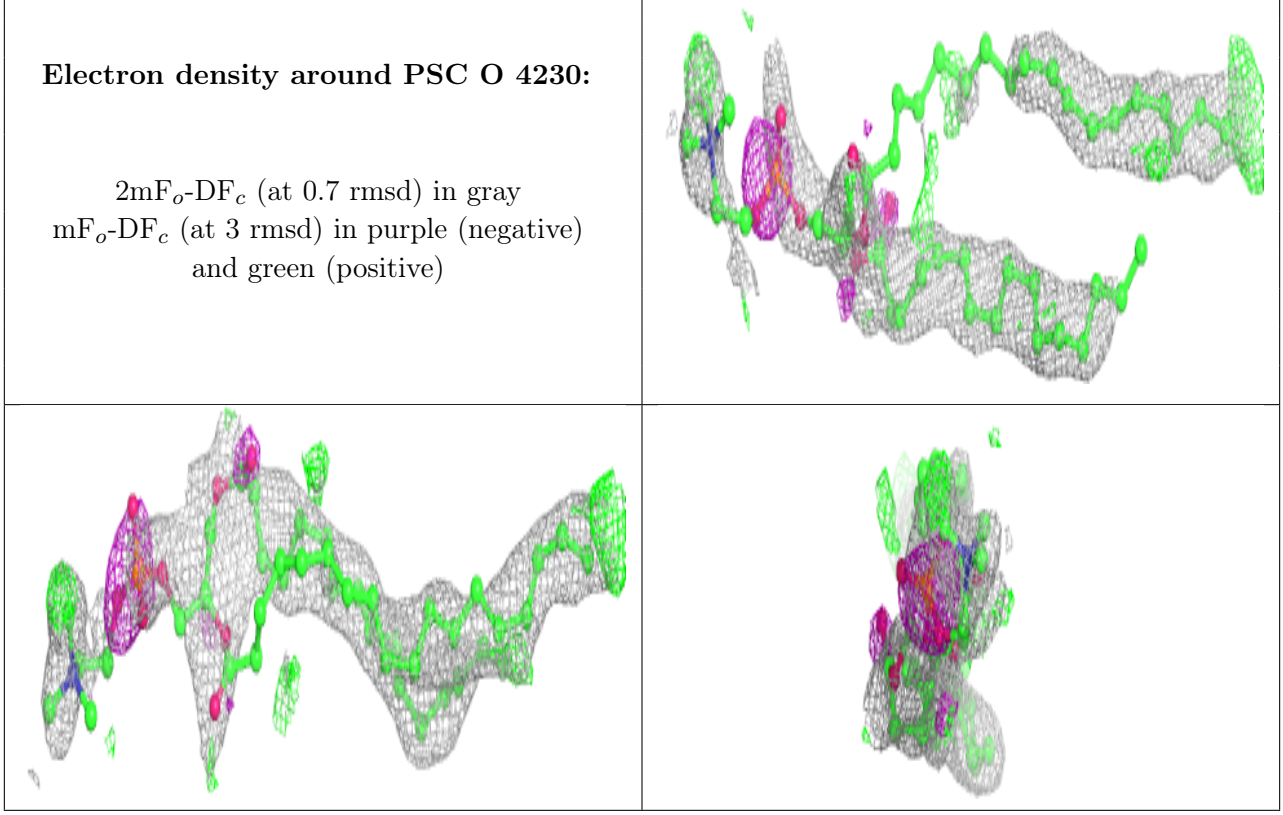
Electron density around CHD W 4060:

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



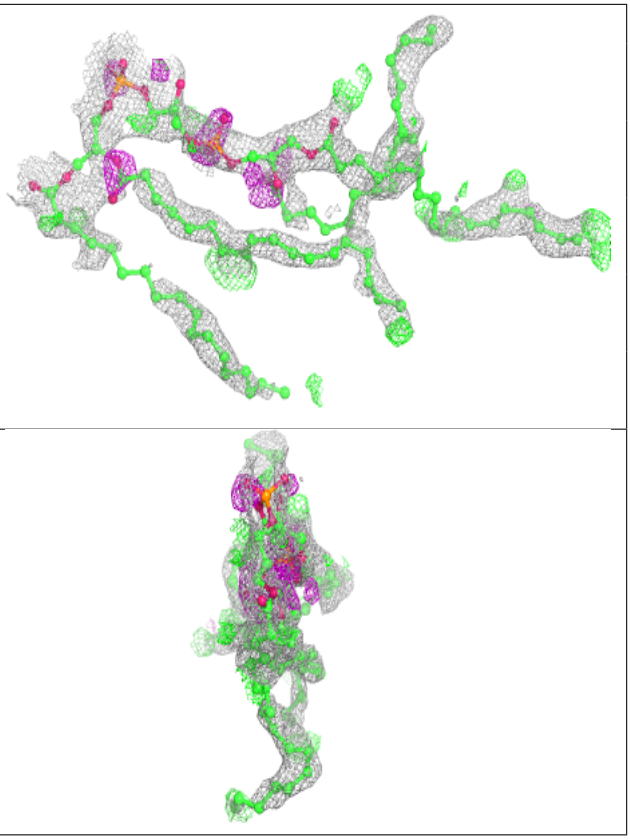
Electron density around PSC O 4230:

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



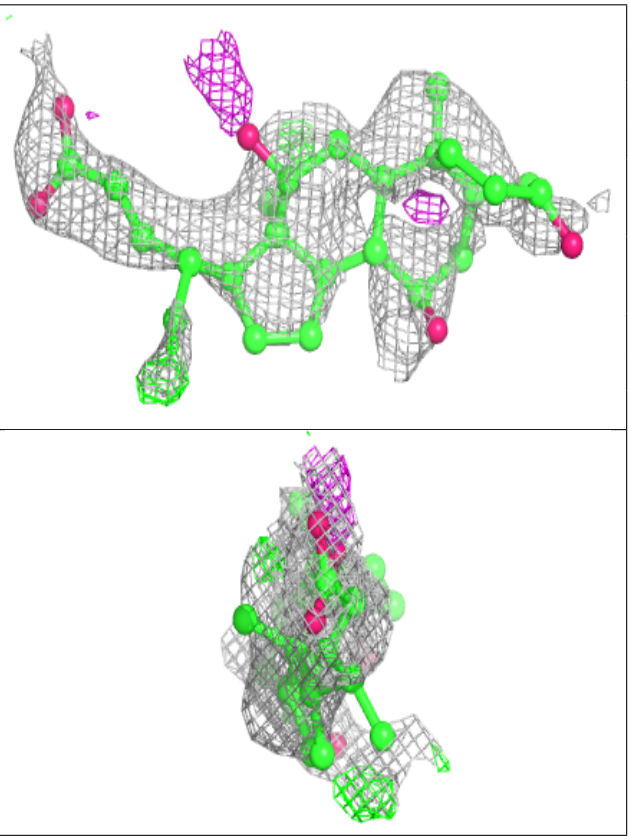
Electron density around CDL G 3269:

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



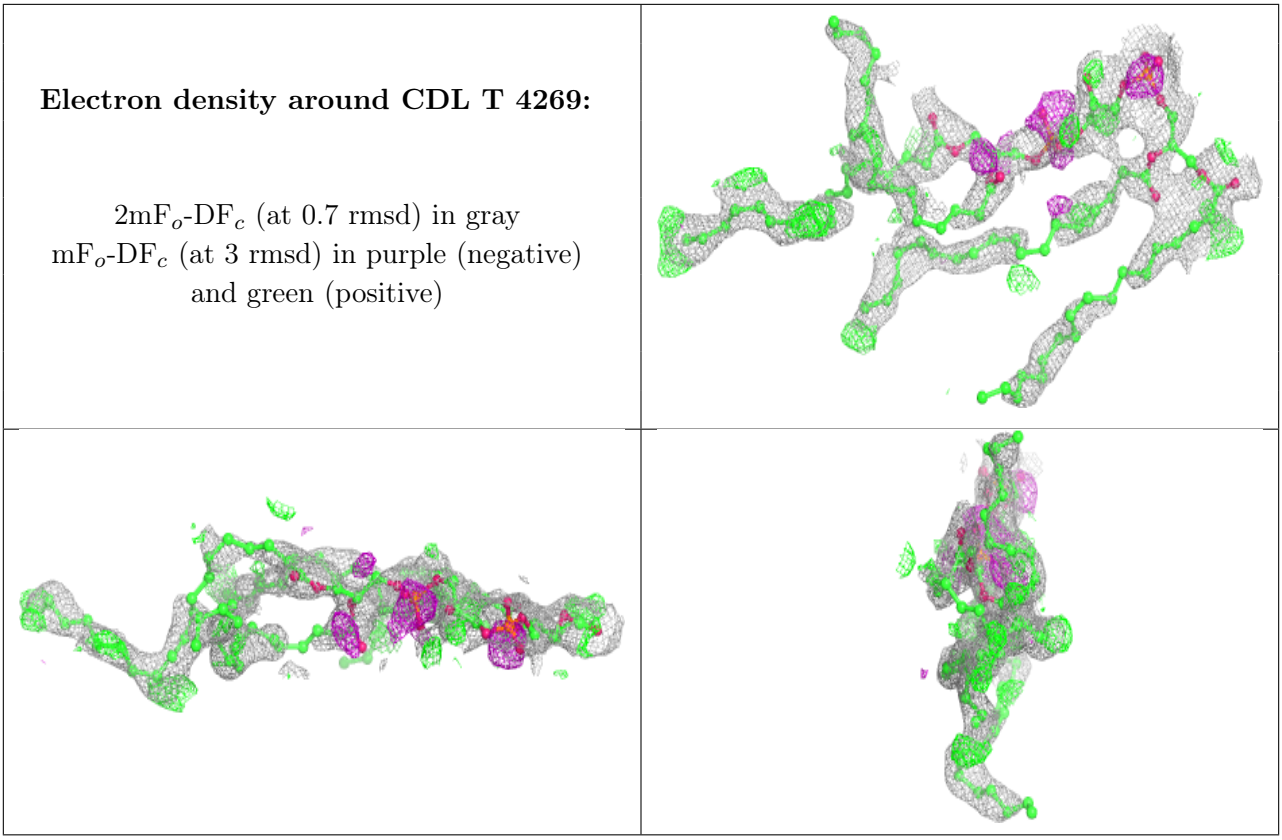
Electron density around CHD J 3060:

