wwPDB EM Validation Summary Report (i)

Oct 14, 2024 – 08:48 AM EDT

PDB ID	:	7SC9
EMDB ID	:	EMD-25030
Title	:	Synechocystis PCC 6803 Phycobilisome core, complex with OCP
Authors	:	Sauer, P.V.; Sutter, M.; Dominguez-Martin, M.A.; Kirst, H.; Kerfeld, C.A.
Deposited on	:	2021-09-27
Resolution	:	2.60 Å(reported)

This is a wwPDB EM 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/EMValidationReportHelp
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:

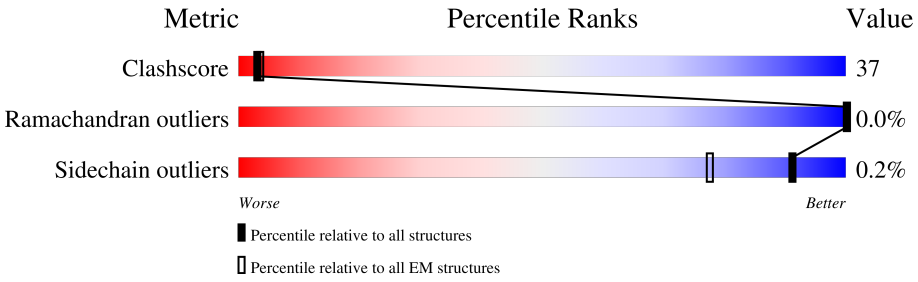
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	161	87% 42% 58%
1	AC	161	87% 37% 61%
1	AH	161	51% 48%
1	AJ	161	50% 50%
1	AN	161	44% 55%
1	AP	161	55% 44%
1	AR	161	42% 58%
1	AV	161	34% 65%

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Mol	Chain	Length	Quality of chain
1	AX	161	48% 52%
1	AZ	161	38% 61%
1	BI	161	60% 50% 50%
1	BK	161	61% 39% 60%
1	BP	161	48% 51%
1	BR	161	50% 50%
1	BV	161	42% 57%
1	BX	161	53% 47%
1	BZ	161	46% 53%
1	CC	161	39% 60%
1	CE	161	34% 66%
1	CG	161	47% 52%
1	CR	161	6% 37% 63%
1	CT	161	48% 51%
1	CV	161	47% 52%
1	CY	161	11% 27% 73%
1	DA	161	47% 52%
1	DC	161	54% 45%
1	DJ	161	8% 32% 66%
1	DL	161	39% 60%
1	DN	161	50% 48%
1	DQ	161	7% 32% 68%
1	DS	161	43% 56%
1	DU	161	49% 50%
2	AB	161	93% 50% 50%

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Mol	Chain	Length	Quality of chain
2	AD	161	92% 37% 63%
2	AF	161	96% 39% 61%
2	AI	161	60% 40%
2	AL	161	45% 55%
2	AO	161	48% 52%
2	AQ	161	59% 41%
2	AS	161	42% 58%
2	AU	161	48% 52%
2	AW	161	46% 54%
2	AY	161	51% 49%
2	BJ	161	58% 50% 50%
2	BL	161	62% 37% 63%
2	BN	161	60% 41% 59%
2	BQ	161	57% 43%
2	BT	161	45% 55%
2	BW	161	50% 50%
2	BY	161	57% 43%
2	CA	161	50% 50%
2	CD	161	48% 52%
2	CF	161	45% 55%
2	CH	161	50% 50%
2	CS	161	5% 35% 65%
2	CU	161	6% 49% 51%
2	CW	161	43% 57%
2	CZ	161	8% 32% 68%

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Mol	Chain	Length	Quality of chain
2	DB	161	47% 53%
2	DD	161	45% 55%
2	DK	161	7% 40% 60%
2	DM	161	49% 51%
2	DO	161	51% 49%
2	DR	161	7% 32% 68%
2	DT	161	40% 60%
2	DV	161	33% 67%
3	AE	161	84% 40% 60%
3	BM	161	46% 39% 60%
4	AK	169	42% 58%
4	BS	169	48% 52%
5	BA	67	84% 34% 64%
5	BB	67	9% 42% 58%
5	CJ	67	31% 45% 55%
5	CK	67	7% 55% 45%
5	DF	67	49% 51%
5	DX	67	46% 54%
6	BD	896	45% 49% 5%
6	CM	896	43% 52% 5%
7	BF	121	10% 20% 70%
7	CO	121	13% 17% 70%
8	BG	249	11% 12% 77%
8	CP	249	12% 10% 77%
8	DG	249	8% 12% 9% 78%

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Mol	Chain	Length	Quality of chain
8	DH	249	13% 8% 78%
8	DY	249	9% 11% 11% 78%
8	DZ	249	12% 10% 78%
9	BH	317	34% 41% 54% 5%
9	CQ	317	29% 41% 53% 5%
9	DI	317	34% 29% 64% 7%
9	EA	317	29% 32% 61% 7%

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
10	CYC	AV	200	-	-	X	-
10	CYC	DD	200	-	-	X	-

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 117470 atoms, of which 208 are hydrogens and 0 are deuteriums.

In the tables below, 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 Allophycocyanin alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	160	Total	C	N	O	S	0	0
			1210	754	207	242	7		
1	AC	160	Total	C	N	O	S	0	0
			1210	754	207	242	7		
1	AH	160	Total	C	N	O	S	0	0
			1210	754	207	242	7		
1	AJ	160	Total	C	N	O	S	0	0
			1210	754	207	242	7		
1	AN	160	Total	C	N	O	S	0	0
			1210	754	207	242	7		
1	AP	160	Total	C	N	O	S	0	0
			1210	754	207	242	7		
1	AR	160	Total	C	N	O	S	0	0
			1210	754	207	242	7		
1	AV	160	Total	C	N	O	S	0	0
			1210	754	207	242	7		
1	AX	160	Total	C	N	O	S	0	0
			1210	754	207	242	7		
1	AZ	160	Total	C	N	O	S	0	0
			1210	754	207	242	7		
1	BI	160	Total	C	N	O	S	0	0
			1210	754	207	242	7		
1	BK	160	Total	C	N	O	S	0	0
			1210	754	207	242	7		
1	BP	160	Total	C	N	O	S	0	0
			1210	754	207	242	7		
1	BR	160	Total	C	N	O	S	0	0
			1210	754	207	242	7		
1	BV	160	Total	C	N	O	S	0	0
			1210	754	207	242	7		
1	BX	160	Total	C	N	O	S	0	0
			1210	754	207	242	7		
1	BZ	160	Total	C	N	O	S	0	0
			1210	754	207	242	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	CC	160	Total	C	N	O	S	0	0
			1210	754	207	242	7		
1	CE	160	Total	C	N	O	S	0	0
			1210	754	207	242	7		
1	CG	160	Total	C	N	O	S	0	0
			1210	754	207	242	7		
1	CR	160	Total	C	N	O	S	0	0
			1210	754	207	242	7		
1	CT	160	Total	C	N	O	S	0	0
			1210	754	207	242	7		
1	CV	160	Total	C	N	O	S	0	0
			1210	754	207	242	7		
1	CY	160	Total	C	N	O	S	0	0
			1210	754	207	242	7		
1	DA	160	Total	C	N	O	S	0	0
			1210	754	207	242	7		
1	DC	160	Total	C	N	O	S	0	0
			1210	754	207	242	7		
1	DJ	160	Total	C	N	O	S	0	0
			1210	754	207	242	7		
1	DL	160	Total	C	N	O	S	0	0
			1210	754	207	242	7		
1	DN	160	Total	C	N	O	S	0	0
			1210	754	207	242	7		
1	DQ	160	Total	C	N	O	S	0	0
			1210	754	207	242	7		
1	DS	160	Total	C	N	O	S	0	0
			1210	754	207	242	7		
1	DU	160	Total	C	N	O	S	0	0
			1210	754	207	242	7		

- Molecule 2 is a protein called Allophycocyanin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AB	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		
2	AD	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		
2	AF	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		
2	AI	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	AL	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		
2	AO	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		
2	AQ	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		
2	AS	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		
2	AU	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		
2	AW	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		
2	AY	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		
2	BJ	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		
2	BL	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		
2	BN	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		
2	BQ	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		
2	BT	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		
2	BW	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		
2	BY	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		
2	CA	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		
2	CD	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		
2	CF	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		
2	CH	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		
2	CS	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		
2	CU	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		
2	CW	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	CZ	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		
2	DB	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		
2	DD	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		
2	DK	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		
2	DM	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		
2	DO	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		
2	DR	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		
2	DT	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		
2	DV	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		

- Molecule 3 is a protein called Allophycocyanin subunit alpha-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AE	160	Total	C	N	O	S	0	0
			1254	797	212	241	4		
3	BM	160	Total	C	N	O	S	0	0
			1254	797	212	241	4		

- Molecule 4 is a protein called Allophycocyanin subunit beta-18.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AK	169	Total	C	N	O	S	0	0
			1322	825	229	259	9		
4	BS	169	Total	C	N	O	S	0	0
			1322	825	229	259	9		

- Molecule 5 is a protein called Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	BA	67	Total	C	N	O	S	0	0
			546	343	104	94	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	BB	67	Total	C	N	O	S	0	0
			546	343	104	94	5		
5	CJ	67	Total	C	N	O	S	0	0
			546	343	104	94	5		
5	CK	67	Total	C	N	O	S	0	0
			546	343	104	94	5		
5	DF	67	Total	C	N	O	S	0	0
			546	343	104	94	5		
5	DX	67	Total	C	N	O	S	0	0
			546	343	104	94	5		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BA	36	TRP	SER	conflict	UNP Q01950
BB	36	TRP	SER	conflict	UNP Q01950
CJ	36	TRP	SER	conflict	UNP Q01950
CK	36	TRP	SER	conflict	UNP Q01950
DF	36	TRP	SER	conflict	UNP Q01950
DX	36	TRP	SER	conflict	UNP Q01950

- Molecule 6 is a protein called Phycobiliprotein ApcE.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	BD	850	Total	C	N	O	S	0	0
			6761	4299	1183	1262	17		
6	CM	850	Total	C	N	O	S	0	0
			6761	4299	1183	1262	17		

- Molecule 7 is a protein called Sll1873 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	BF	36	Total	C	N	O	S	0	0
			277	172	55	49	1		
7	CO	36	Total	C	N	O	S	0	0
			277	172	55	49	1		

- Molecule 8 is a protein called Phycobilisome rod-core linker polypeptide CpcG.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	BG	57	Total	C	N	O	S	0	0
			451	282	87	80	2		

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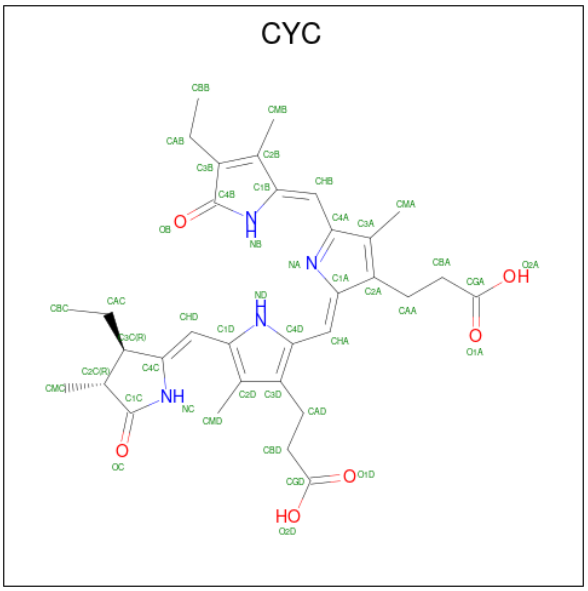
Mol	Chain	Residues	Atoms					AltConf	Trace
8	CP	57	Total	C	N	O	S	0	0
			451	282	87	80	2		
8	DG	54	Total	C	N	O	S	0	0
			426	266	83	75	2		
8	DH	54	Total	C	N	O	S	0	0
			426	266	83	75	2		
8	DY	54	Total	C	N	O	S	0	0
			426	266	83	75	2		
8	DZ	54	Total	C	N	O	S	0	0
			426	266	83	75	2		

- Molecule 9 is a protein called Orange carotenoid-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	BH	300	Total	C	N	O	S	0	0
			2302	1474	388	429	11		
9	CQ	300	Total	C	N	O	S	0	0
			2302	1474	388	429	11		
9	DI	296	Total	C	N	O	S	0	0
			2280	1459	387	423	11		
9	EA	296	Total	C	N	O	S	0	0
			2280	1459	387	423	11		

- Molecule 10 is PHYCOCYANOBILIN (three-letter code: CYC) (formula: $C_{33}H_{40}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
10	AA	1	Total	C	N	O	0
			43	33	4	6	
10	AB	1	Total	C	N	O	0
			43	33	4	6	
10	AC	1	Total	C	N	O	0
			43	33	4	6	
10	AD	1	Total	C	N	O	0
			43	33	4	6	
10	AE	1	Total	C	N	O	0
			43	33	4	6	
10	AF	1	Total	C	N	O	0
			43	33	4	6	
10	AH	1	Total	C	N	O	0
			43	33	4	6	
10	AI	1	Total	C	N	O	0
			43	33	4	6	
10	AJ	1	Total	C	N	O	0
			43	33	4	6	
10	AK	1	Total	C	N	O	0
			43	33	4	6	
10	AL	1	Total	C	N	O	0
			43	33	4	6	
10	AN	1	Total	C	N	O	0
			43	33	4	6	
10	AO	1	Total	C	N	O	0
			43	33	4	6	
10	AP	1	Total	C	N	O	0
			43	33	4	6	
10	AQ	1	Total	C	N	O	0
			43	33	4	6	
10	AR	1	Total	C	N	O	0
			43	33	4	6	
10	AU	1	Total	C	N	O	0
			43	33	4	6	
10	AV	1	Total	C	N	O	0
			43	33	4	6	
10	AW	1	Total	C	N	O	0
			43	33	4	6	
10	AX	1	Total	C	N	O	0
			43	33	4	6	
10	AY	1	Total	C	N	O	0
			43	33	4	6	
10	AZ	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
10	BD	1	Total	C	N	O	0
			43	33	4	6	
10	BD	1	Total	C	N	O	0
			43	33	4	6	
10	BI	1	Total	C	N	O	0
			43	33	4	6	
10	BJ	1	Total	C	N	O	0
			43	33	4	6	
10	BK	1	Total	C	N	O	0
			43	33	4	6	
10	BL	1	Total	C	N	O	0
			43	33	4	6	
10	BM	1	Total	C	N	O	0
			43	33	4	6	
10	BN	1	Total	C	N	O	0
			43	33	4	6	
10	BP	1	Total	C	N	O	0
			43	33	4	6	
10	BQ	1	Total	C	N	O	0
			43	33	4	6	
10	BR	1	Total	C	N	O	0
			43	33	4	6	
10	BS	1	Total	C	N	O	0
			43	33	4	6	
10	BT	1	Total	C	N	O	0
			43	33	4	6	
10	BV	1	Total	C	N	O	0
			43	33	4	6	
10	BW	1	Total	C	N	O	0
			43	33	4	6	
10	BX	1	Total	C	N	O	0
			43	33	4	6	
10	BY	1	Total	C	N	O	0
			43	33	4	6	
10	BZ	1	Total	C	N	O	0
			43	33	4	6	
10	CC	1	Total	C	N	O	0
			43	33	4	6	
10	CD	1	Total	C	N	O	0
			43	33	4	6	
10	CE	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
10	CF	1	Total	C	N	O	0
			43	33	4	6	
10	CG	1	Total	C	N	O	0
			43	33	4	6	
10	CH	1	Total	C	N	O	0
			43	33	4	6	
10	CM	1	Total	C	N	O	0
			43	33	4	6	
10	CM	1	Total	C	N	O	0
			43	33	4	6	
10	CR	1	Total	C	N	O	0
			43	33	4	6	
10	CS	1	Total	C	N	O	0
			43	33	4	6	
10	CT	1	Total	C	N	O	0
			43	33	4	6	
10	CU	1	Total	C	N	O	0
			43	33	4	6	
10	CV	1	Total	C	N	O	0
			43	33	4	6	
10	CW	1	Total	C	N	O	0
			43	33	4	6	
10	CY	1	Total	C	N	O	0
			43	33	4	6	
10	CZ	1	Total	C	N	O	0
			43	33	4	6	
10	DA	1	Total	C	N	O	0
			43	33	4	6	
10	DB	1	Total	C	N	O	0
			43	33	4	6	
10	DC	1	Total	C	N	O	0
			43	33	4	6	
10	DD	1	Total	C	N	O	0
			43	33	4	6	
10	DJ	1	Total	C	N	O	0
			43	33	4	6	
10	DK	1	Total	C	N	O	0
			43	33	4	6	
10	DL	1	Total	C	N	O	0
			43	33	4	6	
10	DM	1	Total	C	N	O	0
			43	33	4	6	

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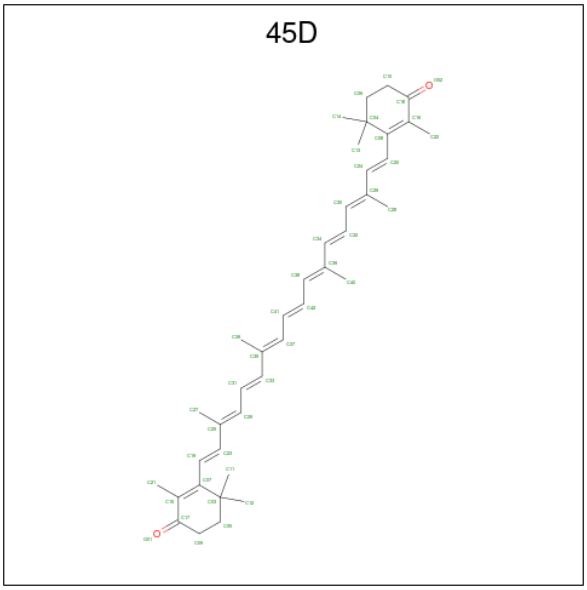
Mol	Chain	Residues	Atoms				AltConf
10	DN	1	Total	C	N	O	0
			43	33	4	6	
10	DO	1	Total	C	N	O	0
			43	33	4	6	
10	DQ	1	Total	C	N	O	0
			43	33	4	6	
10	DR	1	Total	C	N	O	0
			43	33	4	6	
10	DS	1	Total	C	N	O	0
			43	33	4	6	
10	DT	1	Total	C	N	O	0
			43	33	4	6	
10	DU	1	Total	C	N	O	0
			43	33	4	6	
10	DV	1	Total	C	N	O	0
			43	33	4	6	

- Molecule 11 is beta,beta-carotene-4,4'-dione (three-letter code: 45D) (formula: $C_{40}H_{52}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
11	BH	1	Total	C	H	O	0
			94	40	52	2	
11	CQ	1	Total	C	H	O	0
			94	40	52	2	
11	DI	1	Total	C	H	O	0
			94	40	52	2	

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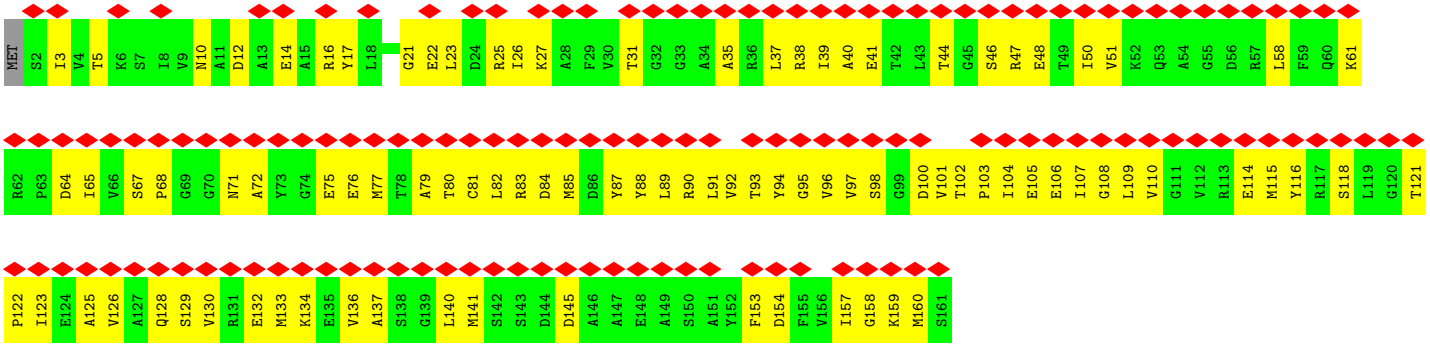
Mol	Chain	Residues	Atoms				AltConf
11	EA	1	Total	C	H	O	0
			94	40	52	2	

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

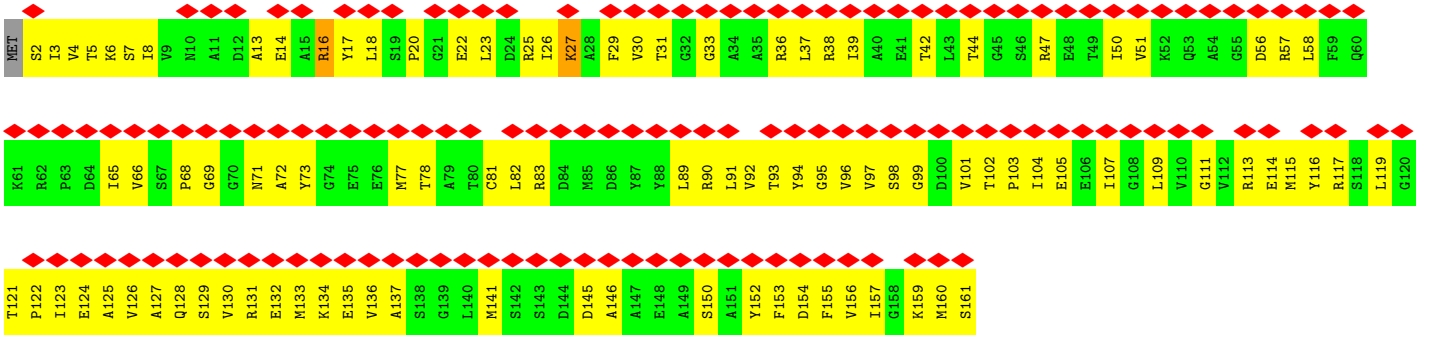
• Molecule 1: Allophycocyanin alpha chain

Chain AA:



• Molecule 1: Allophycocyanin alpha chain

Chain AC:

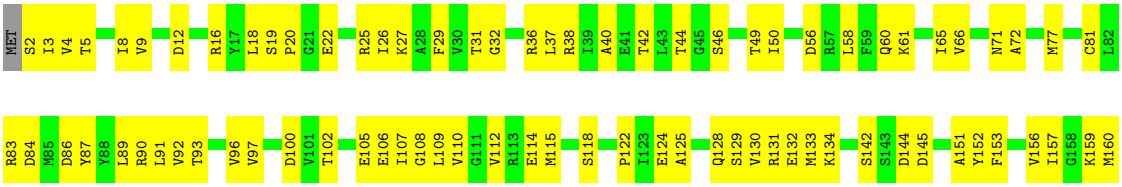


• Molecule 1: Allophycocyanin alpha chain

Chain AH:

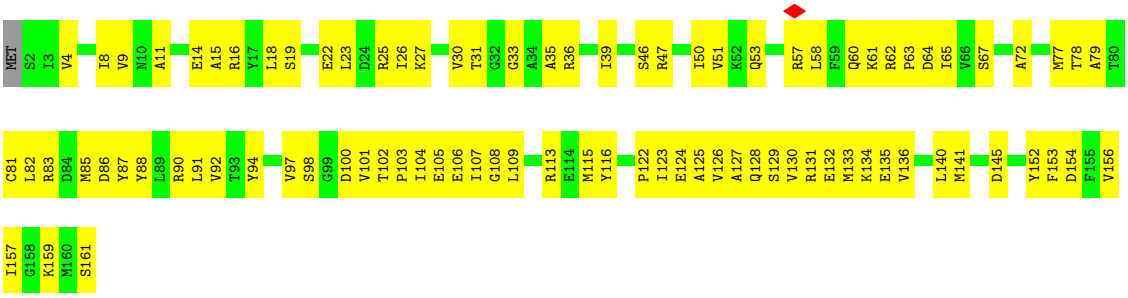
• Molecule 1: Allophycocyanin alpha chain

Chain AJ:



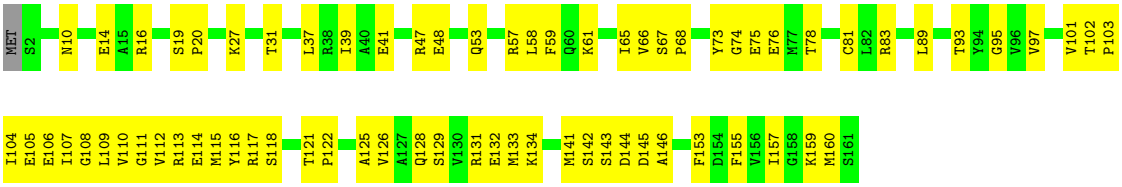
• Molecule 1: Allophycocyanin alpha chain

Chain AN:



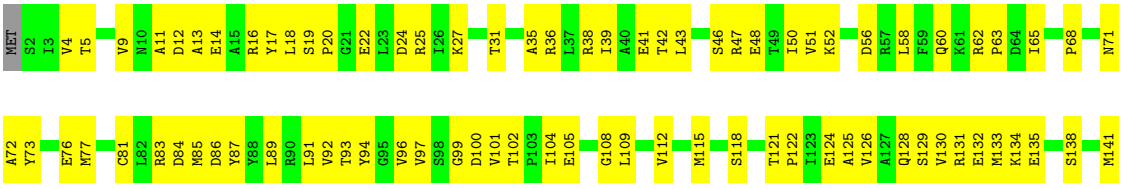
• Molecule 1: Allophycocyanin alpha chain

Chain AP:



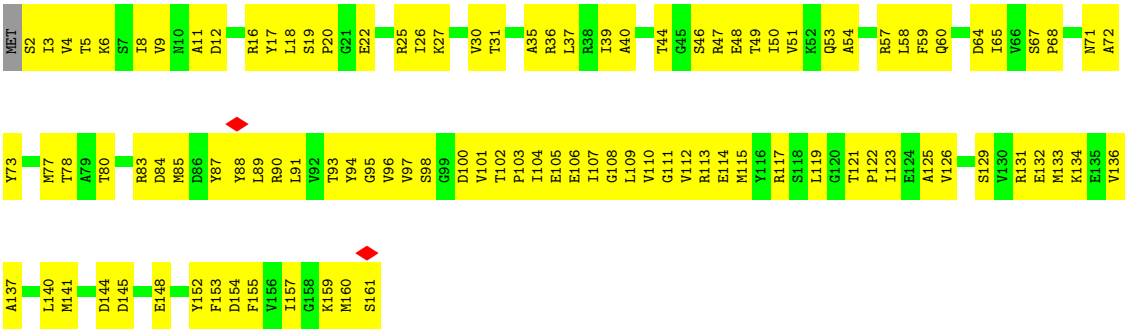
• Molecule 1: Allophycocyanin alpha chain

Chain AR:



• Molecule 1: Allophycocyanin alpha chain

Chain AV:

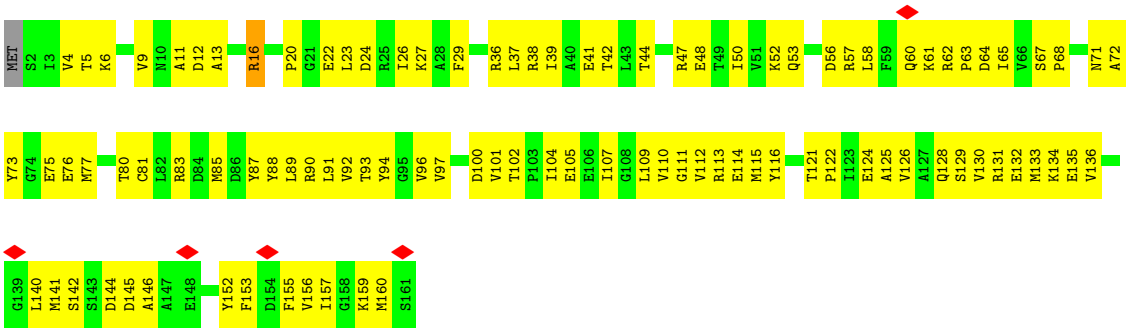


• Molecule 1: Allophycocyanin alpha chain

Chain AX:

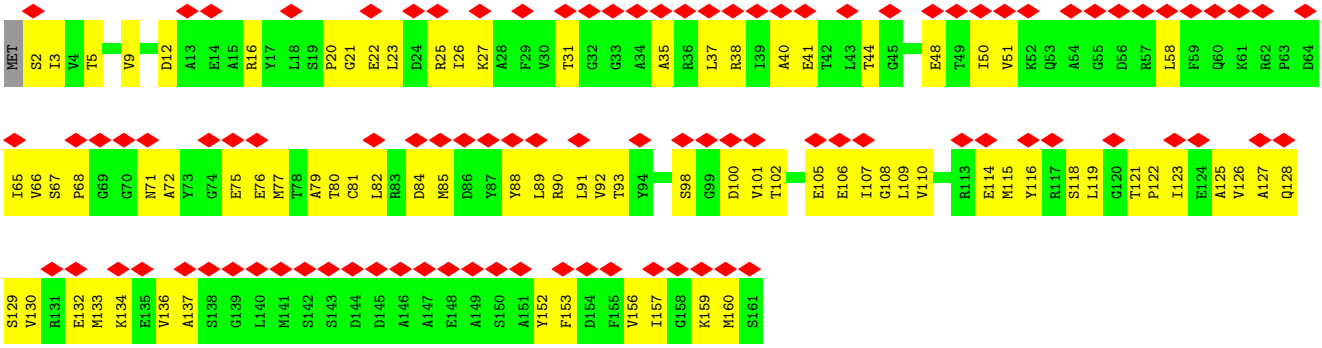
• Molecule 1: Allophycocyanin alpha chain

Chain AZ:

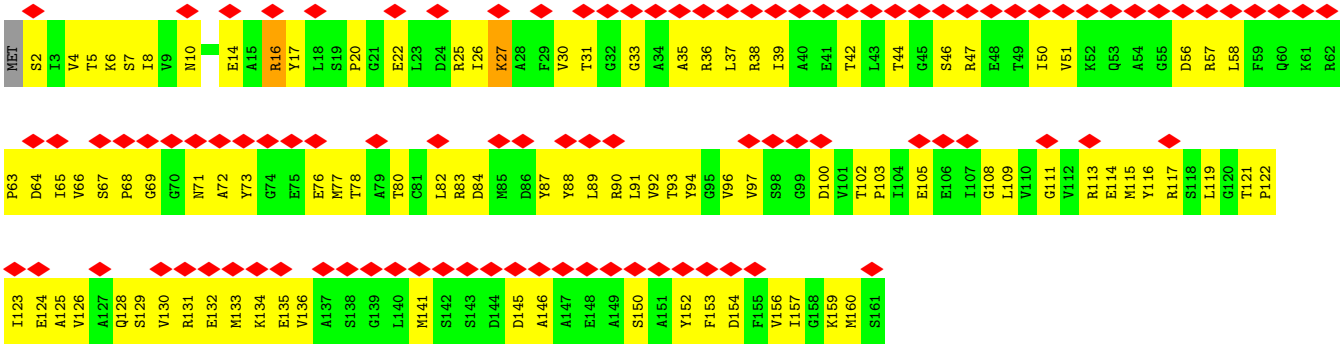


• Molecule 1: Allophycocyanin alpha chain

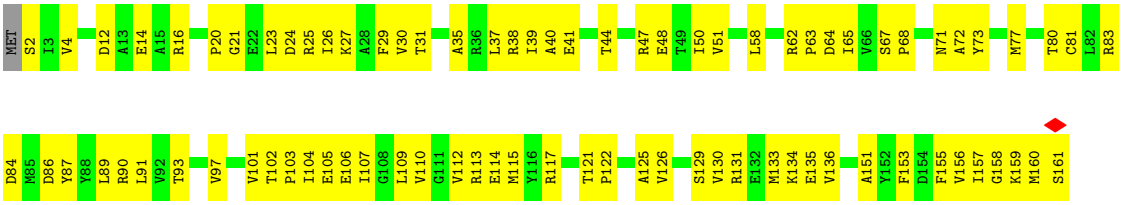
Chain BI:



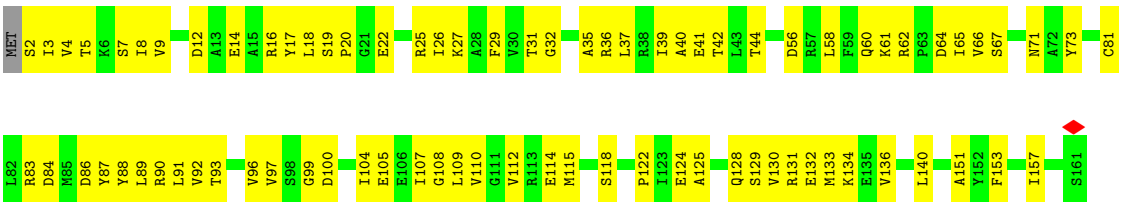
• Molecule 1: Allophycocyanin alpha chain



• Molecule 1: Allophycocyanin alpha chain



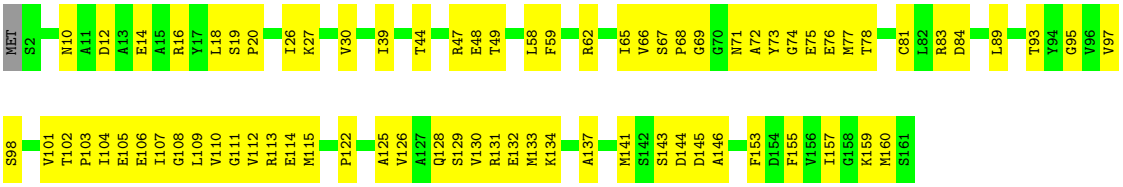
• Molecule 1: Allophycocyanin alpha chain



• Molecule 1: Allophycocyanin alpha chain

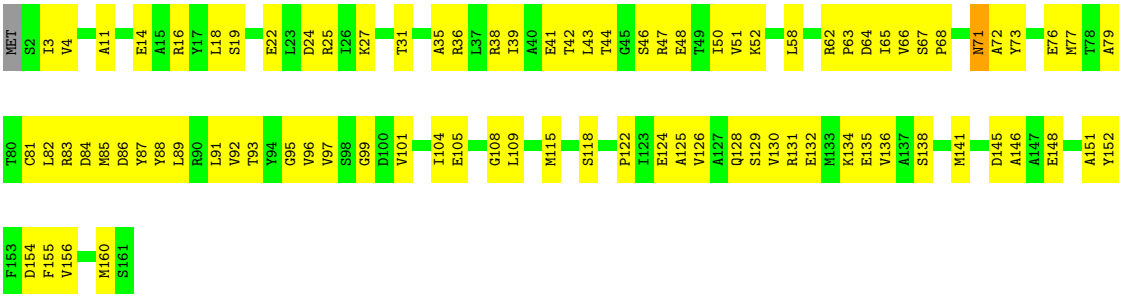
• Molecule 1: Allophycocyanin alpha chain

Chain BX:



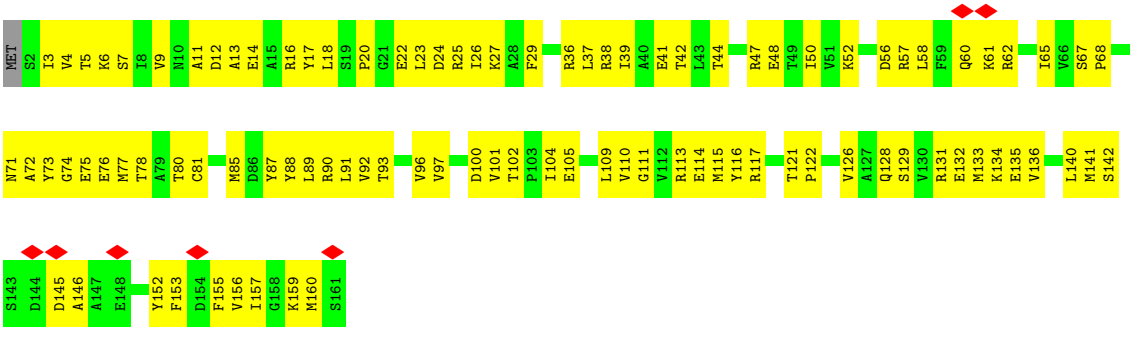
• Molecule 1: Allophycocyanin alpha chain

Chain BZ:



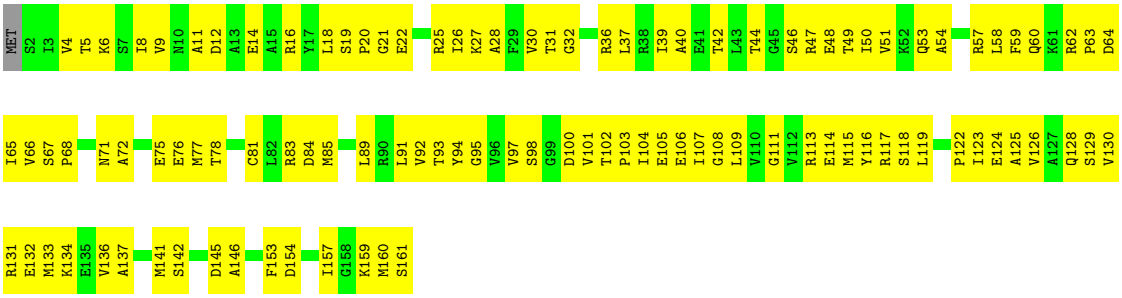
• Molecule 1: Allophycocyanin alpha chain

Chain CC:



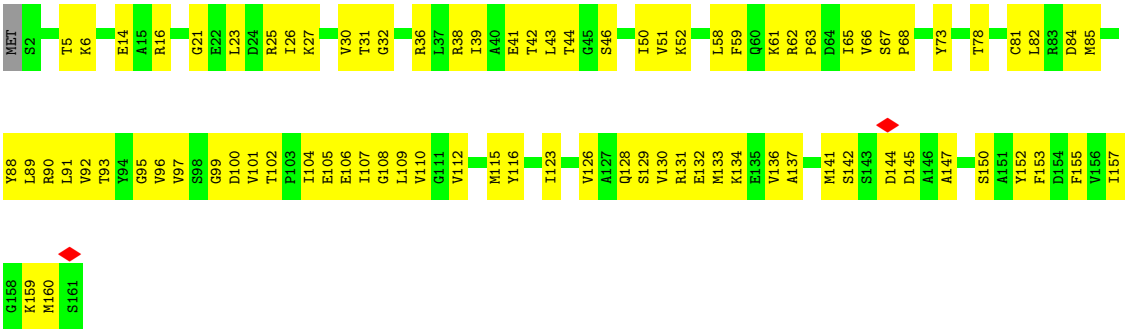
• Molecule 1: Allophycocyanin alpha chain

Chain CE:



• Molecule 1: Allophycocyanin alpha chain

Chain CG:

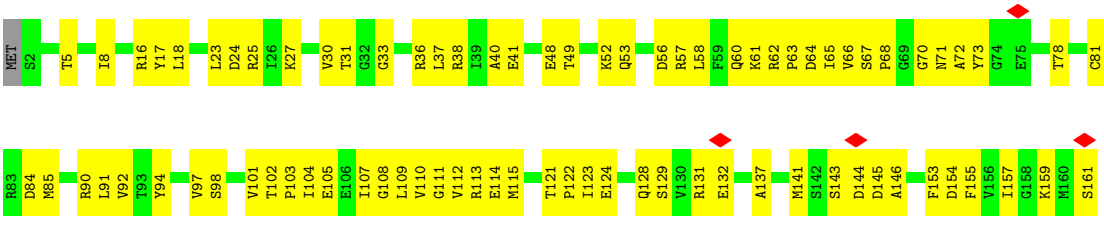


• Molecule 1: Allophycocyanin alpha chain

Chain CR:

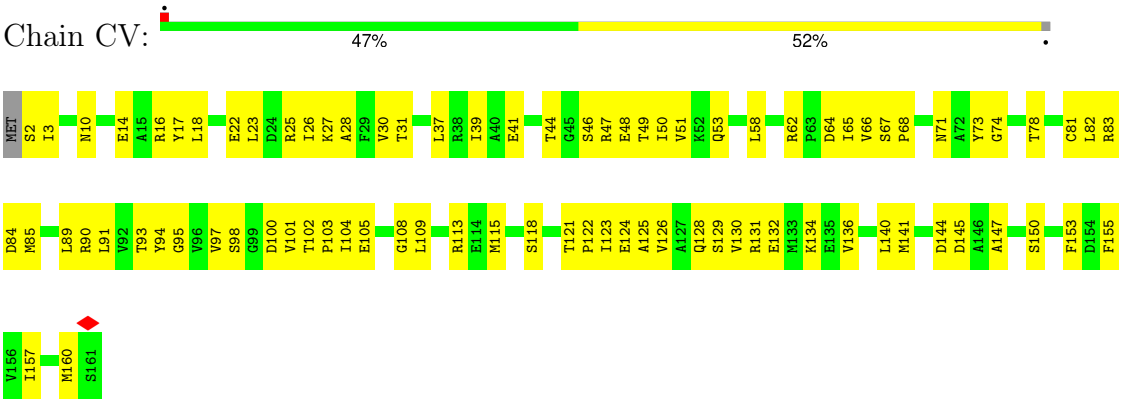
• Molecule 1: Allophycocyanin alpha chain

Chain CT:



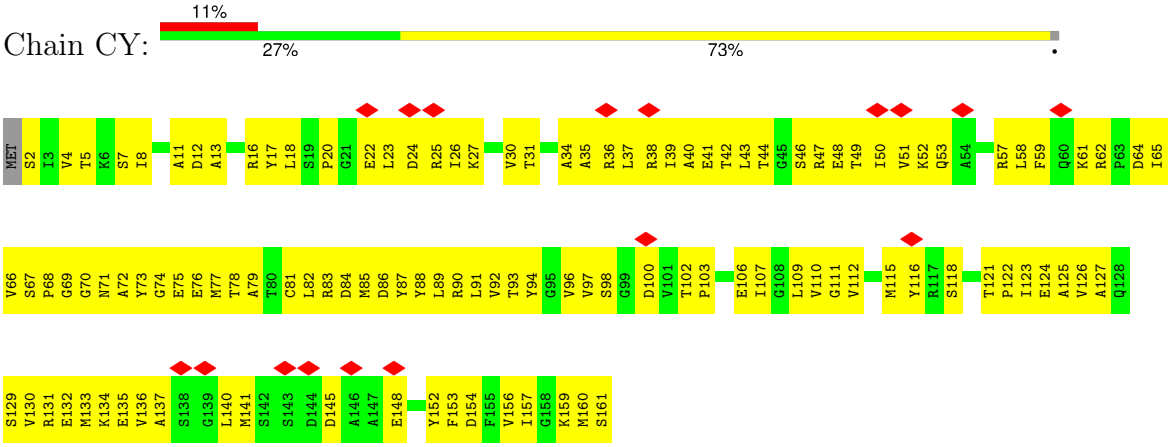
• Molecule 1: Allophycocyanin alpha chain

Chain CV:



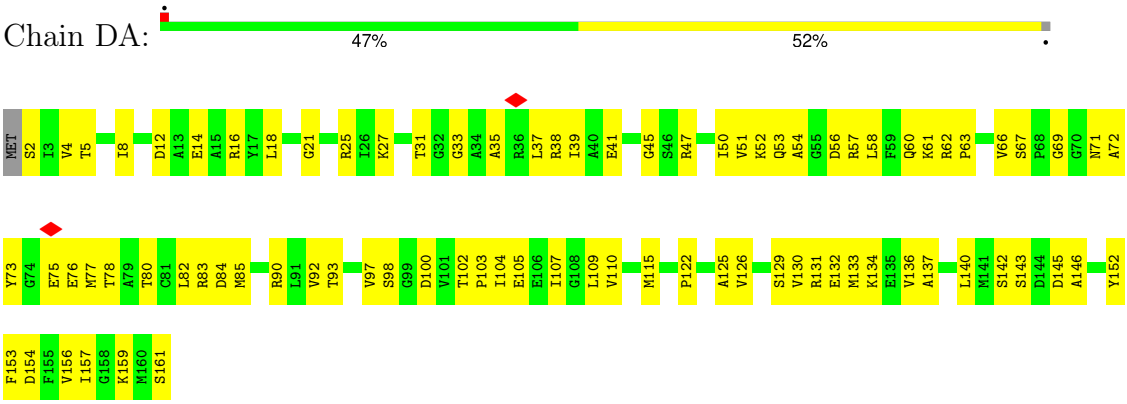
• Molecule 1: Allophycocyanin alpha chain

Chain CY:



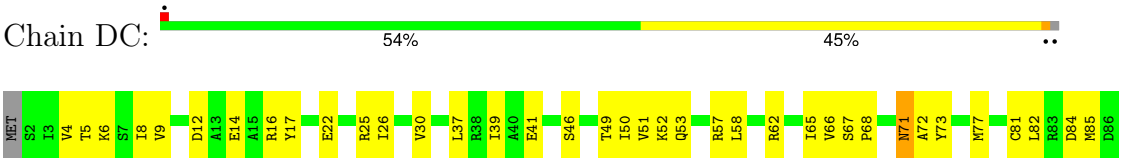
• Molecule 1: Allophycocyanin alpha chain

Chain DA:

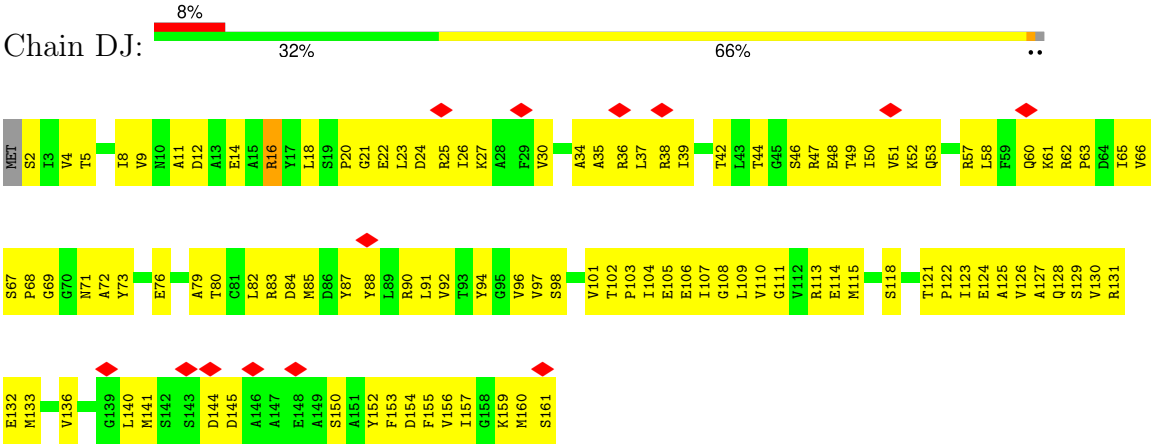


• Molecule 1: Allophycocyanin alpha chain

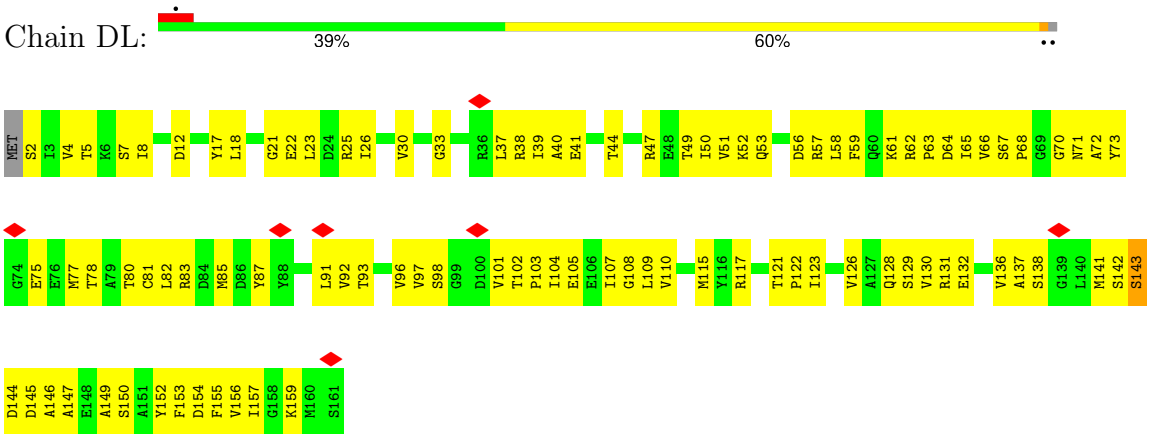
Chain DC:



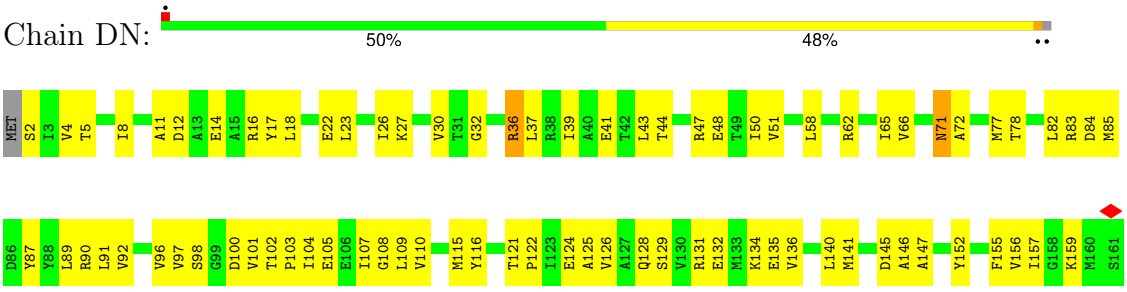
• Molecule 1: Allophycocyanin alpha chain



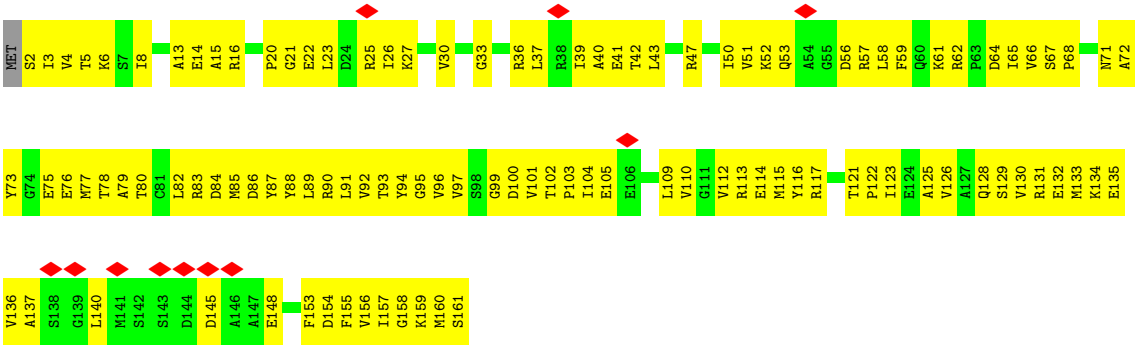
• Molecule 1: Allophycocyanin alpha chain



• Molecule 1: Allophycocyanin alpha chain



• Molecule 1: Allophycocyanin alpha chain



• Molecule 1: Allophycocyanin alpha chain

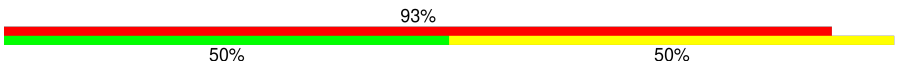
Chain DS:

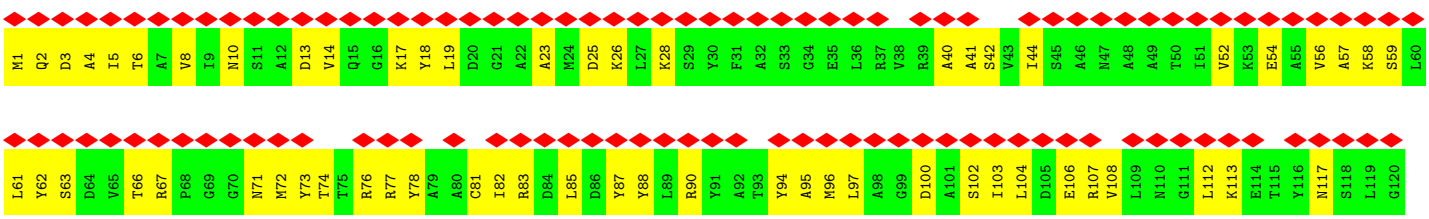
• Molecule 1: Allophycocyanin alpha chain

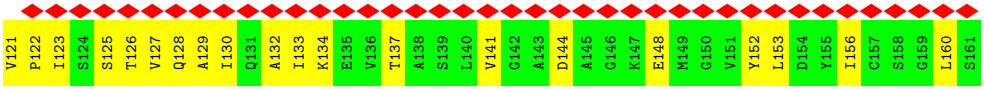
Chain DU:

• Molecule 2: Allophycocyanin beta chain

Chain AB:

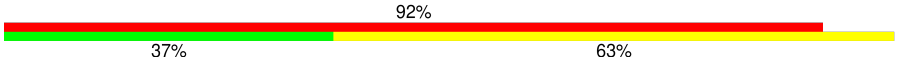


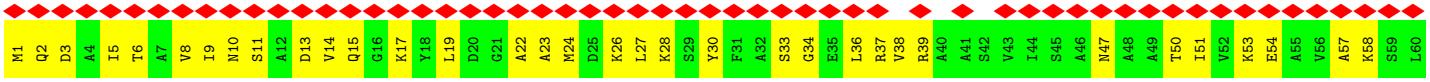


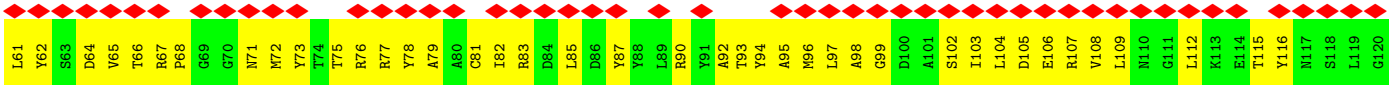


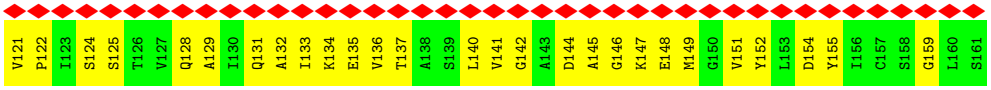
• Molecule 2: Allophycocyanin beta chain

Chain AD:



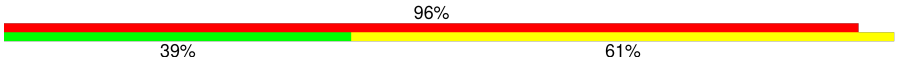


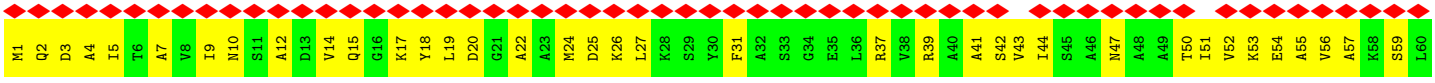


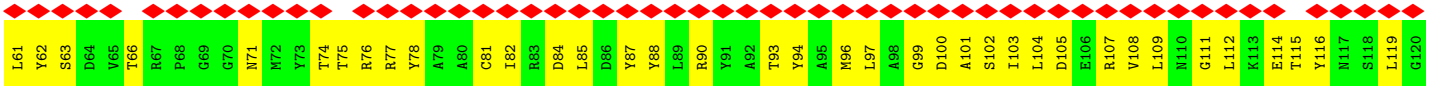


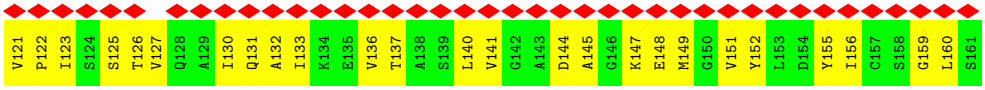
• Molecule 2: Allophycocyanin beta chain

Chain AF:



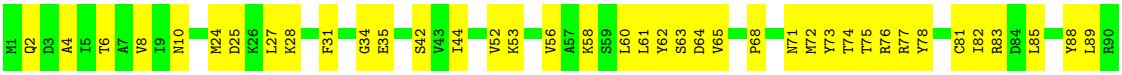


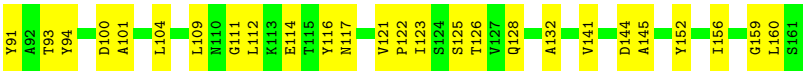




• Molecule 2: Allophycocyanin beta chain

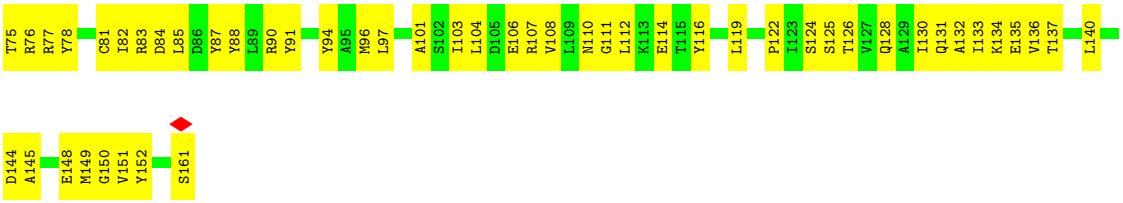
Chain AI:





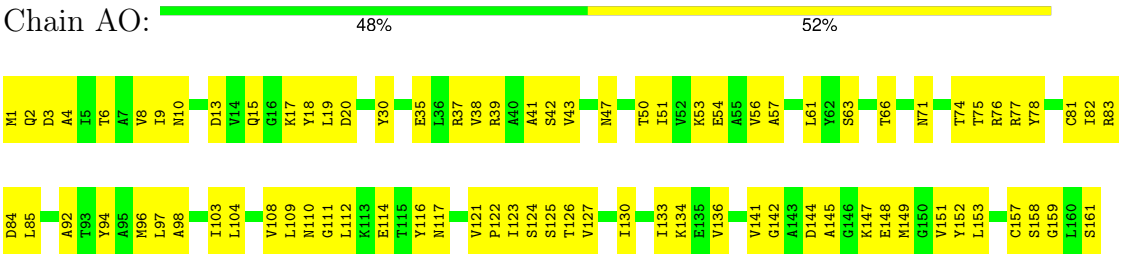
• Molecule 2: Allophycocyanin beta chain

Chain AL:



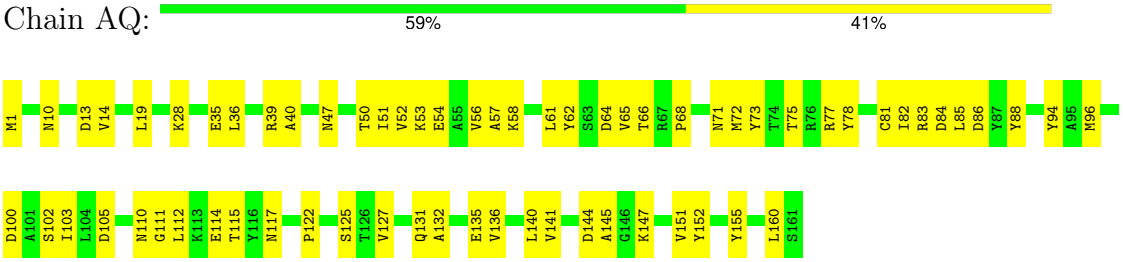
• Molecule 2: Allophycocyanin beta chain

Chain AO:



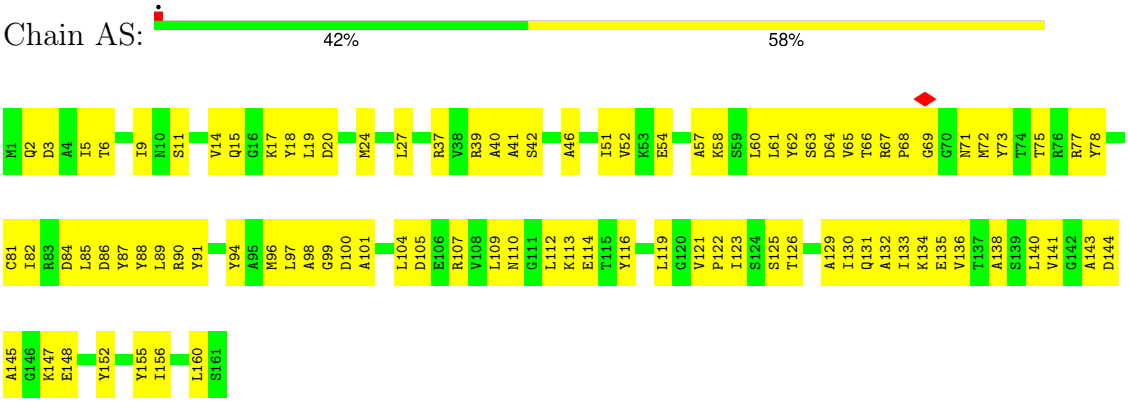
• Molecule 2: Allophycocyanin beta chain

Chain AQ:



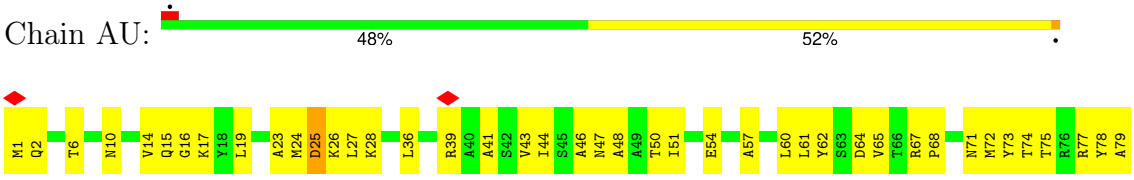
• Molecule 2: Allophycocyanin beta chain

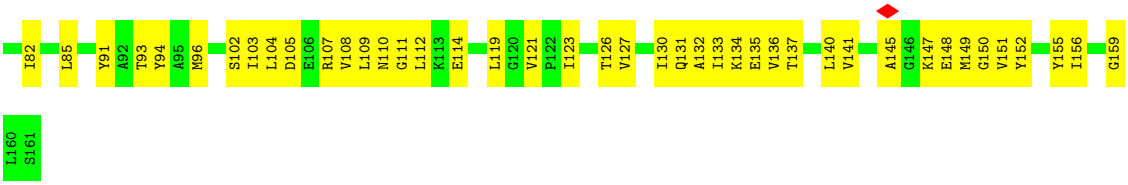
Chain AS:



• Molecule 2: Allophycocyanin beta chain

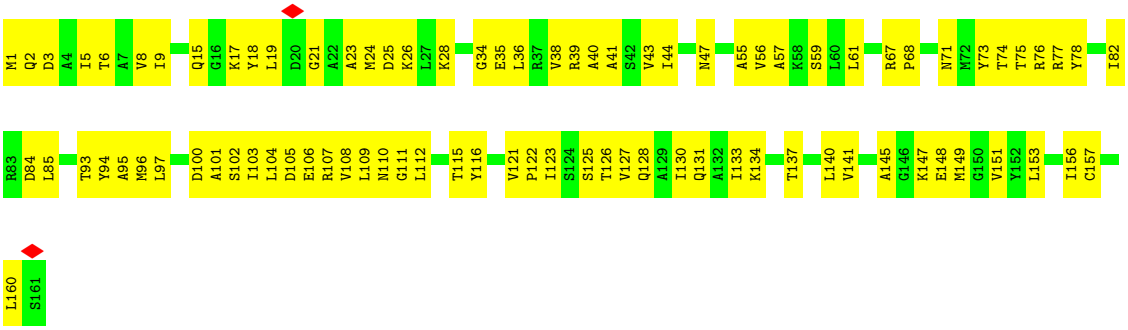
Chain AU:





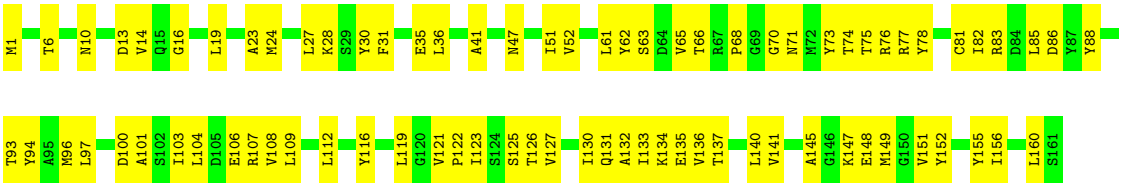
• Molecule 2: Allophycocyanin beta chain

Chain AW:



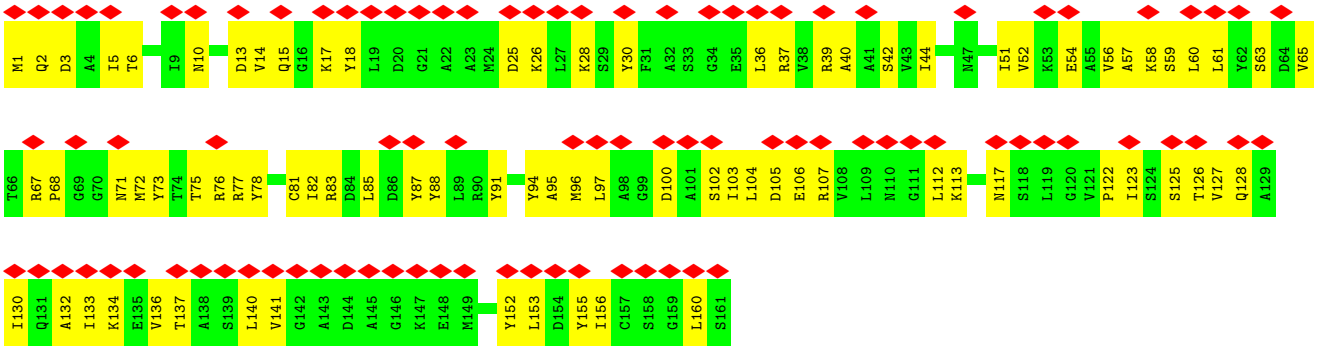
• Molecule 2: Allophycocyanin beta chain

Chain AY:



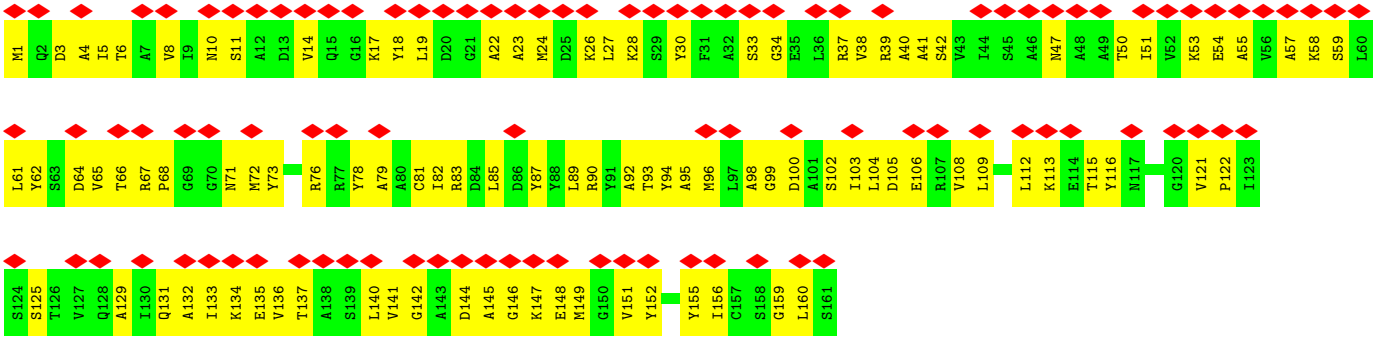
• Molecule 2: Allophycocyanin beta chain

Chain BJ:



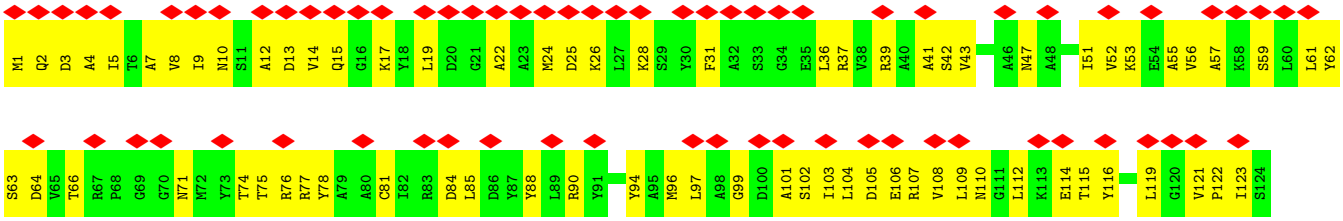
• Molecule 2: Allophycocyanin beta chain

Chain BL:



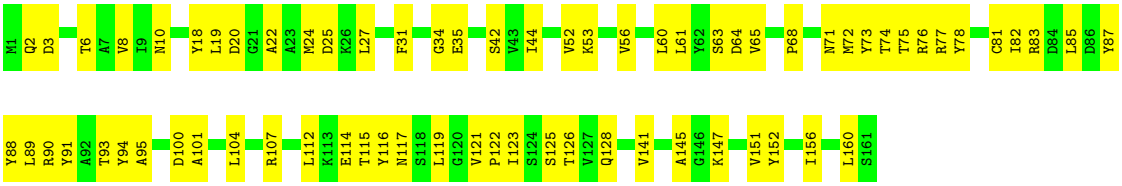
• Molecule 2: Allophycocyanin beta chain

Chain BN:



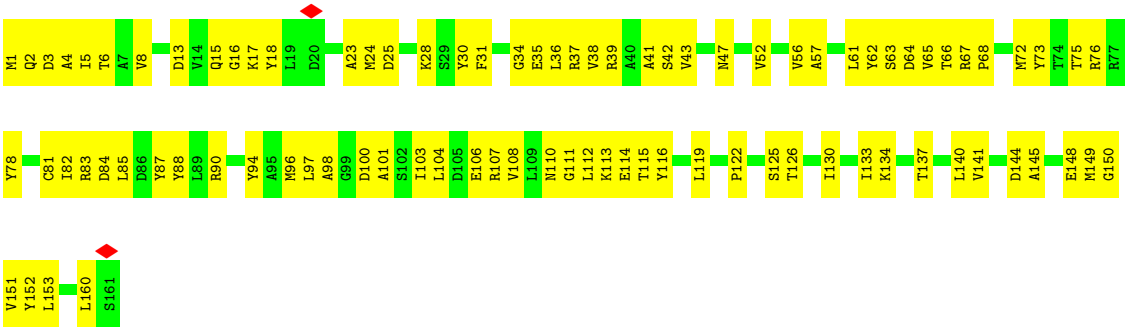
• Molecule 2: Allophycocyanin beta chain

Chain BQ:



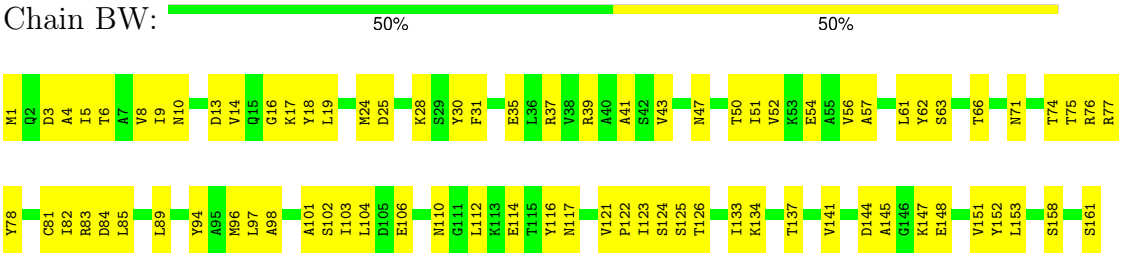
• Molecule 2: Allophycocyanin beta chain

Chain BT:



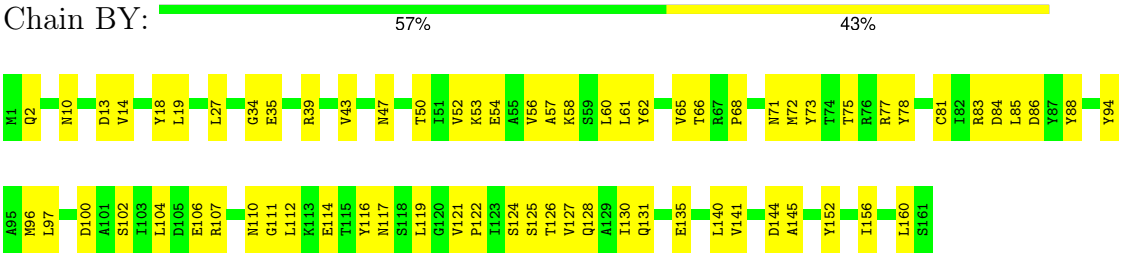
• Molecule 2: Allophycocyanin beta chain

Chain BW:



• Molecule 2: Allophycocyanin beta chain

Chain BY:

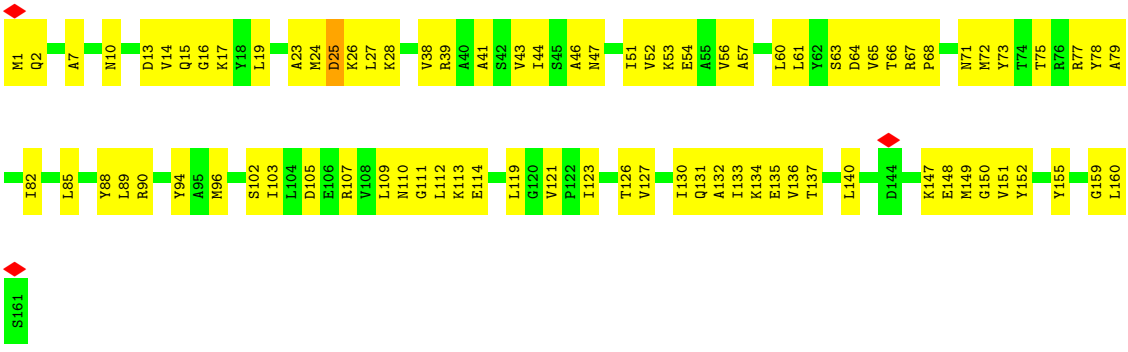


• Molecule 2: Allophycocyanin beta chain

Chain CA:

• Molecule 2: Allophycocyanin beta chain

Chain CD:

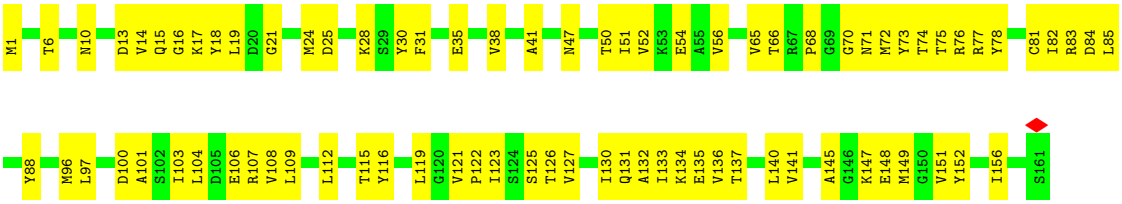


• Molecule 2: Allophycocyanin beta chain

Chain CF:

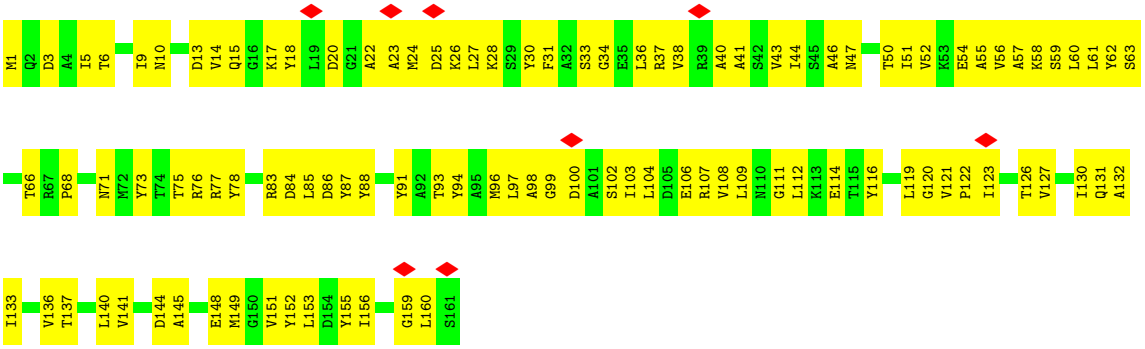
• Molecule 2: Allophycocyanin beta chain

Chain CH:



• Molecule 2: Allophycocyanin beta chain

Chain CS:

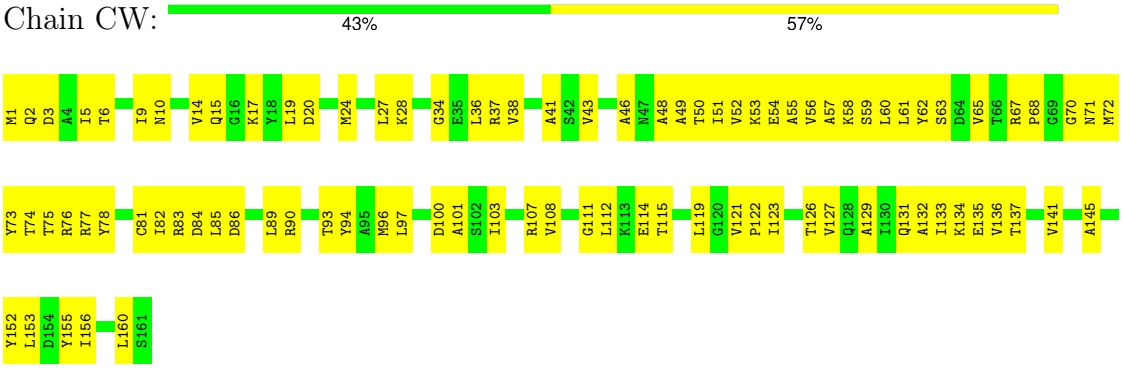


• Molecule 2: Allophycocyanin beta chain

Chain CU:

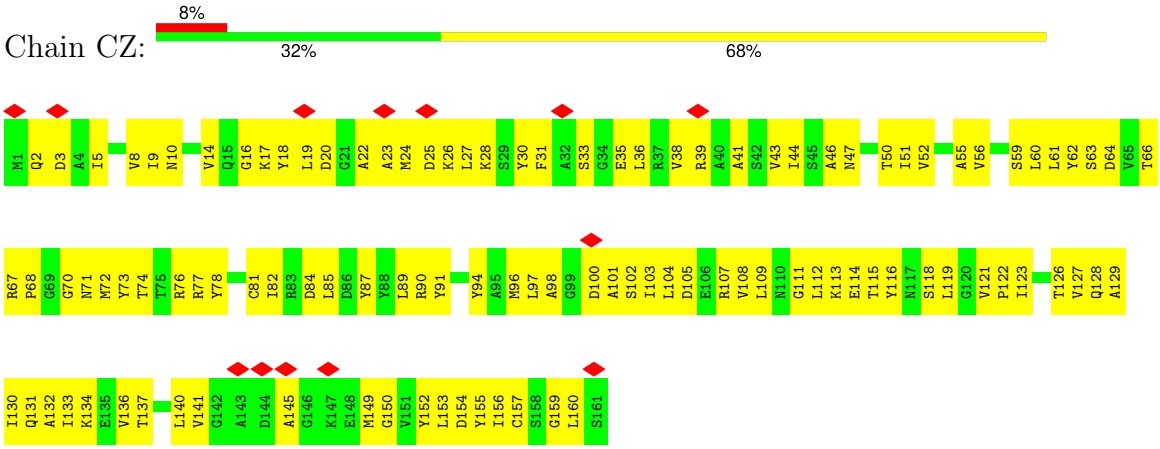
• Molecule 2: Allophycocyanin beta chain

Chain CW:



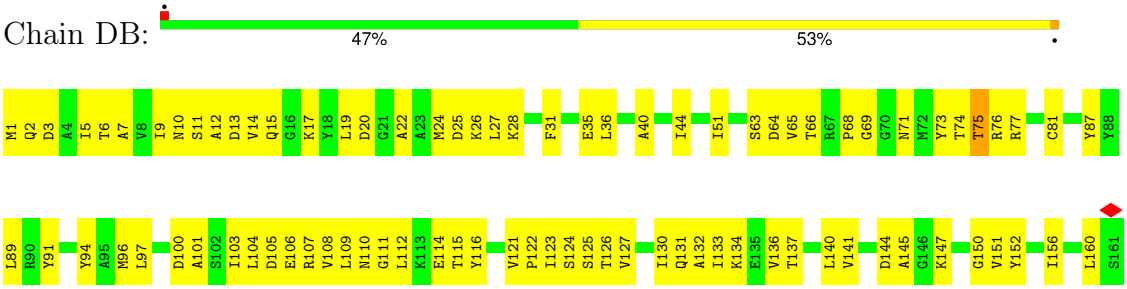
• Molecule 2: Allophycocyanin beta chain

Chain CZ:



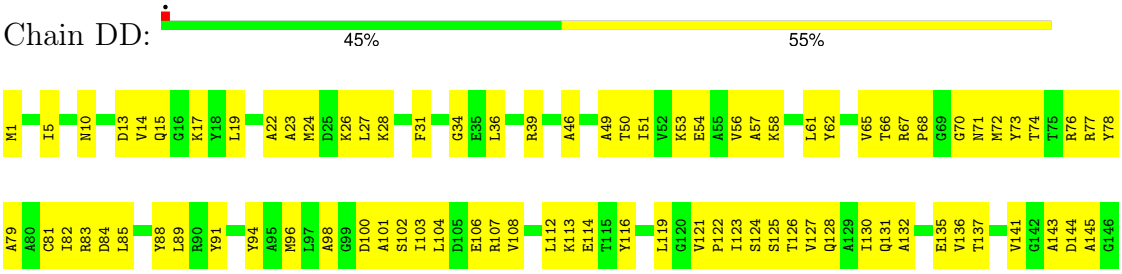
• Molecule 2: Allophycocyanin beta chain

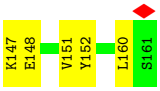
Chain DB:



• Molecule 2: Allophycocyanin beta chain

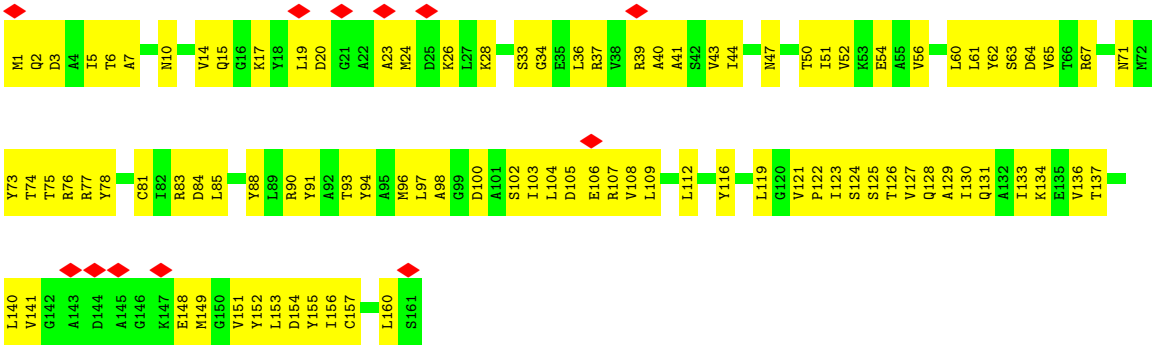
Chain DD:





• Molecule 2: Allophycocyanin beta chain

Chain DK:

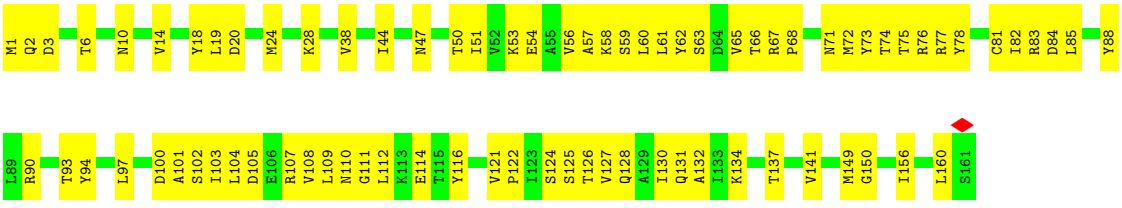


• Molecule 2: Allophycocyanin beta chain

Chain DM:

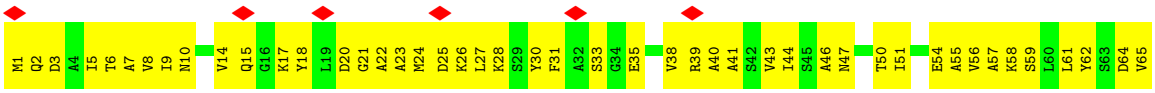
• Molecule 2: Allophycocyanin beta chain

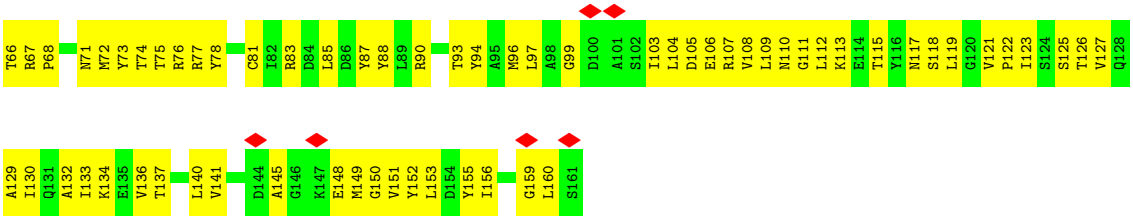
Chain DO:



• Molecule 2: Allophycocyanin beta chain

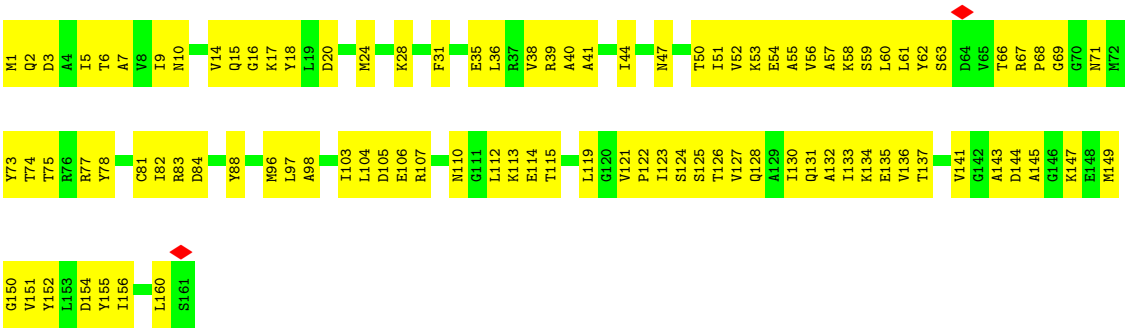
Chain DR:





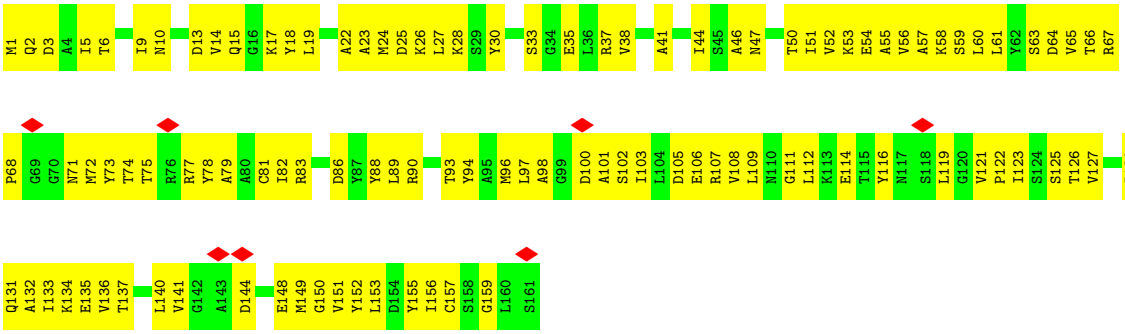
• Molecule 2: Allophycocyanin beta chain

Chain DT:



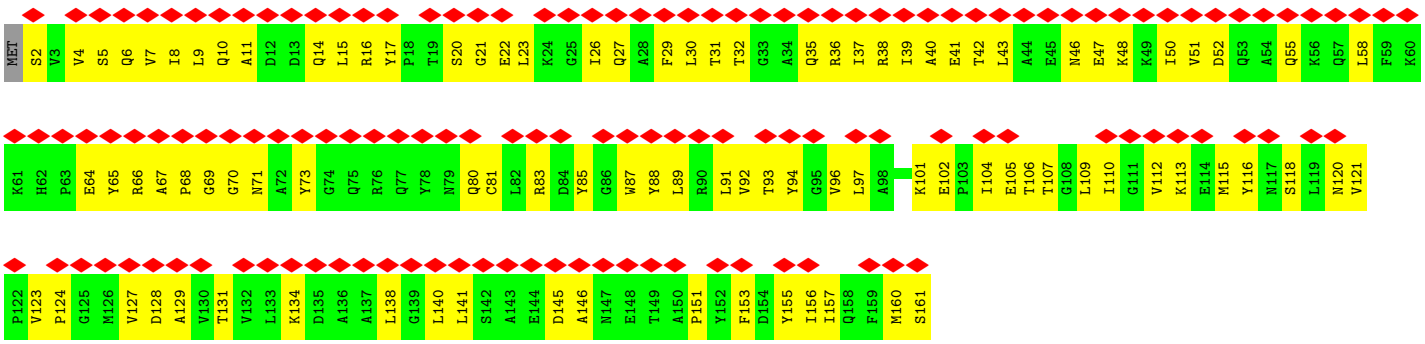
• Molecule 2: Allophycocyanin beta chain

Chain DV:



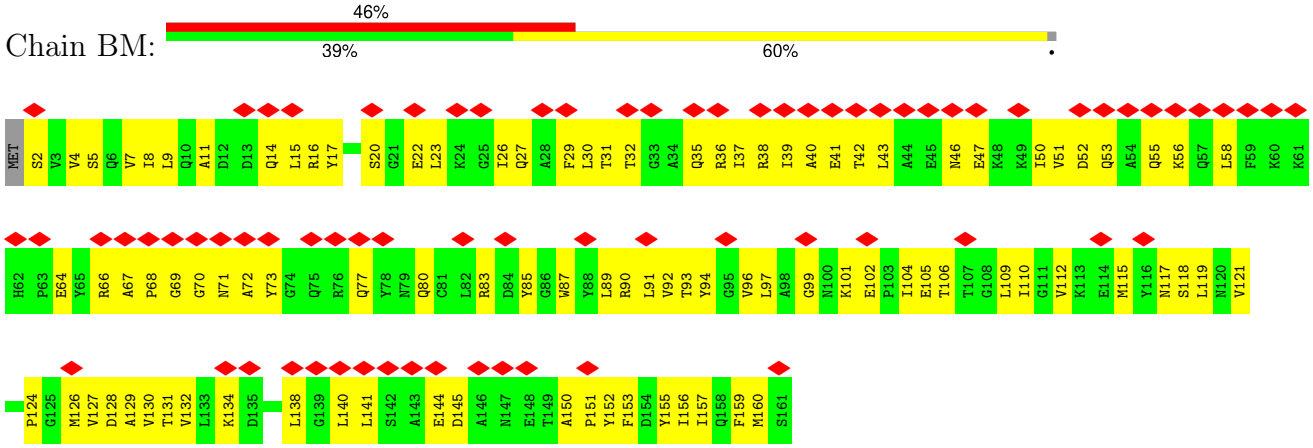
• Molecule 3: Allophycocyanin subunit alpha-B

Chain AE:



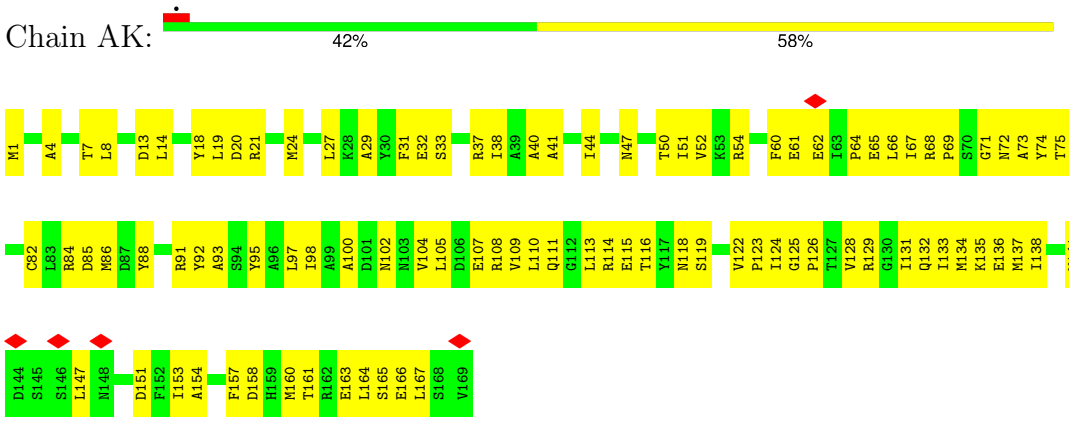
• Molecule 3: Allophycocyanin subunit alpha-B

Chain BM:



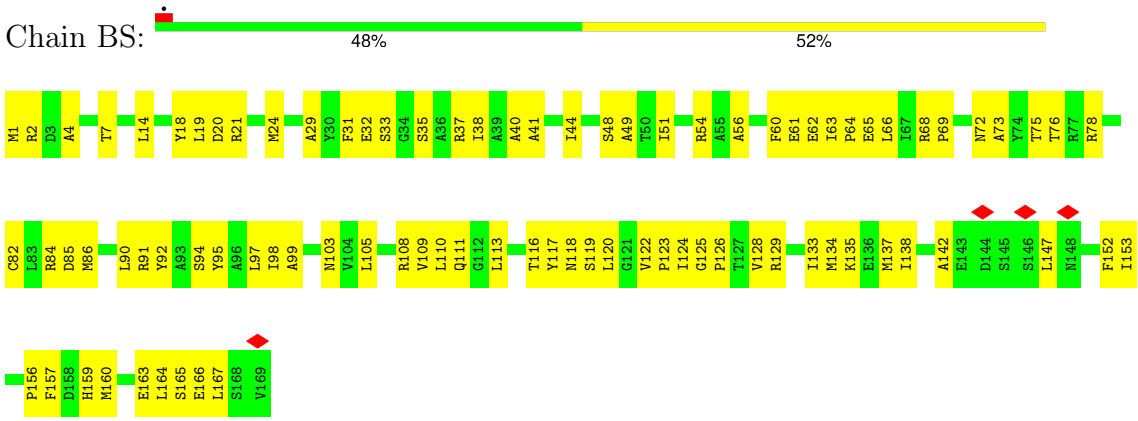
• Molecule 4: Allophycocyanin subunit beta-18

Chain AK:



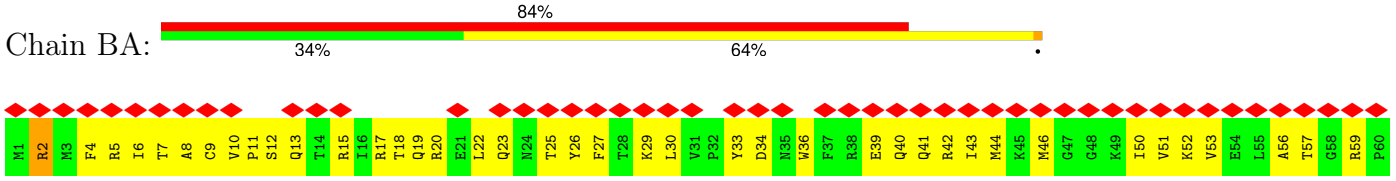
• Molecule 4: Allophycocyanin subunit beta-18

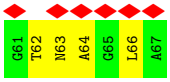
Chain BS:



• Molecule 5: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core

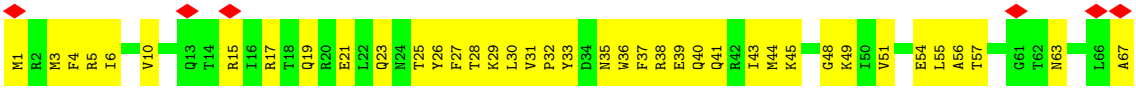
Chain BA:





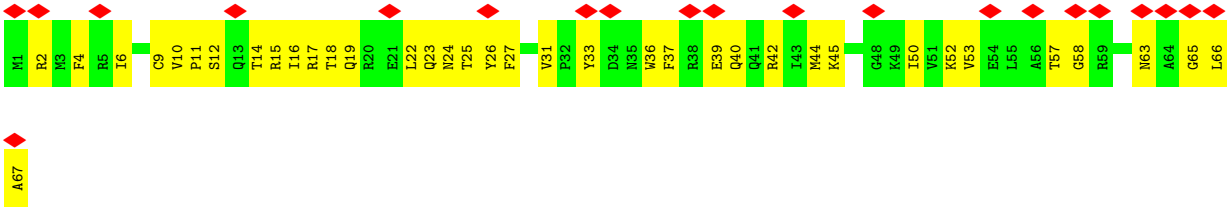
• Molecule 5: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core

Chain BB:



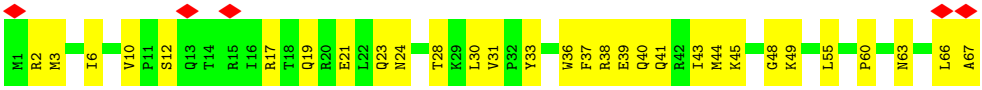
• Molecule 5: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core

Chain CJ:



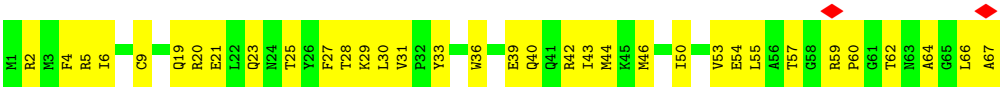
• Molecule 5: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core

Chain CK:



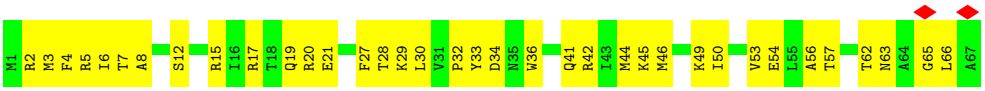
• Molecule 5: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core

Chain DF:



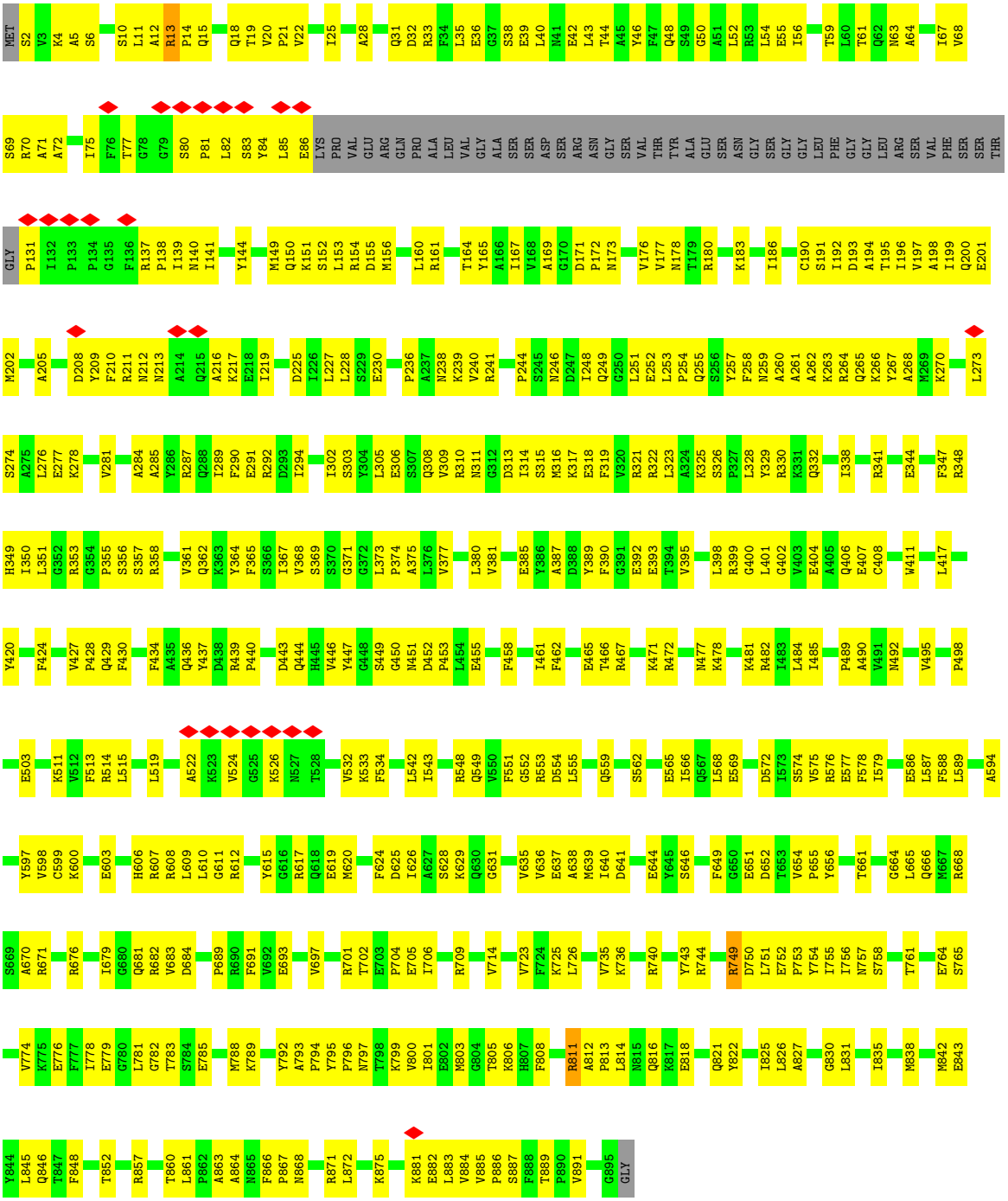
• Molecule 5: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core

Chain DX:



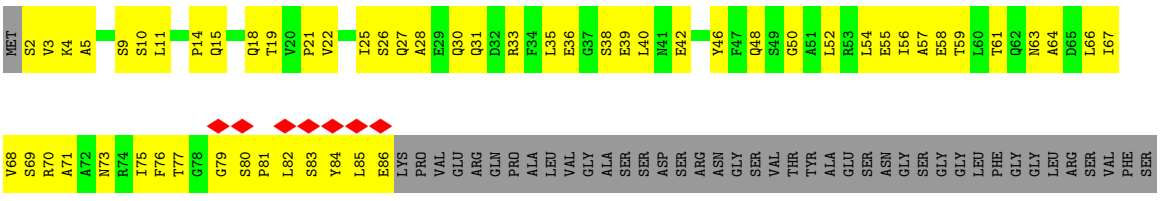
• Molecule 6: Phycobiliprotein ApcE

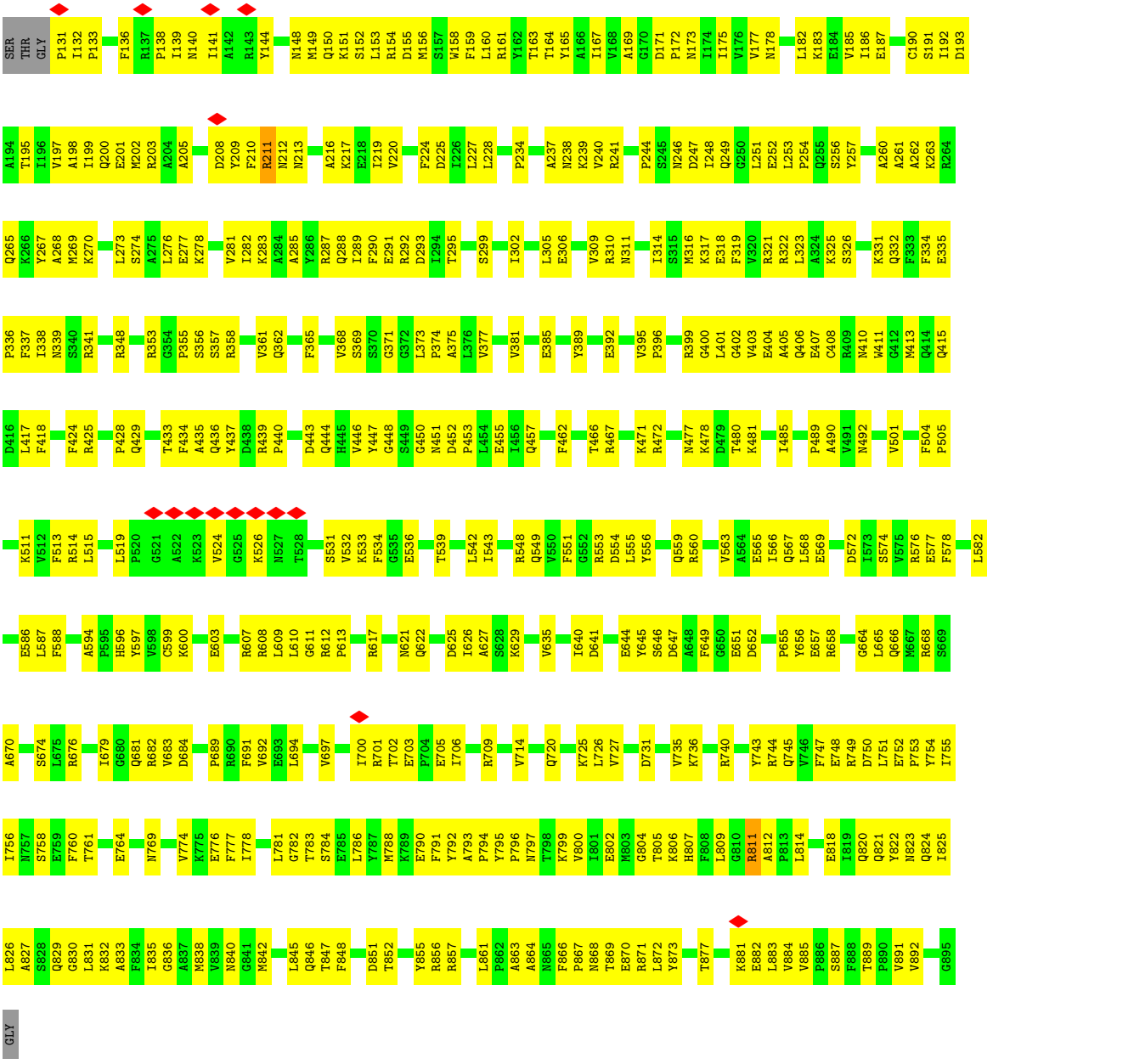
Chain BD:



• Molecule 6: Phycobiliprotein ApcE

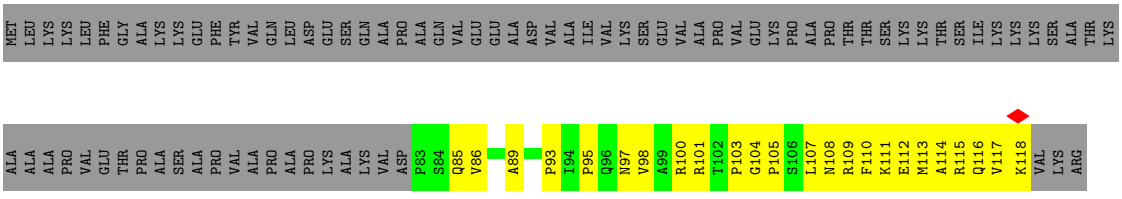
Chain CM:





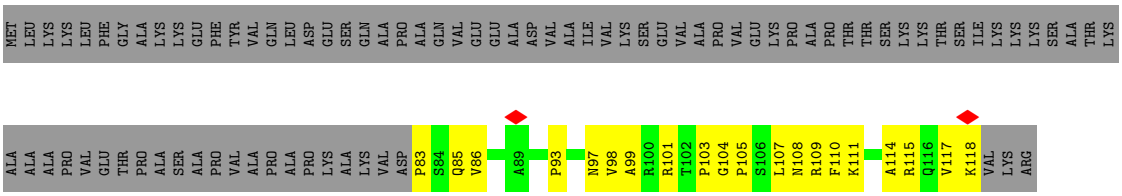
• Molecule 7: Sll1873 protein

Chain BF:



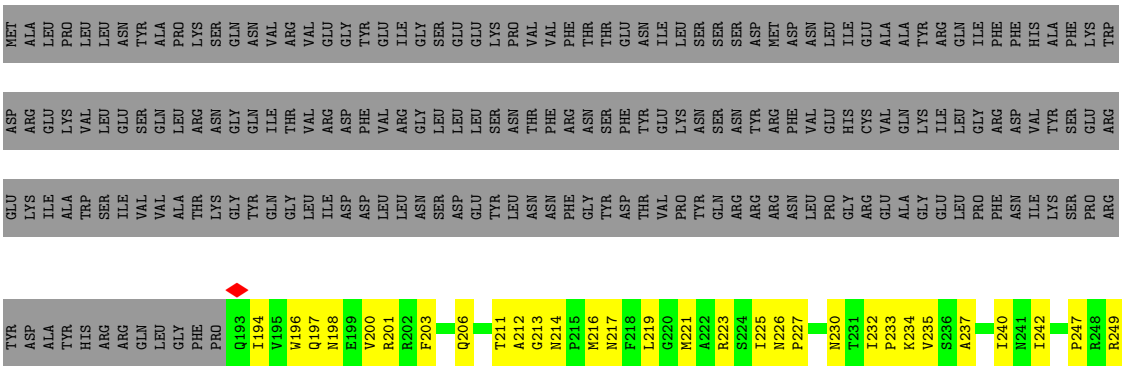
• Molecule 7: Sll1873 protein

Chain CO:



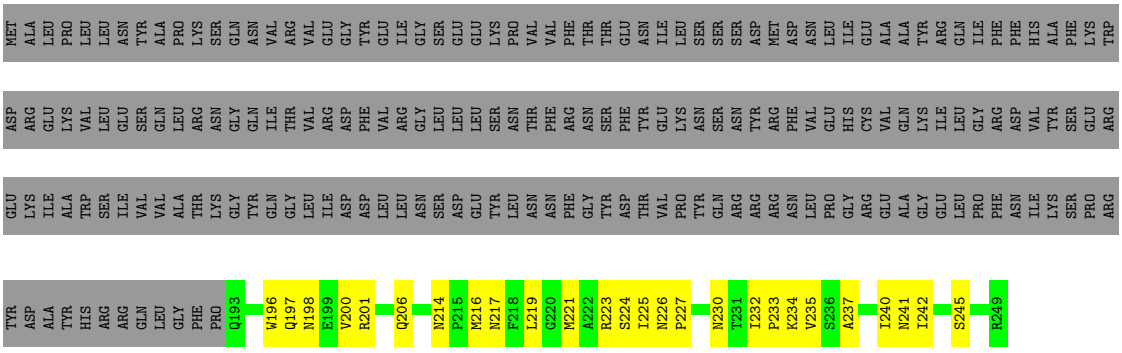
• Molecule 8: Phycobilisome rod-core linker polypeptide CpcG

Chain BG:



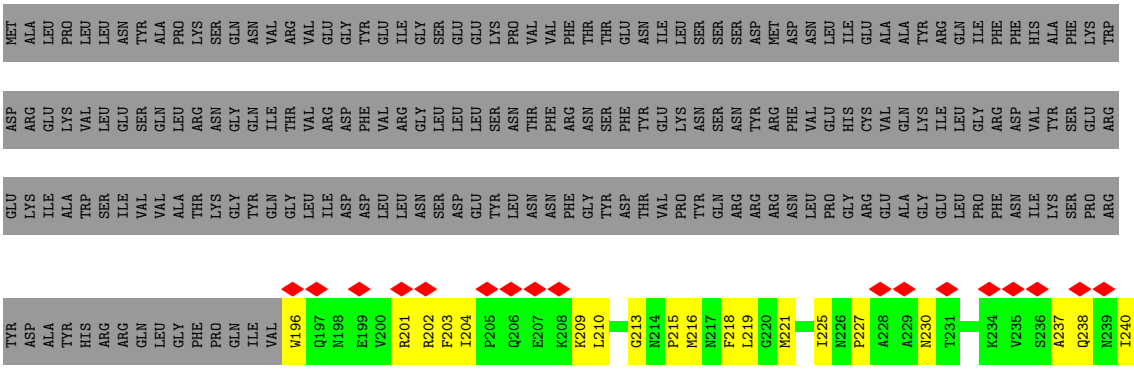
• Molecule 8: Phycobilisome rod-core linker polypeptide CpcG

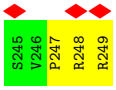
Chain CP:



• Molecule 8: Phycobilisome rod-core linker polypeptide CpcG

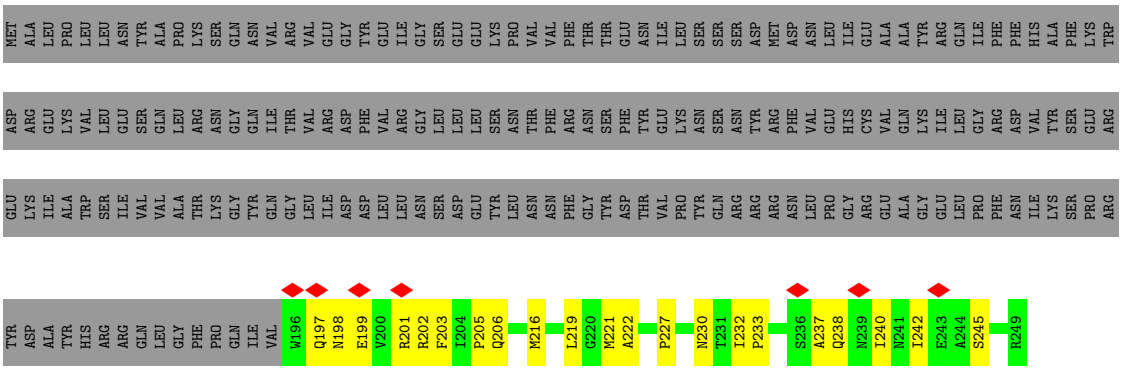
Chain DG:





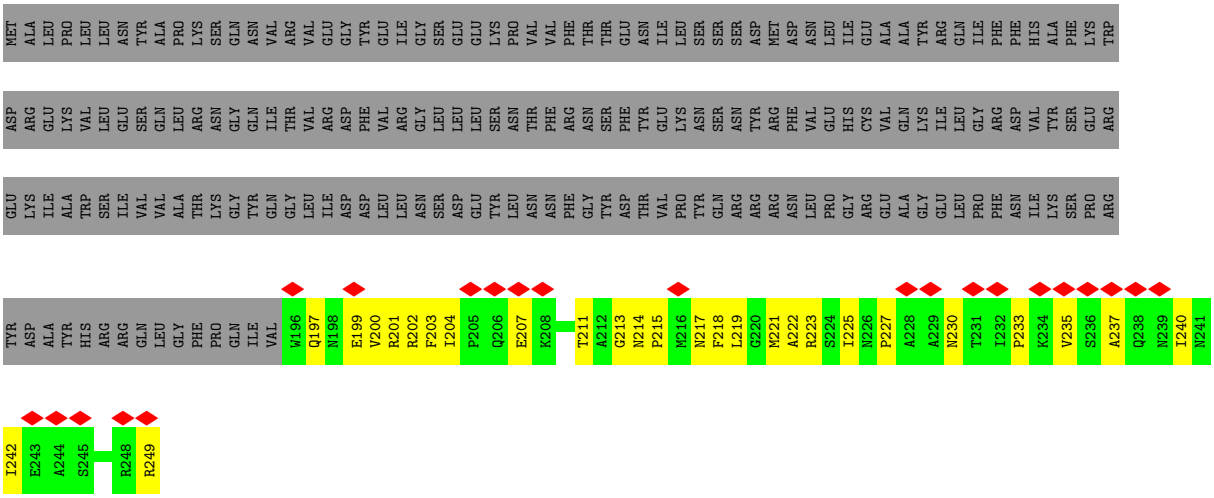
• Molecule 8: Phycobilisome rod-core linker polypeptide CpcG

Chain DH:



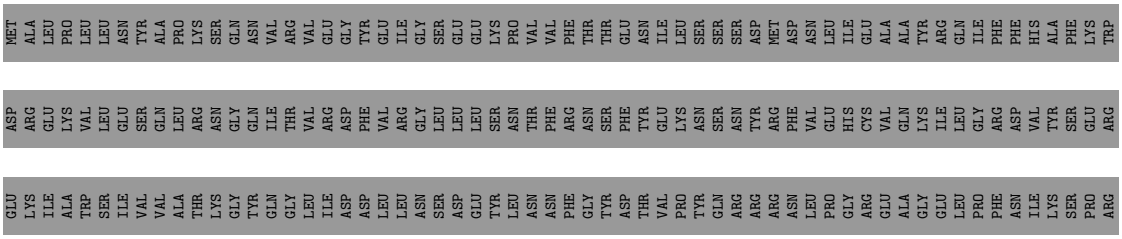
• Molecule 8: Phycobilisome rod-core linker polypeptide CpcG

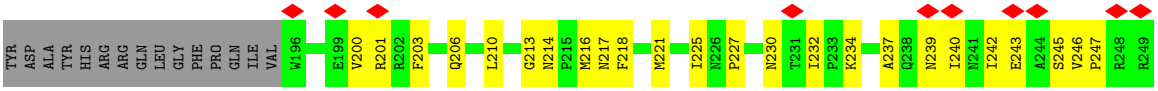
Chain DY:



• Molecule 8: Phycobilisome rod-core linker polypeptide CpcG

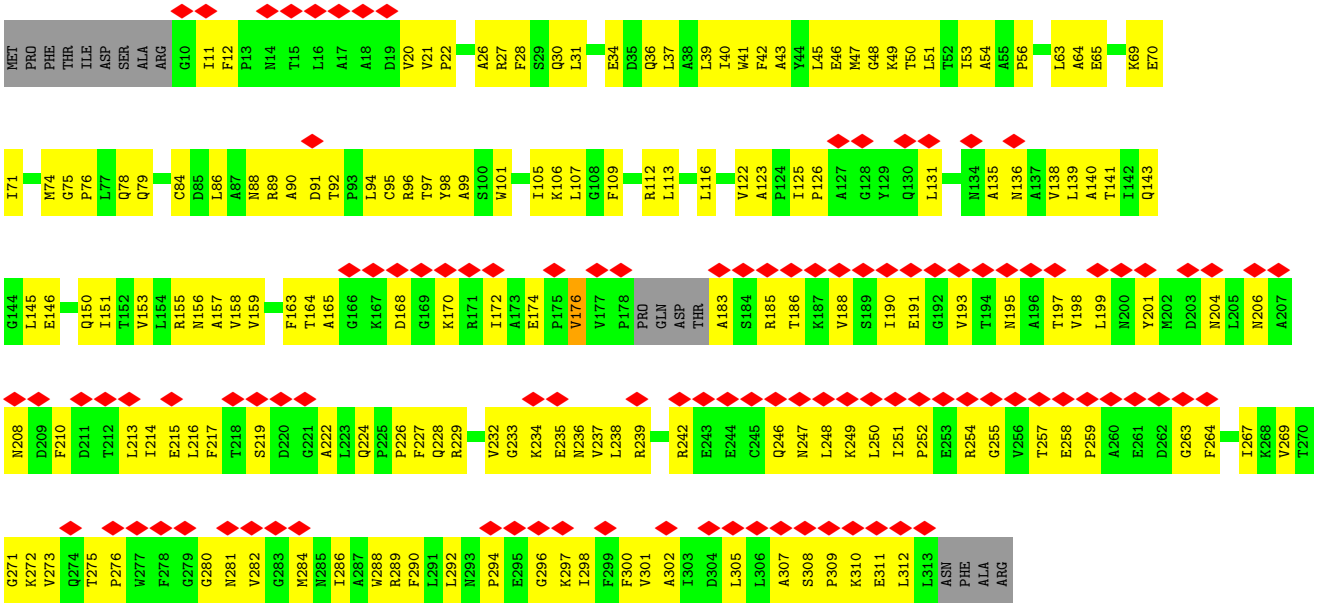
Chain DZ:





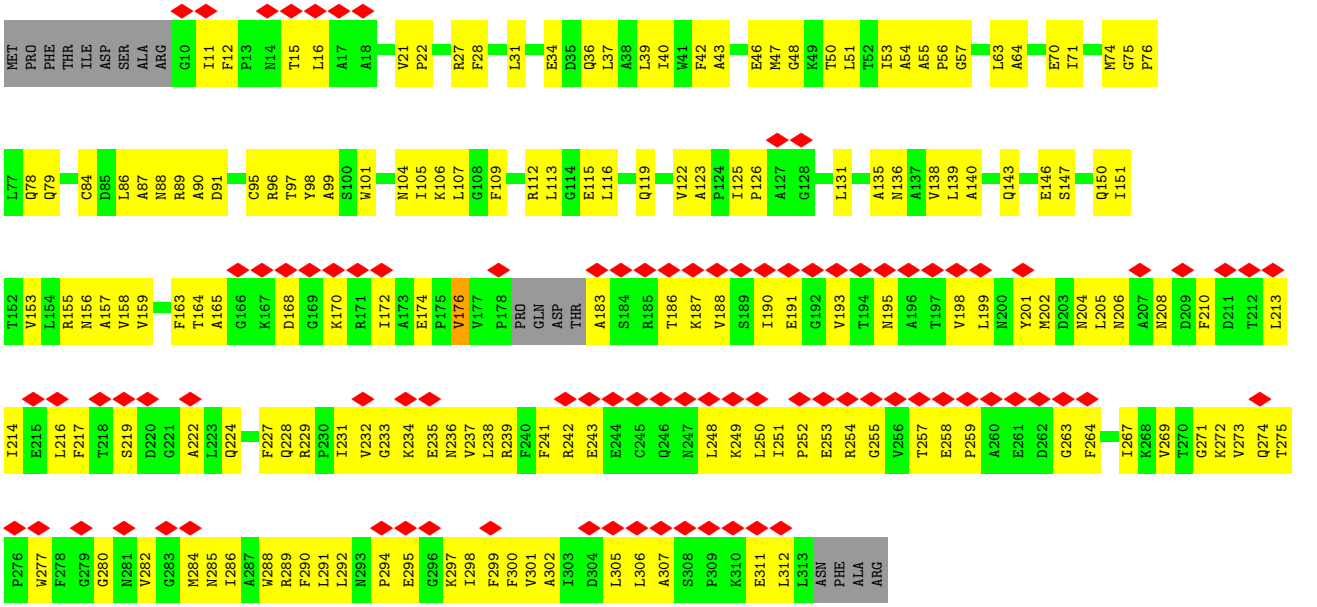
• Molecule 9: Orange carotenoid-binding protein

Chain BH:



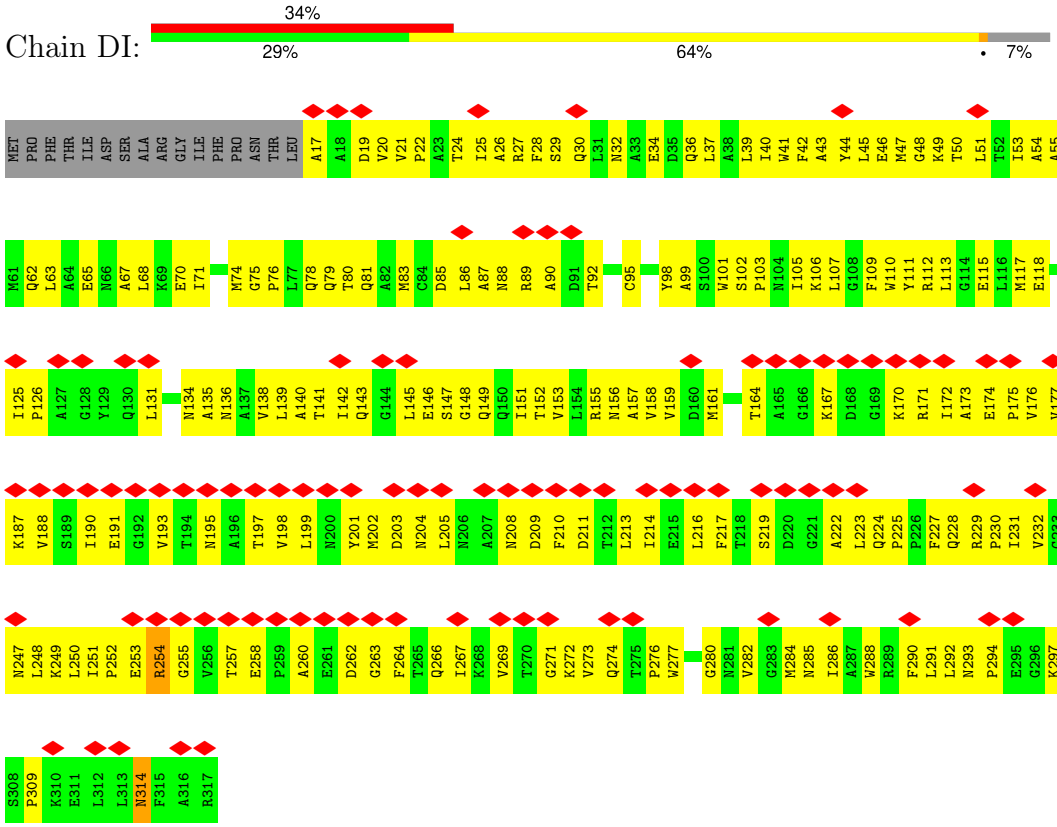
• Molecule 9: Orange carotenoid-binding protein

Chain CQ:



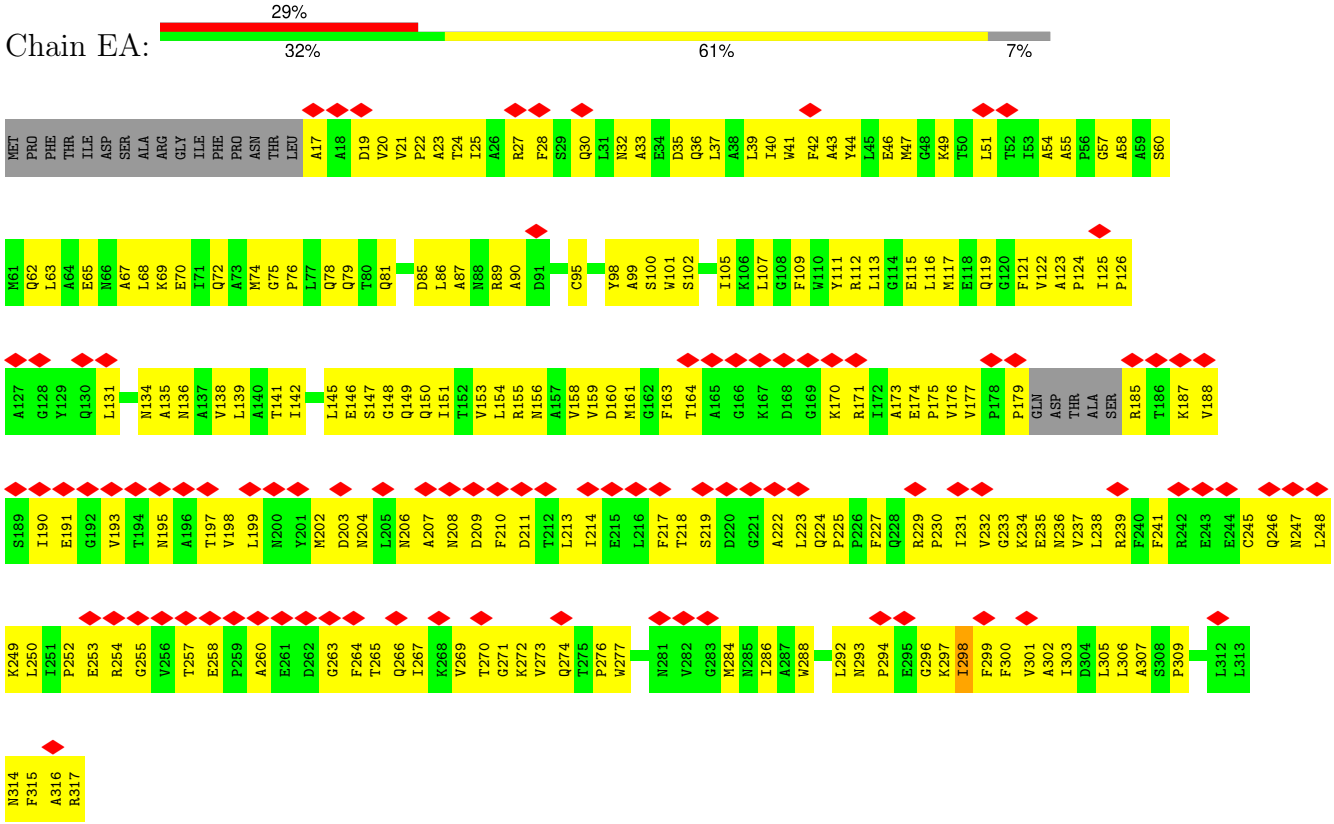
• Molecule 9: Orange carotenoid-binding protein

Chain DI:



• Molecule 9: Orange carotenoid-binding protein

Chain EA:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	340839	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.199	Depositor
Minimum map value	-0.742	Depositor
Average map value	0.021	Depositor
Map value standard deviation	0.113	Depositor
Recommended contour level	0.437	Depositor
Map size (Å)	377.99997, 377.99997, 377.99997	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CYC, 45D

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	AA	0.25	0/1225	0.47	0/1652
1	AC	0.26	0/1225	0.50	0/1652
1	AH	0.28	0/1225	0.48	0/1652
1	AJ	0.31	0/1225	0.49	0/1652
1	AN	0.28	0/1225	0.50	0/1652
1	AP	0.30	0/1225	0.48	0/1652
1	AR	0.28	0/1225	0.48	0/1652
1	AV	0.26	0/1225	0.49	0/1652
1	AX	0.27	0/1225	0.48	0/1652
1	AZ	0.27	0/1225	0.47	0/1652
1	BI	0.25	0/1225	0.47	0/1652
1	BK	0.27	0/1225	0.51	0/1652
1	BP	0.29	0/1225	0.48	0/1652
1	BR	0.31	0/1225	0.49	0/1652
1	BV	0.29	0/1225	0.50	0/1652
1	BX	0.30	0/1225	0.48	0/1652
1	BZ	0.29	0/1225	0.48	0/1652
1	CC	0.27	0/1225	0.47	0/1652
1	CE	0.27	0/1225	0.48	0/1652
1	CG	0.28	0/1225	0.49	0/1652
1	CR	0.28	0/1225	0.49	0/1652
1	CT	0.27	0/1225	0.50	0/1652
1	CV	0.28	0/1225	0.49	0/1652
1	CY	0.28	0/1225	0.52	0/1652
1	DA	0.28	0/1225	0.53	0/1652
1	DC	0.31	0/1225	0.49	0/1652
1	DJ	0.27	0/1225	0.49	0/1652
1	DL	0.27	0/1225	0.49	0/1652
1	DN	0.28	0/1225	0.48	0/1652
1	DQ	0.27	0/1225	0.51	0/1652
1	DS	0.29	0/1225	0.50	0/1652
1	DU	0.31	0/1225	0.49	0/1652

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
2	AB	0.25	0/1220	0.44	0/1650
2	AD	0.26	0/1220	0.46	0/1650
2	AF	0.25	0/1220	0.43	0/1650
2	AI	0.32	0/1220	0.46	0/1650
2	AL	0.29	0/1220	0.46	0/1650
2	AO	0.32	0/1220	0.46	0/1650
2	AQ	0.31	0/1220	0.45	0/1650
2	AS	0.30	0/1220	0.47	0/1650
2	AU	0.28	0/1220	0.49	1/1650 (0.1%)
2	AW	0.27	0/1220	0.45	0/1650
2	AY	0.29	0/1220	0.45	0/1650
2	BJ	0.25	0/1220	0.45	0/1650
2	BL	0.27	0/1220	0.47	0/1650
2	BN	0.26	0/1220	0.44	0/1650
2	BQ	0.32	0/1220	0.46	0/1650
2	BT	0.30	0/1220	0.46	0/1650
2	BW	0.32	0/1220	0.45	0/1650
2	BY	0.31	0/1220	0.45	0/1650
2	CA	0.31	0/1220	0.47	0/1650
2	CD	0.28	0/1220	0.49	1/1650 (0.1%)
2	CF	0.28	0/1220	0.45	0/1650
2	CH	0.28	0/1220	0.44	0/1650
2	CS	0.27	0/1220	0.46	0/1650
2	CU	0.30	0/1220	0.45	0/1650
2	CW	0.28	0/1220	0.45	0/1650
2	CZ	0.29	0/1220	0.48	0/1650
2	DB	0.31	0/1220	0.46	0/1650
2	DD	0.28	0/1220	0.45	0/1650
2	DK	0.27	0/1220	0.45	0/1650
2	DM	0.30	0/1220	0.45	0/1650
2	DO	0.27	0/1220	0.45	0/1650
2	DR	0.28	0/1220	0.46	0/1650
2	DT	0.31	0/1220	0.46	0/1650
2	DV	0.29	0/1220	0.49	0/1650
3	AE	0.26	0/1277	0.45	0/1730
3	BM	0.29	0/1277	0.47	0/1730
4	AK	0.29	0/1341	0.50	0/1813
4	BS	0.30	0/1341	0.50	0/1813
5	BA	0.26	0/555	0.55	0/743
5	BB	0.26	0/555	0.56	0/743
5	CJ	0.26	0/555	0.54	0/743
5	CK	0.26	0/555	0.57	0/743
5	DF	0.28	0/555	0.57	0/743

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
5	DX	0.27	0/555	0.56	0/743
6	BD	0.30	0/6907	0.50	1/9337 (0.0%)
6	CM	0.30	0/6907	0.50	0/9337
7	BF	0.25	0/283	0.51	0/381
7	CO	0.27	0/283	0.50	0/381
8	BG	0.27	0/459	0.50	0/620
8	CP	0.27	0/459	0.51	0/620
8	DG	0.26	0/434	0.53	0/587
8	DH	0.26	0/434	0.52	0/587
8	DY	0.26	0/434	0.53	0/587
8	DZ	0.28	0/434	0.52	0/587
9	BH	0.26	0/2349	0.48	0/3195
9	CQ	0.26	0/2349	0.48	0/3195
9	DI	0.26	0/2327	0.47	0/3164
9	EA	0.26	0/2327	0.47	0/3164
All	All	0.28	0/115632	0.48	3/156250 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	CD	25	ASP	CB-CG-OD1	6.17	123.85	118.30
2	AU	25	ASP	CB-CG-OD1	5.54	123.28	118.30
6	BD	503	GLU	C-N-CA	-5.41	108.19	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	1210	0	1210	100	0
1	AC	1210	0	1210	137	0
1	AH	1210	0	1210	99	0
1	AJ	1210	0	1210	89	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AN	1210	0	1210	115	0
1	AP	1210	0	1210	79	0
1	AR	1210	0	1211	91	0
1	AV	1210	0	1210	125	0
1	AX	1210	0	1210	98	0
1	AZ	1210	0	1210	104	0
1	BI	1210	0	1210	82	0
1	BK	1210	0	1210	139	0
1	BP	1210	0	1210	95	0
1	BR	1210	0	1210	89	0
1	BV	1210	0	1210	116	0
1	BX	1210	0	1210	72	0
1	BZ	1210	0	1210	94	0
1	CC	1210	0	1210	108	0
1	CE	1210	0	1210	129	0
1	CG	1210	0	1210	107	0
1	CR	1210	0	1210	146	0
1	CT	1210	0	1210	97	0
1	CV	1210	0	1210	93	0
1	CY	1210	0	1210	180	0
1	DA	1210	0	1210	132	0
1	DC	1210	0	1210	77	0
1	DJ	1210	0	1210	146	0
1	DL	1210	0	1210	131	0
1	DN	1210	0	1210	83	0
1	DQ	1210	0	1210	167	0
1	DS	1210	0	1210	113	0
1	DU	1210	0	1210	99	0
2	AB	1206	0	1218	84	0
2	AD	1206	0	1218	122	0
2	AF	1206	0	1218	116	0
2	AI	1206	0	1218	72	0
2	AL	1206	0	1218	100	0
2	AO	1206	0	1218	87	0
2	AQ	1206	0	1218	59	0
2	AS	1206	0	1218	108	0
2	AU	1206	0	1218	91	0
2	AW	1206	0	1218	105	0
2	AY	1206	0	1218	87	0
2	BJ	1206	0	1218	80	0
2	BL	1206	0	1218	115	0
2	BN	1206	0	1218	115	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	BQ	1206	0	1218	81	0
2	BT	1206	0	1218	100	0
2	BW	1206	0	1218	92	0
2	BY	1206	0	1218	74	0
2	CA	1206	0	1218	96	0
2	CD	1206	0	1218	93	0
2	CF	1206	0	1218	119	0
2	CH	1206	0	1218	87	0
2	CS	1206	0	1218	131	0
2	CU	1206	0	1218	83	0
2	CW	1206	0	1218	117	0
2	CZ	1206	0	1218	142	0
2	DB	1206	0	1218	109	0
2	DD	1206	0	1218	105	0
2	DK	1206	0	1218	122	0
2	DM	1206	0	1218	99	0
2	DO	1206	0	1218	86	0
2	DR	1206	0	1218	140	0
2	DT	1206	0	1218	107	0
2	DV	1206	0	1218	125	0
3	AE	1254	0	1250	122	0
3	BM	1254	0	1250	123	0
4	AK	1322	0	1311	131	0
4	BS	1322	0	1311	123	0
5	BA	546	0	568	76	0
5	BB	546	0	568	43	0
5	CJ	546	0	568	66	0
5	CK	546	0	568	33	0
5	DF	546	0	568	49	0
5	DX	546	0	568	46	0
6	BD	6761	0	6739	521	0
6	CM	6761	0	6739	526	0
7	BF	277	0	283	36	0
7	CO	277	0	283	36	0
8	BG	451	0	465	33	0
8	CP	451	0	465	26	0
8	DG	426	0	437	45	0
8	DH	426	0	437	46	0
8	DY	426	0	437	39	0
8	DZ	426	0	437	48	0
9	BH	2302	0	2310	199	0
9	CQ	2302	0	2310	195	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	DI	2280	0	2286	257	0
9	EA	2280	0	2286	217	0
10	AA	43	0	37	14	0
10	AB	43	0	37	14	0
10	AC	43	0	37	15	0
10	AD	43	0	37	17	0
10	AE	43	0	37	9	0
10	AF	43	0	37	13	0
10	AH	43	0	37	18	0
10	AI	43	0	37	12	0
10	AJ	43	0	37	11	0
10	AK	43	0	37	20	0
10	AL	43	0	37	11	0
10	AN	43	0	37	10	0
10	AO	43	0	37	8	0
10	AP	43	0	37	10	0
10	AQ	43	0	37	12	0
10	AR	43	0	38	11	0
10	AU	43	0	37	14	0
10	AV	43	0	37	21	0
10	AW	43	0	37	10	0
10	AX	43	0	37	15	0
10	AY	43	0	37	15	0
10	AZ	43	0	37	14	0
10	BD	86	0	74	25	0
10	BI	43	0	37	15	0
10	BJ	43	0	37	13	0
10	BK	43	0	37	17	0
10	BL	43	0	37	17	0
10	BM	43	0	37	9	0
10	BN	43	0	37	16	0
10	BP	43	0	37	17	0
10	BQ	43	0	37	17	0
10	BR	43	0	37	7	0
10	BS	43	0	37	16	0
10	BT	43	0	37	10	0
10	BV	43	0	37	14	0
10	BW	43	0	37	10	0
10	BX	43	0	37	14	0
10	BY	43	0	37	13	0
10	BZ	43	0	37	12	0
10	CC	43	0	37	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	CD	43	0	37	9	0
10	CE	43	0	37	15	0
10	CF	43	0	37	12	0
10	CG	43	0	37	15	0
10	CH	43	0	37	15	0
10	CM	86	0	74	23	0
10	CR	43	0	37	12	0
10	CS	43	0	37	8	0
10	CT	43	0	37	14	0
10	CU	43	0	37	9	0
10	CV	43	0	37	14	0
10	CW	43	0	37	12	0
10	CY	43	0	37	13	0
10	CZ	43	0	37	11	0
10	DA	43	0	37	11	0
10	DB	43	0	37	11	0
10	DC	43	0	37	16	0
10	DD	43	0	37	21	0
10	DJ	43	0	37	14	0
10	DK	43	0	37	13	0
10	DL	43	0	37	13	0
10	DM	43	0	37	11	0
10	DN	43	0	37	15	0
10	DO	43	0	37	7	0
10	DQ	43	0	37	12	0
10	DR	43	0	37	17	0
10	DS	43	0	37	12	0
10	DT	43	0	37	13	0
10	DU	43	0	37	14	0
10	DV	43	0	37	13	0
11	BH	42	52	52	4	0
11	CQ	42	52	52	6	0
11	DI	42	52	52	14	0
11	EA	42	52	52	12	0
All	All	117262	208	117450	8770	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 37.