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



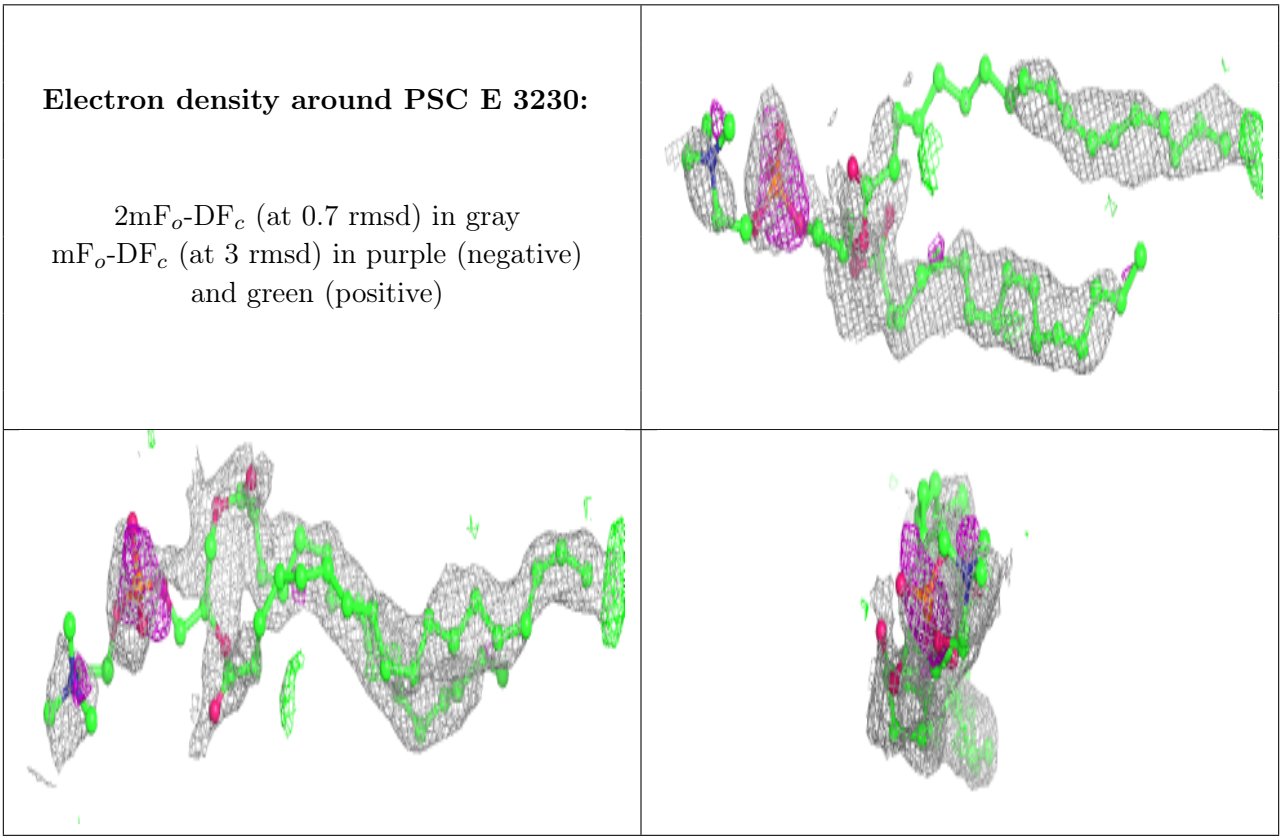
Electron density around CDL T 4269:

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



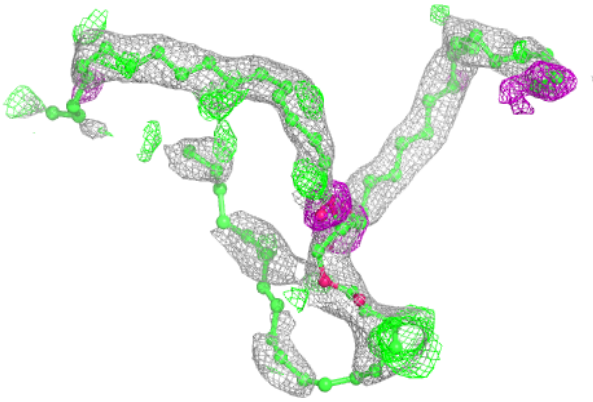
Electron density around PSC E 3230:

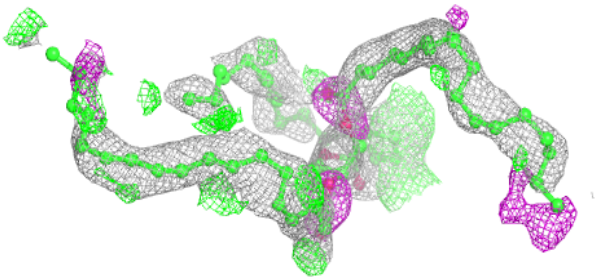
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

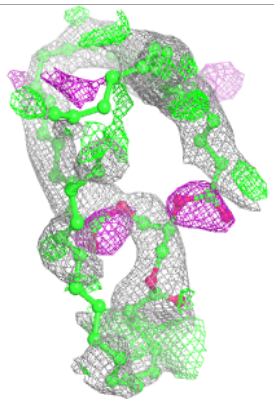


Electron density around TGL N 4522:

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

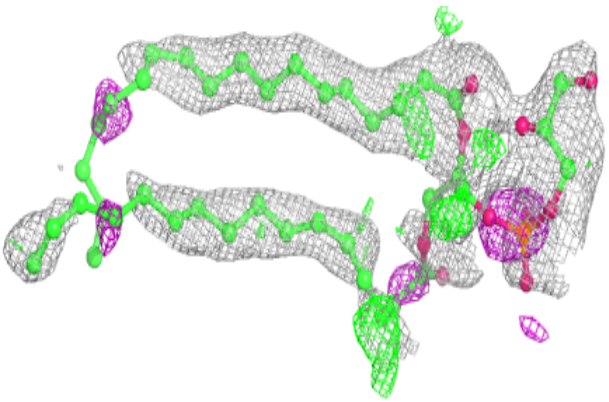


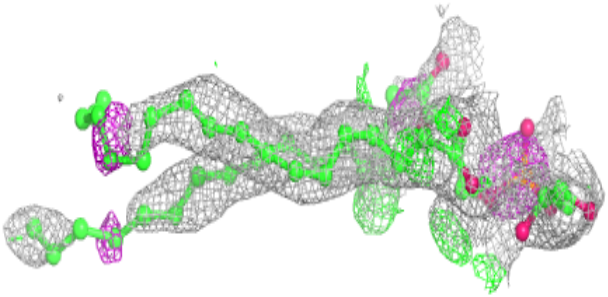


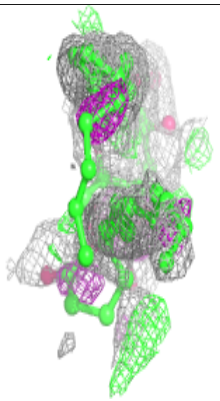


Electron density around PGV N 4524:

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

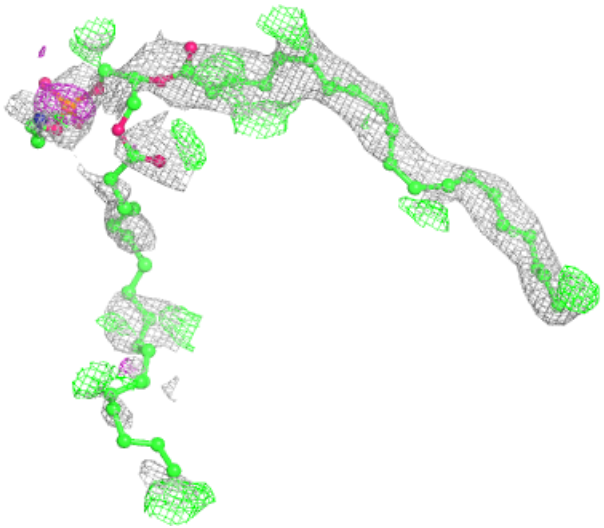


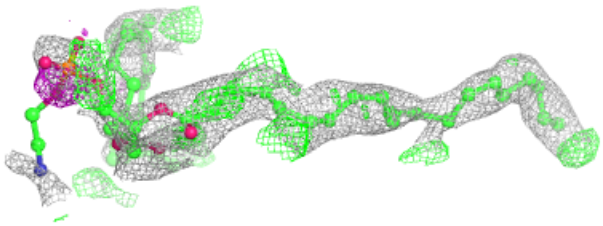


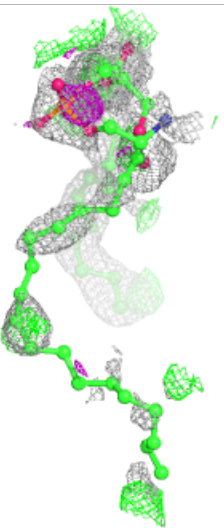


Electron density around PEK G 4263:

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

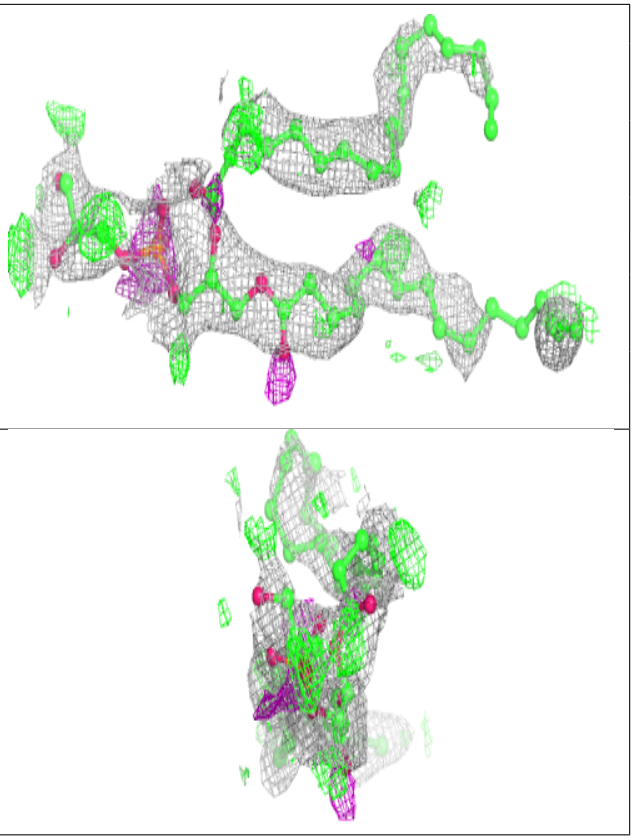






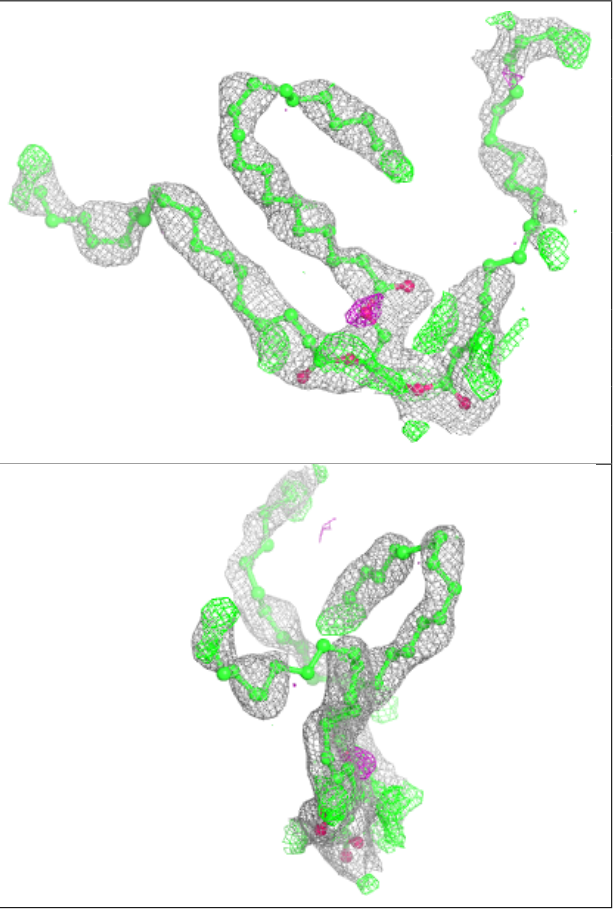
Electron density around PGV C 3268:

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



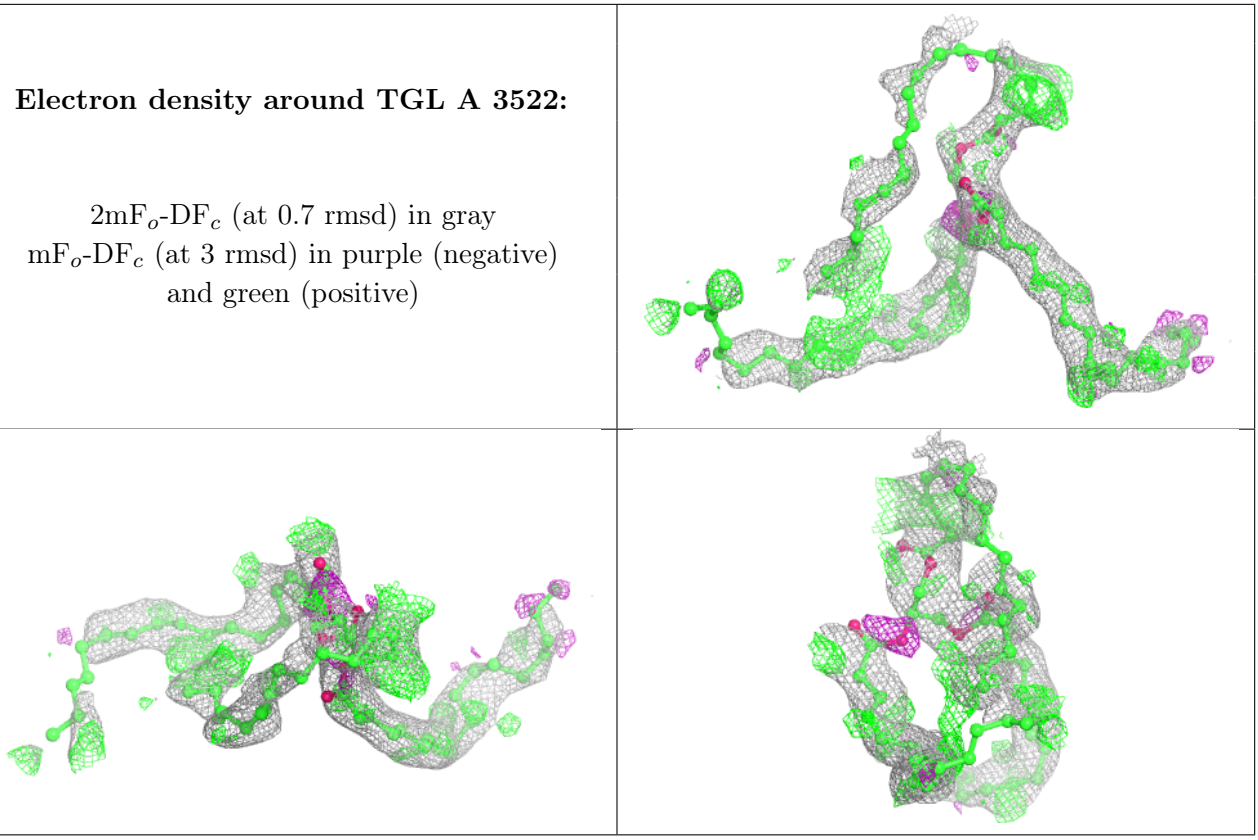
Electron density around TGL Q 4523:

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



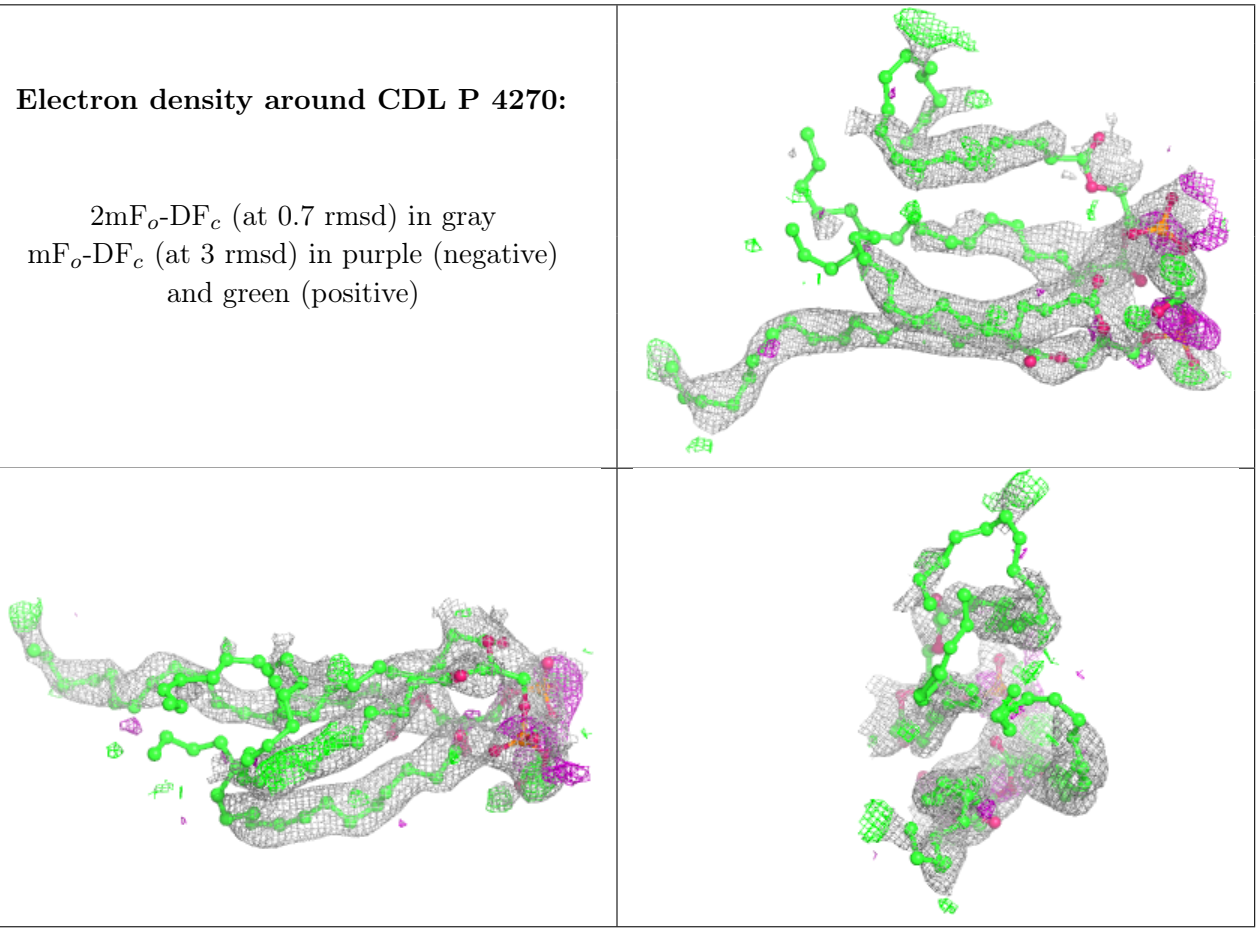
Electron density around TGL A 3522:

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



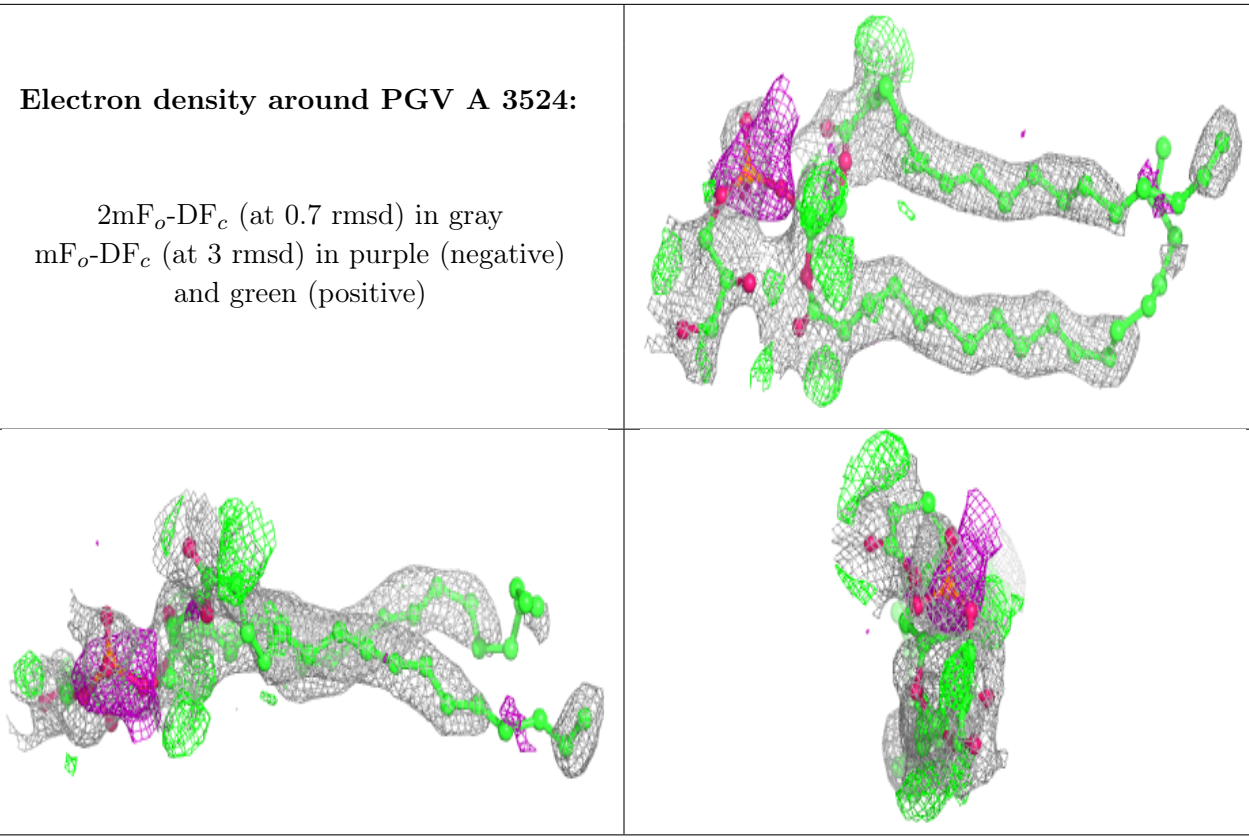
Electron density around CDL P 4270:

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



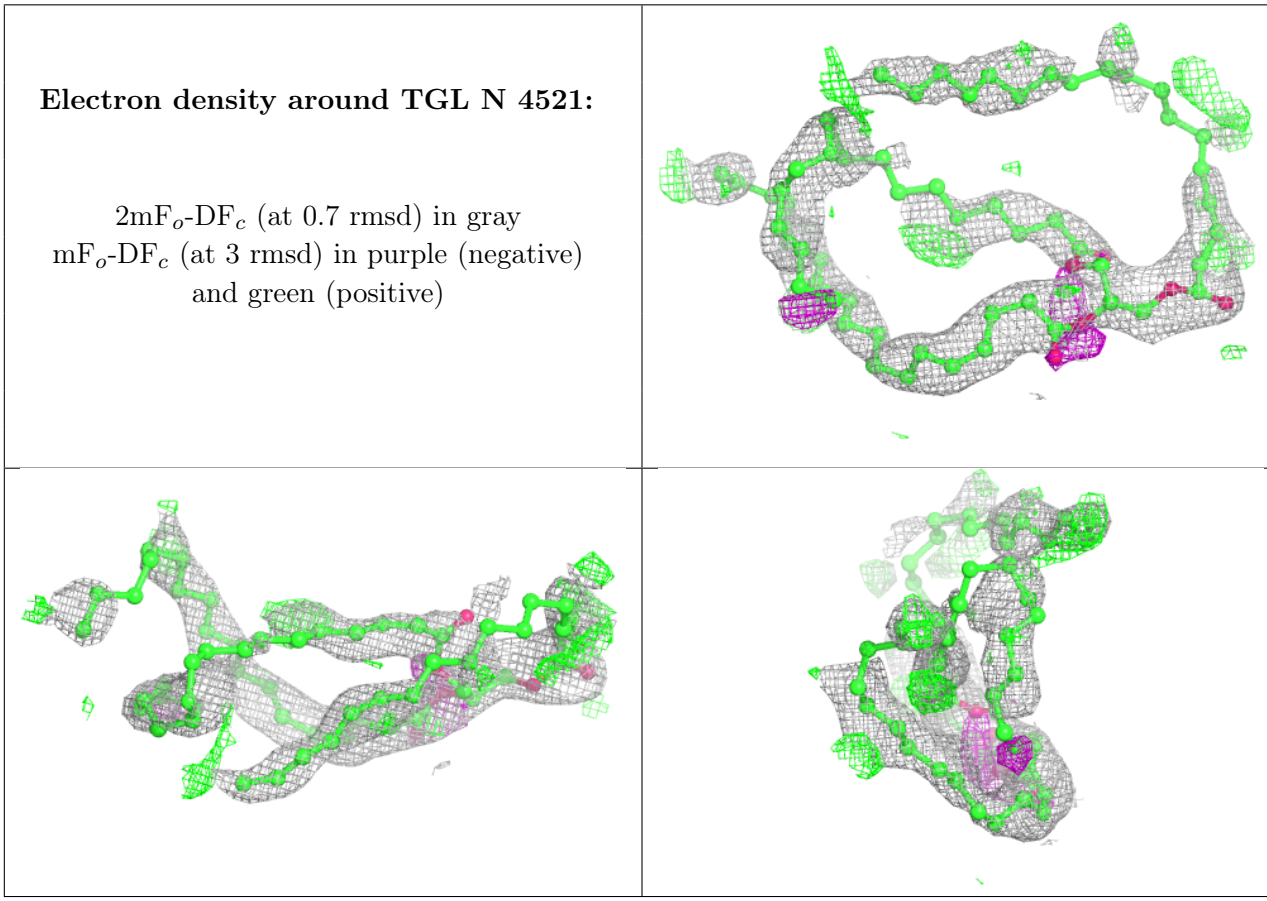
Electron density around PGV A 3524:

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



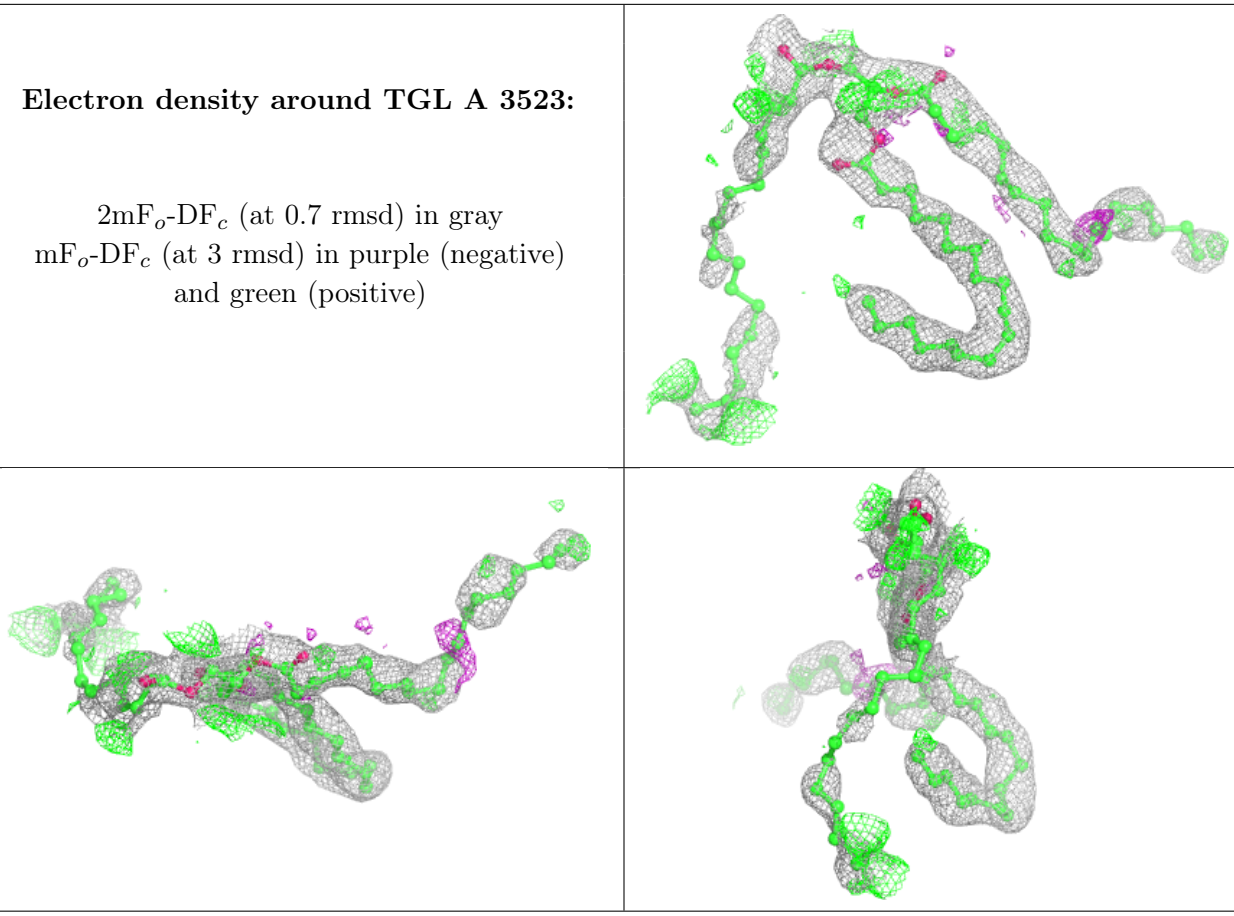
Electron density around TGL N 4521:

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



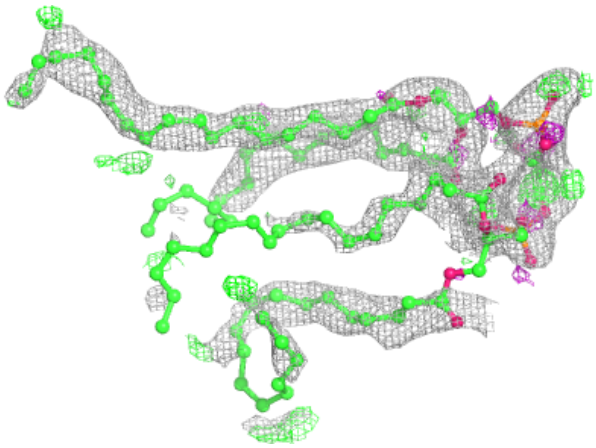
Electron density around TGL A 3523:

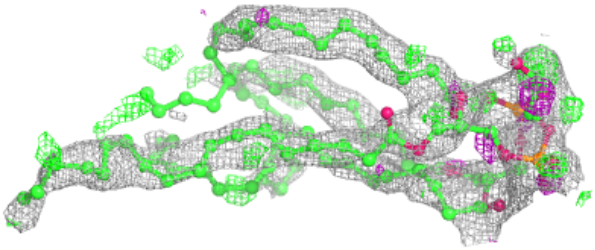
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

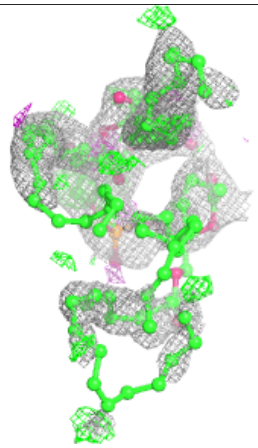


Electron density around CDL C 3270:

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

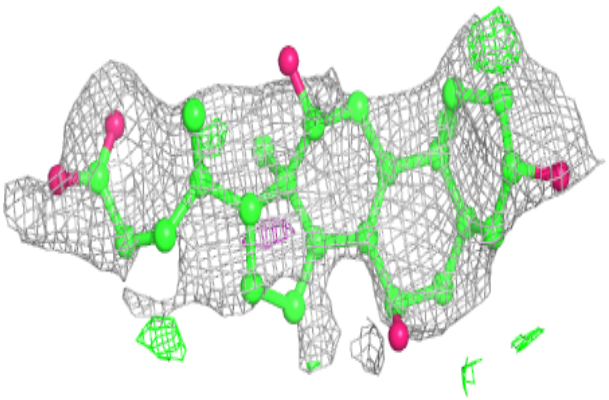


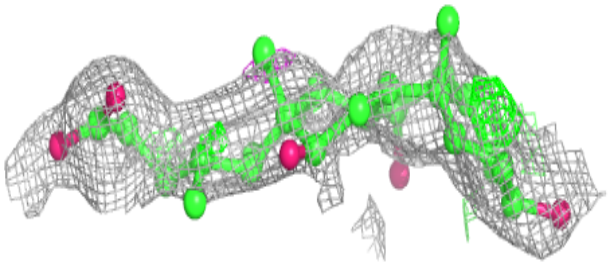


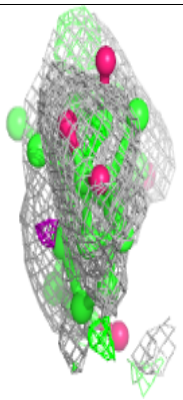


Electron density around CHD P 4271:

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

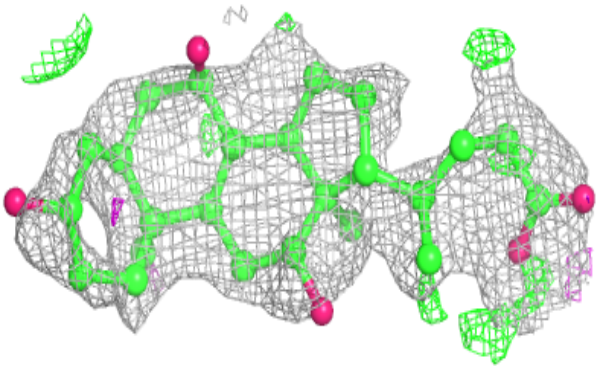


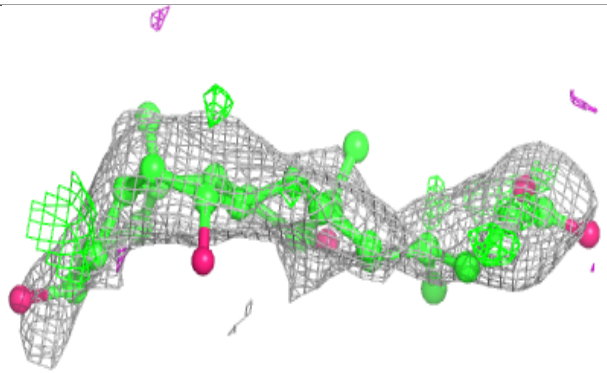


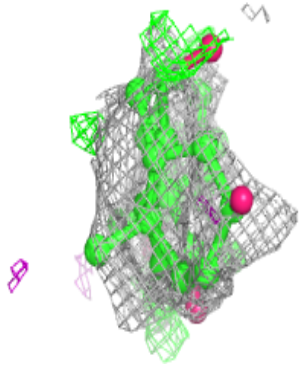


Electron density around CHD C 3271:

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

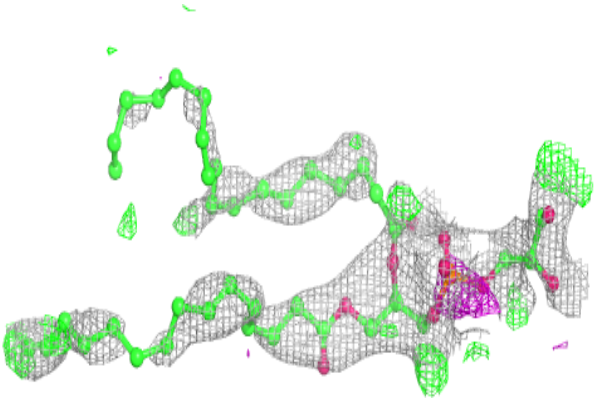


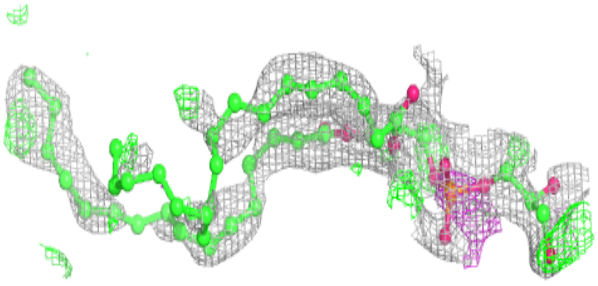


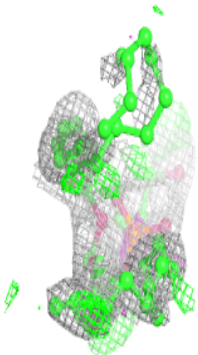


Electron density around PGV P 4268:

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

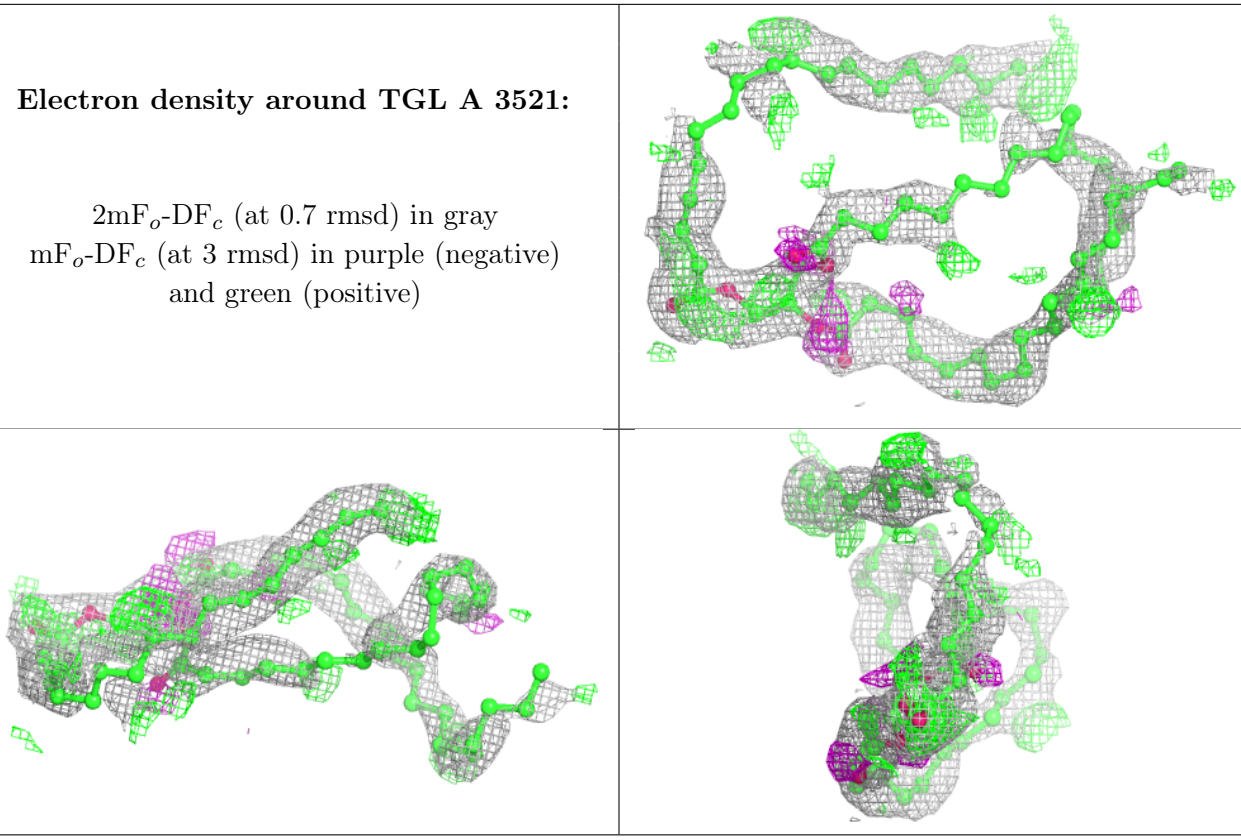






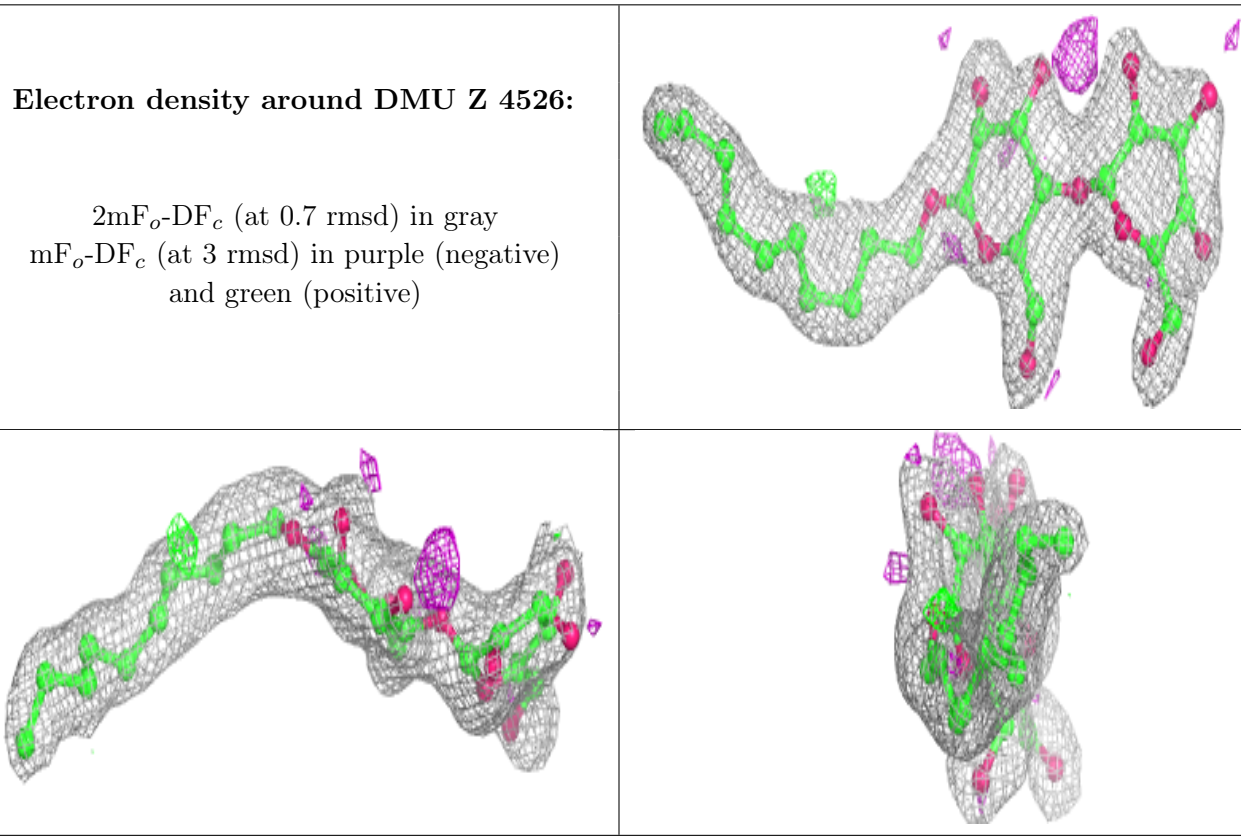
Electron density around TGL A 3521:

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



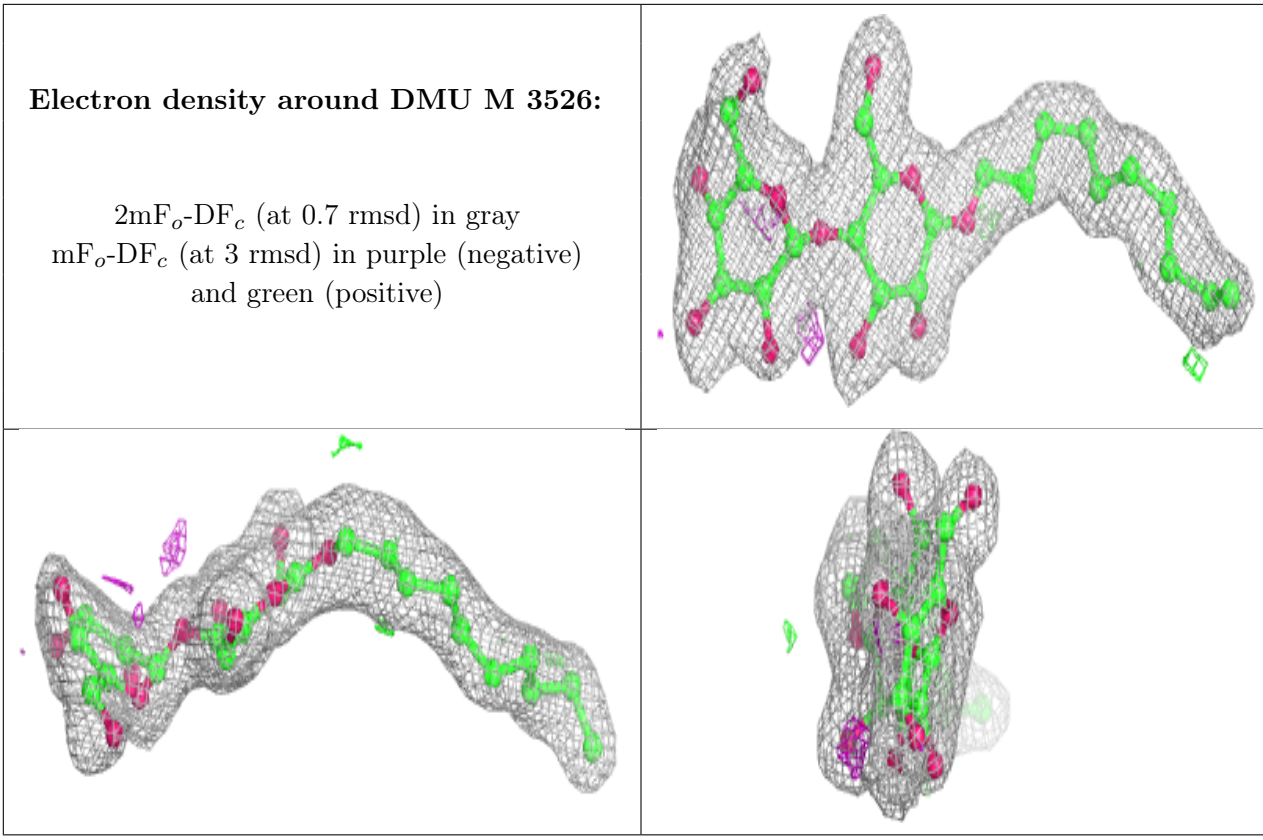
Electron density around DMU Z 4526:

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



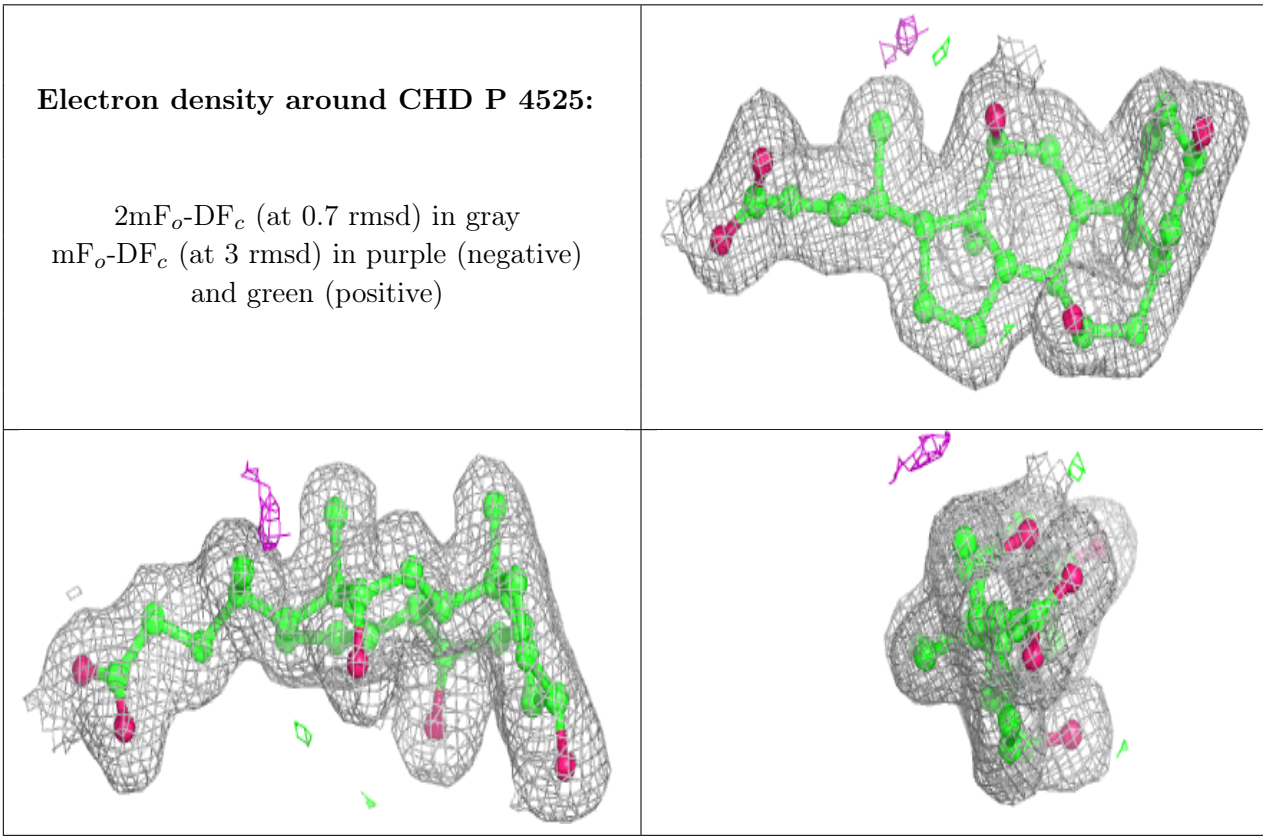
Electron density around DMU M 3526:

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



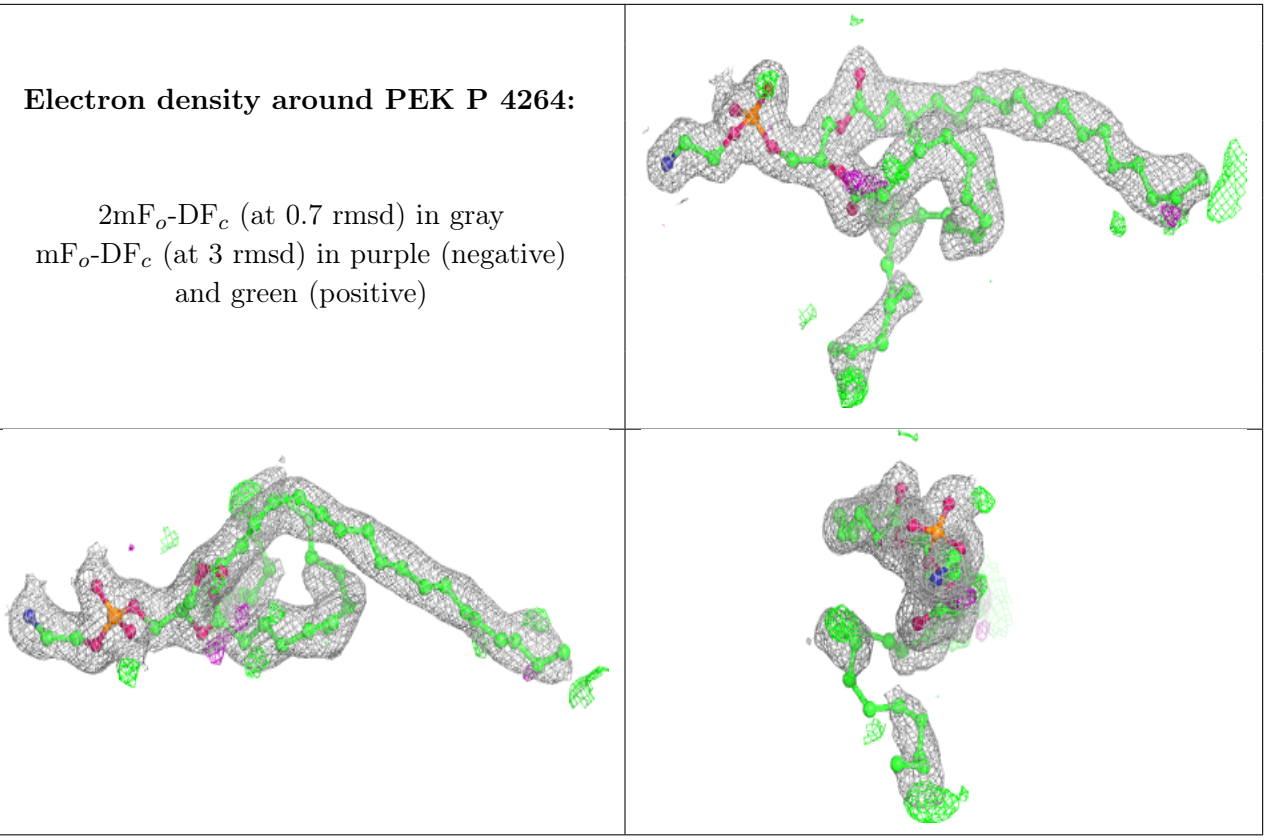
Electron density around CHD P 4525:

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



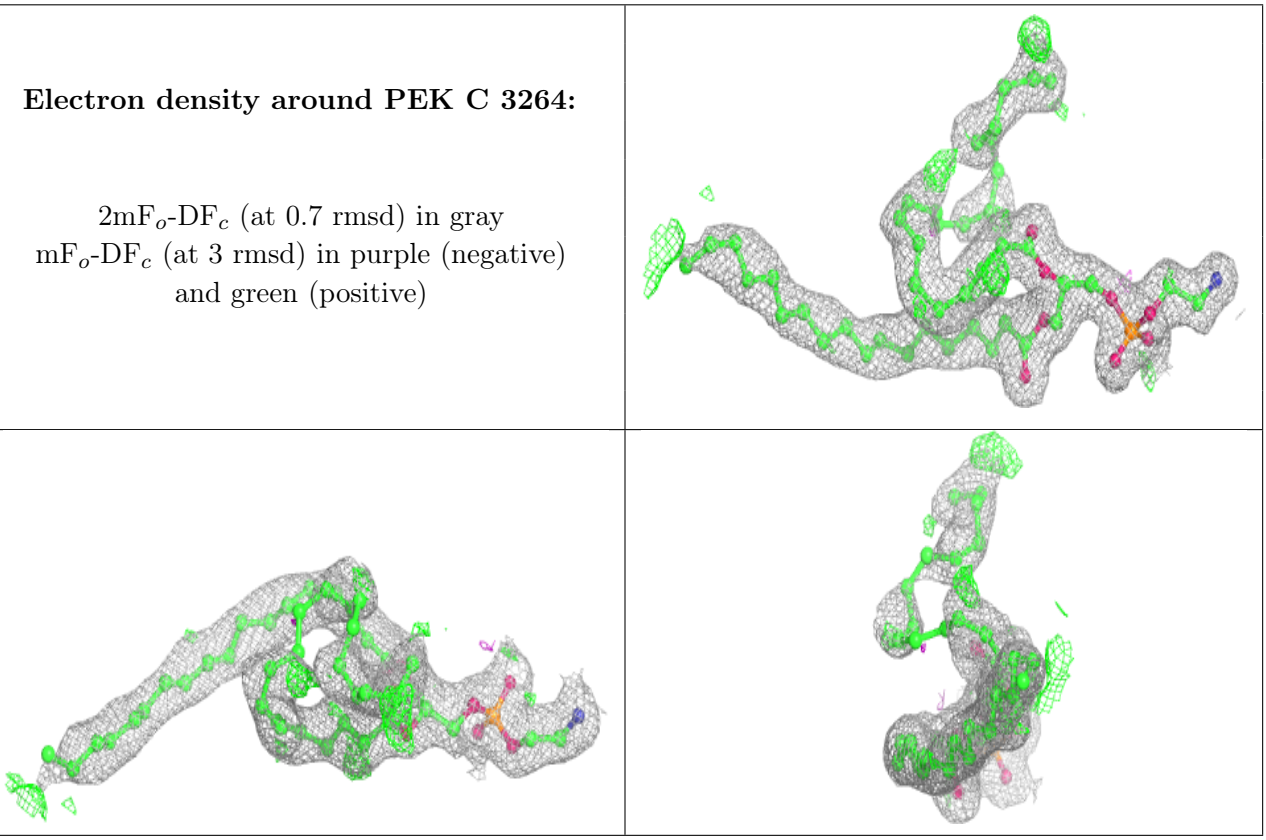
Electron density around PEK P 4264:

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



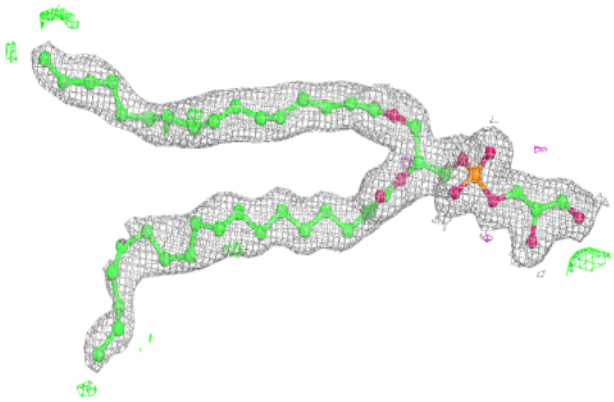
Electron density around PEK C 3264:

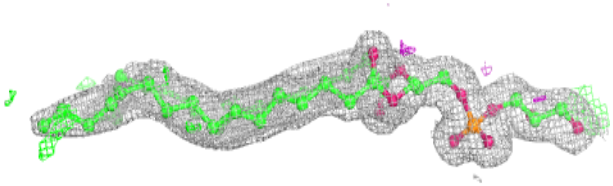
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

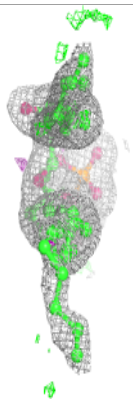


Electron density around PGV P 4267:

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

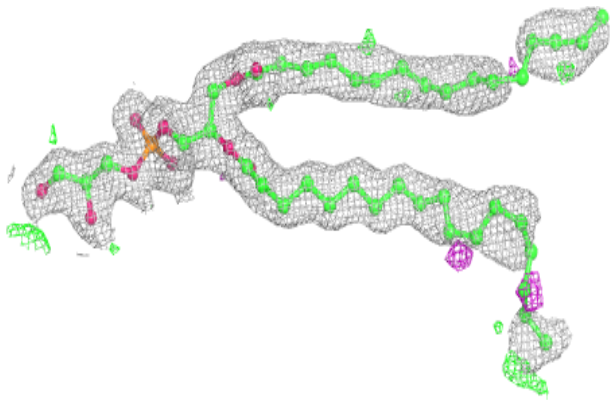


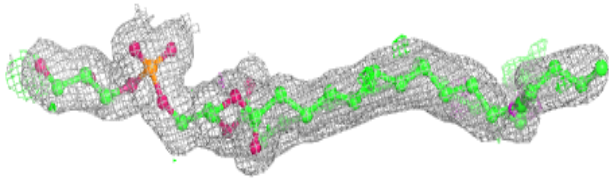


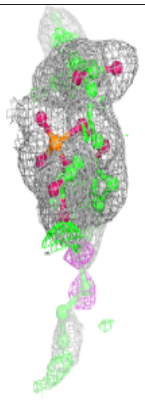


Electron density around PGV C 3267:

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

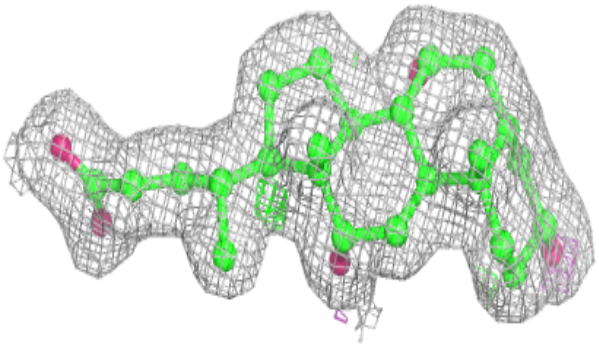


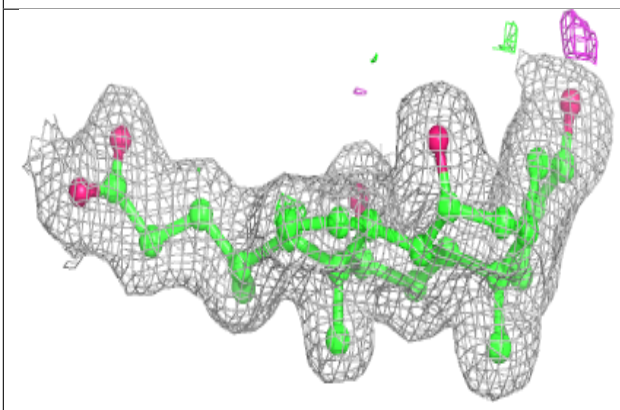


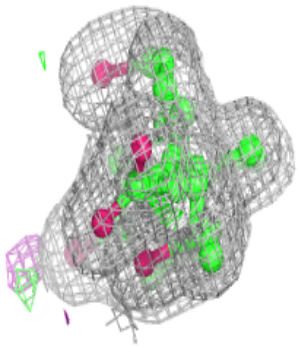


Electron density around CHD C 3525:

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

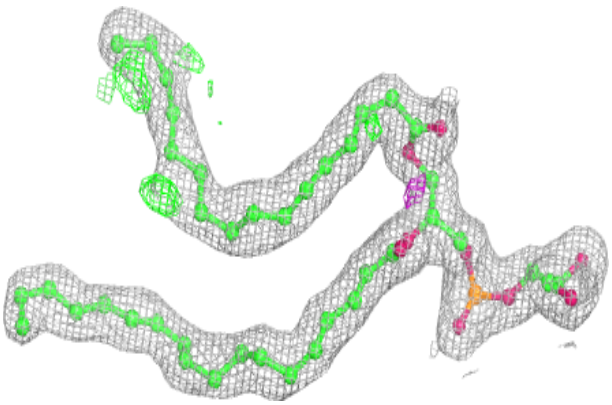


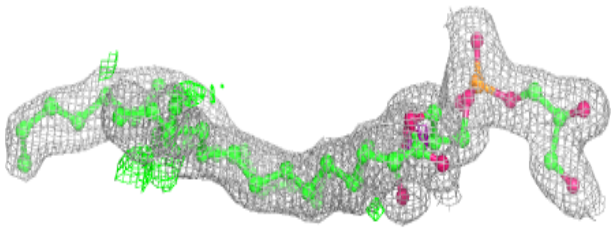


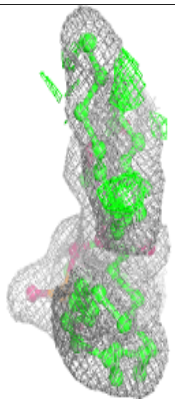


Electron density around PGV N 4266:

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

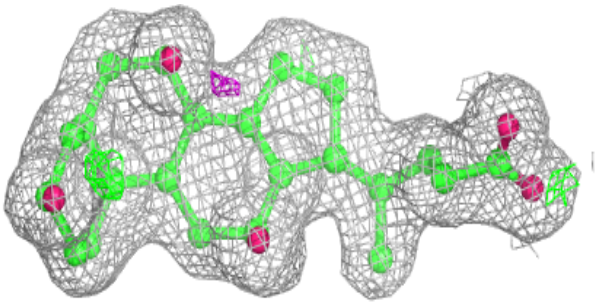


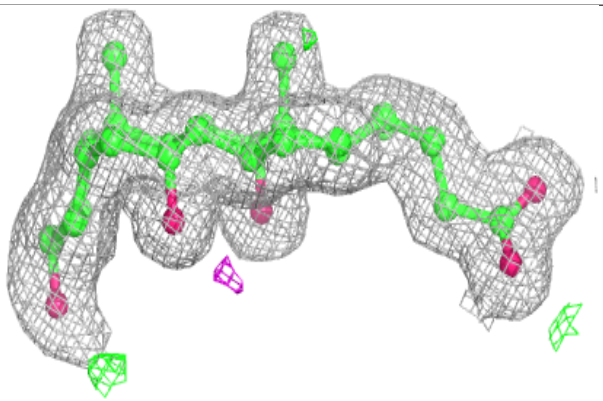


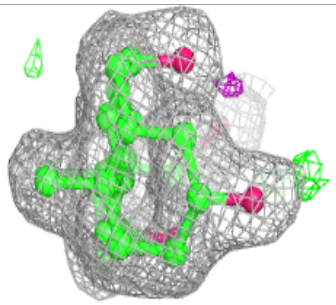


Electron density around CHD B 4085:

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

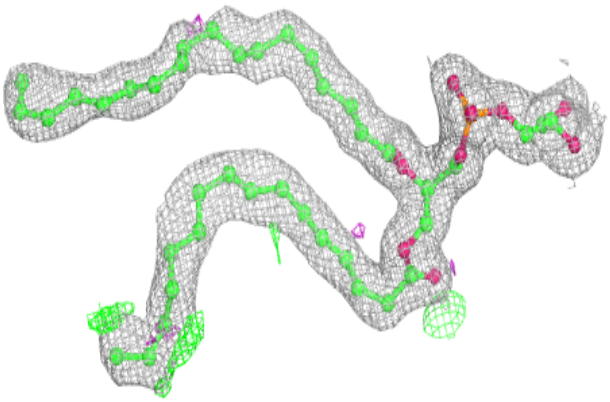


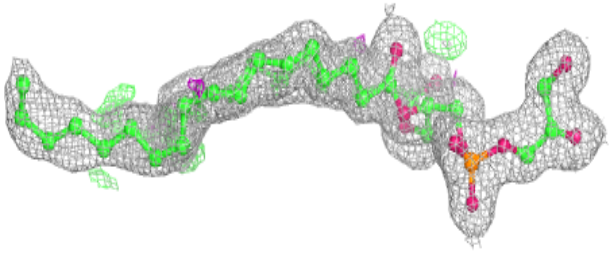


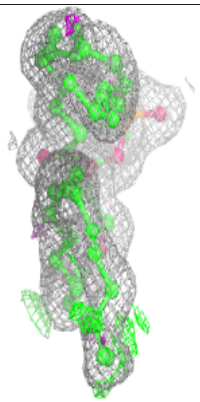


Electron density around PGV A 3266:

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

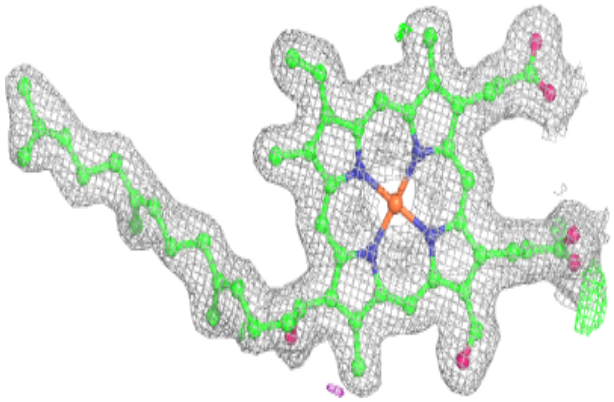


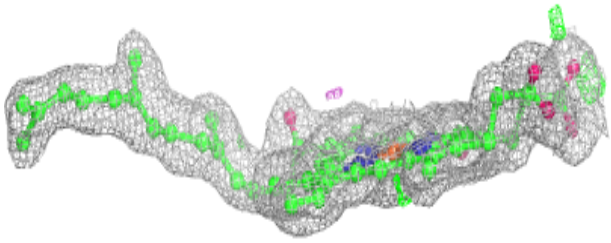


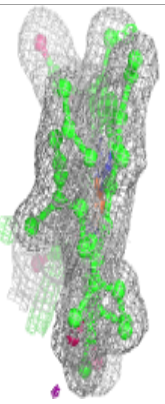


Electron density around HEA N 515:

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

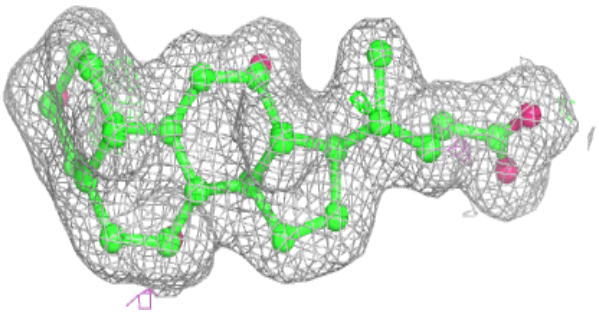


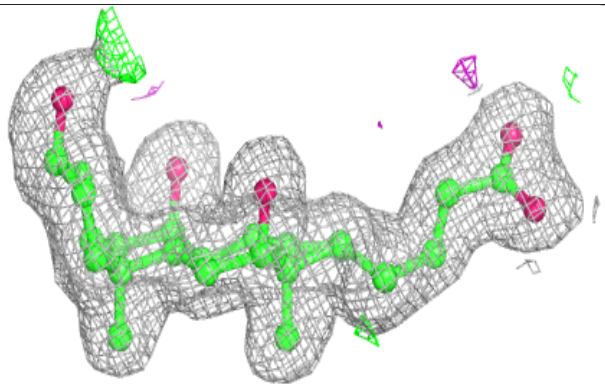


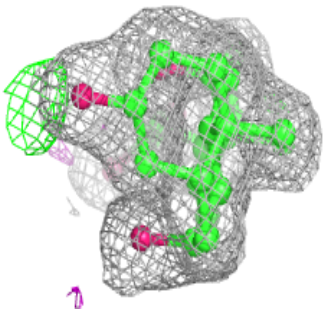


Electron density around CHD O 3085:

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

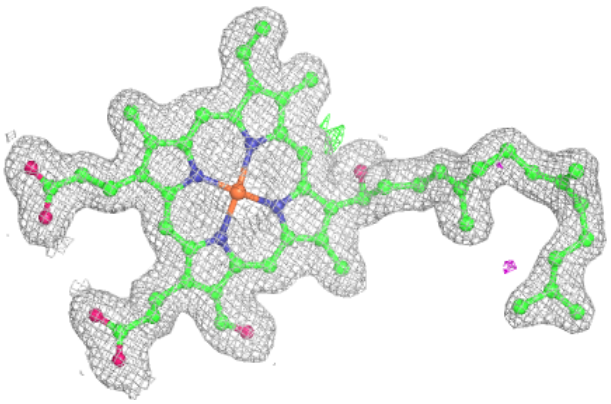


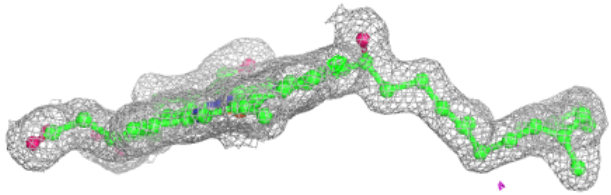


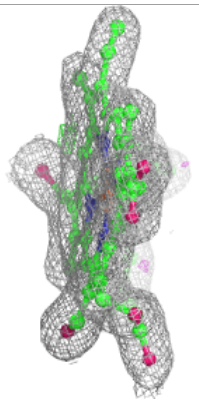


Electron density around HEA N 516:

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

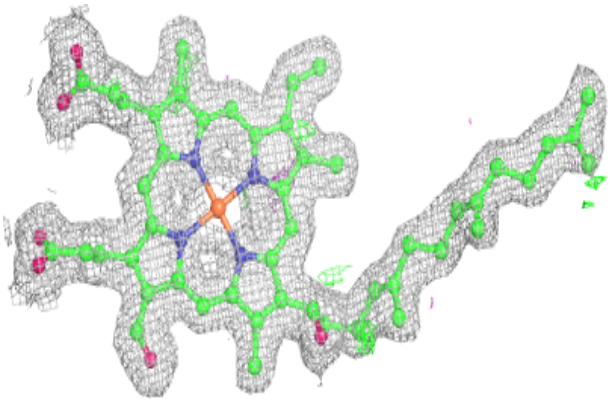


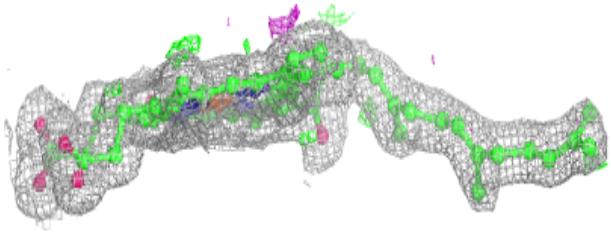


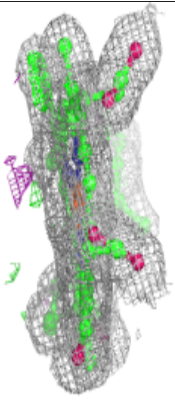


Electron density around HEA A 515:

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

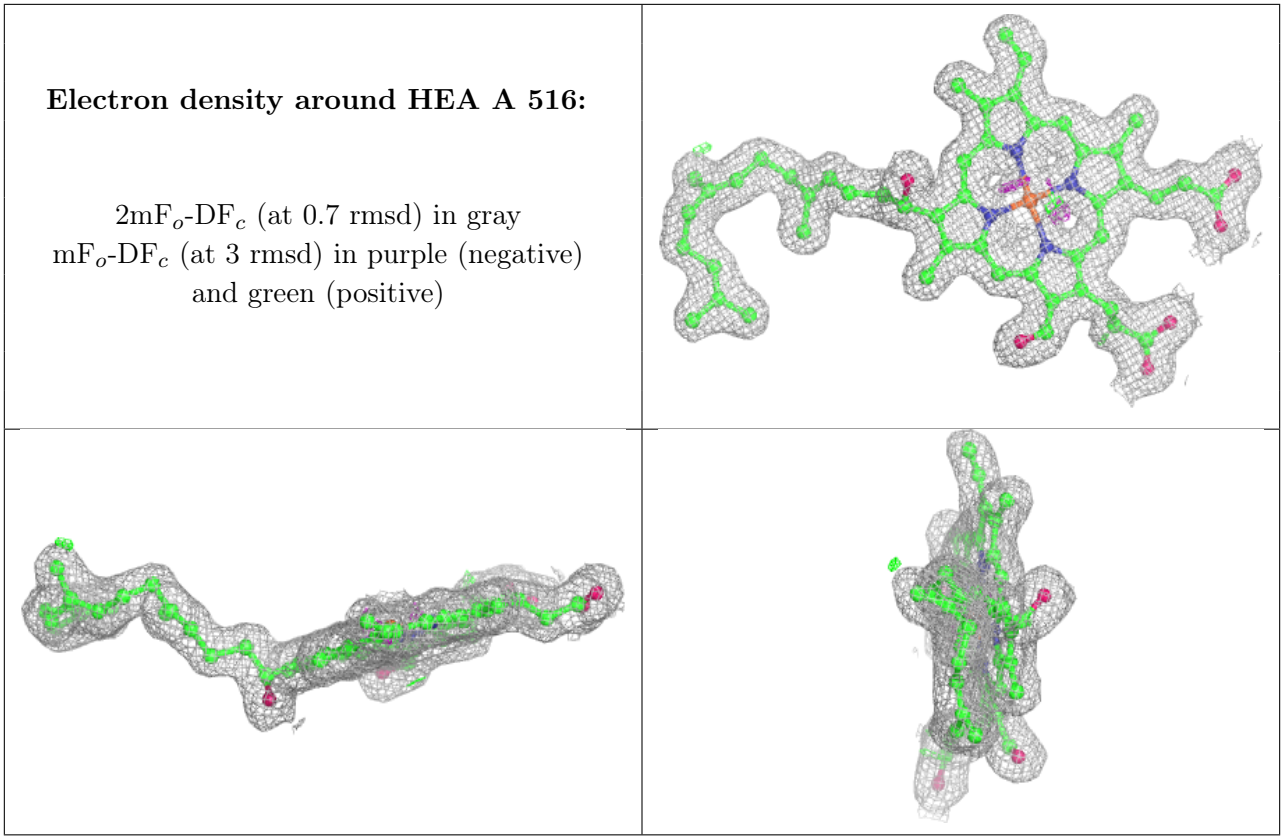






Electron density around HEA A 516:

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



6.5 Other polymers (i)

There are no such residues in this entry.