The worst 5 of 8770 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)
9:BH:214:ILE:HD13	9:BH:238:LEU:HD22	1.27	1.12
9:CQ:214:ILE:HD13	9:CQ:238:LEU:HD22	1.28	1.12
6:CM:700:ILE:HG21	2:DB:147:LYS:HE2	1.36	1.06
2:DV:41:ALA:HB2	2:DV:97:LEU:HD21	1.37	1.04
1:CR:50:ILE:HD13	1:CR:136:VAL:HG12	1.39	1.04

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 PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AA	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
1	AC	158/161 (98%)	153 (97%)	5 (3%)	0	100	100
1	AH	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
1	AJ	158/161 (98%)	158 (100%)	0	0	100	100
1	AN	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
1	AP	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
1	AR	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
1	AV	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
1	AX	158/161 (98%)	158 (100%)	0	0	100	100
1	AZ	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
1	BI	158/161 (98%)	158 (100%)	0	0	100	100
1	BK	158/161 (98%)	152 (96%)	6 (4%)	0	100	100
1	BP	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
1	BR	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
1	BV	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
1	BX	158/161 (98%)	156 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BZ	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
1	CC	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
1	CE	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
1	CG	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
1	CR	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
1	CT	158/161 (98%)	153 (97%)	5 (3%)	0	100	100
1	CV	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
1	CY	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
1	DA	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
1	DC	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
1	DJ	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
1	DL	158/161 (98%)	151 (96%)	6 (4%)	1 (1%)	22	43
1	DN	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
1	DQ	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
1	DS	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
1	DU	158/161 (98%)	153 (97%)	5 (3%)	0	100	100
2	AB	159/161 (99%)	159 (100%)	0	0	100	100
2	AD	159/161 (99%)	155 (98%)	4 (2%)	0	100	100
2	AF	159/161 (99%)	158 (99%)	1 (1%)	0	100	100
2	AI	159/161 (99%)	154 (97%)	5 (3%)	0	100	100
2	AL	159/161 (99%)	155 (98%)	4 (2%)	0	100	100
2	AO	159/161 (99%)	156 (98%)	3 (2%)	0	100	100
2	AQ	159/161 (99%)	154 (97%)	5 (3%)	0	100	100
2	AS	159/161 (99%)	156 (98%)	3 (2%)	0	100	100
2	AU	159/161 (99%)	153 (96%)	6 (4%)	0	100	100
2	AW	159/161 (99%)	156 (98%)	3 (2%)	0	100	100
2	AY	159/161 (99%)	159 (100%)	0	0	100	100
2	BJ	159/161 (99%)	159 (100%)	0	0	100	100
2	BL	159/161 (99%)	155 (98%)	4 (2%)	0	100	100
2	BN	159/161 (99%)	157 (99%)	2 (1%)	0	100	100
2	BQ	159/161 (99%)	156 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	BT	159/161 (99%)	155 (98%)	4 (2%)	0	100	100
2	BW	159/161 (99%)	157 (99%)	2 (1%)	0	100	100
2	BY	159/161 (99%)	153 (96%)	6 (4%)	0	100	100
2	CA	159/161 (99%)	154 (97%)	5 (3%)	0	100	100
2	CD	159/161 (99%)	157 (99%)	2 (1%)	0	100	100
2	CF	159/161 (99%)	157 (99%)	2 (1%)	0	100	100
2	CH	159/161 (99%)	158 (99%)	1 (1%)	0	100	100
2	CS	159/161 (99%)	156 (98%)	3 (2%)	0	100	100
2	CU	159/161 (99%)	154 (97%)	5 (3%)	0	100	100
2	CW	159/161 (99%)	153 (96%)	6 (4%)	0	100	100
2	CZ	159/161 (99%)	147 (92%)	12 (8%)	0	100	100
2	DB	159/161 (99%)	149 (94%)	9 (6%)	1 (1%)	22	43
2	DD	159/161 (99%)	154 (97%)	5 (3%)	0	100	100
2	DK	159/161 (99%)	156 (98%)	3 (2%)	0	100	100
2	DM	159/161 (99%)	156 (98%)	3 (2%)	0	100	100
2	DO	159/161 (99%)	156 (98%)	3 (2%)	0	100	100
2	DR	159/161 (99%)	151 (95%)	8 (5%)	0	100	100
2	DT	159/161 (99%)	150 (94%)	8 (5%)	1 (1%)	22	43
2	DV	159/161 (99%)	156 (98%)	3 (2%)	0	100	100
3	AE	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
3	BM	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
4	AK	167/169 (99%)	164 (98%)	3 (2%)	0	100	100
4	BS	167/169 (99%)	161 (96%)	6 (4%)	0	100	100
5	BA	65/67 (97%)	64 (98%)	1 (2%)	0	100	100
5	BB	65/67 (97%)	65 (100%)	0	0	100	100
5	CJ	65/67 (97%)	64 (98%)	1 (2%)	0	100	100
5	CK	65/67 (97%)	65 (100%)	0	0	100	100
5	DF	65/67 (97%)	62 (95%)	3 (5%)	0	100	100
5	DX	65/67 (97%)	63 (97%)	2 (3%)	0	100	100
6	BD	846/896 (94%)	803 (95%)	43 (5%)	0	100	100
6	CM	846/896 (94%)	794 (94%)	52 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	BF	34/121 (28%)	30 (88%)	4 (12%)	0	100	100
7	CO	34/121 (28%)	34 (100%)	0	0	100	100
8	BG	55/249 (22%)	52 (94%)	3 (6%)	0	100	100
8	CP	55/249 (22%)	51 (93%)	4 (7%)	0	100	100
8	DG	52/249 (21%)	45 (86%)	7 (14%)	0	100	100
8	DH	52/249 (21%)	47 (90%)	5 (10%)	0	100	100
8	DY	52/249 (21%)	45 (86%)	7 (14%)	0	100	100
8	DZ	52/249 (21%)	46 (88%)	6 (12%)	0	100	100
9	BH	296/317 (93%)	283 (96%)	12 (4%)	1 (0%)	37	59
9	CQ	296/317 (93%)	282 (95%)	13 (4%)	1 (0%)	37	59
9	DI	292/317 (92%)	279 (96%)	12 (4%)	1 (0%)	37	59
9	EA	292/317 (92%)	279 (96%)	12 (4%)	1 (0%)	37	59
All	All	14756/16484 (90%)	14347 (97%)	402 (3%)	7 (0%)	100	100

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	BH	176	VAL
9	CQ	176	VAL
1	DL	143	SER
2	DB	75	THR
2	DT	75	THR

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 PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AA	128/129 (99%)	128 (100%)	0	100	100
1	AC	128/129 (99%)	126 (98%)	2 (2%)	58	79
1	AH	128/129 (99%)	128 (100%)	0	100	100
1	AJ	128/129 (99%)	127 (99%)	1 (1%)	79	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AN	128/129 (99%)	128 (100%)	0	100	100
1	AP	128/129 (99%)	128 (100%)	0	100	100
1	AR	128/129 (99%)	127 (99%)	1 (1%)	79	91
1	AV	128/129 (99%)	128 (100%)	0	100	100
1	AX	128/129 (99%)	128 (100%)	0	100	100
1	AZ	128/129 (99%)	127 (99%)	1 (1%)	79	91
1	BI	128/129 (99%)	128 (100%)	0	100	100
1	BK	128/129 (99%)	126 (98%)	2 (2%)	58	79
1	BP	128/129 (99%)	128 (100%)	0	100	100
1	BR	128/129 (99%)	127 (99%)	1 (1%)	79	91
1	BV	128/129 (99%)	128 (100%)	0	100	100
1	BX	128/129 (99%)	128 (100%)	0	100	100
1	BZ	128/129 (99%)	127 (99%)	1 (1%)	79	91
1	CC	128/129 (99%)	128 (100%)	0	100	100
1	CE	128/129 (99%)	128 (100%)	0	100	100
1	CG	128/129 (99%)	128 (100%)	0	100	100
1	CR	128/129 (99%)	128 (100%)	0	100	100
1	CT	128/129 (99%)	128 (100%)	0	100	100
1	CV	128/129 (99%)	128 (100%)	0	100	100
1	CY	128/129 (99%)	128 (100%)	0	100	100
1	DA	128/129 (99%)	127 (99%)	1 (1%)	79	91
1	DC	128/129 (99%)	127 (99%)	1 (1%)	79	91
1	DJ	128/129 (99%)	127 (99%)	1 (1%)	79	91
1	DL	128/129 (99%)	128 (100%)	0	100	100
1	DN	128/129 (99%)	126 (98%)	2 (2%)	58	79
1	DQ	128/129 (99%)	128 (100%)	0	100	100
1	DS	128/129 (99%)	127 (99%)	1 (1%)	79	91
1	DU	128/129 (99%)	128 (100%)	0	100	100
2	AB	125/125 (100%)	125 (100%)	0	100	100
2	AD	125/125 (100%)	125 (100%)	0	100	100
2	AF	125/125 (100%)	125 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AI	125/125 (100%)	125 (100%)	0	100	100
2	AL	125/125 (100%)	125 (100%)	0	100	100
2	AO	125/125 (100%)	125 (100%)	0	100	100
2	AQ	125/125 (100%)	125 (100%)	0	100	100
2	AS	125/125 (100%)	125 (100%)	0	100	100
2	AU	125/125 (100%)	125 (100%)	0	100	100
2	AW	125/125 (100%)	125 (100%)	0	100	100
2	AY	125/125 (100%)	125 (100%)	0	100	100
2	BJ	125/125 (100%)	125 (100%)	0	100	100
2	BL	125/125 (100%)	125 (100%)	0	100	100
2	BN	125/125 (100%)	125 (100%)	0	100	100
2	BQ	125/125 (100%)	125 (100%)	0	100	100
2	BT	125/125 (100%)	125 (100%)	0	100	100
2	BW	125/125 (100%)	125 (100%)	0	100	100
2	BY	125/125 (100%)	125 (100%)	0	100	100
2	CA	125/125 (100%)	125 (100%)	0	100	100
2	CD	125/125 (100%)	125 (100%)	0	100	100
2	CF	125/125 (100%)	125 (100%)	0	100	100
2	CH	125/125 (100%)	125 (100%)	0	100	100
2	CS	125/125 (100%)	125 (100%)	0	100	100
2	CU	125/125 (100%)	125 (100%)	0	100	100
2	CW	125/125 (100%)	125 (100%)	0	100	100
2	CZ	125/125 (100%)	125 (100%)	0	100	100
2	DB	125/125 (100%)	125 (100%)	0	100	100
2	DD	125/125 (100%)	125 (100%)	0	100	100
2	DK	125/125 (100%)	125 (100%)	0	100	100
2	DM	125/125 (100%)	125 (100%)	0	100	100
2	DO	125/125 (100%)	125 (100%)	0	100	100
2	DR	125/125 (100%)	125 (100%)	0	100	100
2	DT	125/125 (100%)	125 (100%)	0	100	100
2	DV	125/125 (100%)	125 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	AE	132/133 (99%)	132 (100%)	0	100	100
3	BM	132/133 (99%)	132 (100%)	0	100	100
4	AK	140/140 (100%)	140 (100%)	0	100	100
4	BS	140/140 (100%)	140 (100%)	0	100	100
5	BA	58/58 (100%)	57 (98%)	1 (2%)	56	78
5	BB	58/58 (100%)	58 (100%)	0	100	100
5	CJ	58/58 (100%)	58 (100%)	0	100	100
5	CK	58/58 (100%)	58 (100%)	0	100	100
5	DF	58/58 (100%)	58 (100%)	0	100	100
5	DX	58/58 (100%)	58 (100%)	0	100	100
6	BD	719/753 (96%)	716 (100%)	3 (0%)	89	96
6	CM	719/753 (96%)	717 (100%)	2 (0%)	91	97
7	BF	30/98 (31%)	30 (100%)	0	100	100
7	CO	30/98 (31%)	30 (100%)	0	100	100
8	BG	49/221 (22%)	49 (100%)	0	100	100
8	CP	49/221 (22%)	49 (100%)	0	100	100
8	DG	46/221 (21%)	45 (98%)	1 (2%)	47	72
8	DH	46/221 (21%)	46 (100%)	0	100	100
8	DY	46/221 (21%)	46 (100%)	0	100	100
8	DZ	46/221 (21%)	46 (100%)	0	100	100
9	BH	242/257 (94%)	241 (100%)	1 (0%)	89	96
9	CQ	242/257 (94%)	242 (100%)	0	100	100
9	DI	239/257 (93%)	237 (99%)	2 (1%)	79	91
9	EA	239/257 (93%)	239 (100%)	0	100	100
All	All	11980/13328 (90%)	11955 (100%)	25 (0%)	91	98

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	CM	211	ARG
1	DC	71	ASN
1	DS	71	ASN
1	DA	71	ASN
8	DG	209	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 66 such sidechains are listed below:

Mol	Chain	Res	Type
2	DR	71	ASN
2	DT	71	ASN
9	EA	224	GLN
2	BQ	71	ASN
2	BN	128	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

76 ligands 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	$\#\|Z\| > 2$
10	CYC	AL	200	2	42,46,46	0.47	1 (2%)	52,67,67	0.79	3 (5%)
10	CYC	DO	200	2	42,46,46	0.53	1 (2%)	52,67,67	1.03	4 (7%)
10	CYC	DK	200	2	42,46,46	0.52	1 (2%)	52,67,67	0.75	3 (5%)
10	CYC	CV	200	1	42,46,46	0.51	1 (2%)	52,67,67	0.76	3 (5%)
10	CYC	DL	200	1	42,46,46	0.57	1 (2%)	52,67,67	0.84	2 (3%)
10	CYC	BK	200	1	42,46,46	0.51	1 (2%)	52,67,67	0.60	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
10	CYC	BP	200	1	42,46,46	0.52	1 (2%)	52,67,67	0.87	4 (7%)
10	CYC	AE	200	3	42,46,46	0.53	1 (2%)	52,67,67	0.80	3 (5%)
10	CYC	DC	200	1	42,46,46	0.45	1 (2%)	52,67,67	0.87	3 (5%)
10	CYC	CG	200	1	42,46,46	0.49	1 (2%)	52,67,67	0.86	4 (7%)
10	CYC	AF	200	2	42,46,46	0.57	1 (2%)	52,67,67	1.07	4 (7%)
10	CYC	CE	200	1	42,46,46	0.53	1 (2%)	52,67,67	0.92	4 (7%)
10	CYC	DV	200	2	42,46,46	0.47	1 (2%)	52,67,67	0.70	3 (5%)
10	CYC	CW	200	2	42,46,46	0.58	1 (2%)	52,67,67	1.09	4 (7%)
10	CYC	AO	200	2	42,46,46	0.48	1 (2%)	52,67,67	1.02	4 (7%)
10	CYC	CF	200	2	42,46,46	0.60	1 (2%)	52,67,67	1.10	5 (9%)
10	CYC	CC	200	1	42,46,46	0.52	1 (2%)	52,67,67	0.71	3 (5%)
10	CYC	CM	902	6	42,46,46	0.60	1 (2%)	52,67,67	0.89	3 (5%)
10	CYC	DU	200	1	42,46,46	0.47	1 (2%)	52,67,67	0.88	3 (5%)
10	CYC	BV	200	1	42,46,46	0.52	1 (2%)	52,67,67	0.85	3 (5%)
10	CYC	DA	200	1	42,46,46	0.62	1 (2%)	52,67,67	0.91	3 (5%)
10	CYC	AY	200	2	42,46,46	0.52	1 (2%)	52,67,67	0.73	3 (5%)
10	CYC	DJ	200	1	42,46,46	0.54	1 (2%)	52,67,67	0.57	2 (3%)
10	CYC	AR	200	-	42,46,46	0.51	1 (2%)	52,67,67	0.74	2 (3%)
10	CYC	BT	200	2	42,46,46	0.43	1 (2%)	52,67,67	0.97	3 (5%)
10	CYC	BM	200	3	42,46,46	0.55	1 (2%)	52,67,67	0.91	4 (7%)
10	CYC	BN	200	2	42,46,46	0.57	1 (2%)	52,67,67	1.08	4 (7%)
10	CYC	BI	200	1	42,46,46	0.51	1 (2%)	52,67,67	0.61	2 (3%)
10	CYC	AN	200	1	42,46,46	0.56	1 (2%)	52,67,67	0.89	4 (7%)
10	CYC	AQ	200	2	42,46,46	0.49	1 (2%)	52,67,67	1.01	4 (7%)
10	CYC	BJ	200	2	42,46,46	0.48	1 (2%)	52,67,67	0.78	3 (5%)
10	CYC	CY	200	1	42,46,46	0.52	1 (2%)	52,67,67	0.83	3 (5%)
10	CYC	BW	200	2	42,46,46	0.46	1 (2%)	52,67,67	0.95	3 (5%)
10	CYC	CU	200	2	42,46,46	0.50	1 (2%)	52,67,67	0.99	4 (7%)
10	CYC	AZ	200	1	42,46,46	0.52	1 (2%)	52,67,67	0.69	3 (5%)
10	CYC	AH	200	1	42,46,46	0.47	1 (2%)	52,67,67	0.83	4 (7%)
10	CYC	BD	901	2	42,46,46	0.45	1 (2%)	52,67,67	1.04	4 (7%)
10	CYC	BD	902	6	42,46,46	0.55	1 (2%)	52,67,67	0.85	3 (5%)
10	CYC	BL	200	2	42,46,46	0.51	1 (2%)	52,67,67	1.03	4 (7%)
10	CYC	CM	901	2	42,46,46	0.53	1 (2%)	52,67,67	1.14	4 (7%)
10	CYC	CZ	200	2	42,46,46	0.46	1 (2%)	52,67,67	1.03	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
10	CYC	DD	200	2	42,46,46	0.49	1 (2%)	52,67,67	0.71	3 (5%)
10	CYC	CR	200	1	42,46,46	0.51	1 (2%)	52,67,67	0.86	4 (7%)
10	CYC	AX	200	1	42,46,46	0.51	1 (2%)	52,67,67	0.88	4 (7%)
10	CYC	AK	200	4	42,46,46	0.49	1 (2%)	52,67,67	1.00	4 (7%)
10	CYC	AW	200	2	42,46,46	0.57	1 (2%)	52,67,67	1.10	3 (5%)
10	CYC	DM	200	2	42,46,46	0.48	1 (2%)	52,67,67	0.89	4 (7%)
10	CYC	CS	200	2	42,46,46	0.53	1 (2%)	52,67,67	0.83	3 (5%)
10	CYC	AC	200	1	42,46,46	0.55	1 (2%)	52,67,67	0.73	2 (3%)
10	CYC	DR	200	2	42,46,46	0.48	1 (2%)	52,67,67	1.15	4 (7%)
10	CYC	BS	200	4	42,46,46	0.39	0	52,67,67	1.08	4 (7%)
10	CYC	AU	200	2	42,46,46	0.51	1 (2%)	52,67,67	1.32	4 (7%)
10	CYC	AI	200	2	42,46,46	0.45	1 (2%)	52,67,67	0.97	4 (7%)
10	CYC	CH	200	2	42,46,46	0.51	1 (2%)	52,67,67	0.80	3 (5%)
10	CYC	CT	200	1	42,46,46	0.51	1 (2%)	52,67,67	0.87	3 (5%)
10	CYC	DN	200	1	42,46,46	0.53	1 (2%)	52,67,67	0.85	3 (5%)
10	CYC	BY	200	2	42,46,46	0.53	1 (2%)	52,67,67	1.03	4 (7%)
10	CYC	AD	200	2	42,46,46	0.49	1 (2%)	52,67,67	0.79	3 (5%)
10	CYC	AV	200	1	42,46,46	0.48	1 (2%)	52,67,67	0.87	3 (5%)
10	CYC	BR	200	1	42,46,46	0.47	1 (2%)	52,67,67	0.83	4 (7%)
10	CYC	BZ	200	1	42,46,46	0.50	1 (2%)	52,67,67	0.88	4 (7%)
10	CYC	DQ	200	1	42,46,46	0.53	1 (2%)	52,67,67	0.63	2 (3%)
10	CYC	AJ	200	1	42,46,46	0.49	1 (2%)	52,67,67	0.83	4 (7%)
10	CYC	BQ	200	2	42,46,46	0.51	1 (2%)	52,67,67	1.09	4 (7%)
10	CYC	AB	200	2	42,46,46	0.50	1 (2%)	52,67,67	0.82	3 (5%)
10	CYC	DS	200	1	42,46,46	0.54	1 (2%)	52,67,67	0.89	3 (5%)
10	CYC	DT	200	2	42,46,46	0.56	1 (2%)	52,67,67	0.94	5 (9%)
11	45D	DI	400	-	43,43,43	0.96	2 (4%)	54,60,60	1.50	12 (22%)
10	CYC	AA	200	1	42,46,46	0.53	1 (2%)	52,67,67	0.78	4 (7%)
10	CYC	CD	200	2	42,46,46	0.52	1 (2%)	52,67,67	1.32	4 (7%)
10	CYC	DB	200	2	42,46,46	0.55	1 (2%)	52,67,67	1.03	5 (9%)
11	45D	EA	400	-	43,43,43	1.00	3 (6%)	54,60,60	1.49	10 (18%)
10	CYC	AP	200	1	42,46,46	0.53	1 (2%)	52,67,67	0.84	4 (7%)
10	CYC	BX	200	1	42,46,46	0.52	1 (2%)	52,67,67	0.89	4 (7%)
11	45D	CQ	400	-	43,43,43	0.97	1 (2%)	54,60,60	1.50	14 (25%)
11	45D	BH	400	-	43,43,43	0.97	2 (4%)	54,60,60	1.57	12 (22%)

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
10	CYC	AL	200	2	-	9/25/74/74	0/4/4/4
10	CYC	DO	200	2	-	7/25/74/74	0/4/4/4
10	CYC	DK	200	2	-	7/25/74/74	0/4/4/4
10	CYC	CV	200	1	-	3/25/74/74	0/4/4/4
10	CYC	DL	200	1	-	10/25/74/74	0/4/4/4
10	CYC	BK	200	1	-	6/25/74/74	0/4/4/4
10	CYC	BP	200	1	-	7/25/74/74	0/4/4/4
10	CYC	AE	200	3	-	12/25/74/74	0/4/4/4
10	CYC	DC	200	1	-	10/25/74/74	0/4/4/4
10	CYC	CG	200	1	-	8/25/74/74	0/4/4/4
10	CYC	AF	200	2	-	5/25/74/74	0/4/4/4
10	CYC	CE	200	1	-	8/25/74/74	0/4/4/4
10	CYC	DV	200	2	-	8/25/74/74	0/4/4/4
10	CYC	CW	200	2	-	9/25/74/74	0/4/4/4
10	CYC	AO	200	2	-	7/25/74/74	0/4/4/4
10	CYC	CF	200	2	-	9/25/74/74	0/4/4/4
10	CYC	CC	200	1	-	6/25/74/74	0/4/4/4
10	CYC	CM	902	6	-	7/25/74/74	0/4/4/4
10	CYC	DU	200	1	-	9/25/74/74	0/4/4/4
10	CYC	BV	200	1	-	11/25/74/74	0/4/4/4
10	CYC	DA	200	1	-	6/25/74/74	0/4/4/4
10	CYC	AY	200	2	-	9/25/74/74	0/4/4/4
10	CYC	DJ	200	1	-	10/25/74/74	0/4/4/4
10	CYC	AR	200	-	-	11/25/74/74	0/4/4/4
10	CYC	BT	200	2	-	13/25/74/74	0/4/4/4
10	CYC	BM	200	3	-	7/25/74/74	0/4/4/4
10	CYC	BN	200	2	-	5/25/74/74	0/4/4/4
10	CYC	BI	200	1	-	10/25/74/74	0/4/4/4
10	CYC	AN	200	1	-	8/25/74/74	0/4/4/4
10	CYC	AQ	200	2	-	11/25/74/74	0/4/4/4
10	CYC	BJ	200	2	-	5/25/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CYC	CY	200	1	-	12/25/74/74	0/4/4/4
10	CYC	BW	200	2	-	8/25/74/74	0/4/4/4
10	CYC	CU	200	2	-	10/25/74/74	0/4/4/4
10	CYC	AZ	200	1	-	8/25/74/74	0/4/4/4
10	CYC	AH	200	1	-	10/25/74/74	0/4/4/4
10	CYC	BD	901	2	-	10/25/74/74	0/4/4/4
10	CYC	BD	902	6	-	8/25/74/74	0/4/4/4
10	CYC	BL	200	2	-	14/25/74/74	0/4/4/4
10	CYC	CM	901	2	-	13/25/74/74	0/4/4/4
10	CYC	CZ	200	2	-	12/25/74/74	0/4/4/4
10	CYC	DD	200	2	-	5/25/74/74	0/4/4/4
10	CYC	CR	200	1	-	10/25/74/74	0/4/4/4
10	CYC	AX	200	1	-	7/25/74/74	0/4/4/4
10	CYC	AK	200	4	-	8/25/74/74	0/4/4/4
10	CYC	AW	200	2	-	11/25/74/74	0/4/4/4
10	CYC	DM	200	2	-	9/25/74/74	0/4/4/4
10	CYC	CS	200	2	-	7/25/74/74	0/4/4/4
10	CYC	AC	200	1	-	7/25/74/74	0/4/4/4
10	CYC	DR	200	2	-	10/25/74/74	0/4/4/4
10	CYC	BS	200	4	-	9/25/74/74	0/4/4/4
10	CYC	AU	200	2	-	8/25/74/74	0/4/4/4
10	CYC	AI	200	2	-	6/25/74/74	0/4/4/4
10	CYC	CH	200	2	-	8/25/74/74	0/4/4/4
10	CYC	CT	200	1	-	12/25/74/74	0/4/4/4
10	CYC	DN	200	1	-	7/25/74/74	0/4/4/4
10	CYC	BY	200	2	-	9/25/74/74	0/4/4/4
10	CYC	AD	200	2	-	9/25/74/74	0/4/4/4
10	CYC	AV	200	1	-	6/25/74/74	0/4/4/4
10	CYC	BR	200	1	-	7/25/74/74	0/4/4/4
10	CYC	BZ	200	1	-	7/25/74/74	0/4/4/4
10	CYC	DQ	200	1	-	13/25/74/74	0/4/4/4
10	CYC	AJ	200	1	-	8/25/74/74	0/4/4/4
10	CYC	BQ	200	2	-	7/25/74/74	0/4/4/4
10	CYC	AB	200	2	-	7/25/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CYC	DS	200	1	-	7/25/74/74	0/4/4/4
10	CYC	DT	200	2	-	10/25/74/74	0/4/4/4
11	45D	DI	400	-	-	15/29/69/69	0/2/2/2
10	CYC	AA	200	1	-	7/25/74/74	0/4/4/4
10	CYC	CD	200	2	-	12/25/74/74	0/4/4/4
10	CYC	DB	200	2	-	10/25/74/74	0/4/4/4
11	45D	EA	400	-	-	16/29/69/69	0/2/2/2
10	CYC	AP	200	1	-	7/25/74/74	0/4/4/4
10	CYC	BX	200	1	-	7/25/74/74	0/4/4/4
11	45D	CQ	400	-	-	15/29/69/69	0/2/2/2
11	45D	BH	400	-	-	16/29/69/69	0/2/2/2

The worst 5 of 79 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	EA	400	45D	C34-C36	3.69	1.53	1.46
10	DA	200	CYC	CHA-C1A	3.52	1.38	1.35
11	DI	400	45D	C34-C36	3.51	1.53	1.46
11	BH	400	45D	C34-C36	3.50	1.53	1.46
10	CF	200	CYC	CHA-C1A	3.49	1.38	1.35

The worst 5 of 296 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	AU	200	CYC	C1D-CHD-C4C	6.61	137.54	128.47
10	CD	200	CYC	C1D-CHD-C4C	6.59	137.52	128.47
10	DR	200	CYC	C1D-CHD-C4C	6.52	137.42	128.47
10	AW	200	CYC	C1D-CHD-C4C	5.95	136.63	128.47
10	BL	200	CYC	C1D-CHD-C4C	5.82	136.46	128.47

There are no chirality outliers.

5 of 677 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	AA	200	CYC	NA-C4A-CHB-C1B
10	AA	200	CYC	C3A-C4A-CHB-C1B
10	AB	200	CYC	NA-C4A-CHB-C1B
10	AB	200	CYC	C3A-C4A-CHB-C1B
10	AB	200	CYC	NC-C4C-CHD-C1D

There are no ring outliers.

76 monomers are involved in 977 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	AL	200	CYC	11	0
10	DO	200	CYC	7	0
10	DK	200	CYC	13	0
10	CV	200	CYC	14	0
10	DL	200	CYC	13	0
10	BK	200	CYC	17	0
10	BP	200	CYC	17	0
10	AE	200	CYC	9	0
10	DC	200	CYC	16	0
10	CG	200	CYC	15	0
10	AF	200	CYC	13	0
10	CE	200	CYC	15	0
10	DV	200	CYC	13	0
10	CW	200	CYC	12	0
10	AO	200	CYC	8	0
10	CF	200	CYC	12	0
10	CC	200	CYC	10	0
10	CM	902	CYC	13	0
10	DU	200	CYC	14	0
10	BV	200	CYC	14	0
10	DA	200	CYC	11	0
10	AY	200	CYC	15	0
10	DJ	200	CYC	14	0
10	AR	200	CYC	11	0
10	BT	200	CYC	10	0
10	BM	200	CYC	9	0
10	BN	200	CYC	16	0
10	BI	200	CYC	15	0
10	AN	200	CYC	10	0
10	AQ	200	CYC	12	0
10	BJ	200	CYC	13	0
10	CY	200	CYC	13	0
10	BW	200	CYC	10	0
10	CU	200	CYC	9	0
10	AZ	200	CYC	14	0
10	AH	200	CYC	18	0
10	BD	901	CYC	12	0
10	BD	902	CYC	13	0
10	BL	200	CYC	17	0
10	CM	901	CYC	10	0

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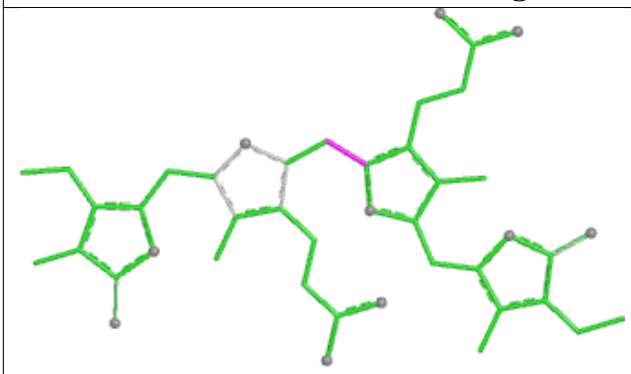
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	CZ	200	CYC	11	0
10	DD	200	CYC	21	0
10	CR	200	CYC	12	0
10	AX	200	CYC	15	0
10	AK	200	CYC	20	0
10	AW	200	CYC	10	0
10	DM	200	CYC	11	0
10	CS	200	CYC	8	0
10	AC	200	CYC	15	0
10	DR	200	CYC	17	0
10	BS	200	CYC	16	0
10	AU	200	CYC	14	0
10	AI	200	CYC	12	0
10	CH	200	CYC	15	0
10	CT	200	CYC	14	0
10	DN	200	CYC	15	0
10	BY	200	CYC	13	0
10	AD	200	CYC	17	0
10	AV	200	CYC	21	0
10	BR	200	CYC	7	0
10	BZ	200	CYC	12	0
10	DQ	200	CYC	12	0
10	AJ	200	CYC	11	0
10	BQ	200	CYC	17	0
10	AB	200	CYC	14	0
10	DS	200	CYC	12	0
10	DT	200	CYC	13	0
11	DI	400	45D	14	0
10	AA	200	CYC	14	0
10	CD	200	CYC	9	0
10	DB	200	CYC	11	0
11	EA	400	45D	12	0
10	AP	200	CYC	10	0
10	BX	200	CYC	14	0
11	CQ	400	45D	6	0
11	BH	400	45D	4	0

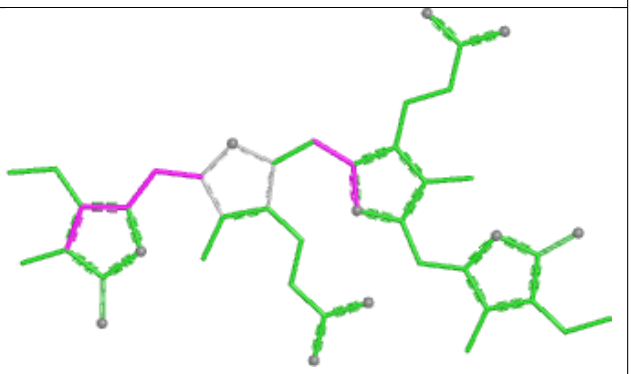
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

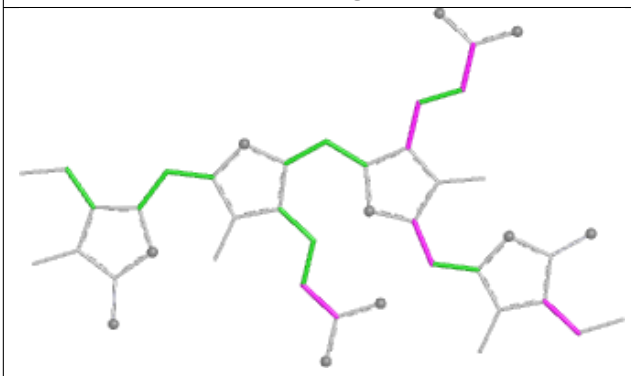
Ligand CYC AL 200



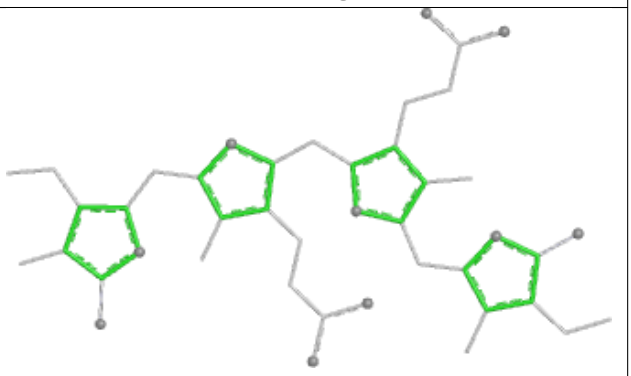
Bond lengths



Bond angles

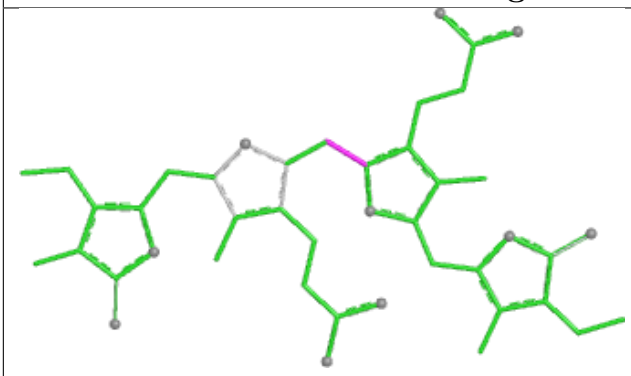


Torsions

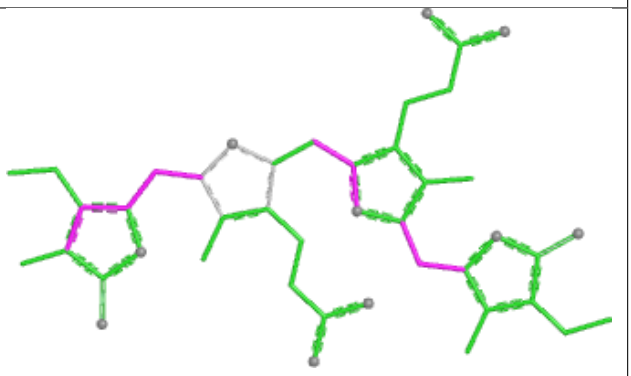


Rings

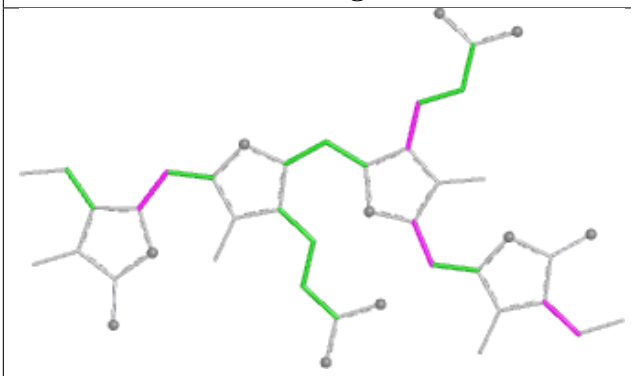
Ligand CYC DO 200



Bond lengths



Bond angles



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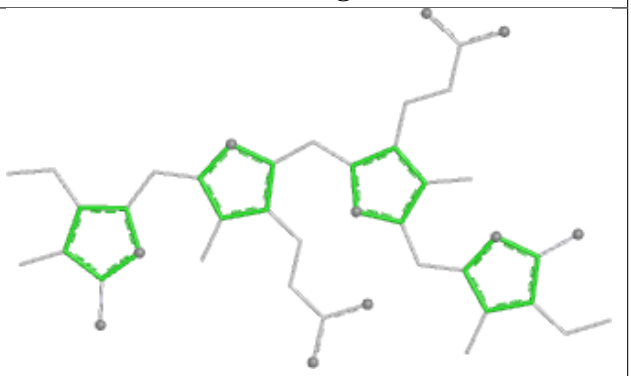
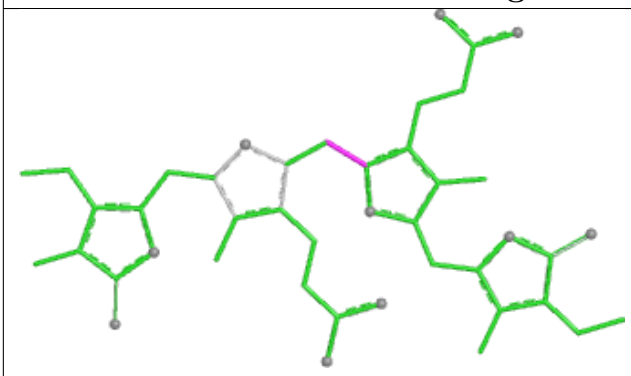
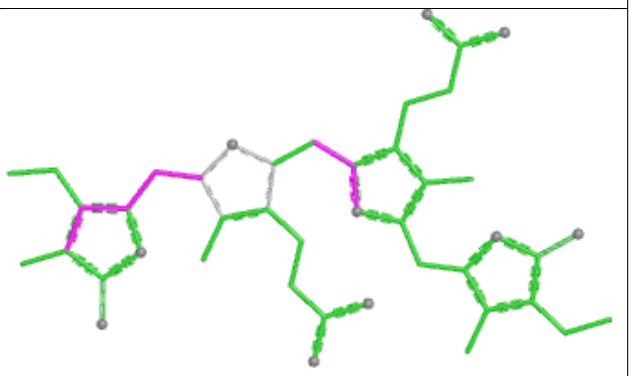


Rings

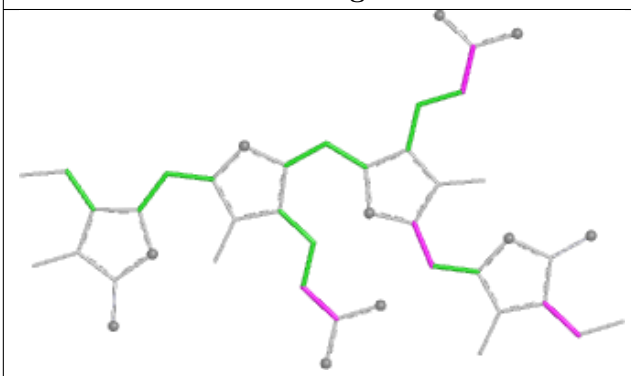
Ligand CYC DK 200



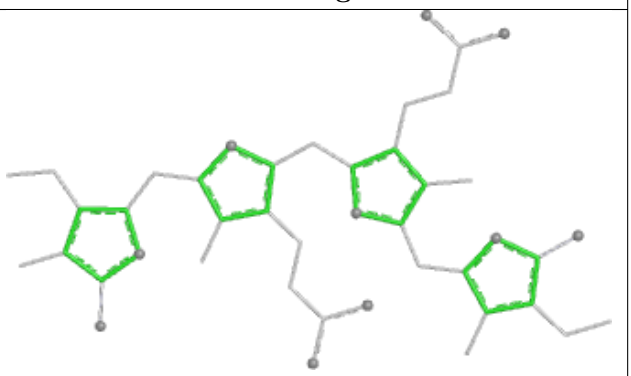
Bond lengths



Bond angles

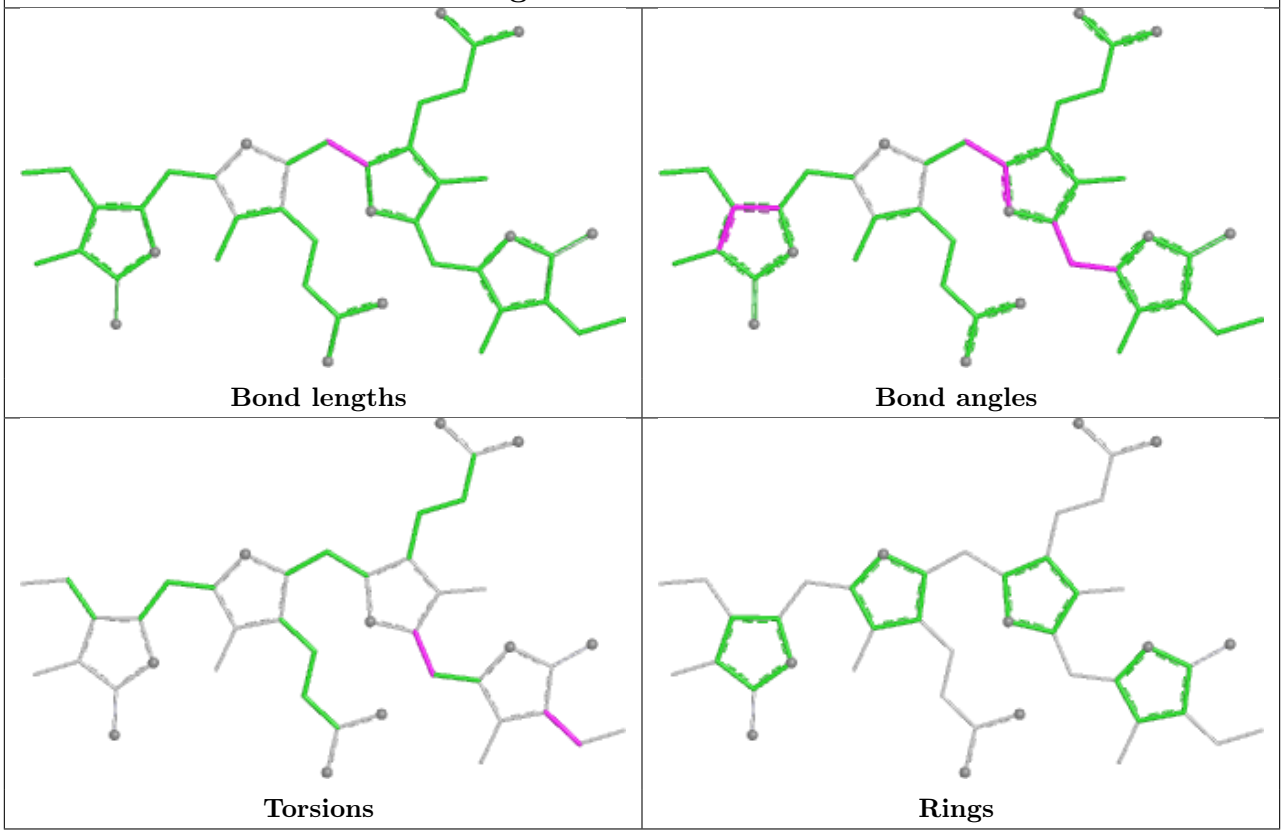


Torsions



Rings

Ligand CYC CV 200



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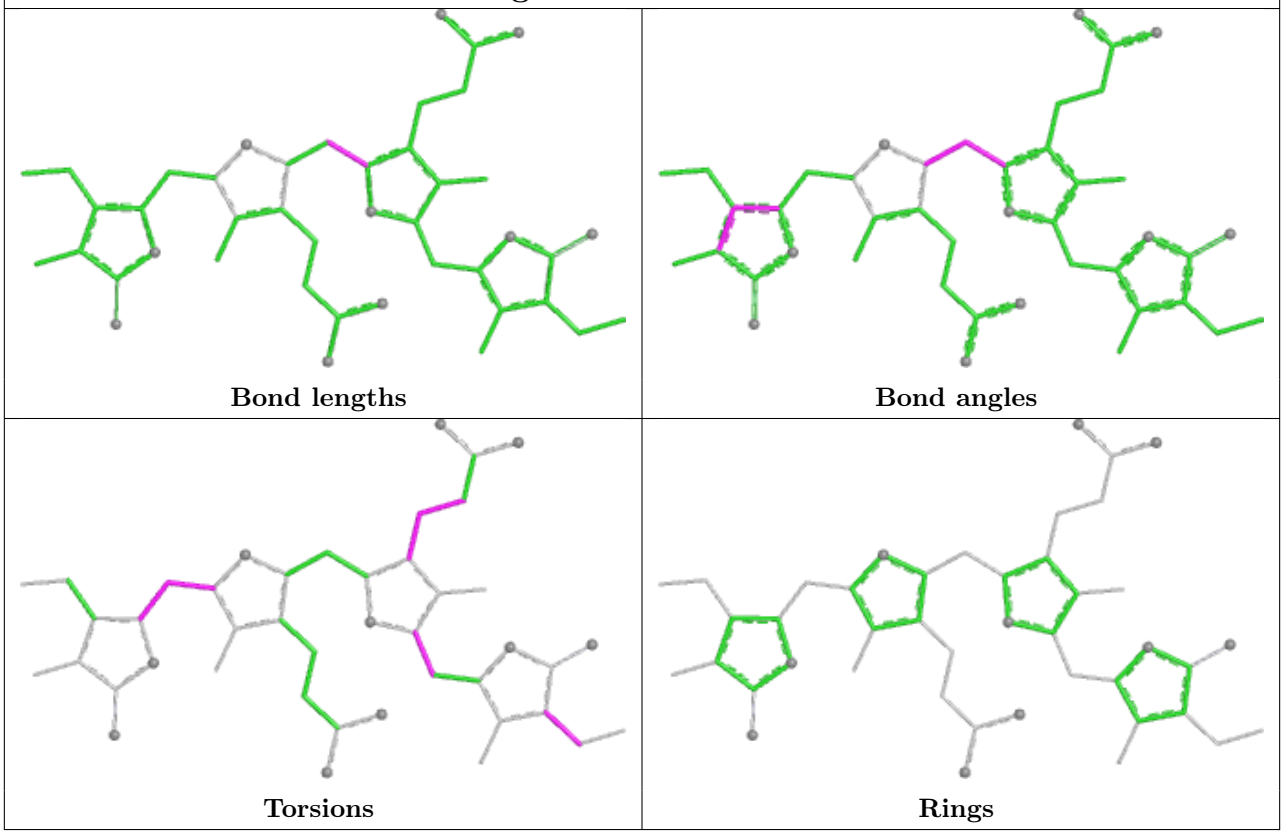
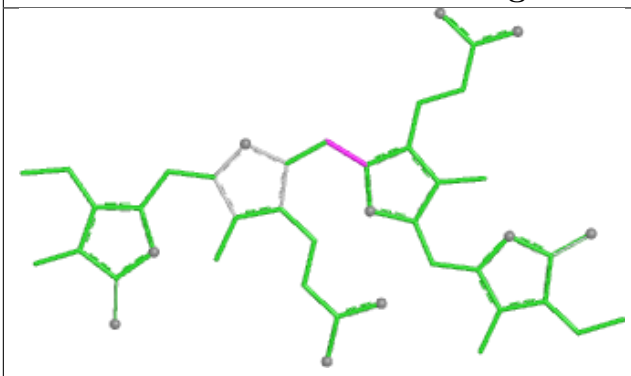
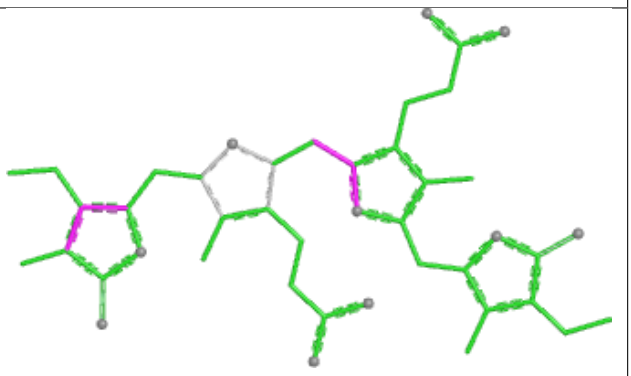


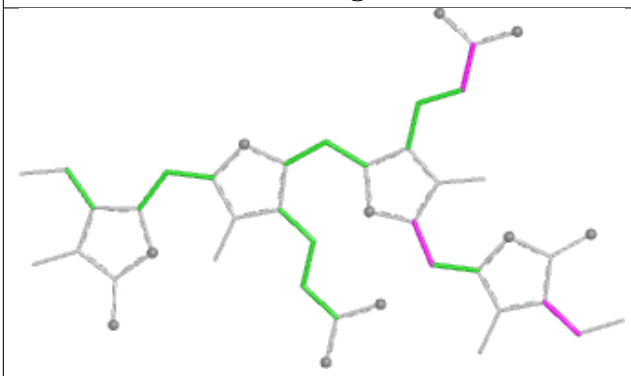
Ligand CYC BK 200



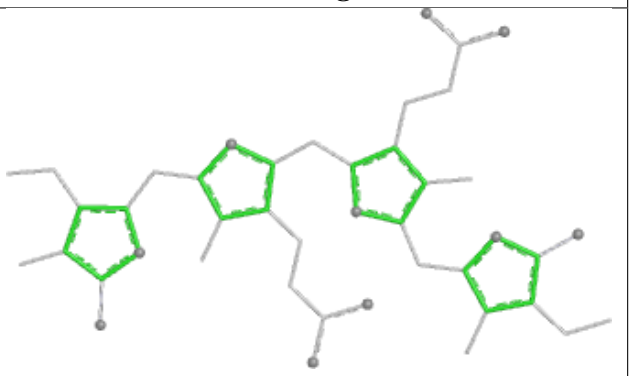
Bond lengths



Bond angles



Torsions



Rings

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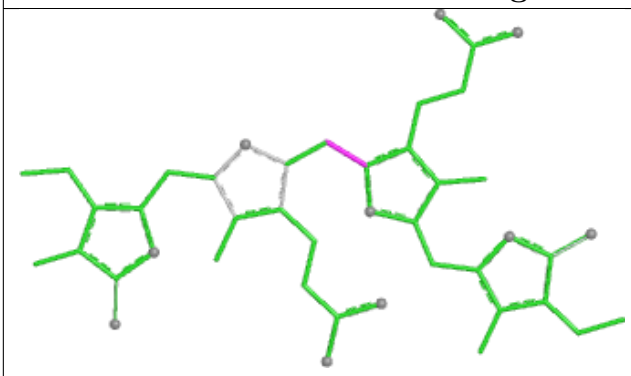
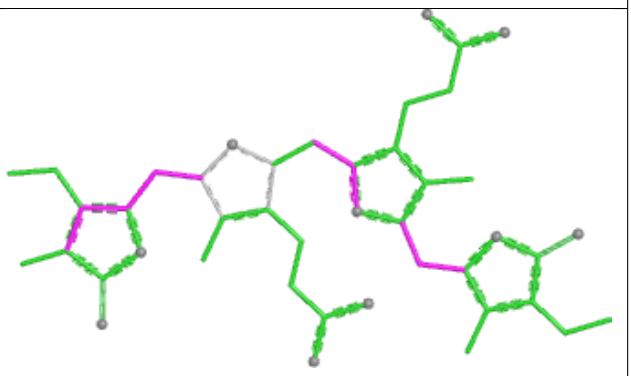
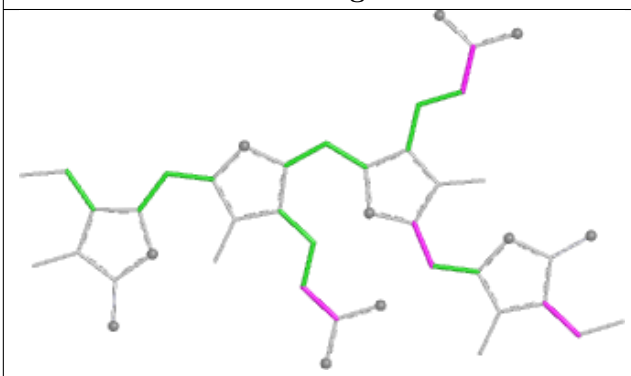


Bond lengths



Bond angles



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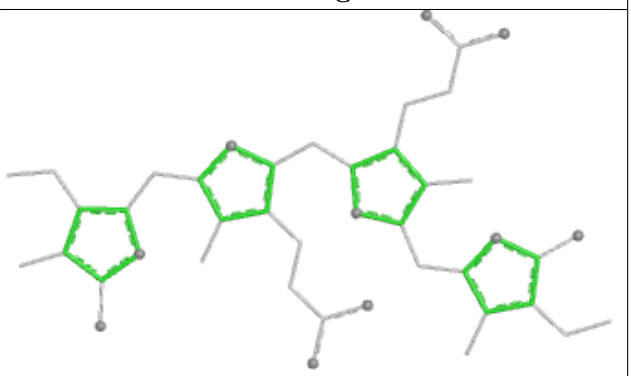
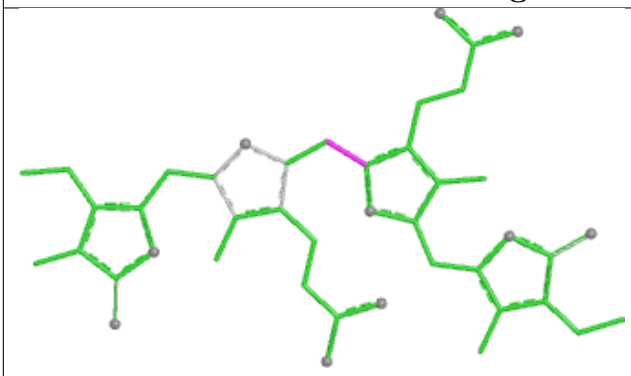
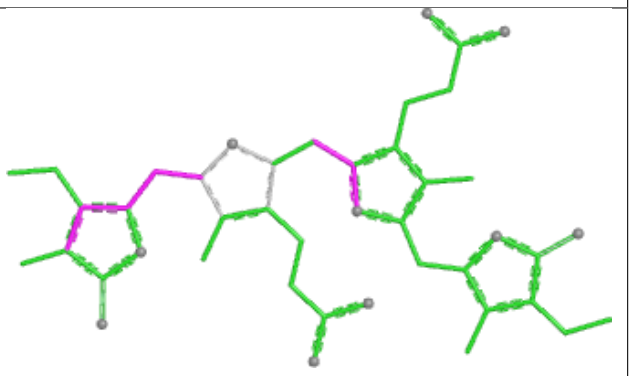


Rings

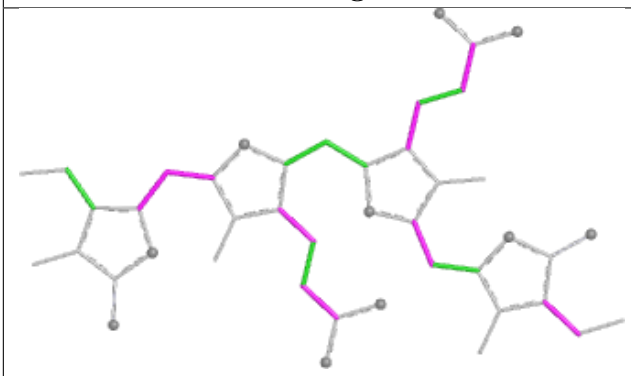
Ligand CYC AE 200



Bond lengths



Bond angles



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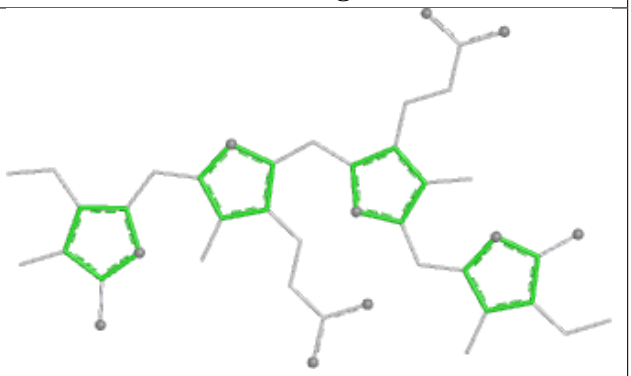
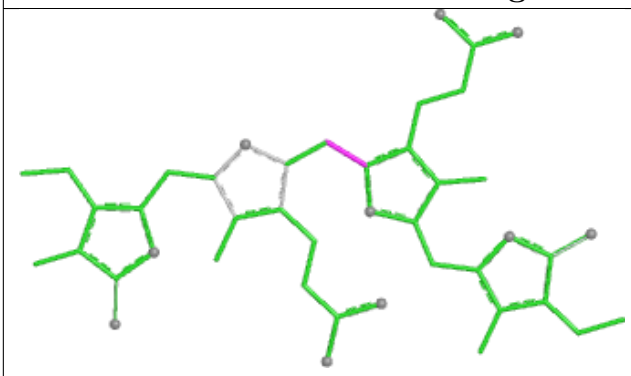
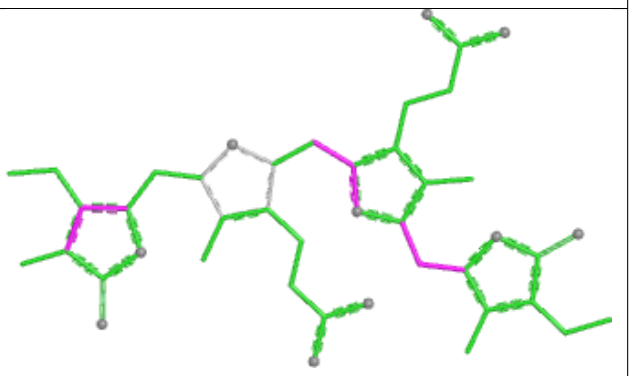


Rings

Ligand CYC DC 200



Bond lengths



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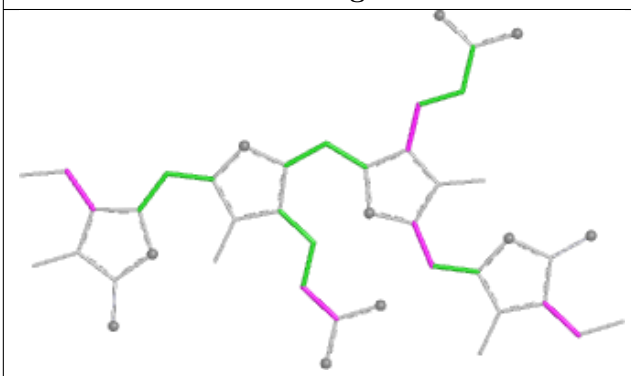

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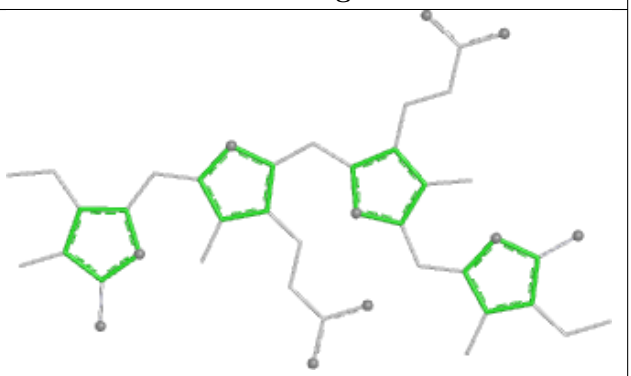
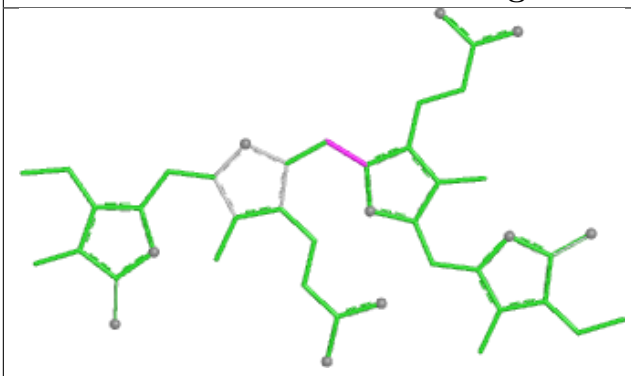
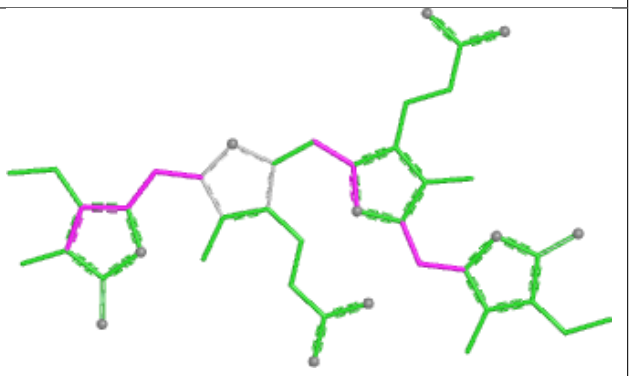


Rings

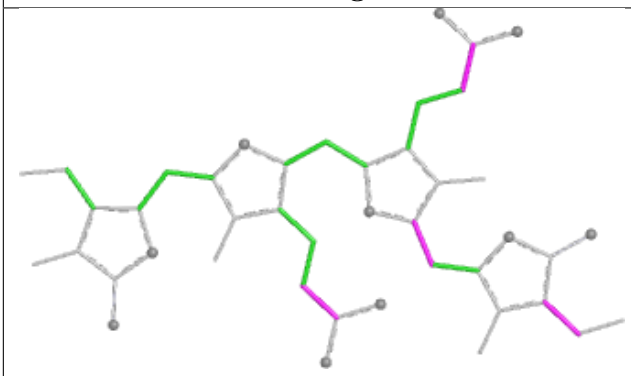
Ligand CYC CG 200



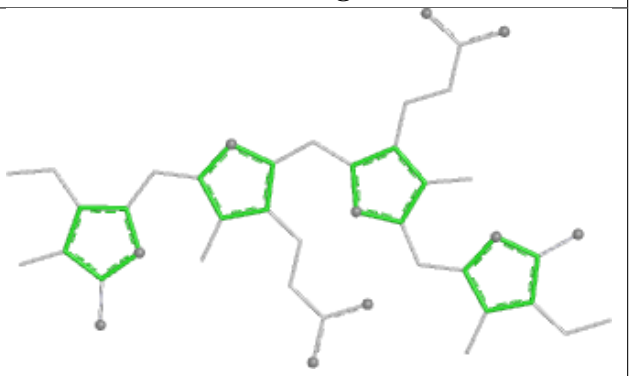
Bond lengths



Bond angles

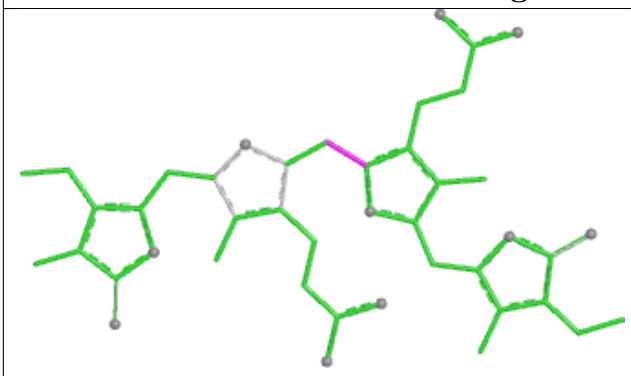


Torsions

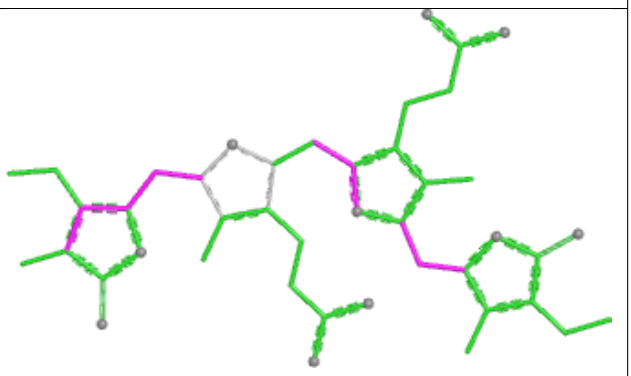


Rings

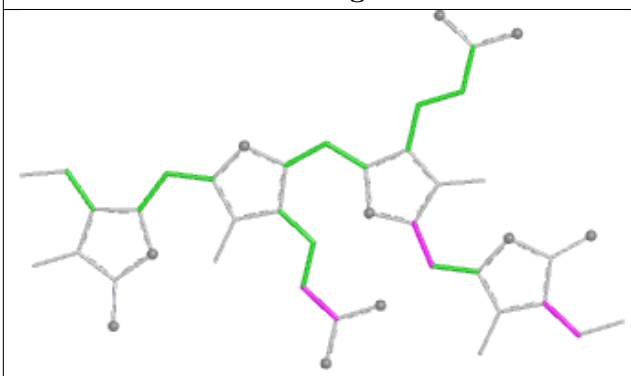
Ligand CYC AF 200



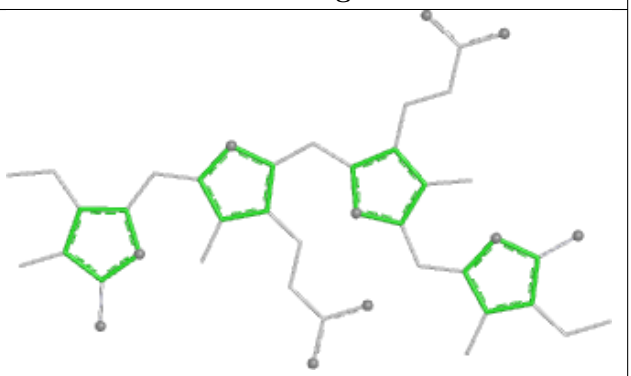
Bond lengths



Bond angles

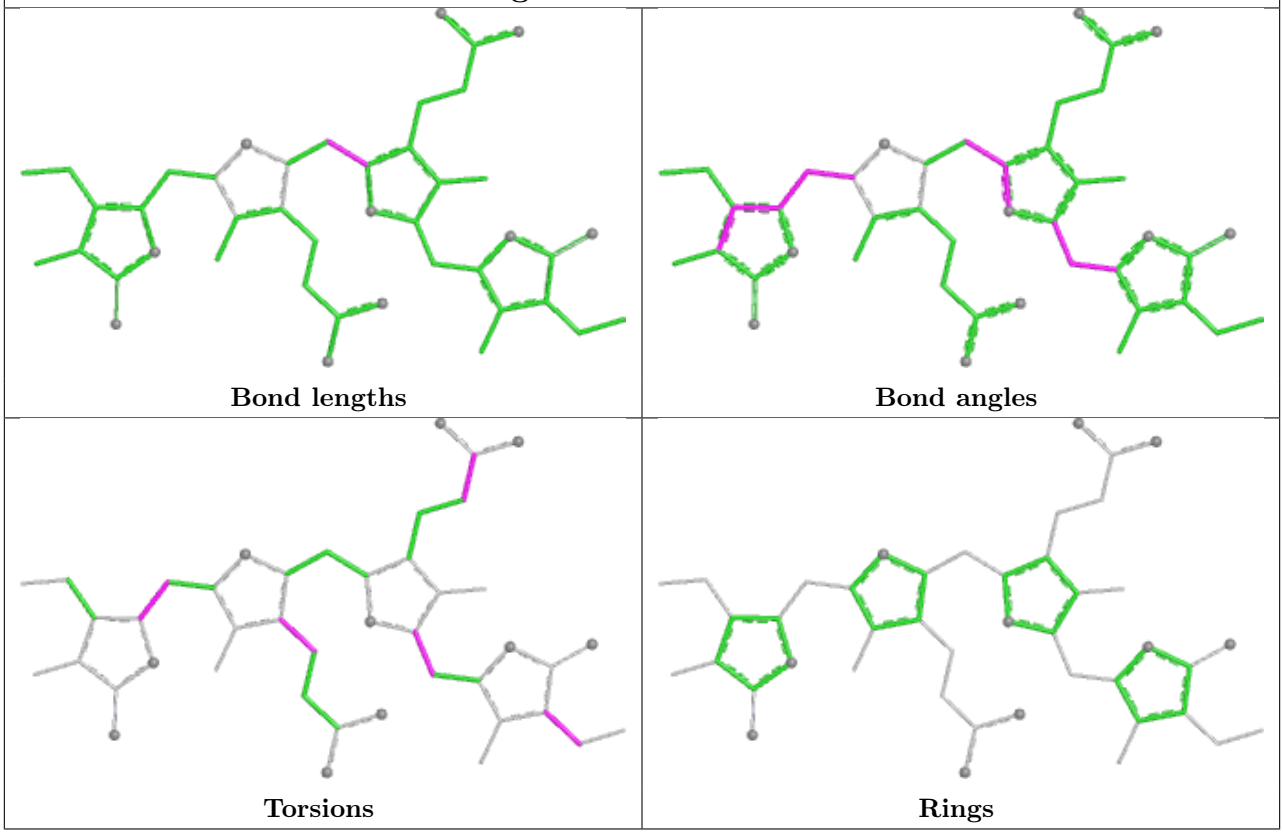


Torsions

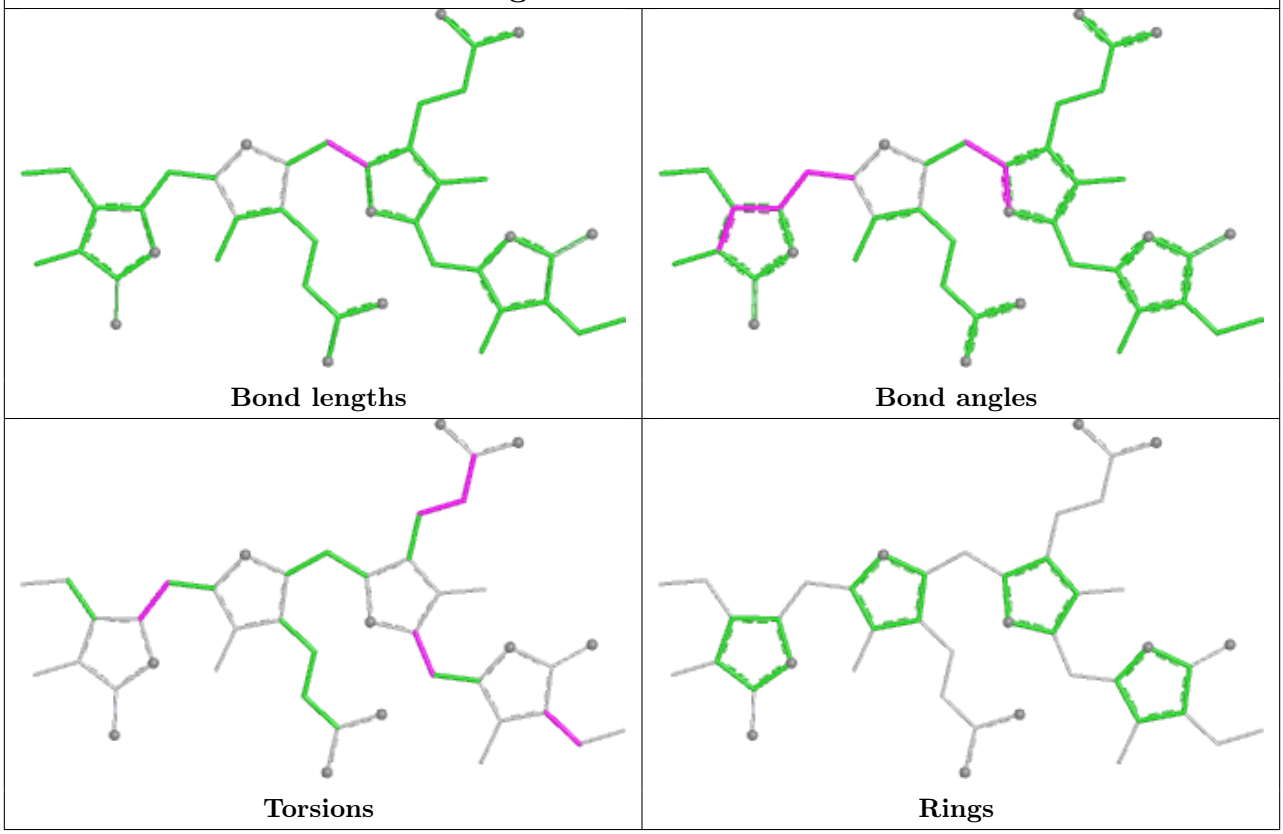


Rings

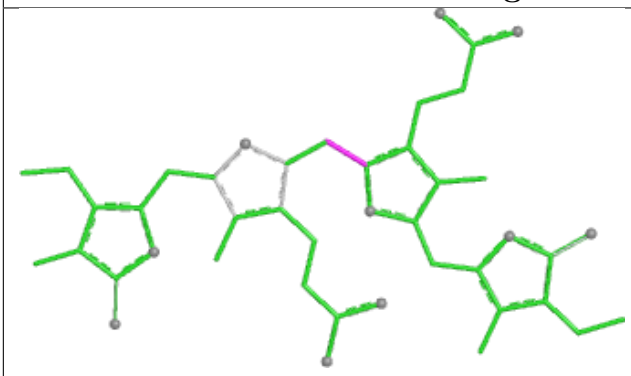
Ligand CYC CE 200



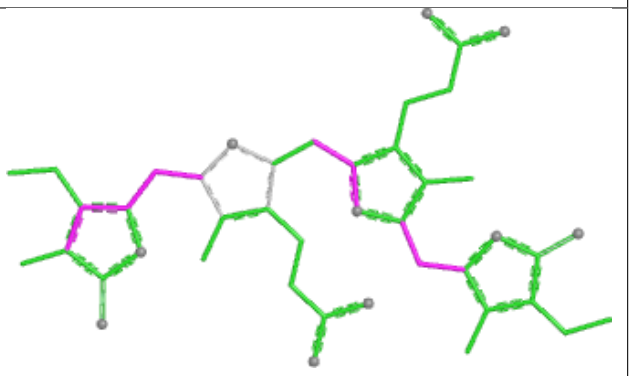
Ligand CYC DV 200



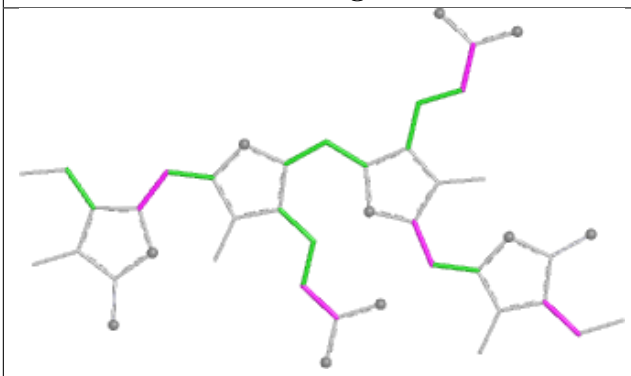
Ligand CYC CW 200



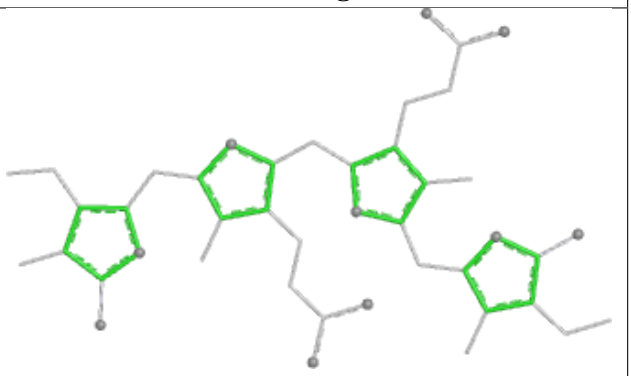
Bond lengths



Bond angles

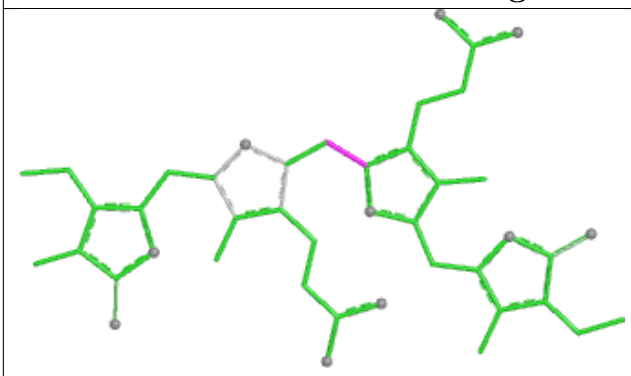


Torsions

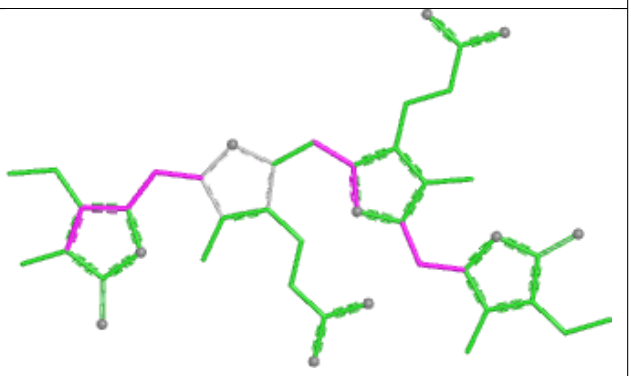


Rings

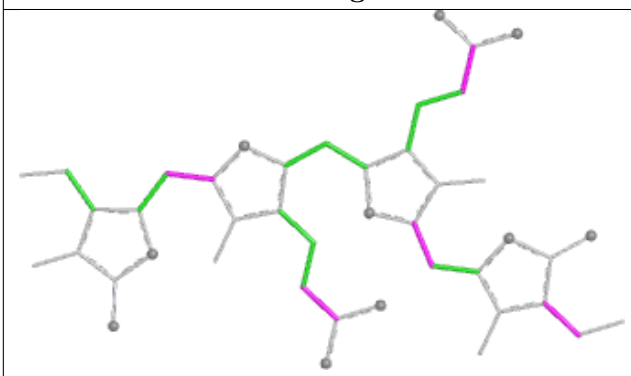
Ligand CYC AO 200



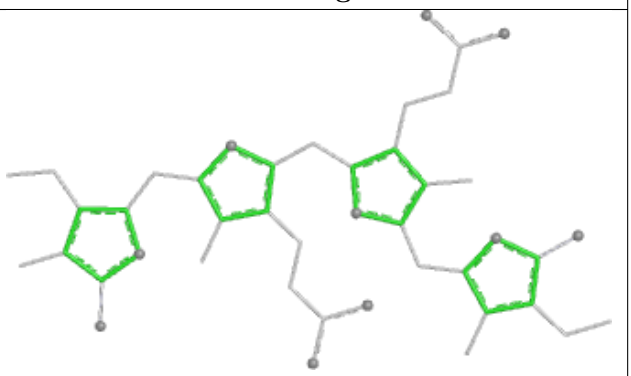
Bond lengths



Bond angles



Torsions



Rings

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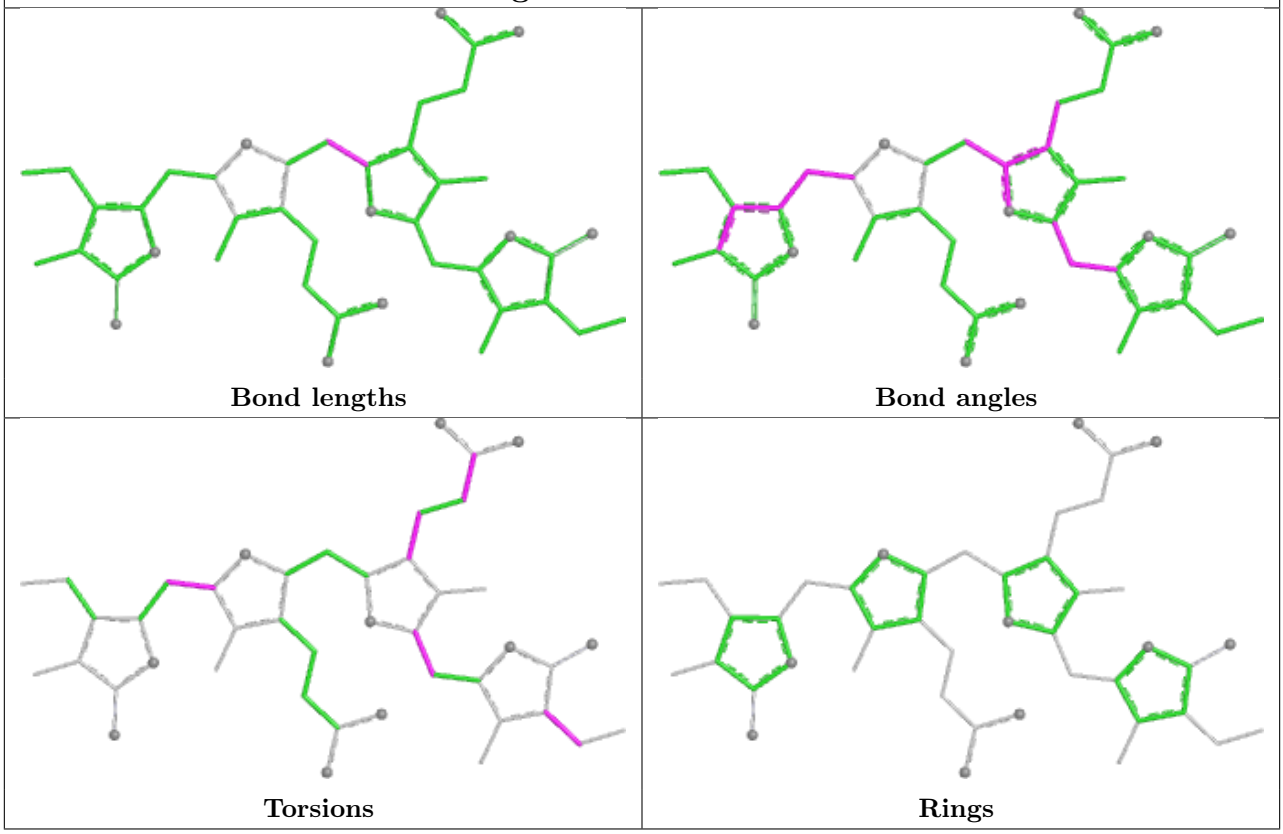
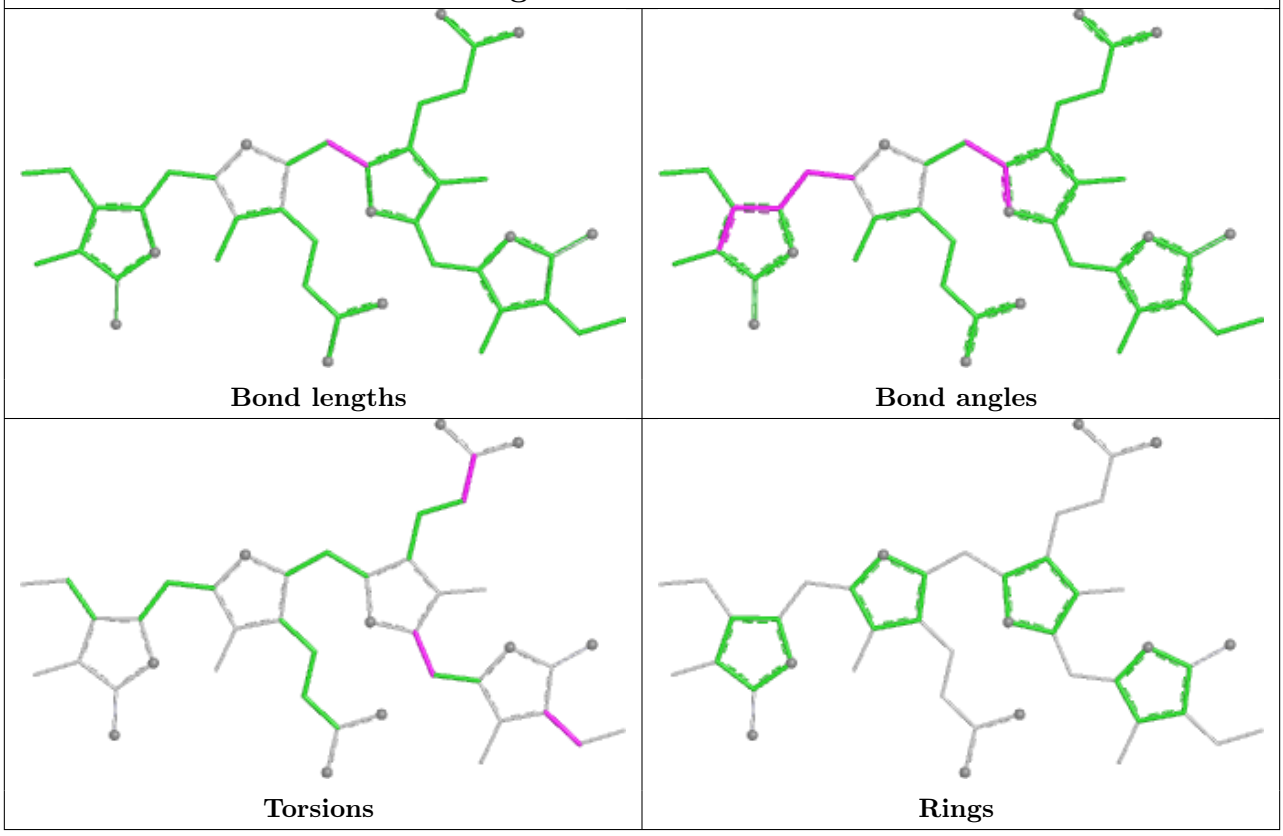
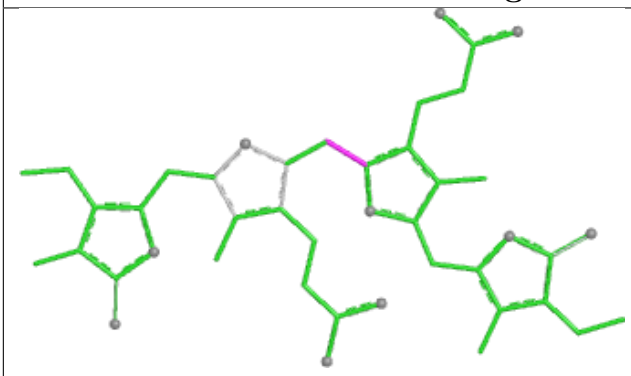


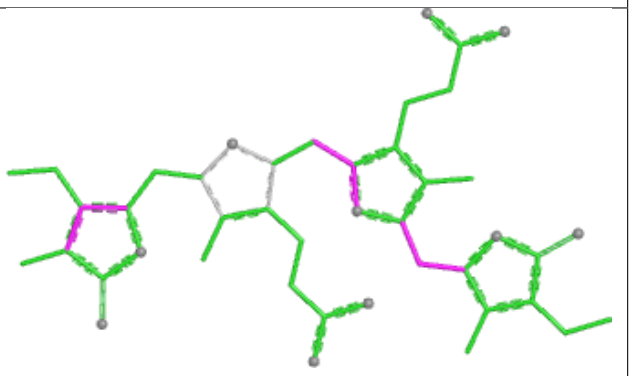
Ligand CYC CC 200



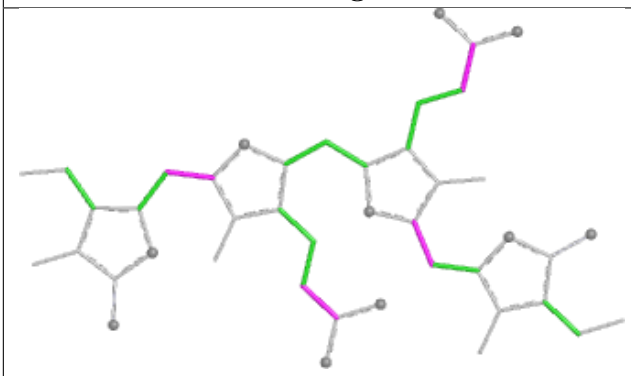
Ligand CYC CM 902



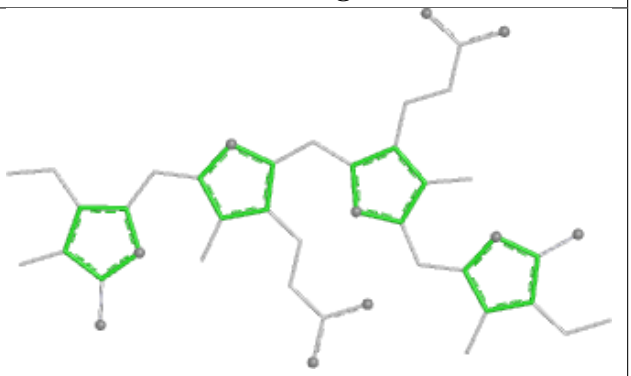
Bond lengths



Bond angles

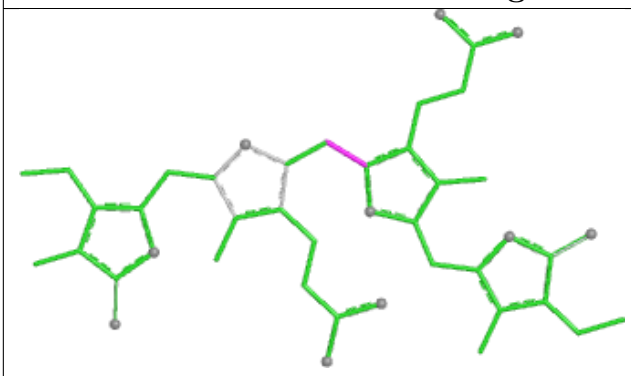


Torsions

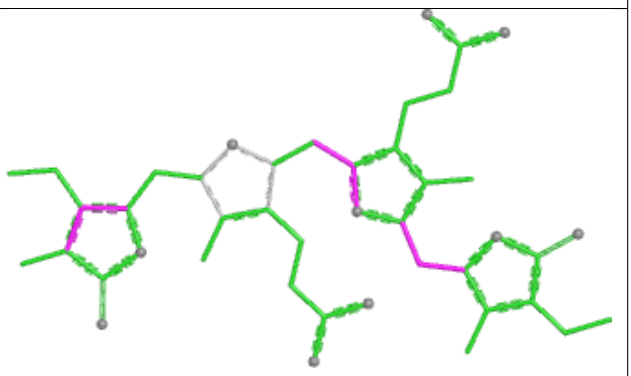


Rings

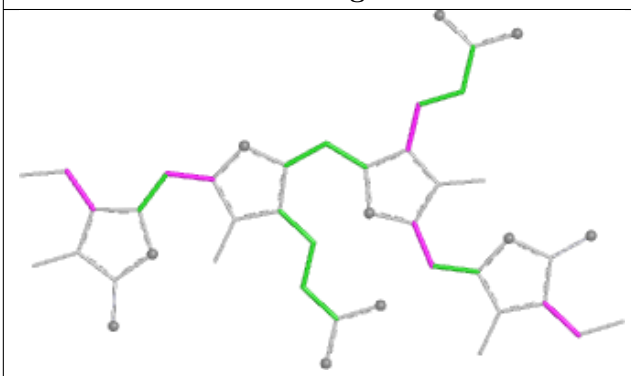
Ligand CYC DU 200



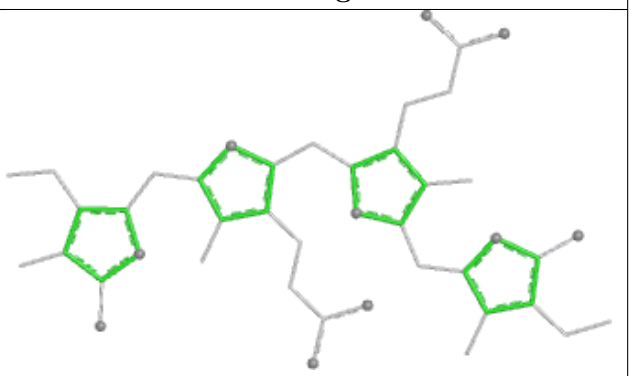
Bond lengths



Bond angles



Torsions



Rings

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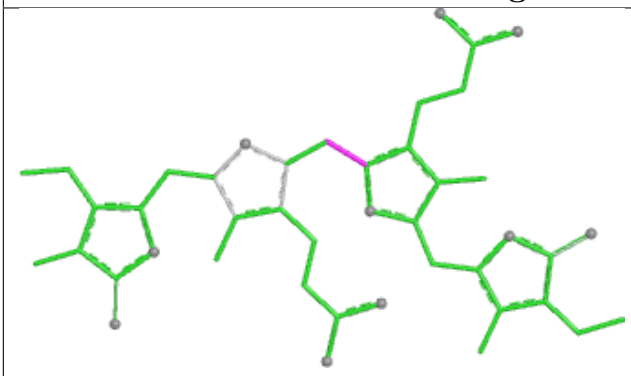
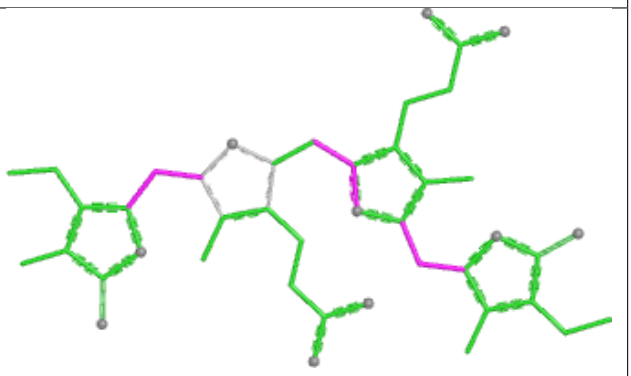
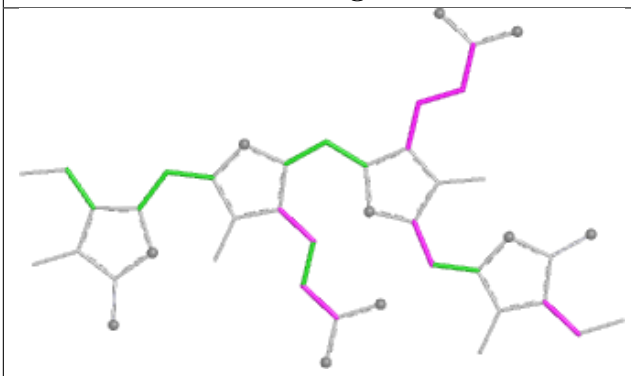


Bond lengths



Bond angles



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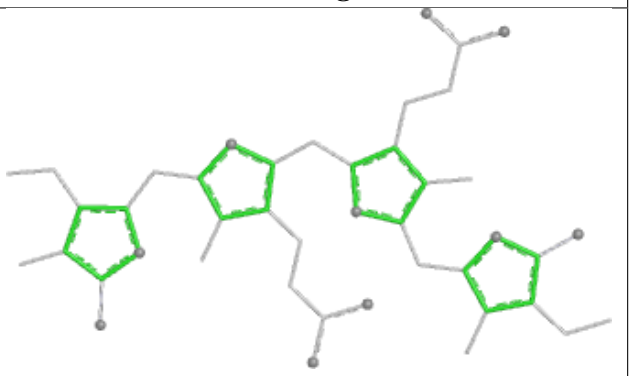
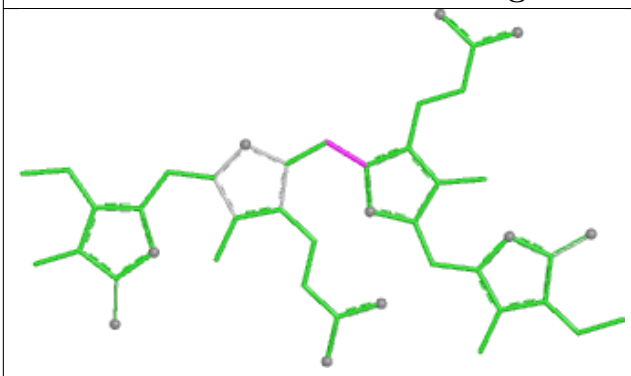
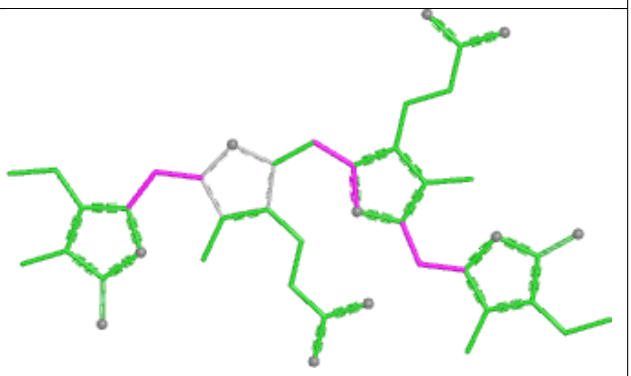


Rings

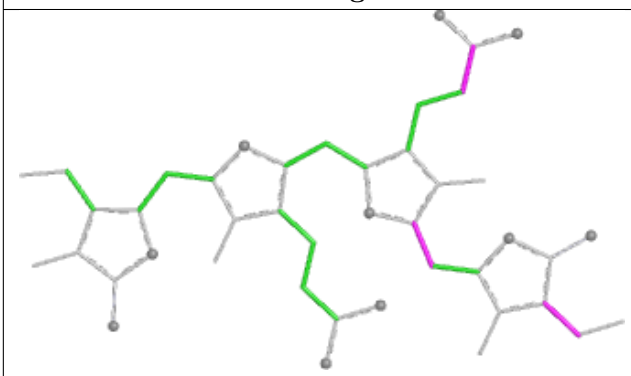
Ligand CYC DA 200



Bond lengths



Bond angles



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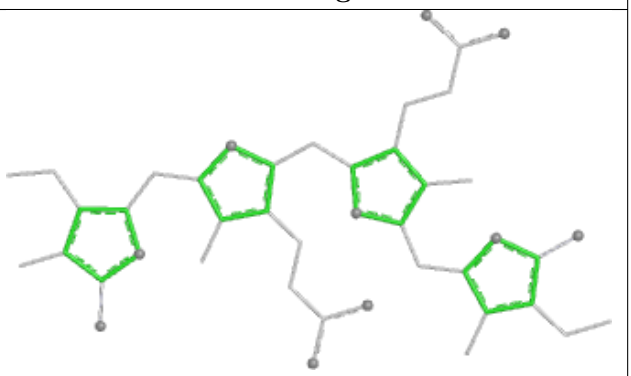
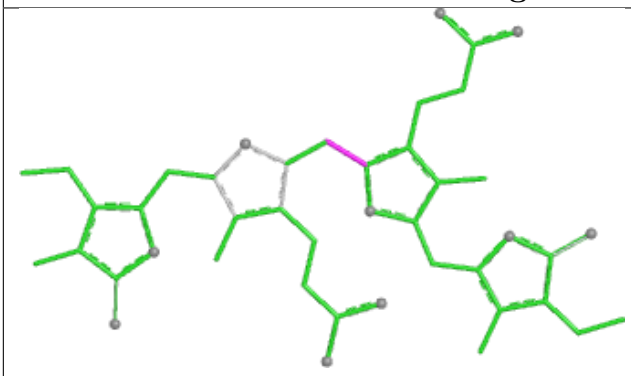
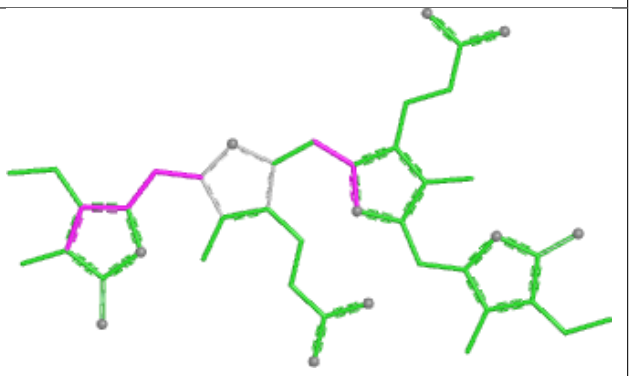


Rings

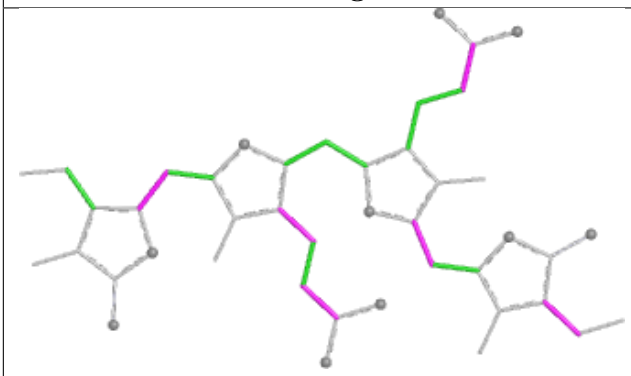
Ligand CYC AY 200



Bond lengths



Bond angles



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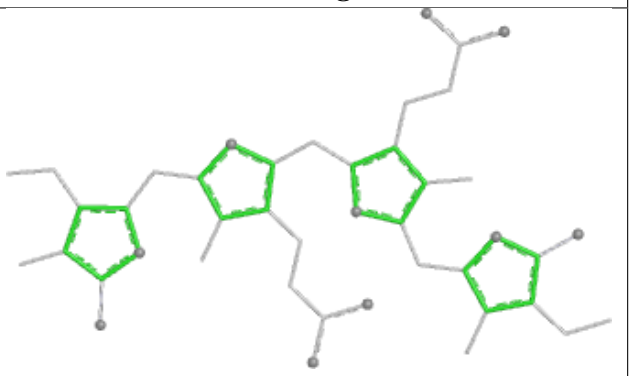
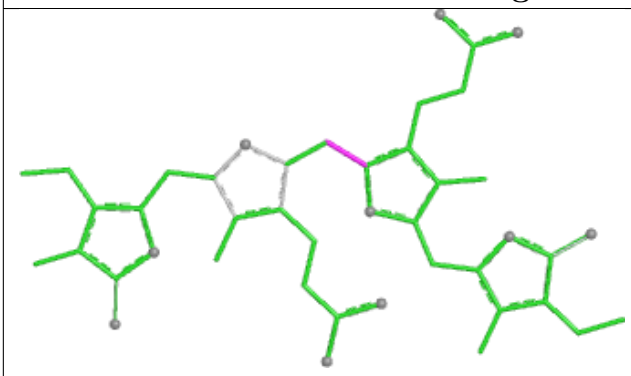
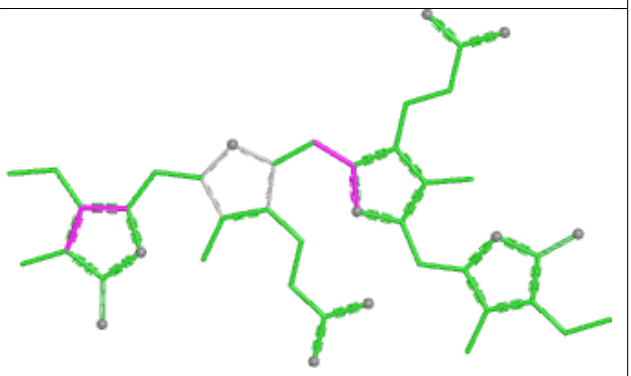


Rings

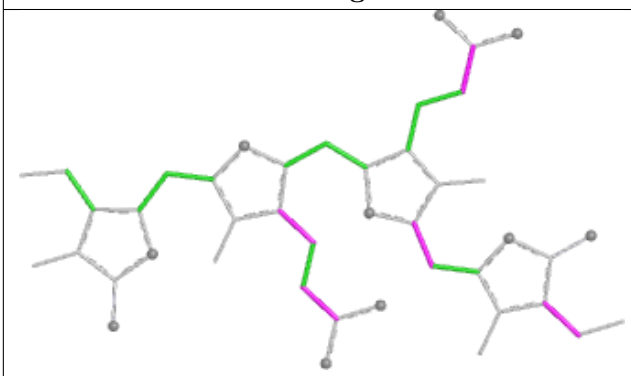
Ligand CYC DJ 200



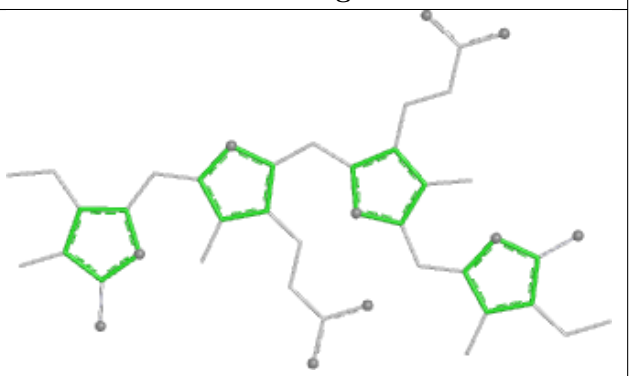
Bond lengths



Bond angles

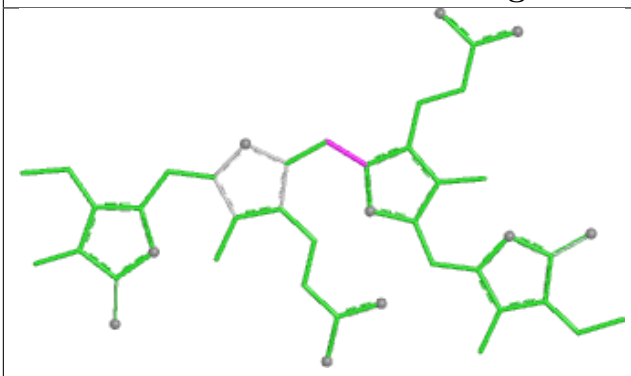


Torsions

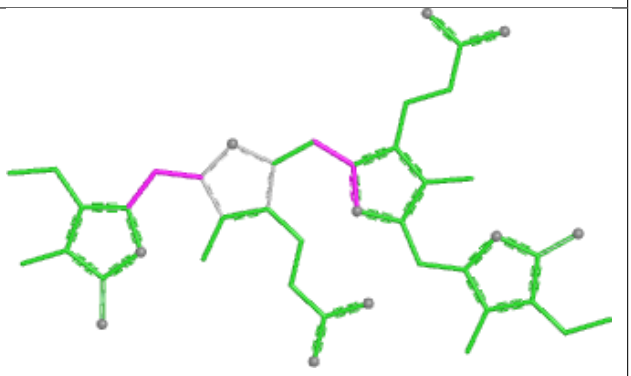


Rings

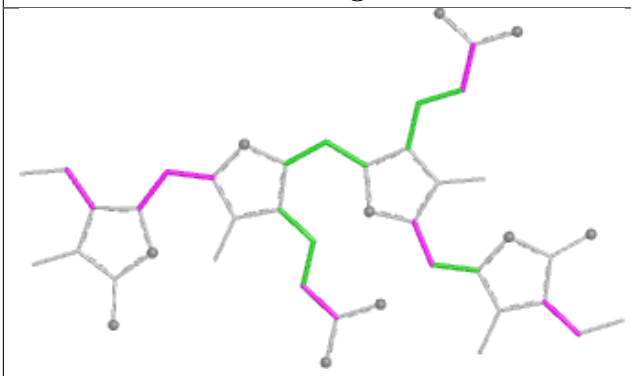
Ligand CYC AR 200



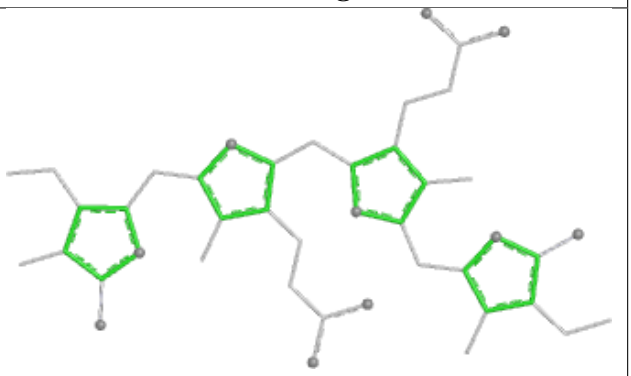
Bond lengths



Bond angles

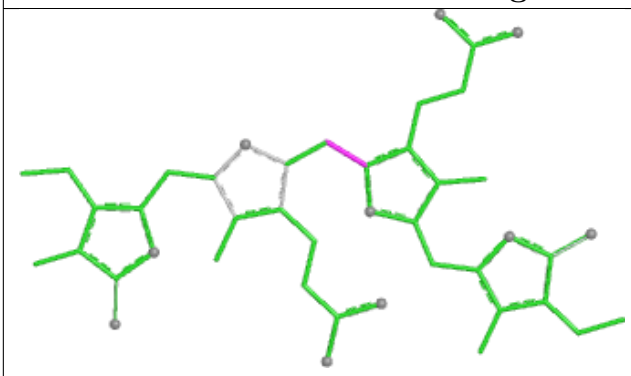


Torsions

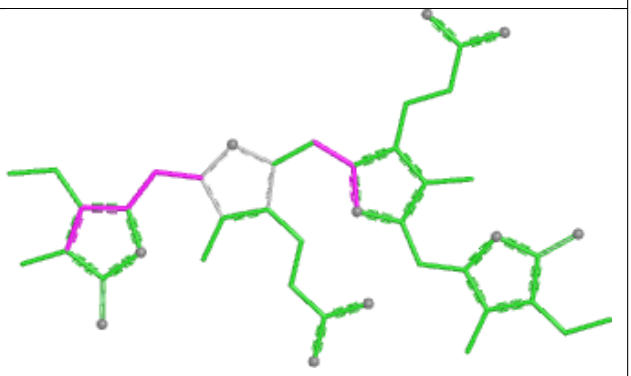


Rings

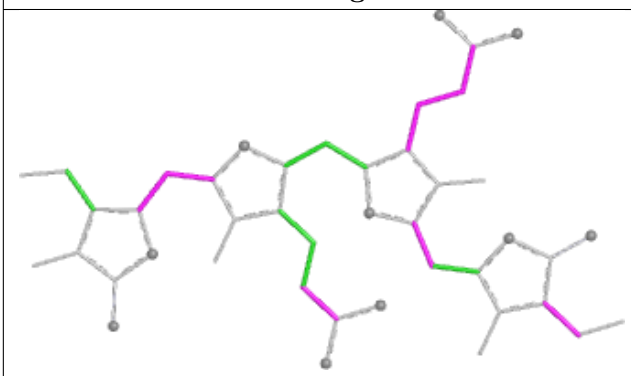
Ligand CYC BT 200



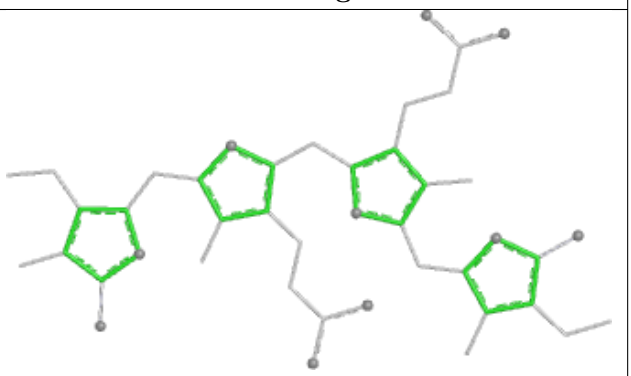
Bond lengths



Bond angles

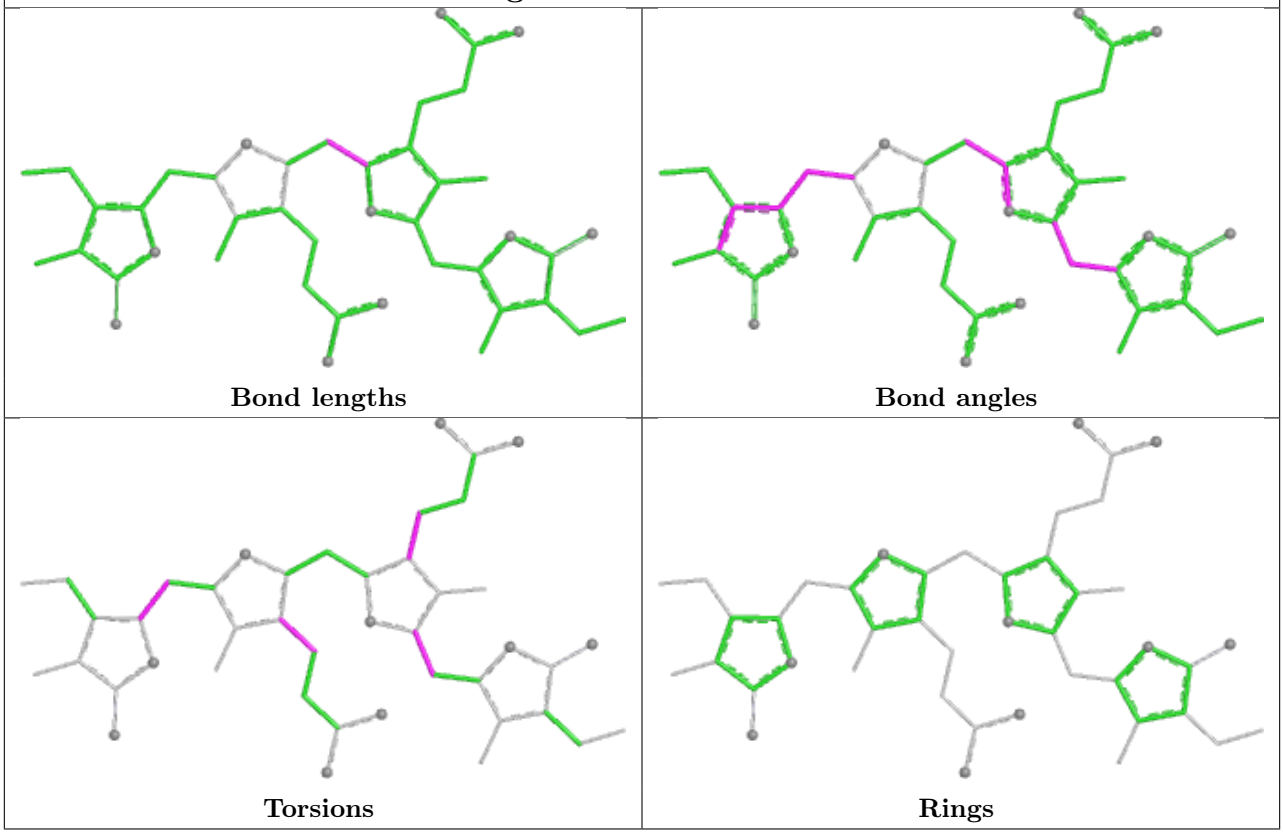


Torsions

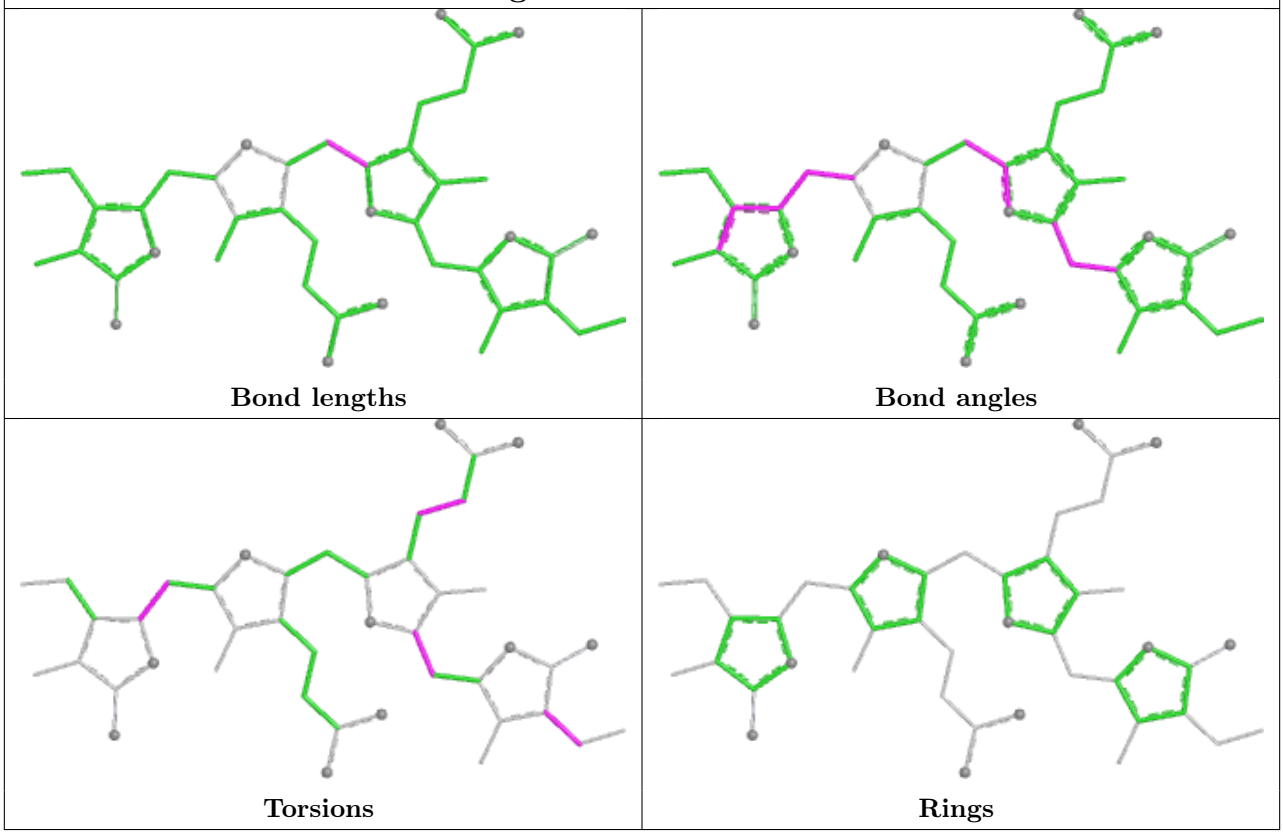


Rings

Ligand CYC BM 200



Ligand CYC BN 200



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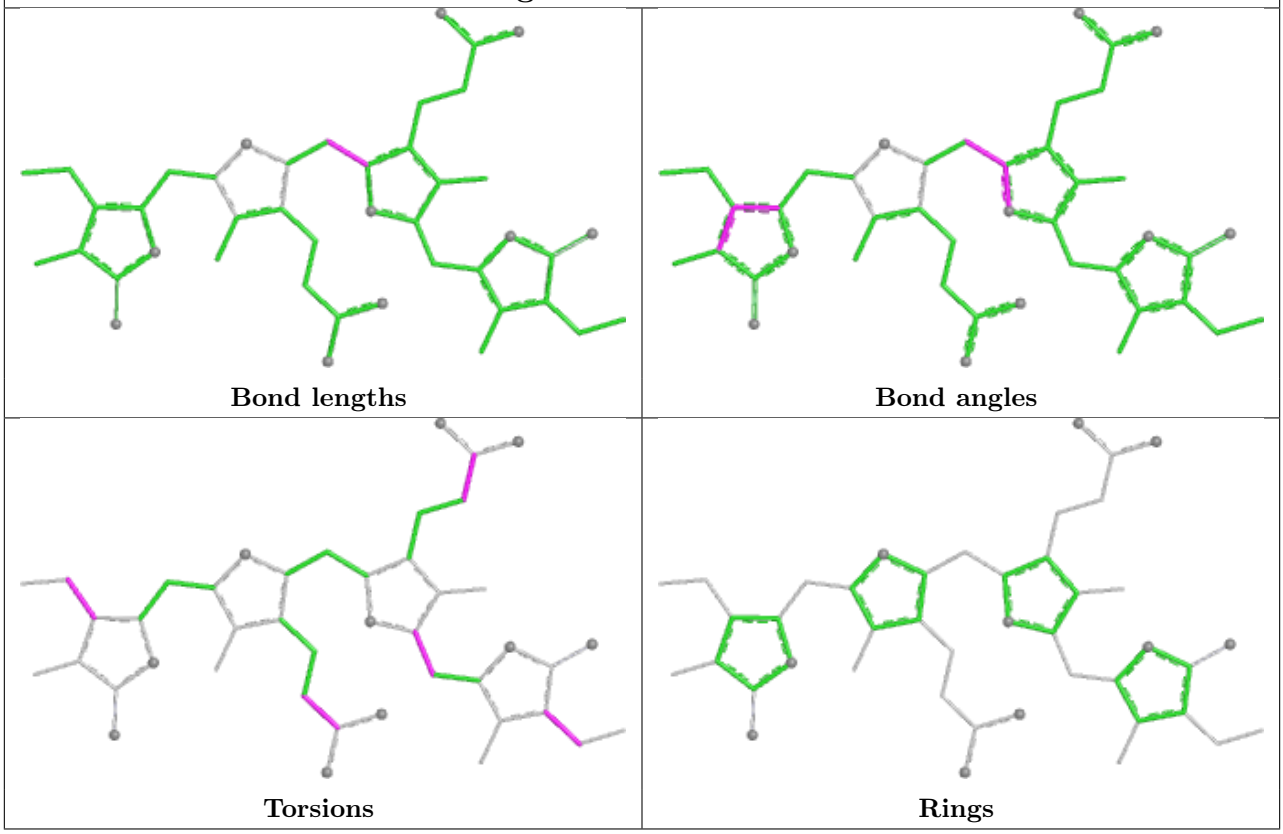
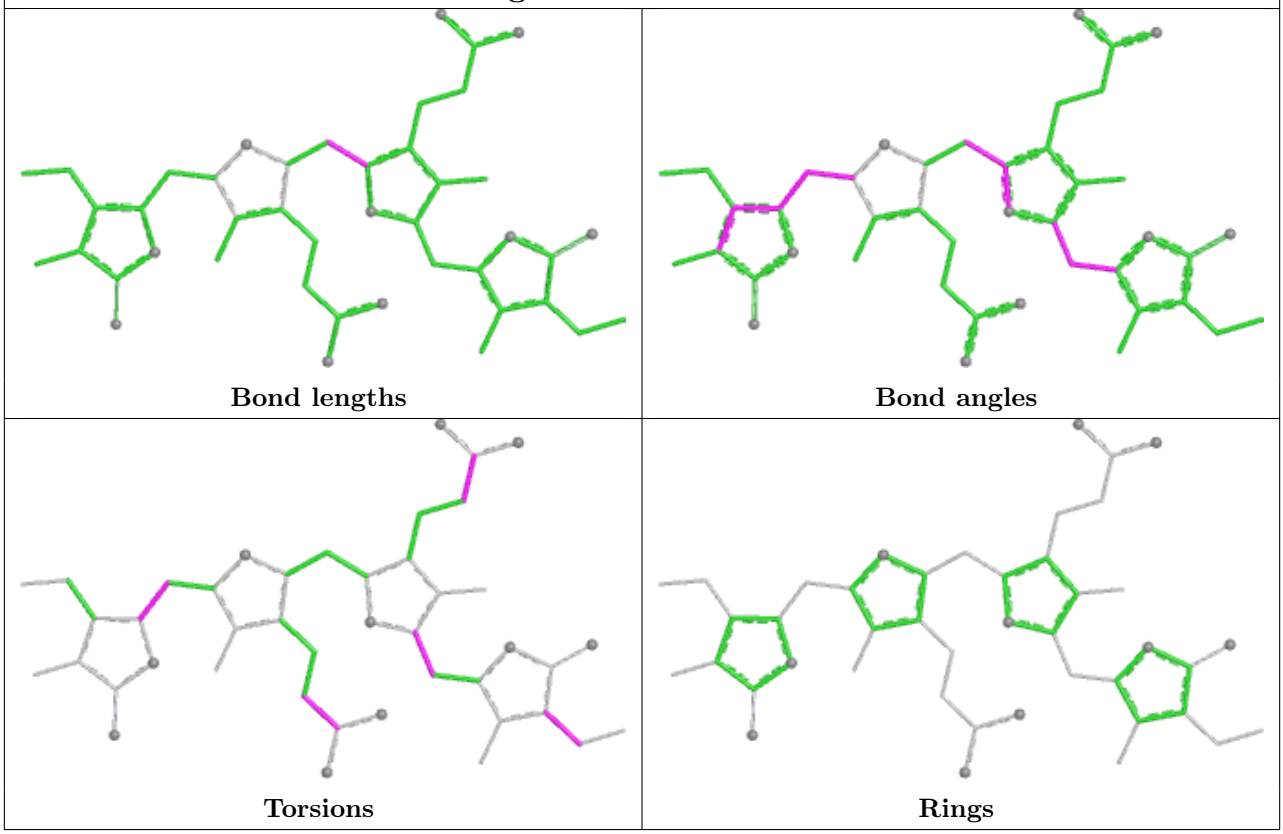
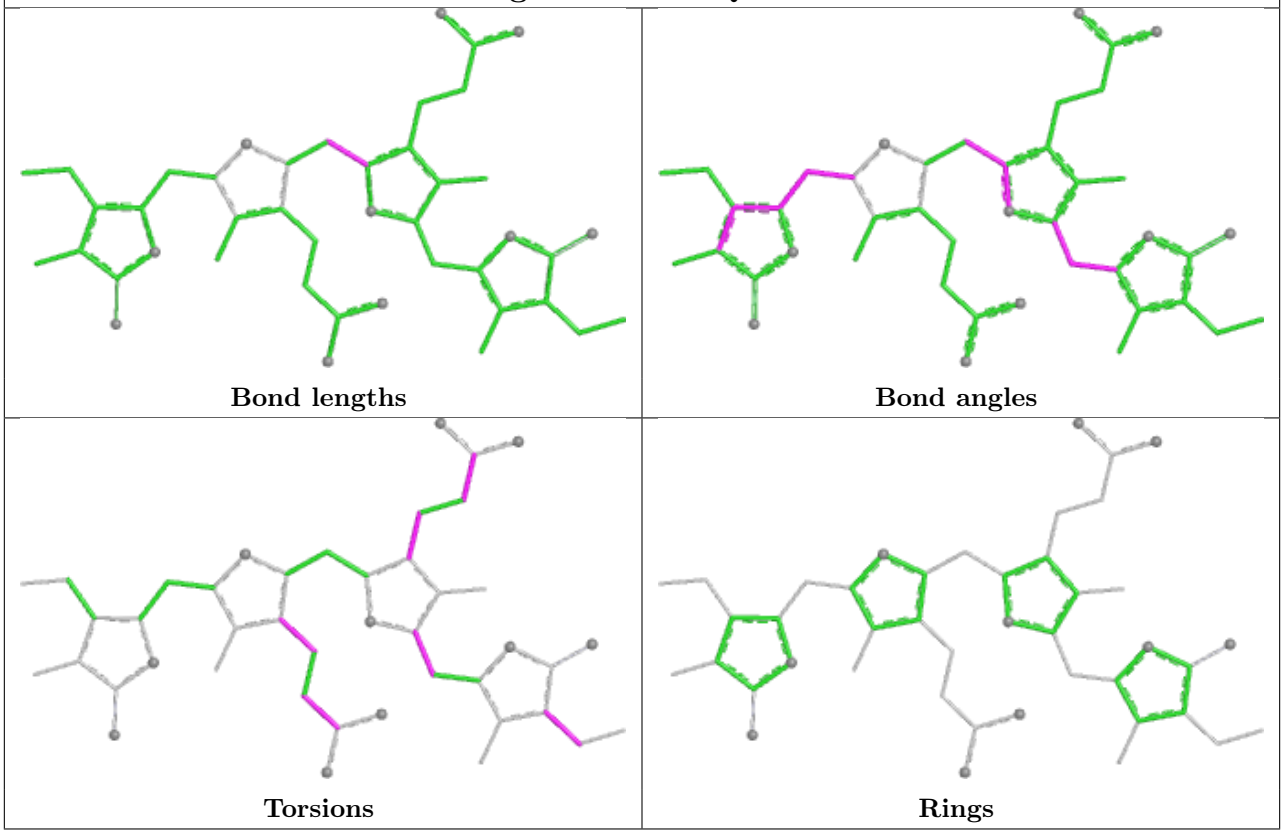


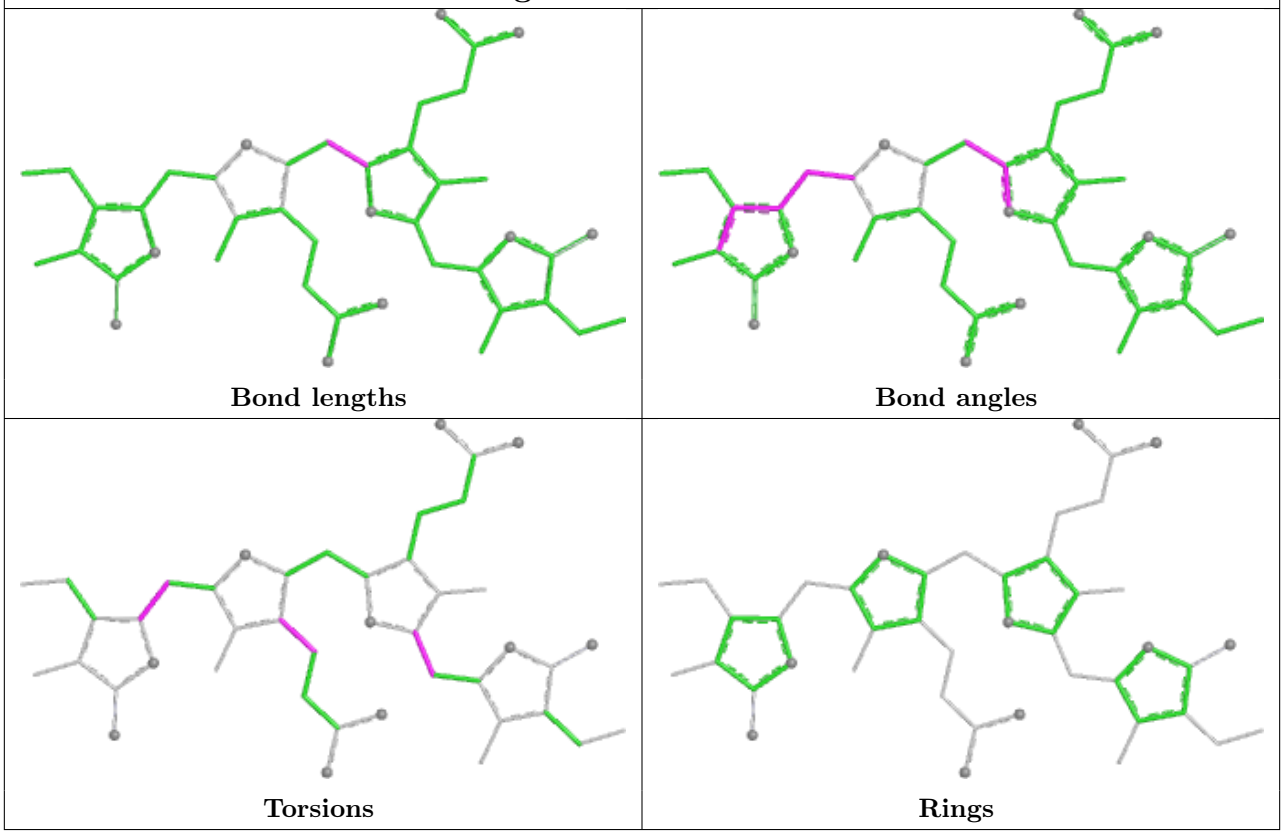
Ligand CYC AN 200



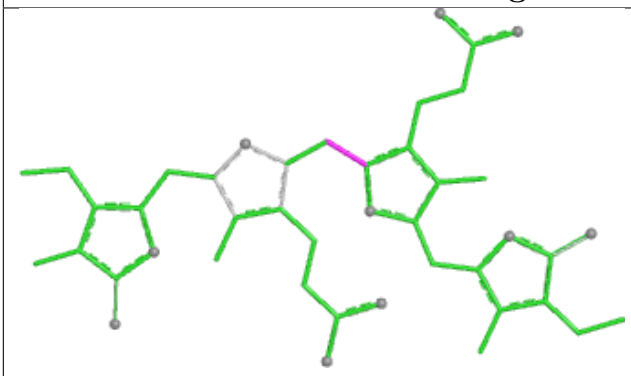
Ligand CYC AQ 200



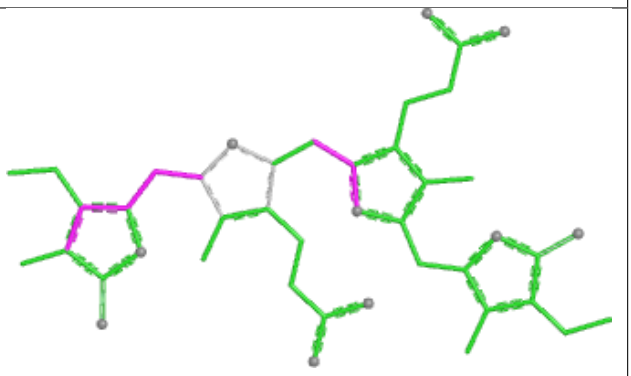
Ligand CYC BJ 200



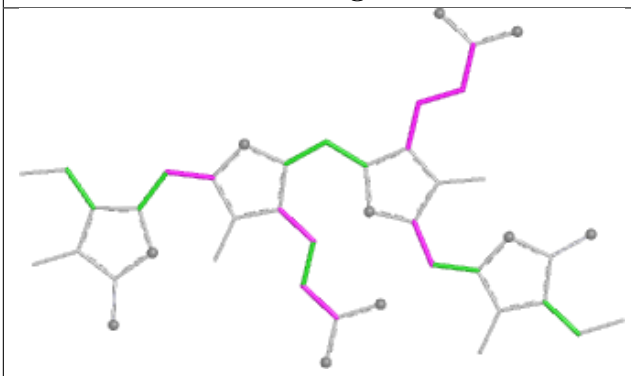
Ligand CYC CY 200



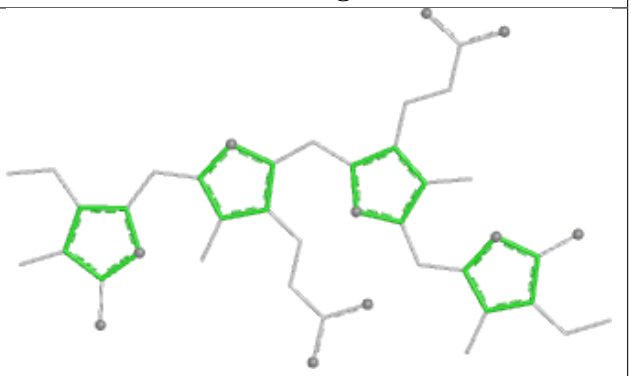
Bond lengths



Bond angles

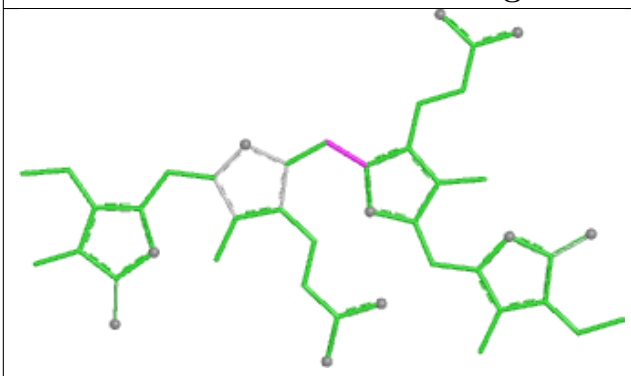


Torsions

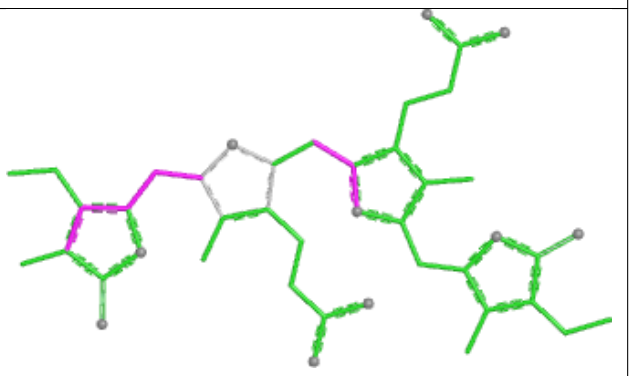


Rings

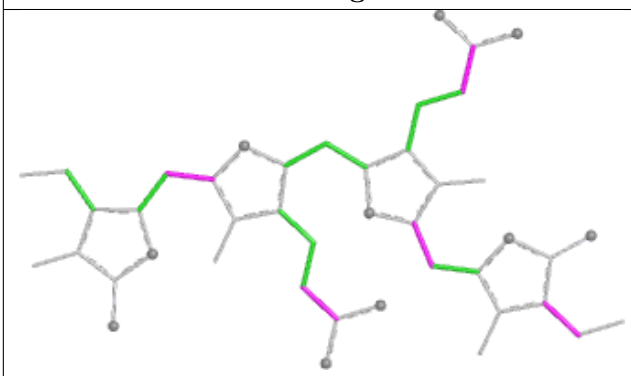
Ligand CYC BW 200



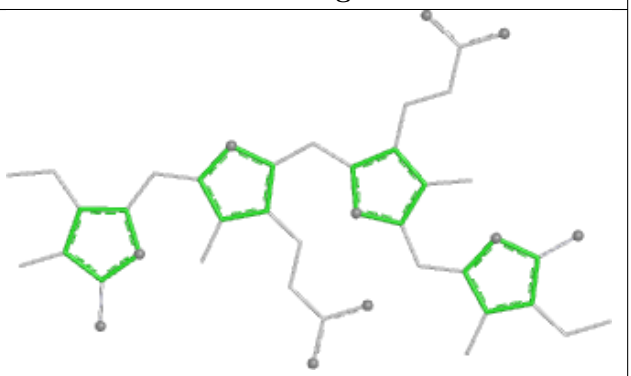
Bond lengths



Bond angles

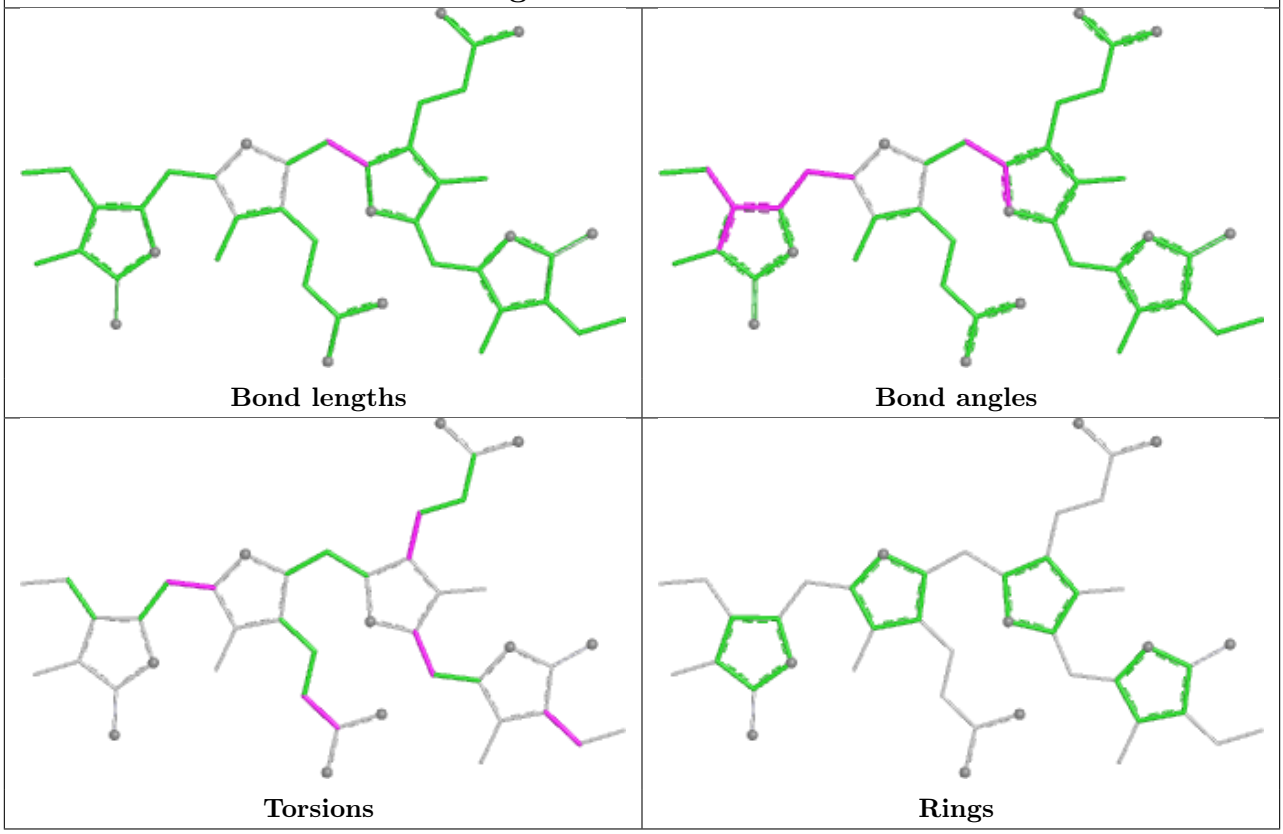


Torsions

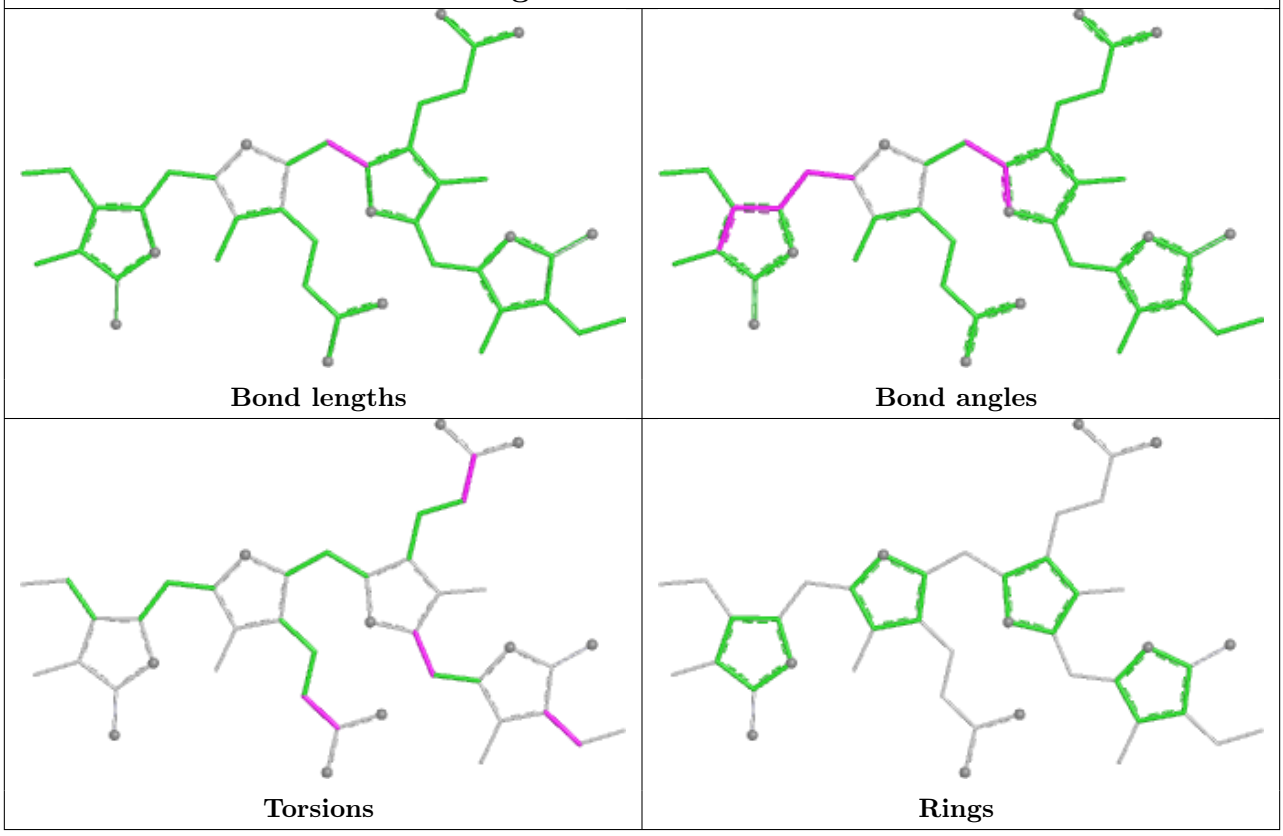


Rings

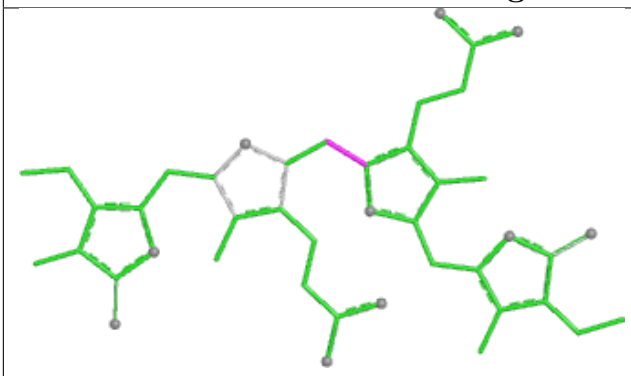
Ligand CYC CU 200



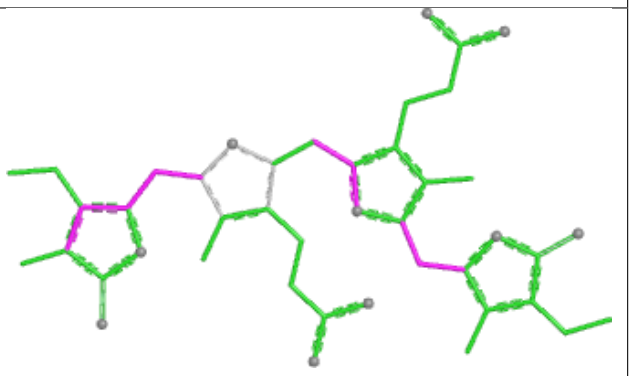
Ligand CYC AZ 200



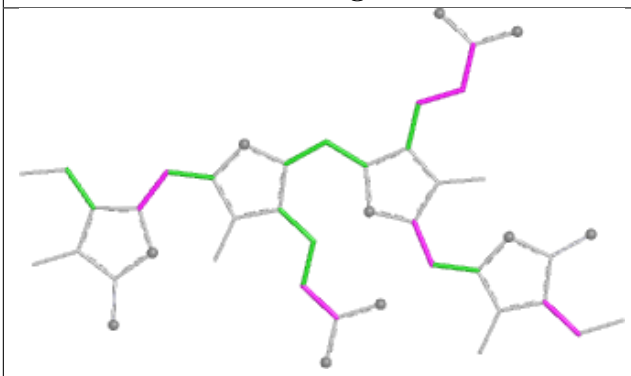
Ligand CYC AH 200



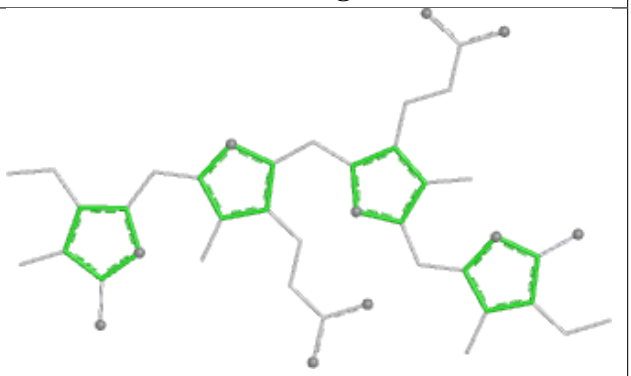
Bond lengths



Bond angles

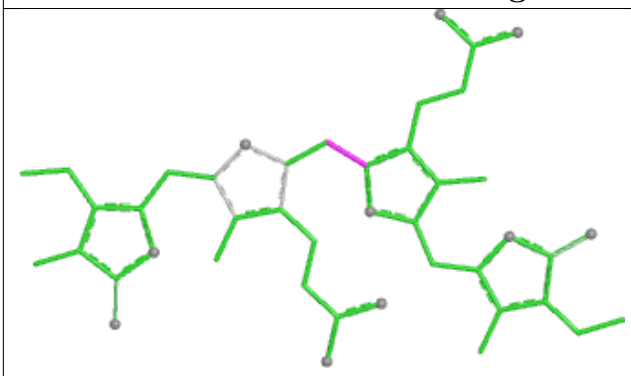


Torsions

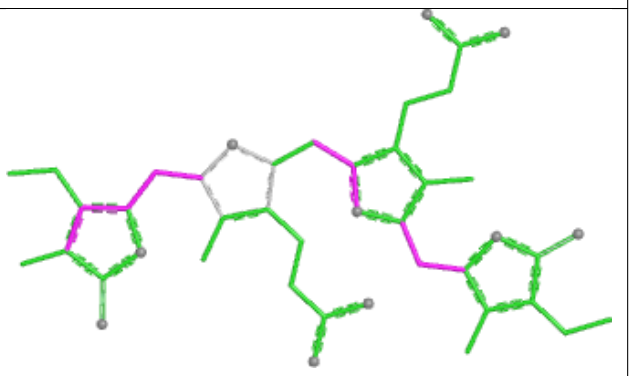


Rings

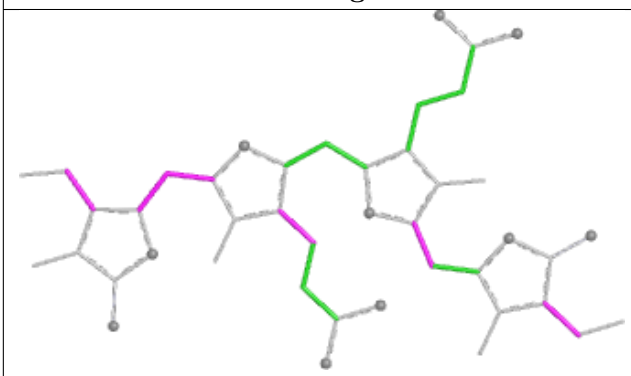
Ligand CYC BD 901



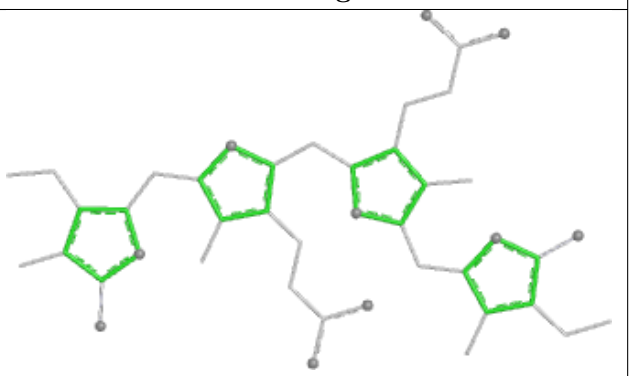
Bond lengths



Bond angles

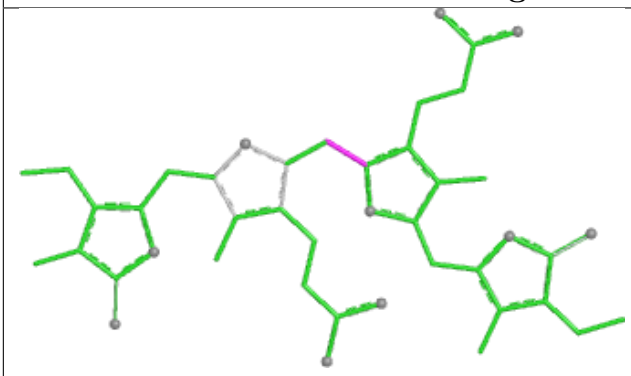


Torsions

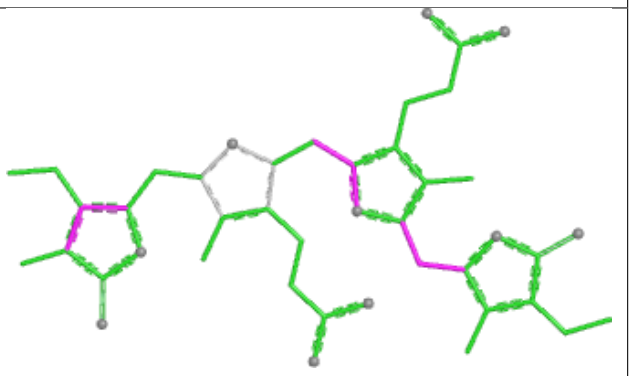


Rings

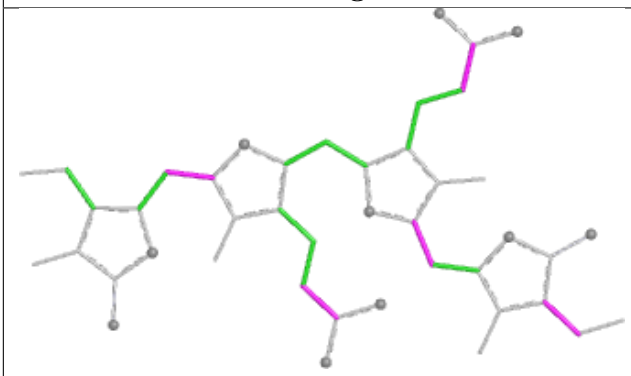
Ligand CYC BD 902



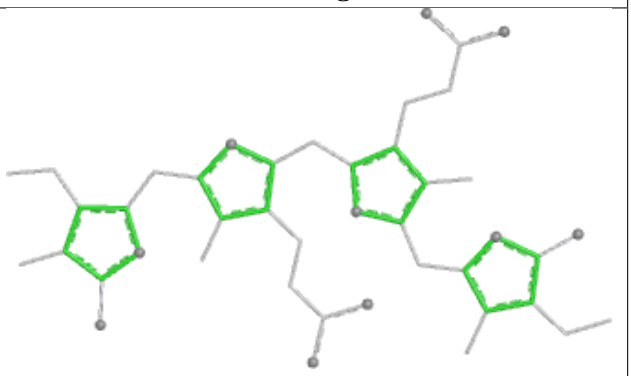
Bond lengths



Bond angles

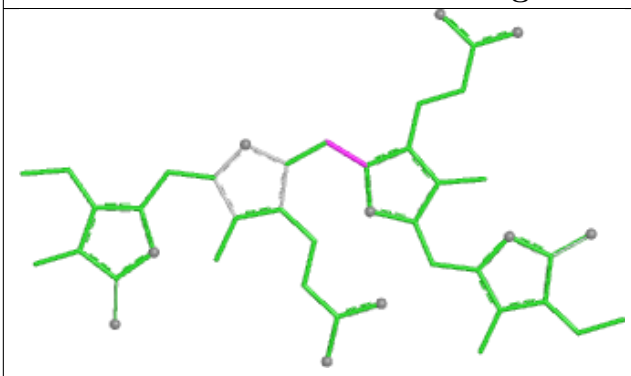


Torsions

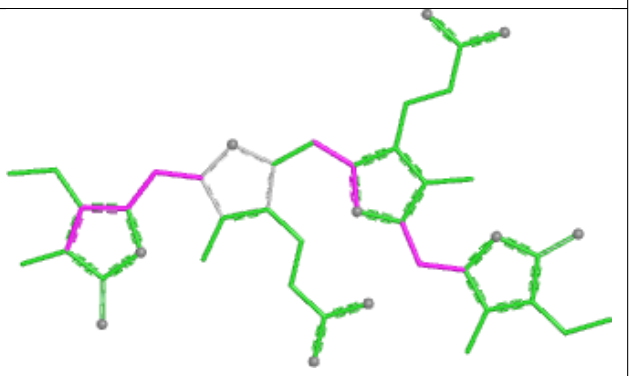


Rings

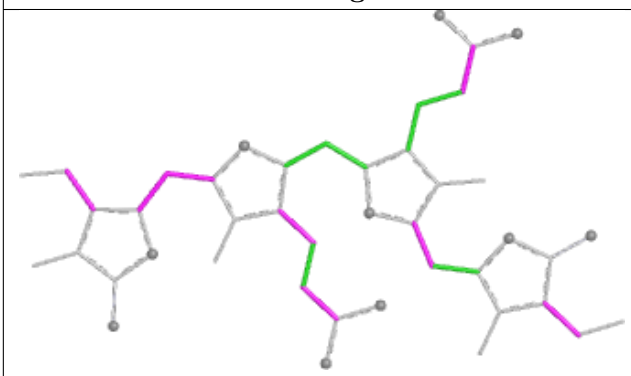
Ligand CYC BL 200



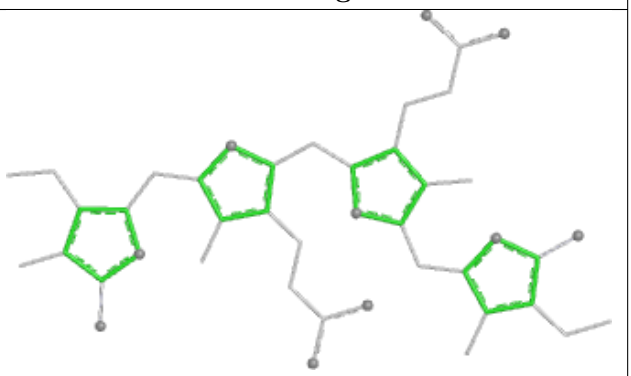
Bond lengths



Bond angles

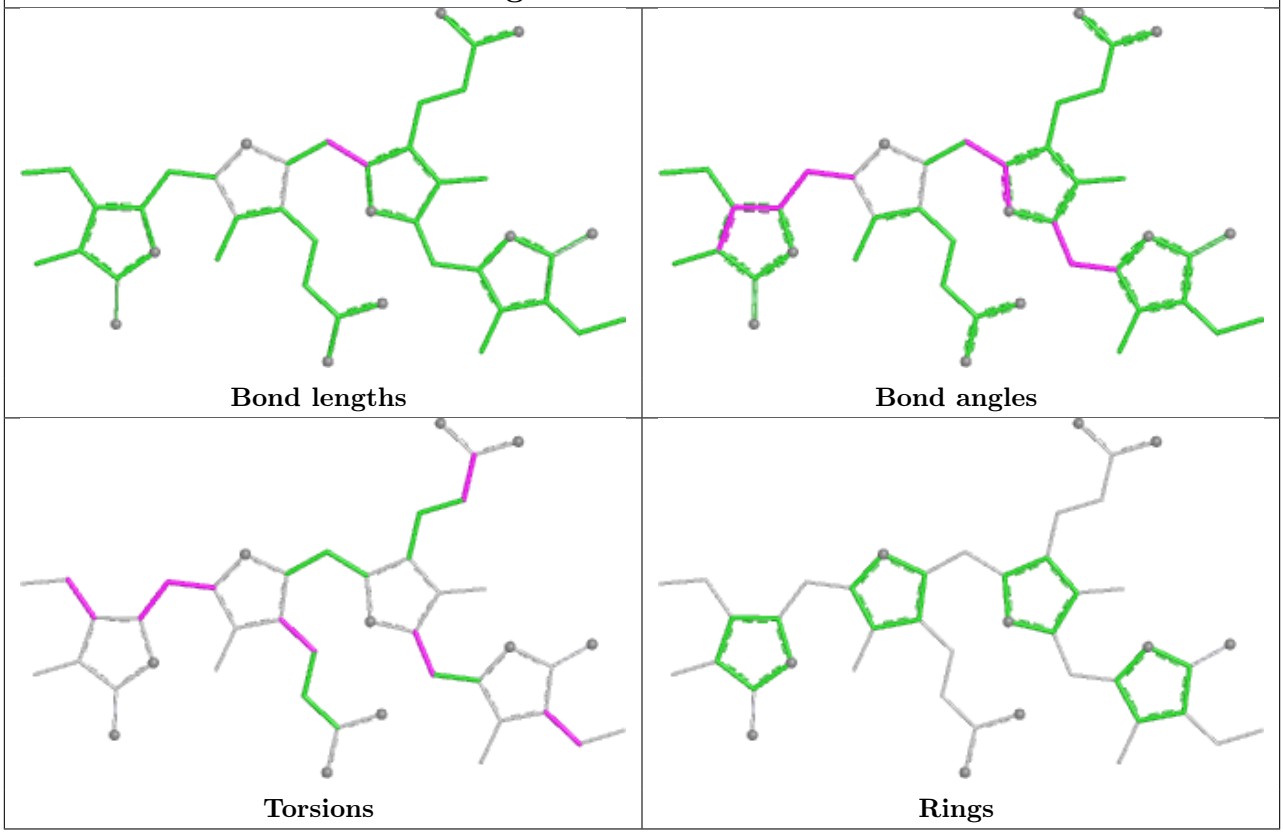


Torsions

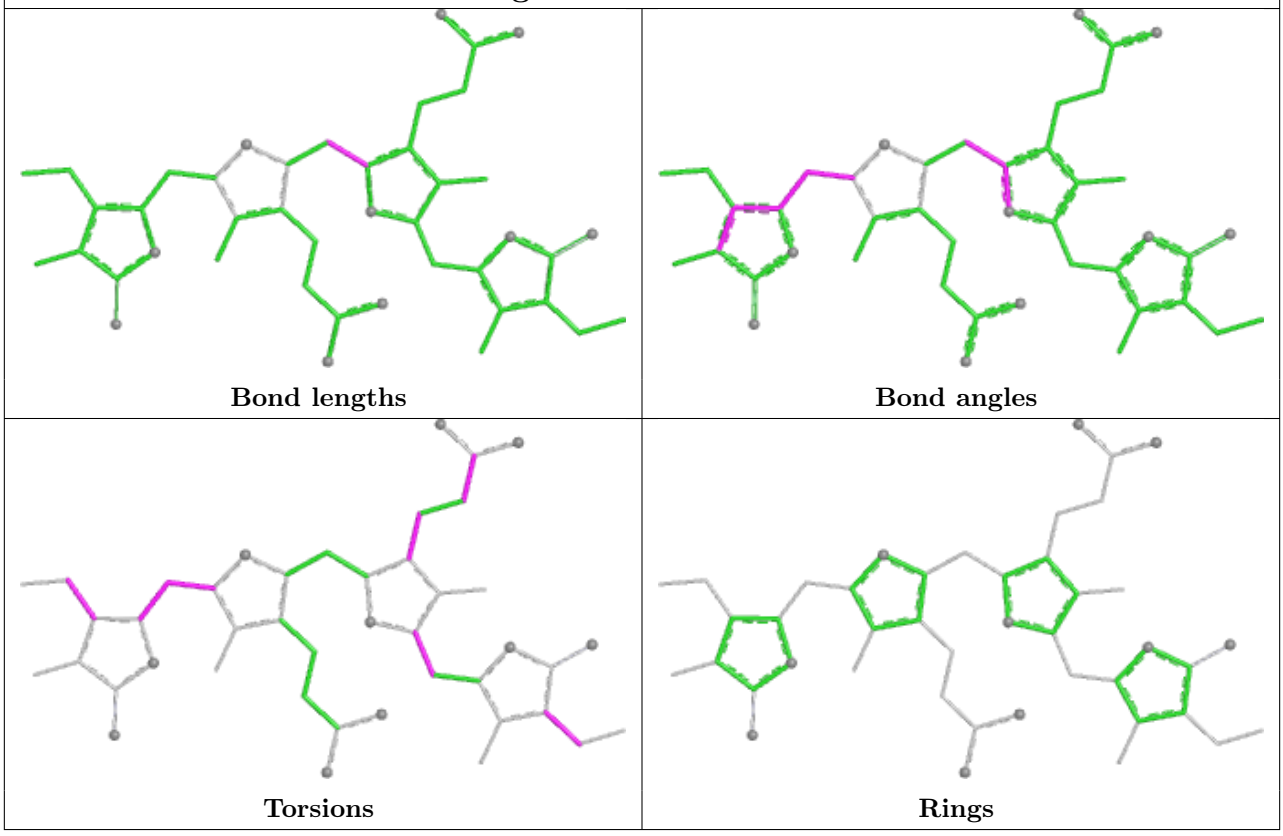


Rings

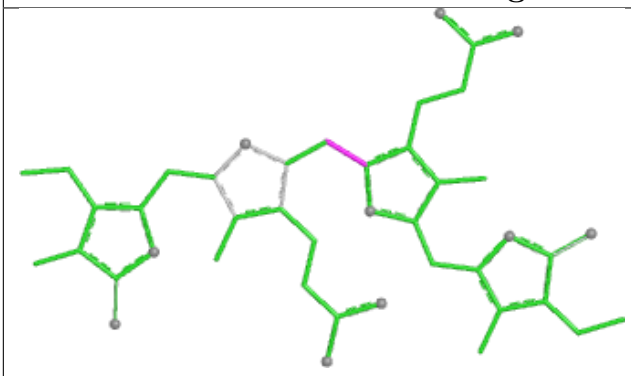
Ligand CYC CM 901



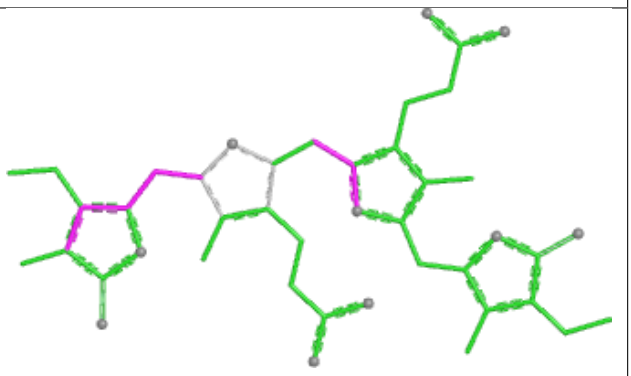
Ligand CYC CZ 200



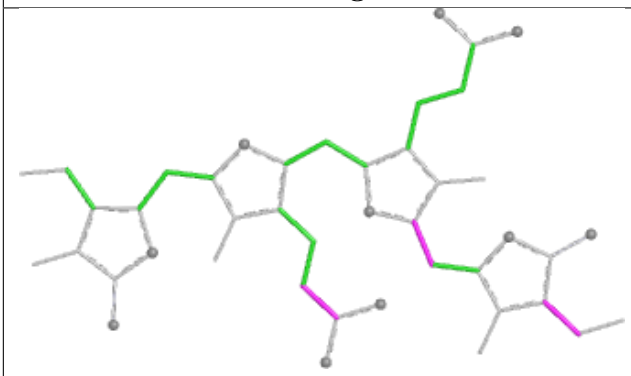
Ligand CYC DD 200



Bond lengths



Bond angles



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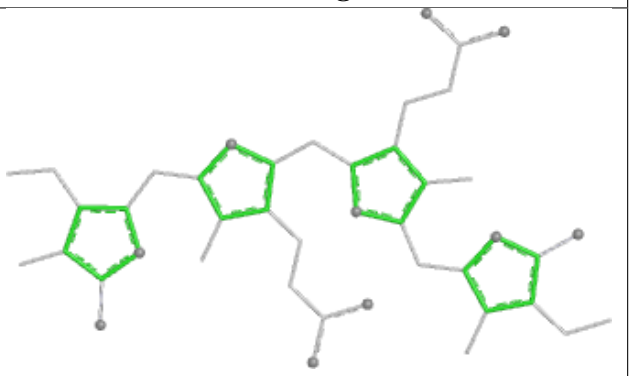
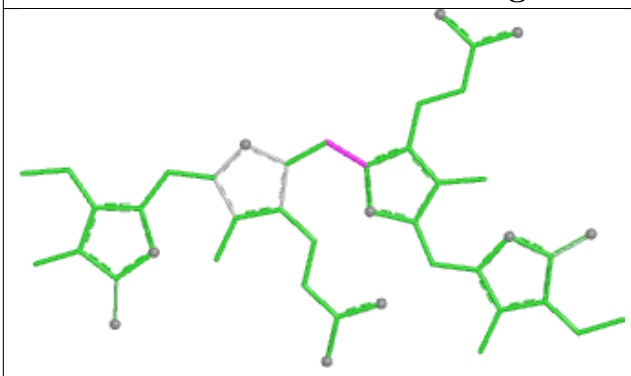
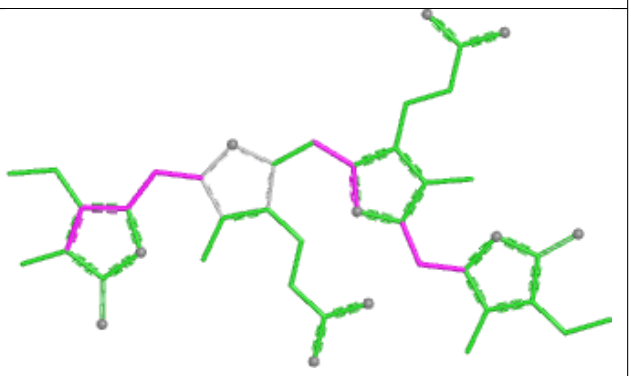


Rings

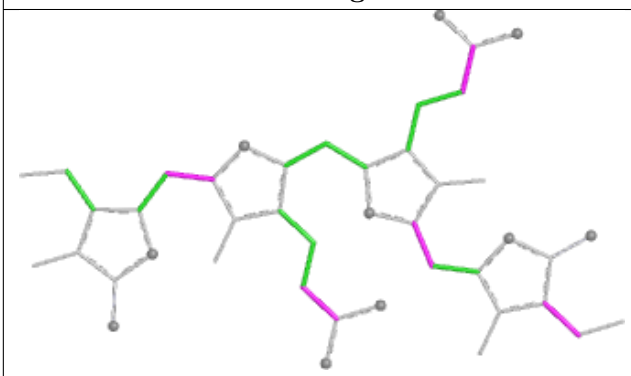
Ligand CYC CR 200



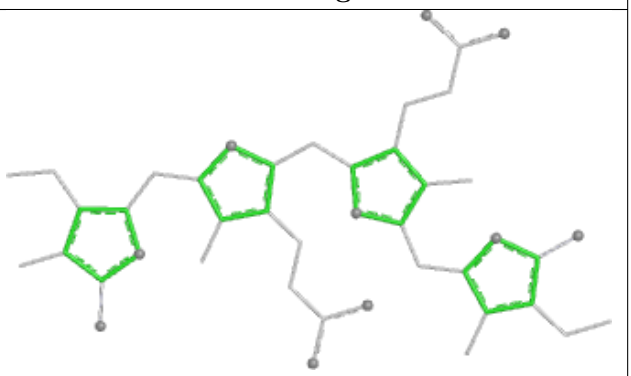
Bond lengths



Bond angles

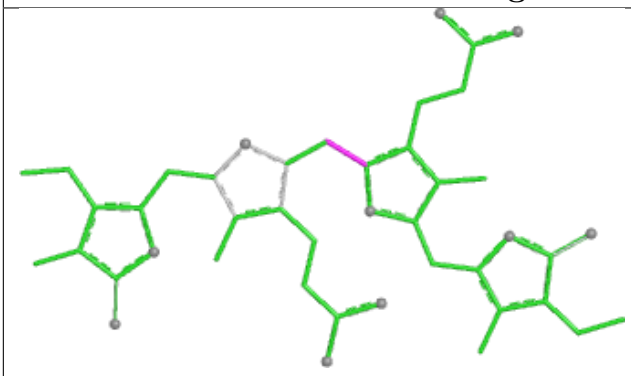


Torsions

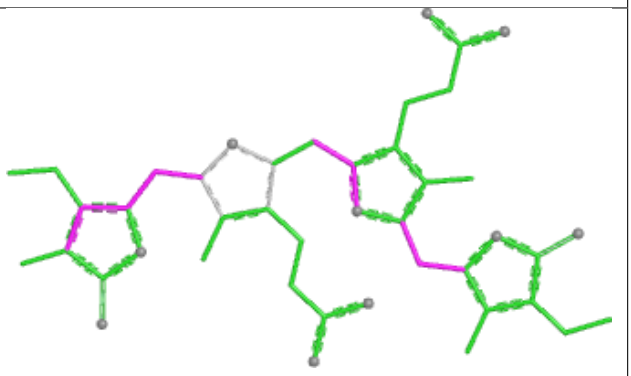


Rings

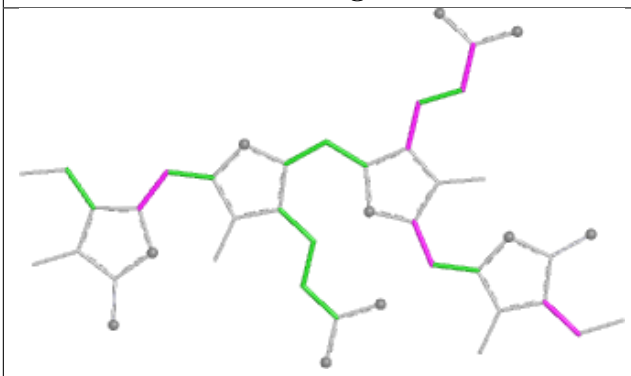
Ligand CYC AX 200



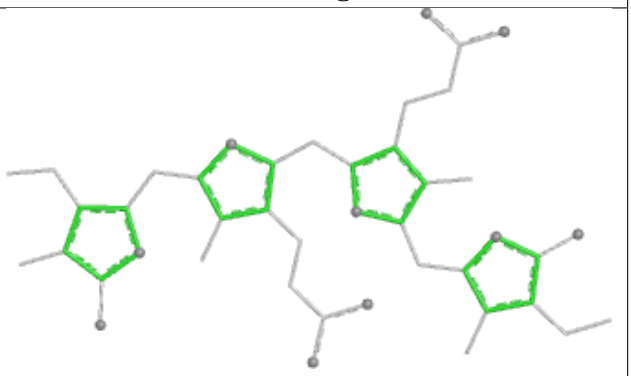
Bond lengths



Bond angles

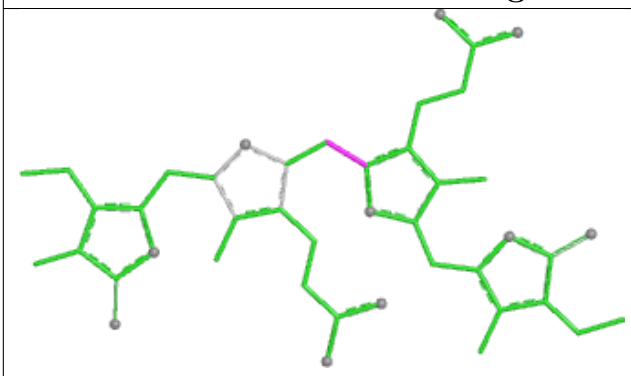


Torsions

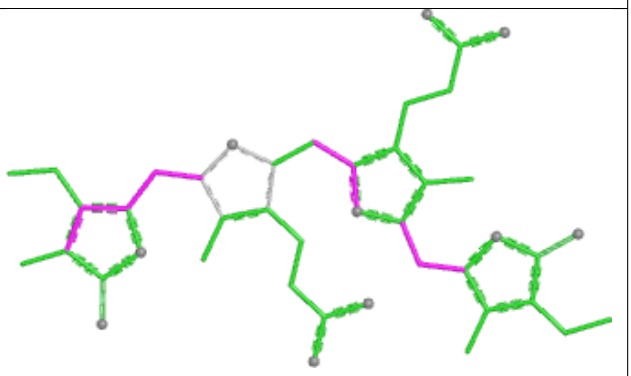


Rings

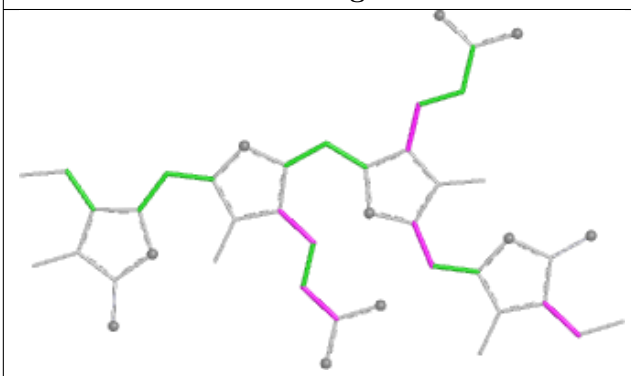
Ligand CYC AK 200



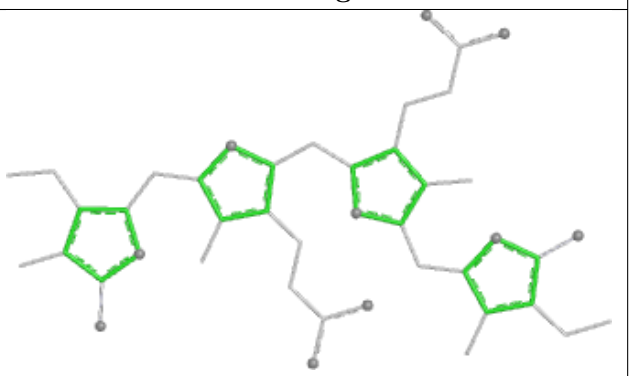
Bond lengths



Bond angles

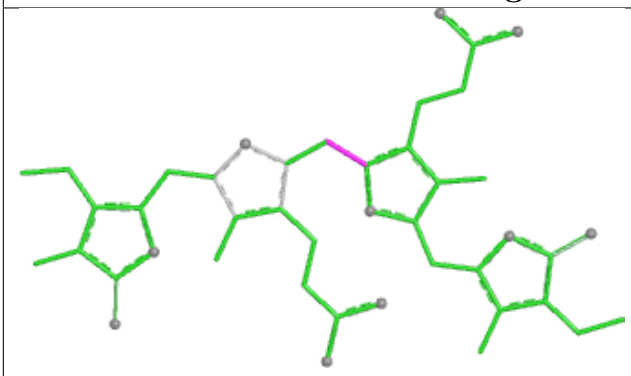


Torsions

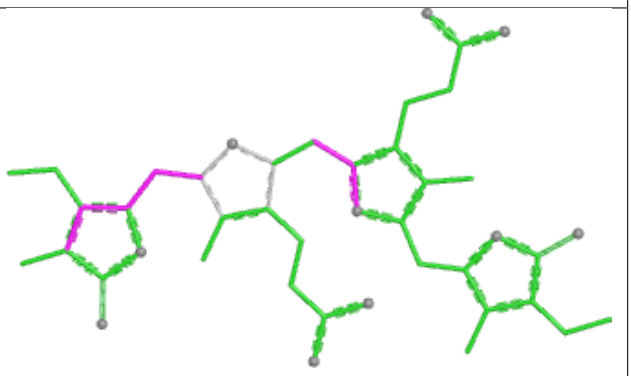


Rings

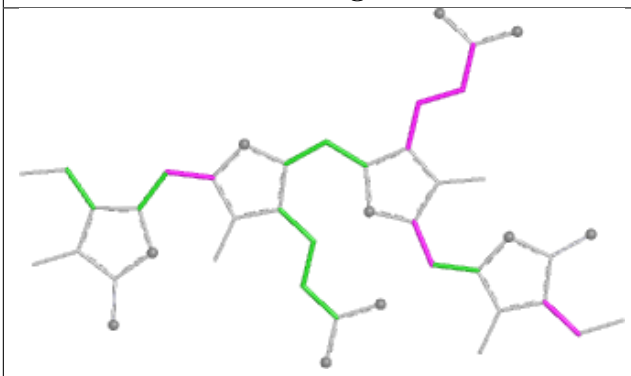
Ligand CYC AW 200



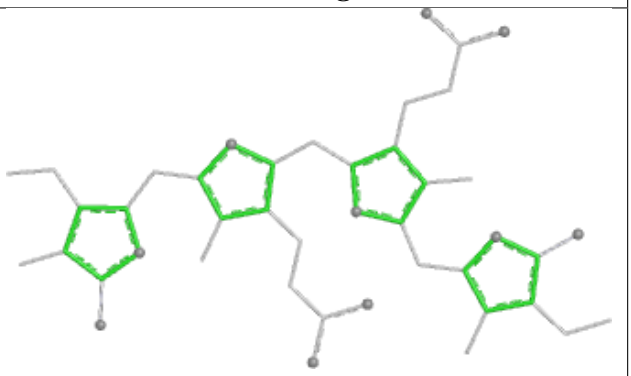
Bond lengths



Bond angles

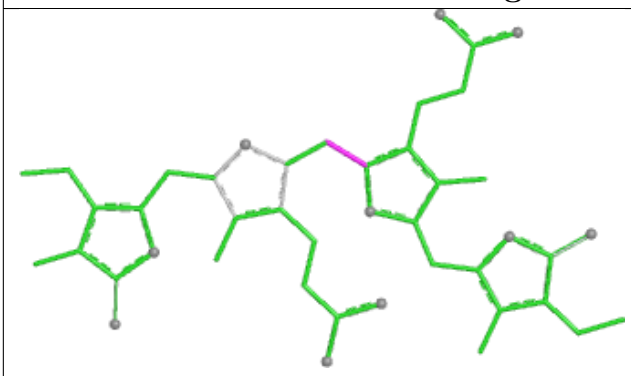


Torsions

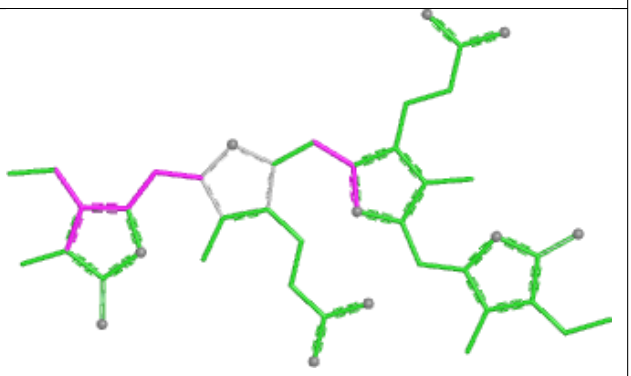


Rings

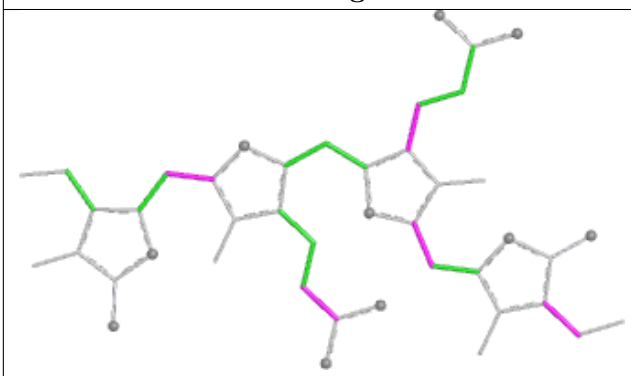
Ligand CYC DM 200



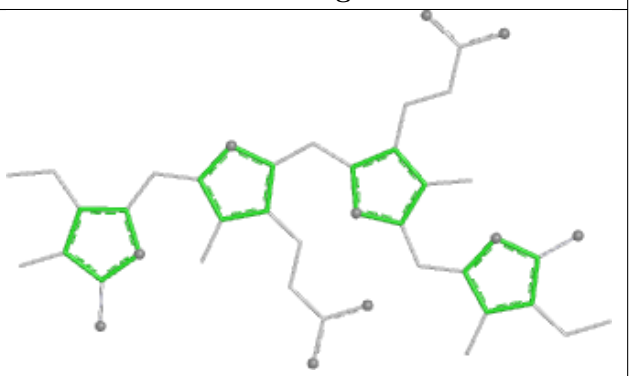
Bond lengths



Bond angles



Torsions



Rings

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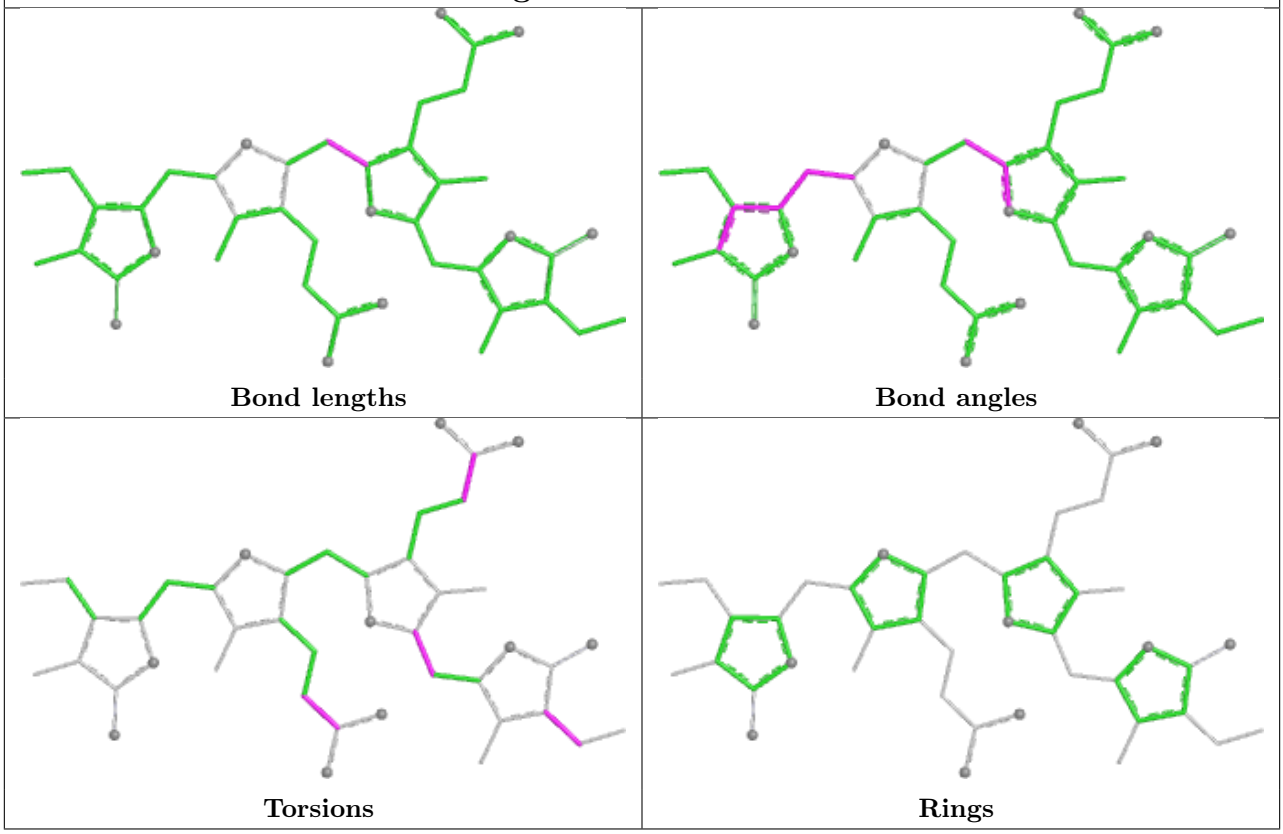
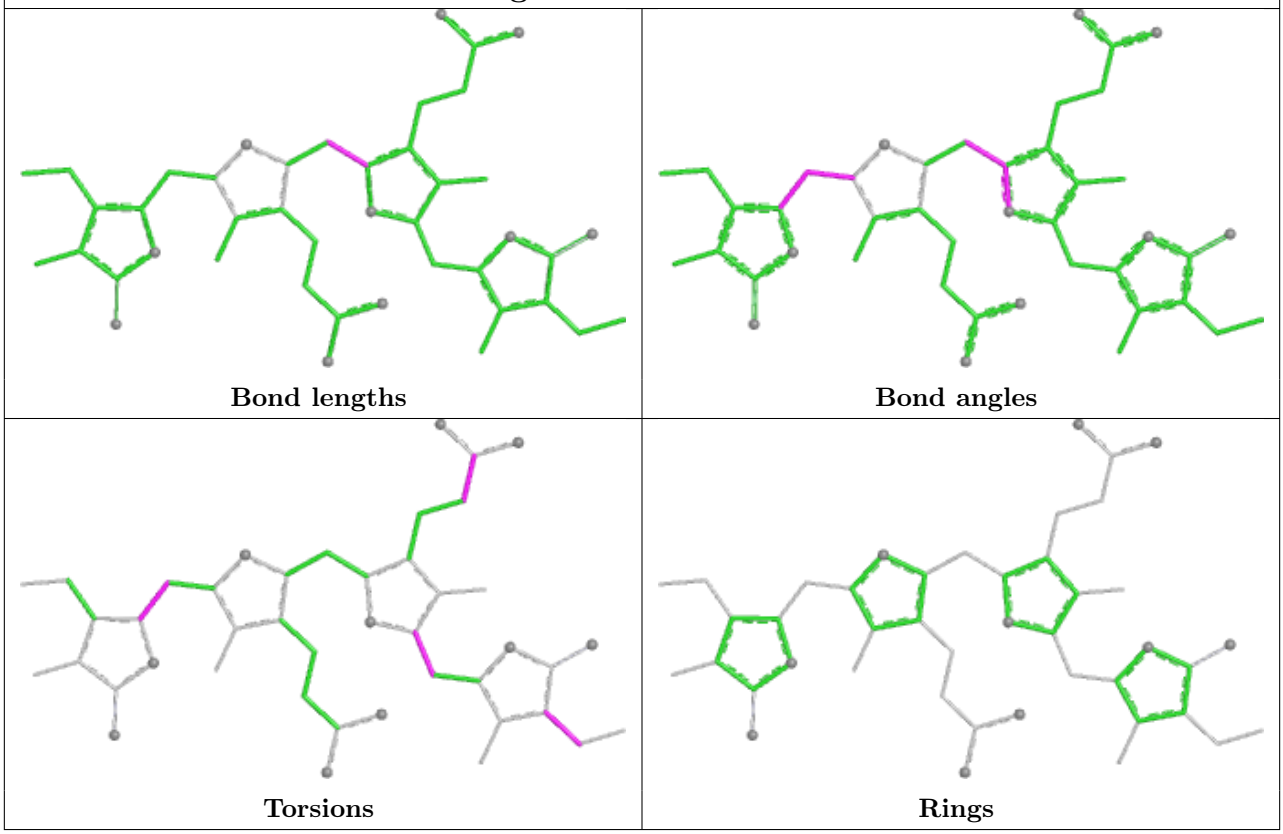
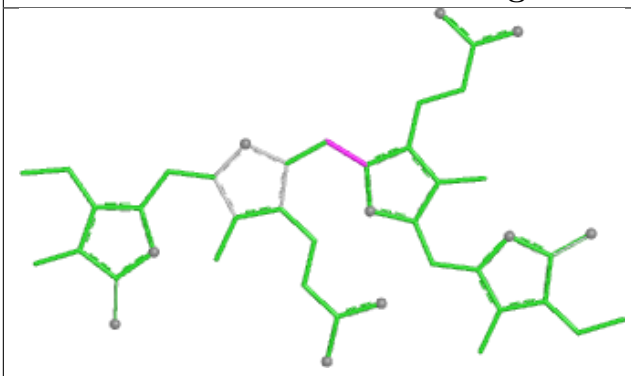


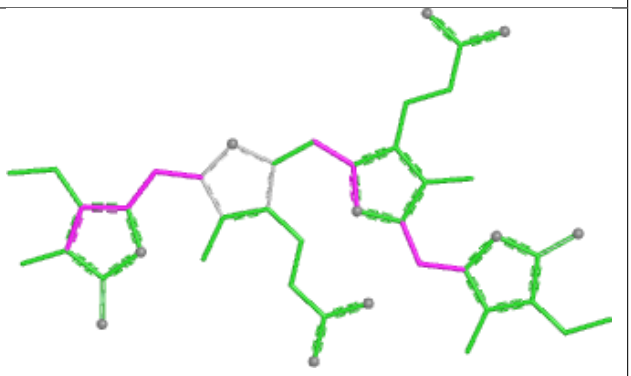
Ligand CYC AC 200



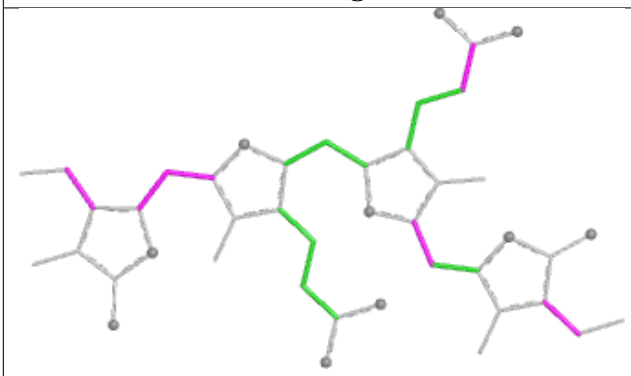
Ligand CYC DR 200



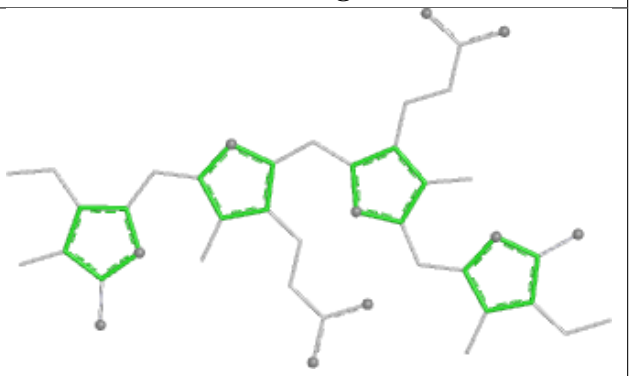
Bond lengths



Bond angles

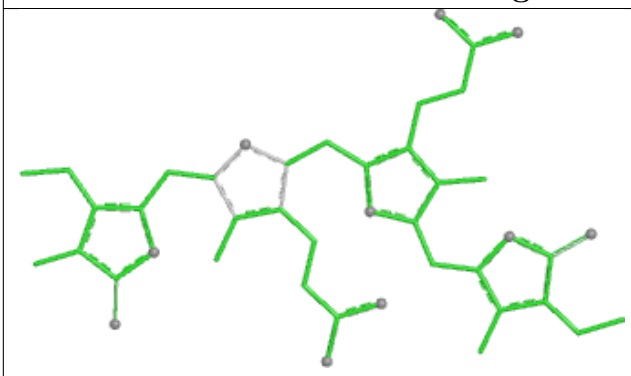


Torsions

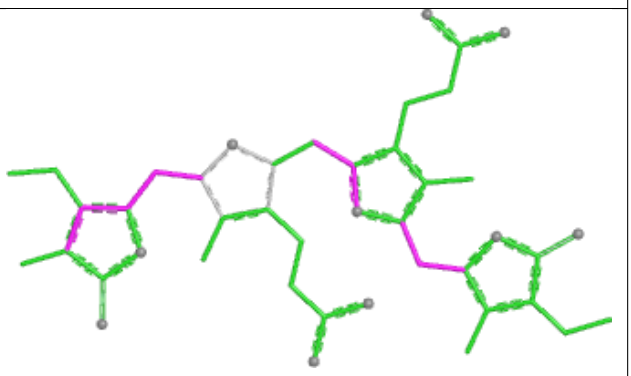


Rings

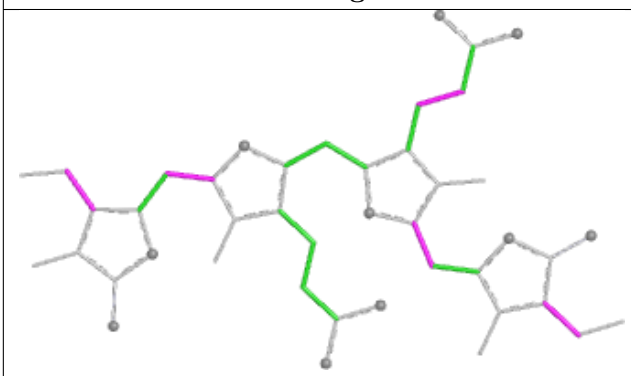
Ligand CYC BS 200



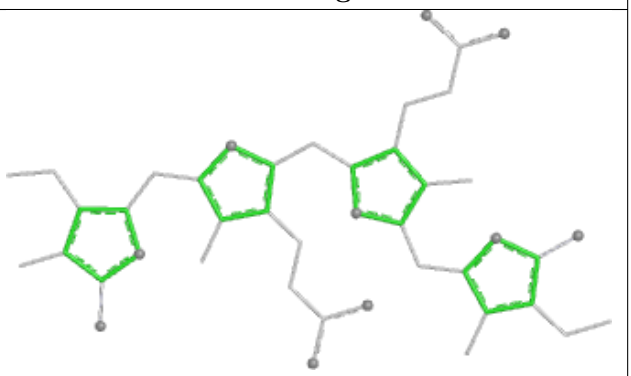
Bond lengths



Bond angles



Torsions



Rings

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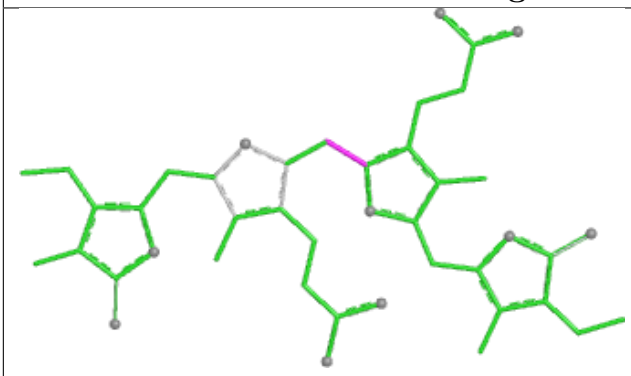
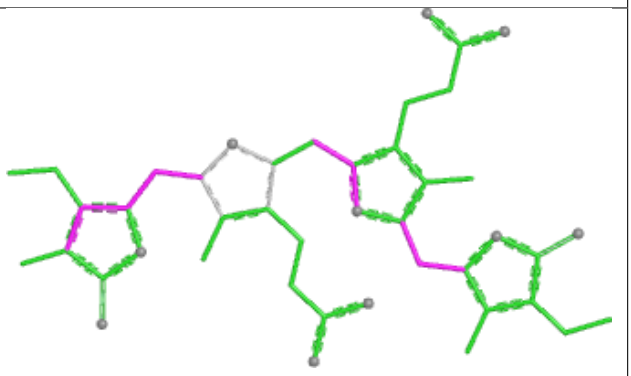
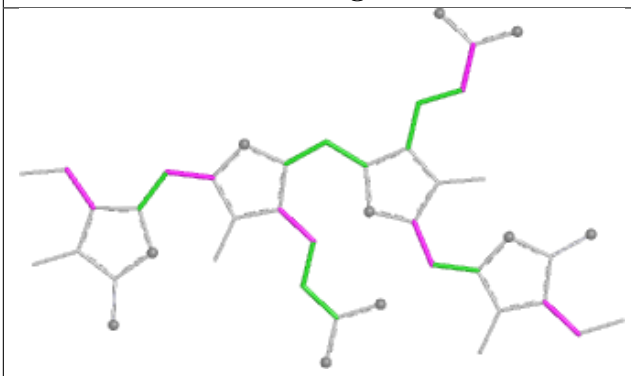


Bond lengths



Bond angles



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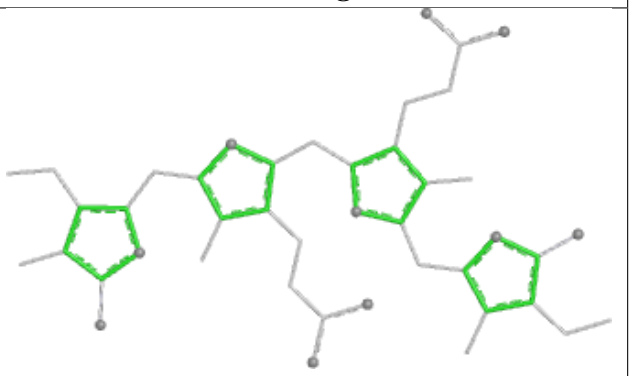
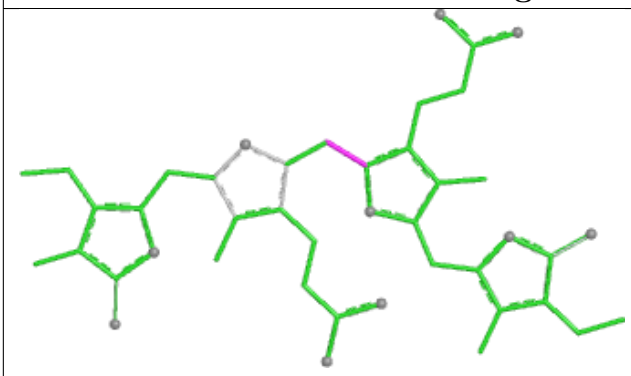
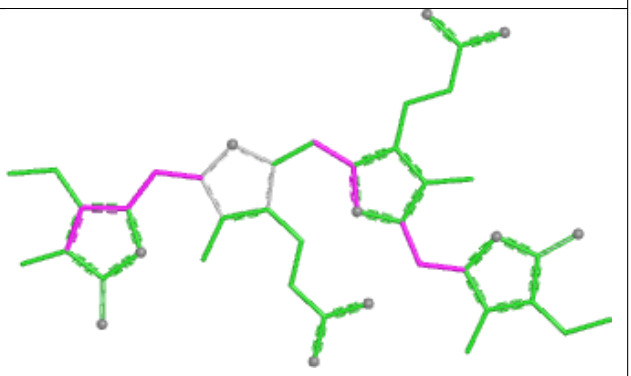


Rings

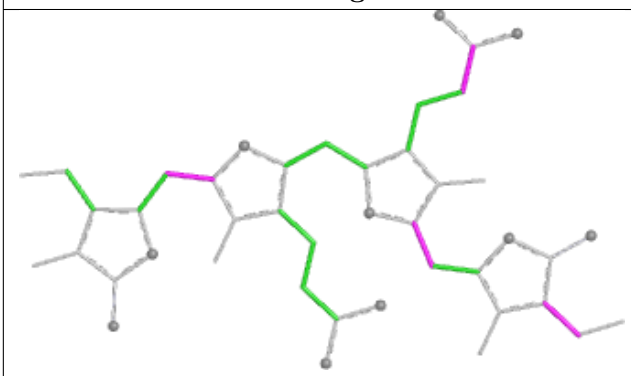
Ligand CYC AI 200



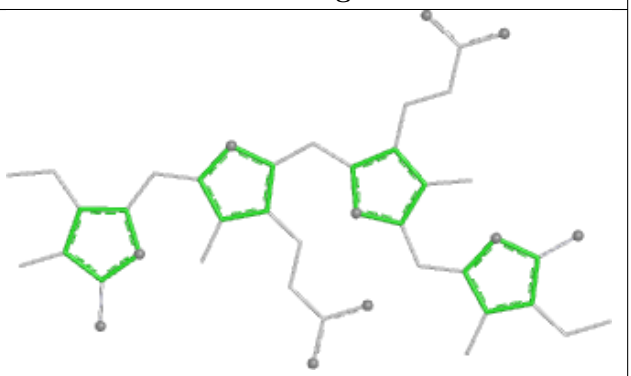
Bond lengths



Bond angles

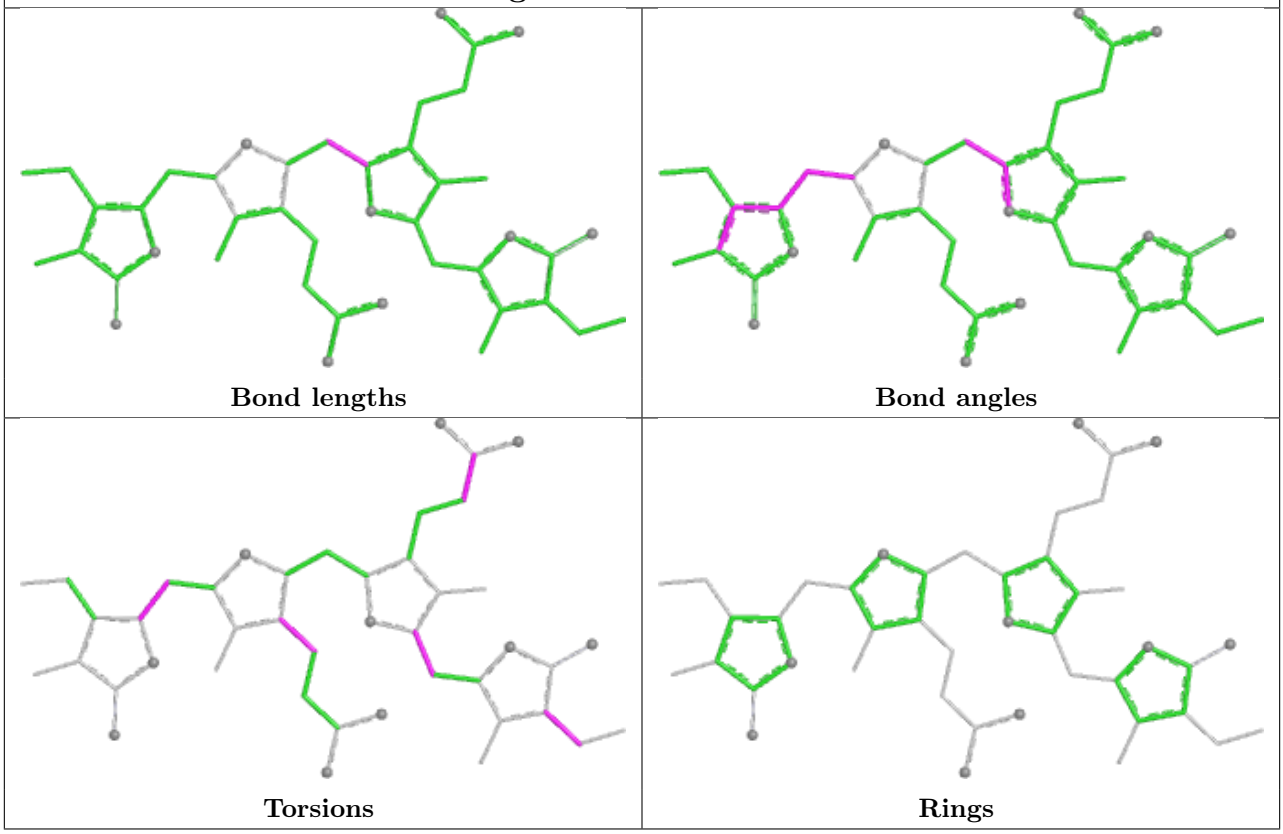


Torsions

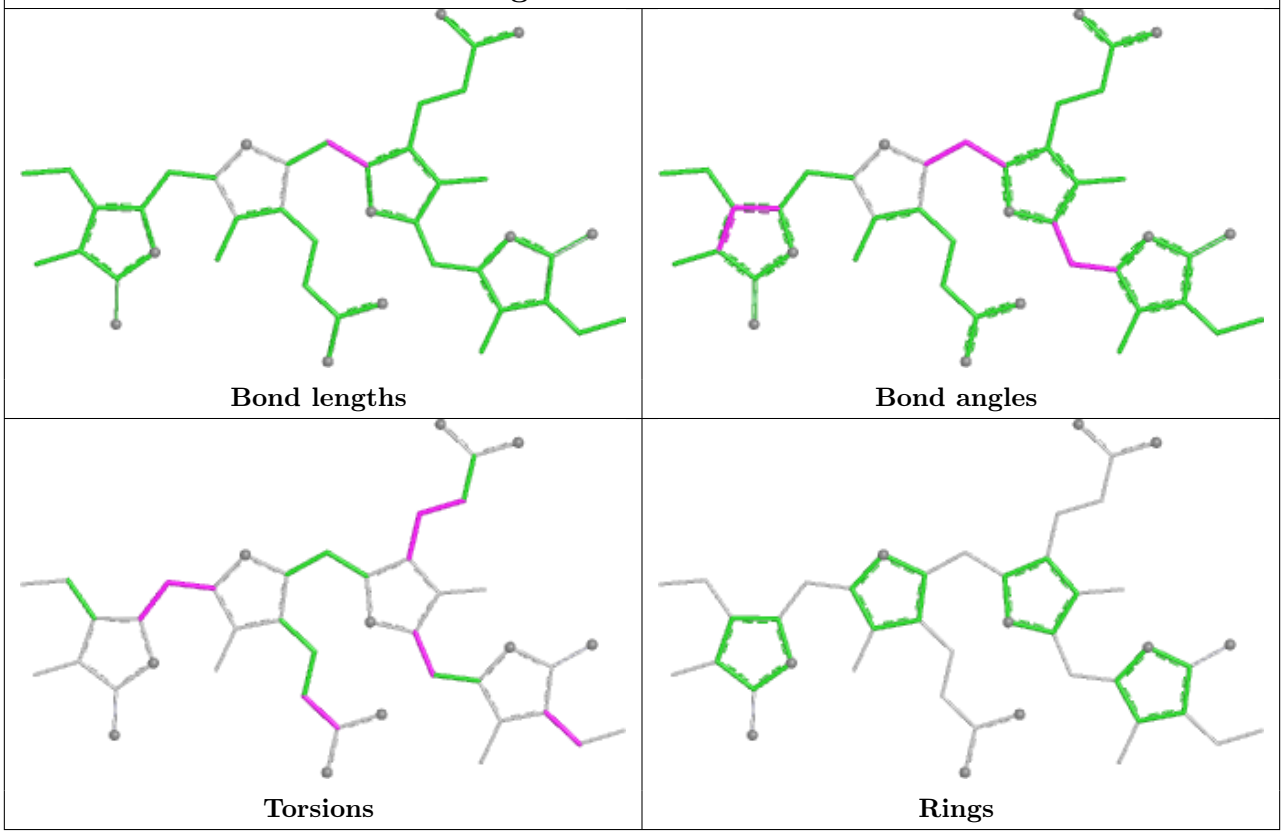


Rings

Ligand CYC CH 200



Ligand CYC CT 200



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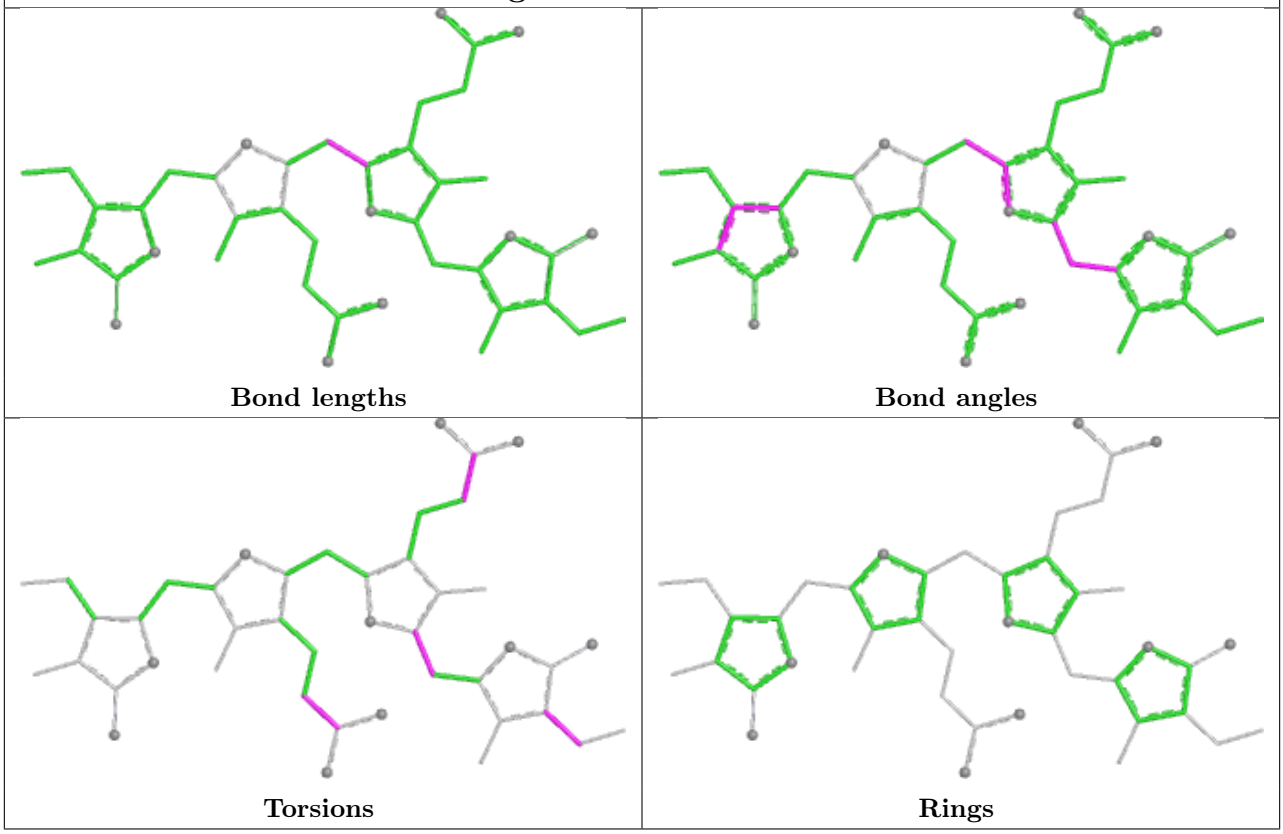

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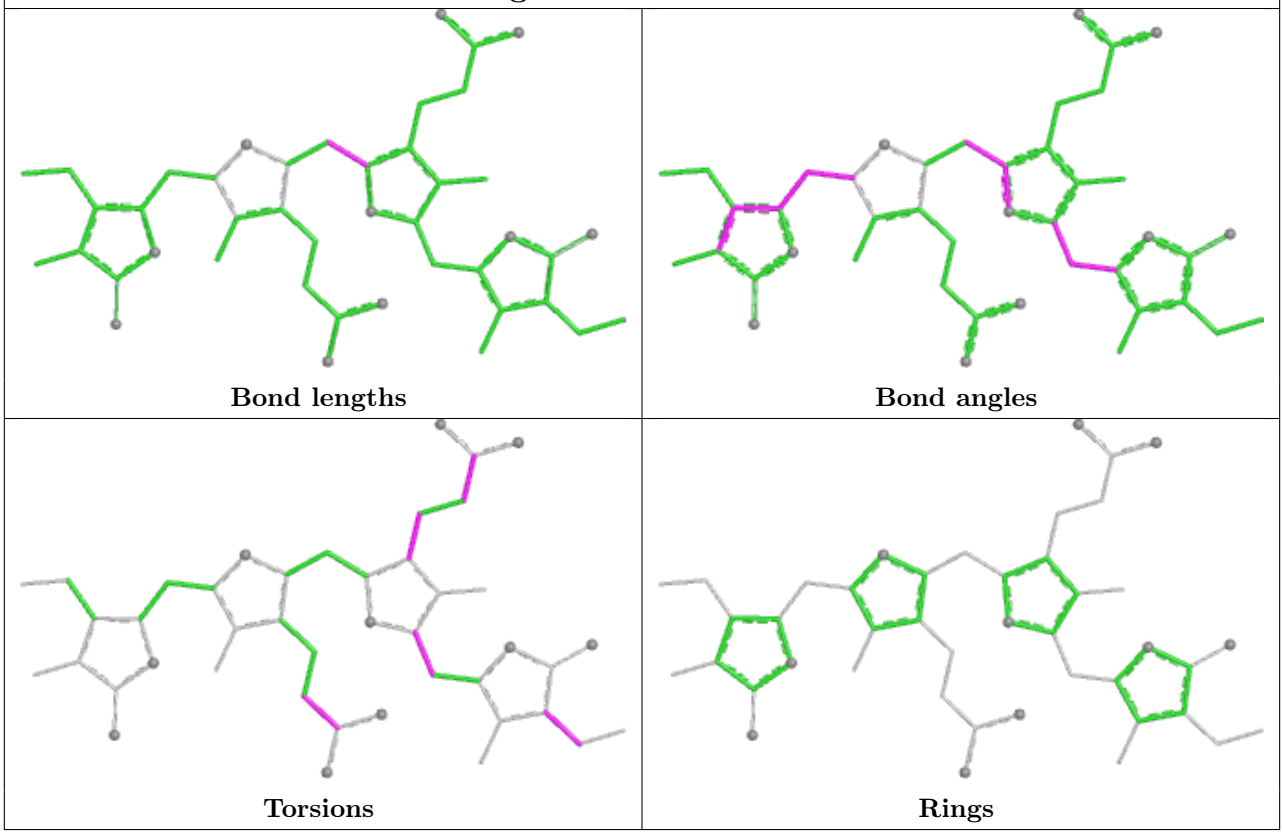

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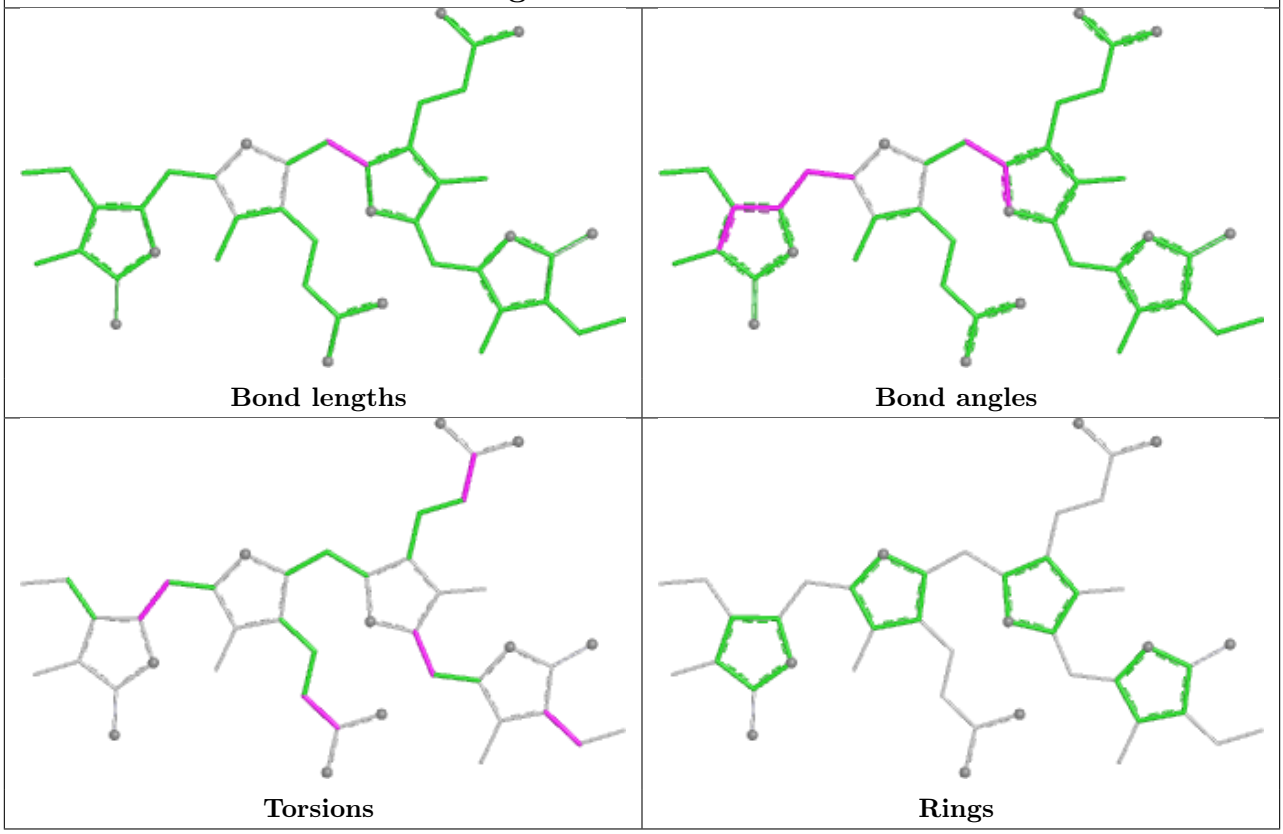
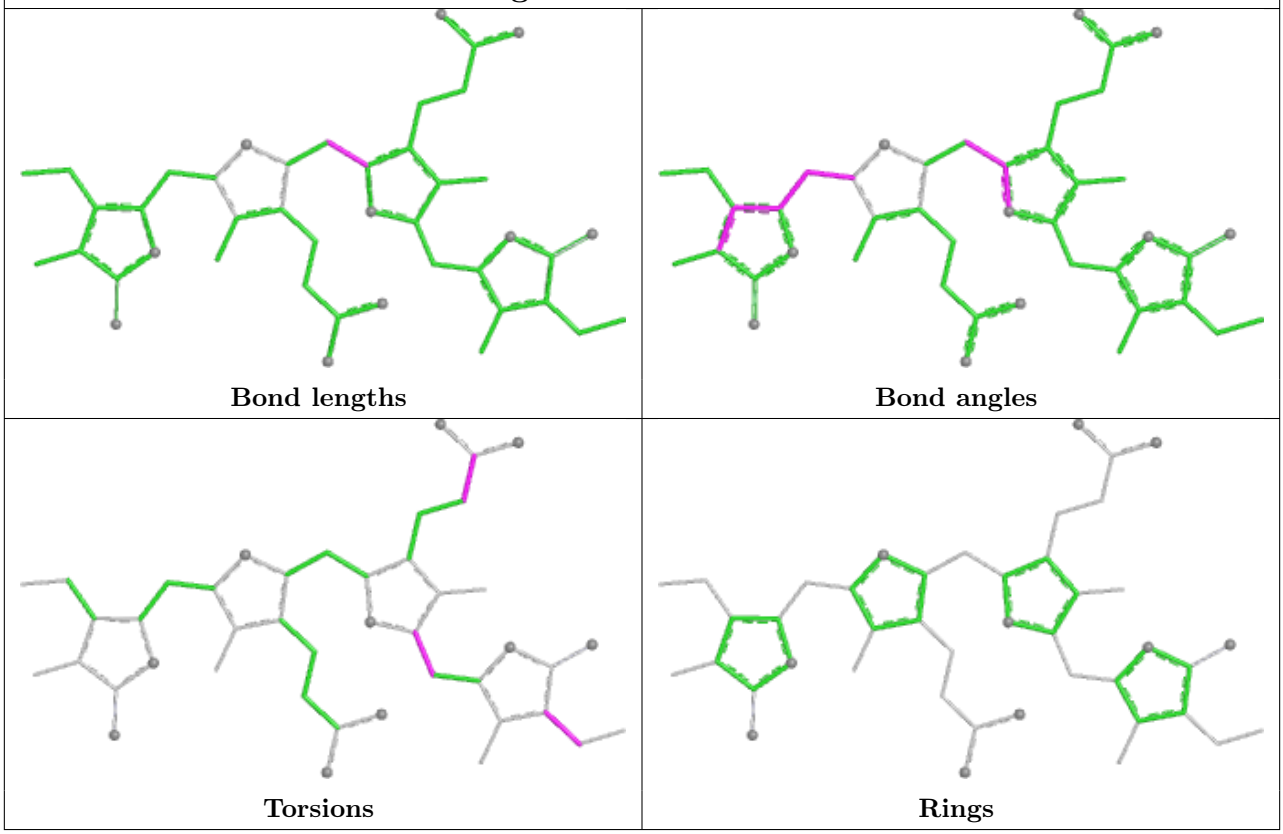


Ligand CYC AV 200



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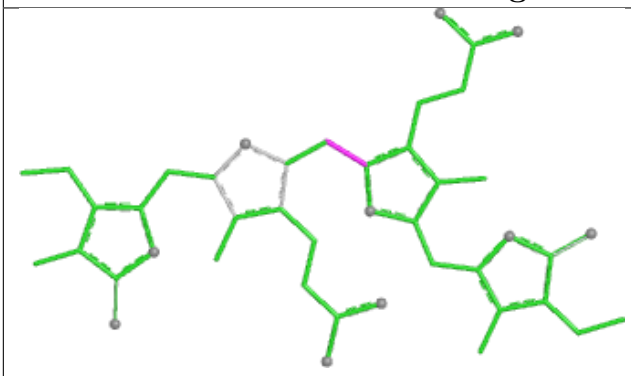
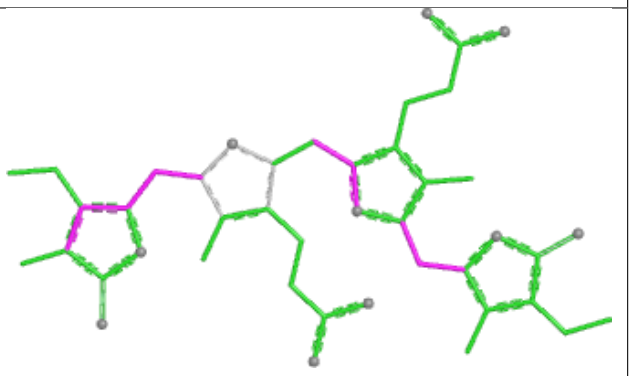
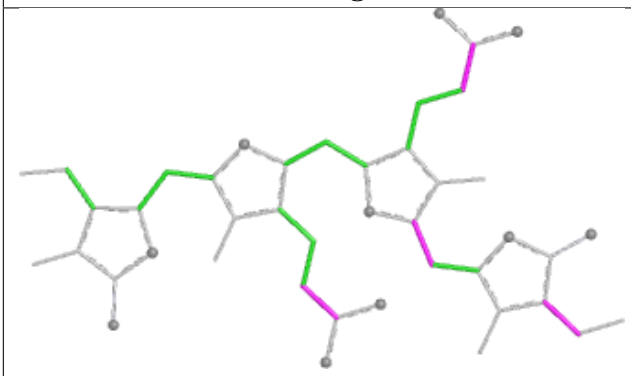


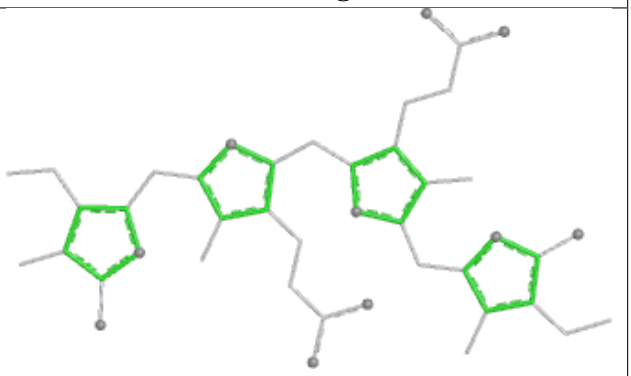
Bond lengths



Bond angles

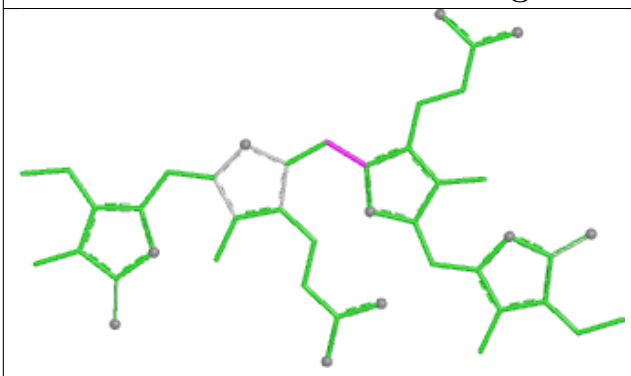


Torsions

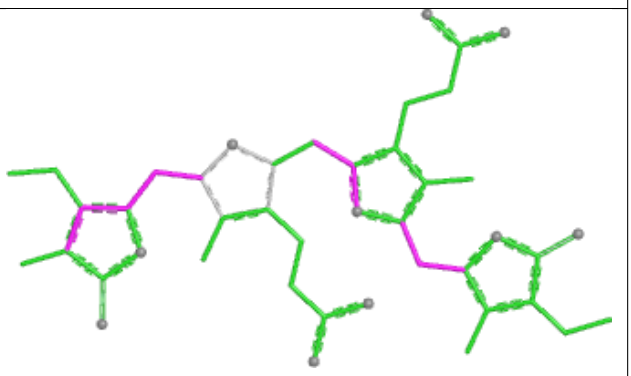


Rings

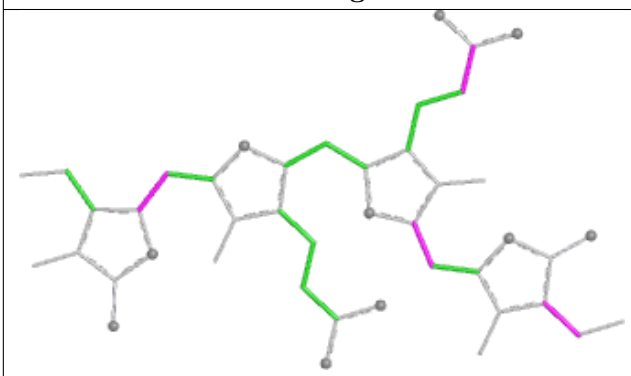
Ligand CYC BZ 200



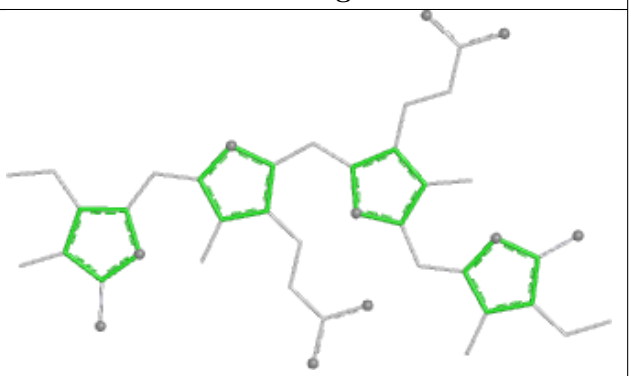
Bond lengths



Bond angles

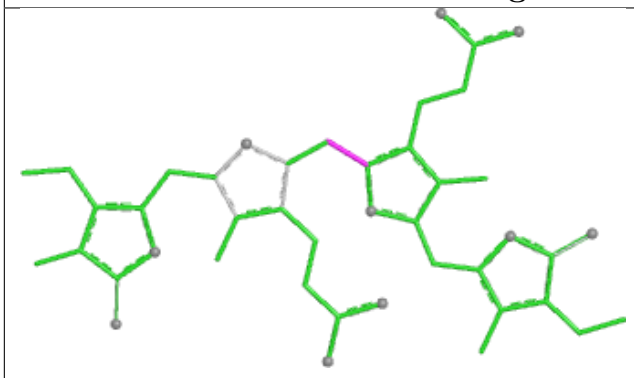


Torsions

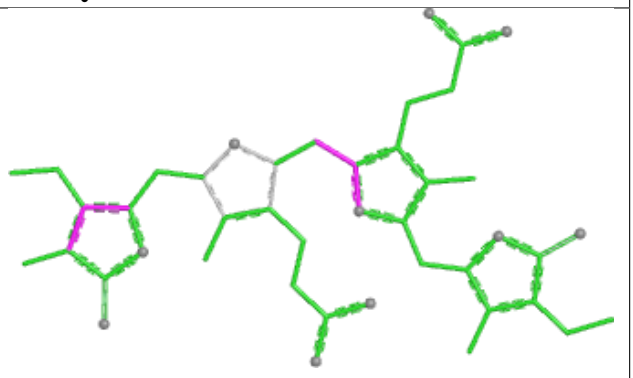


Rings

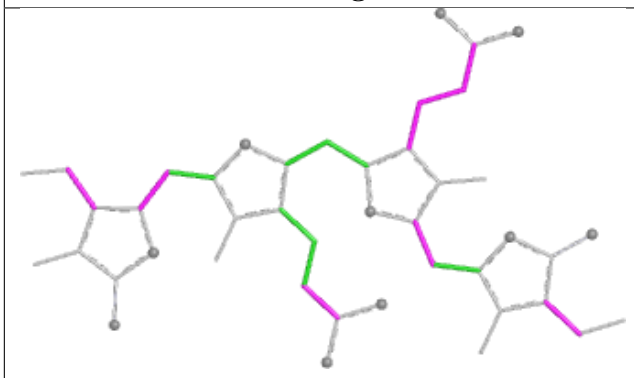
Ligand CYC DQ 200



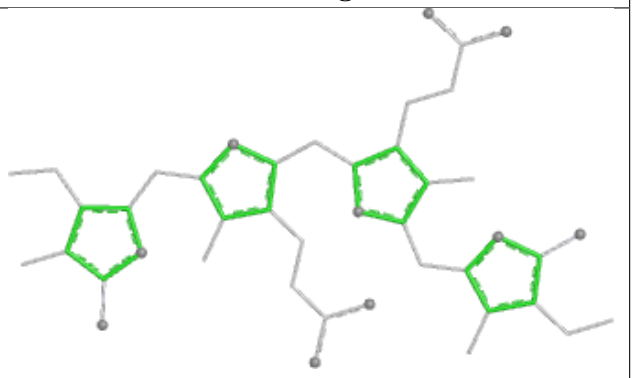
Bond lengths



Bond angles

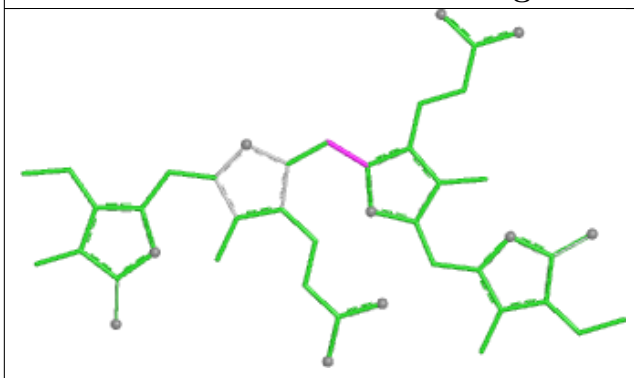


Torsions

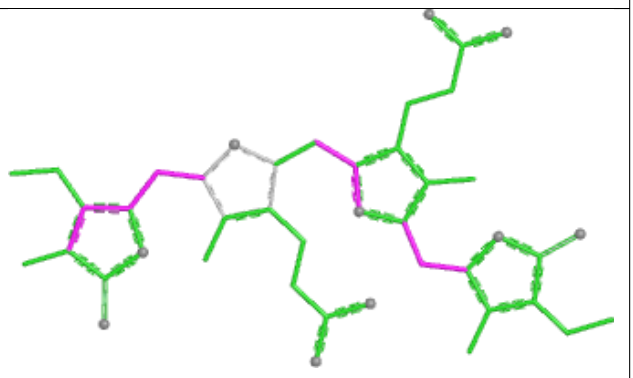


Rings

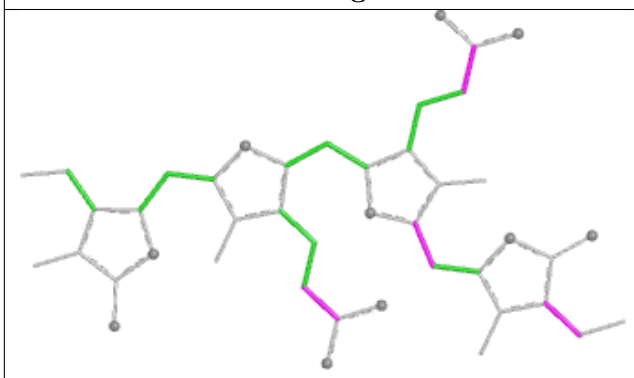
Ligand CYC AJ 200



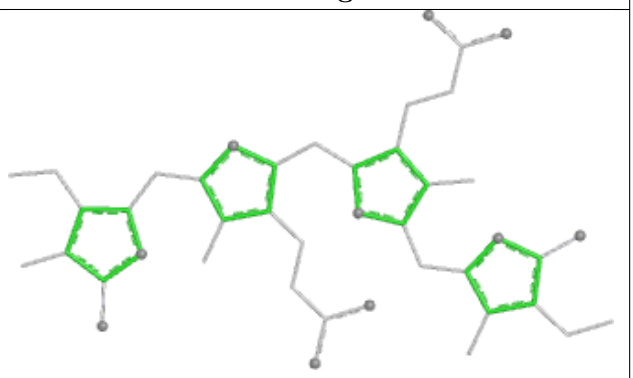
Bond lengths



Bond angles

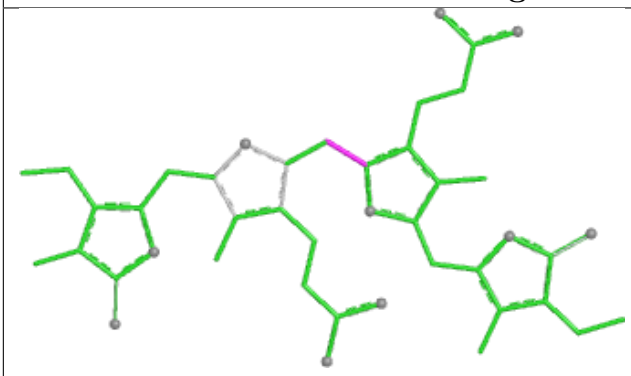


Torsions

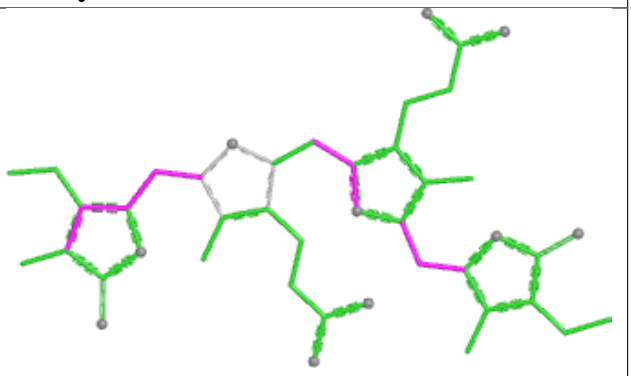


Rings

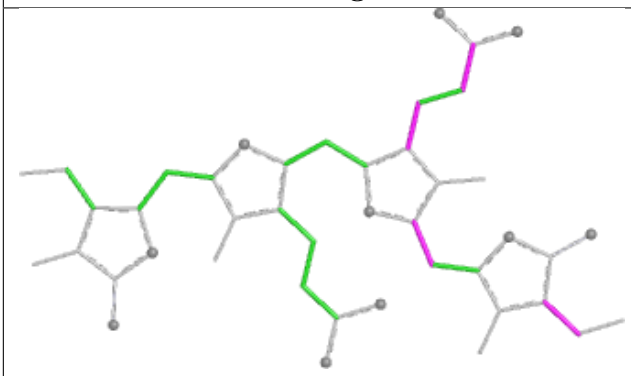
Ligand CYC BQ 200



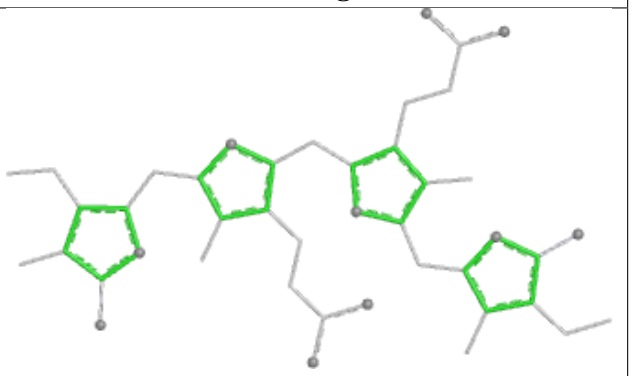
Bond lengths



Bond angles

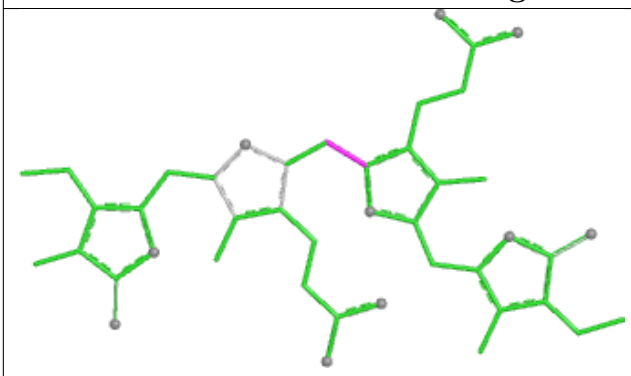


Torsions

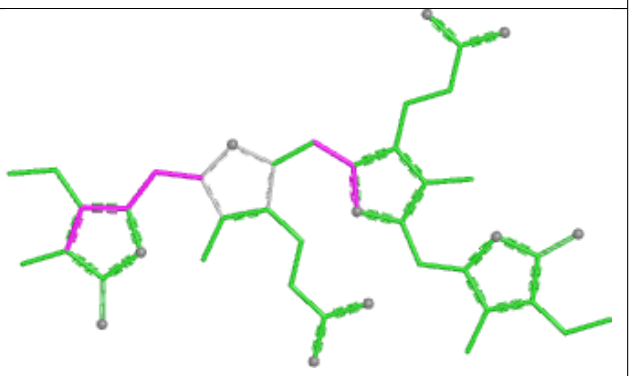


Rings

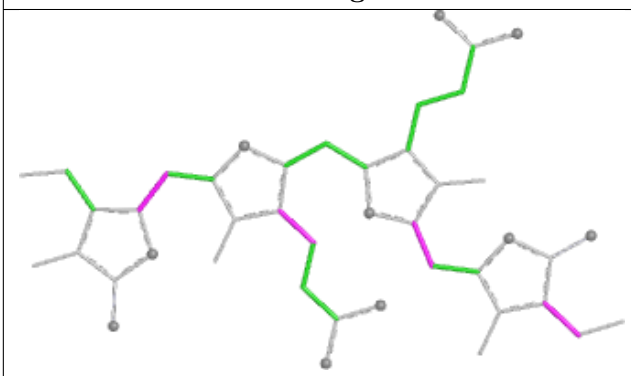
Ligand CYC AB 200



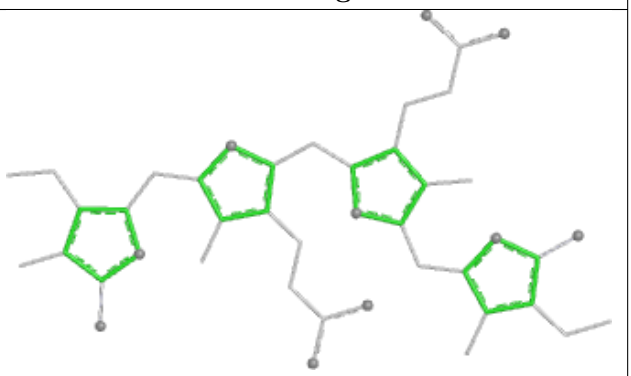
Bond lengths



Bond angles

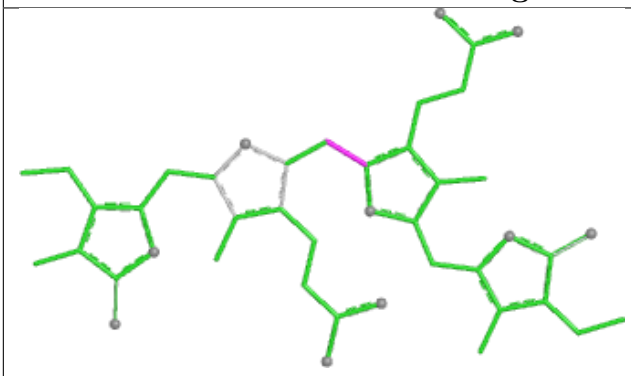


Torsions

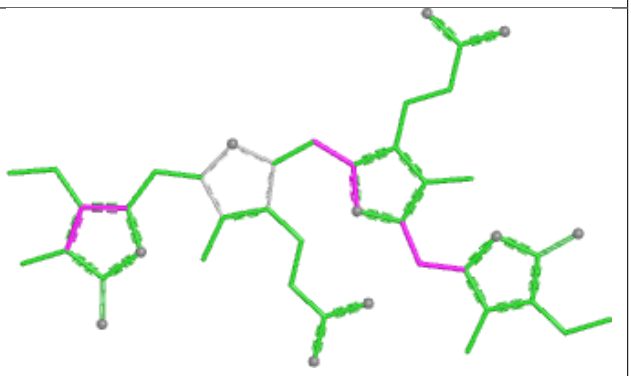


Rings

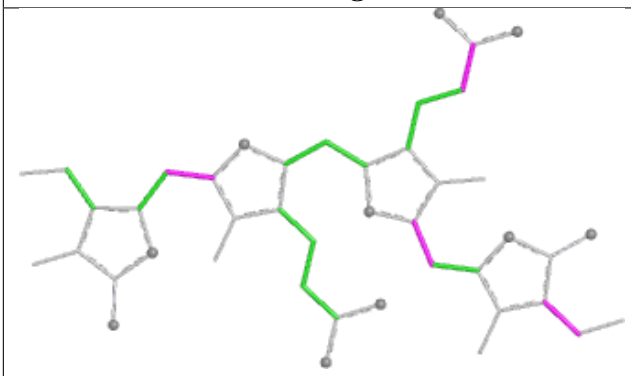
Ligand CYC DS 200



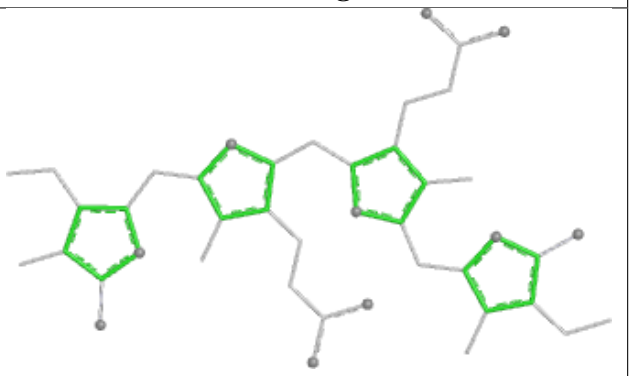
Bond lengths



Bond angles

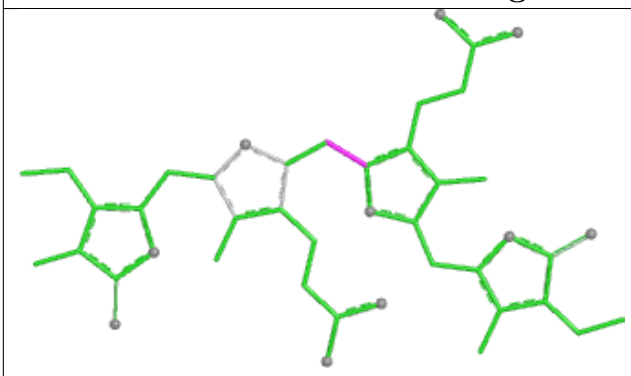


Torsions

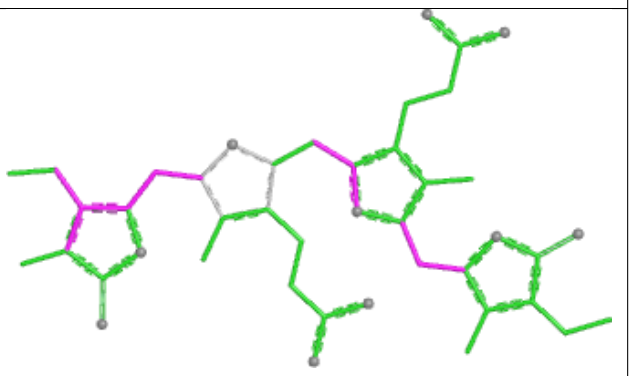


Rings

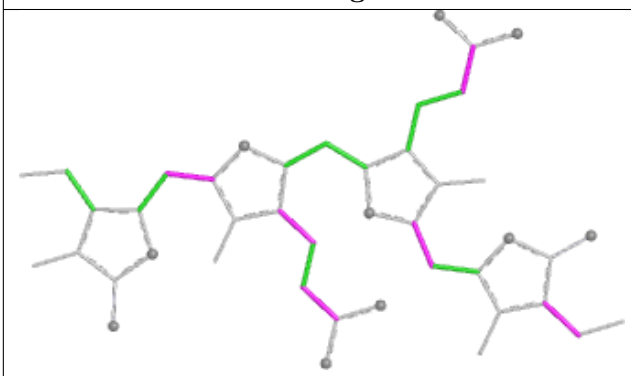
Ligand CYC DT 200



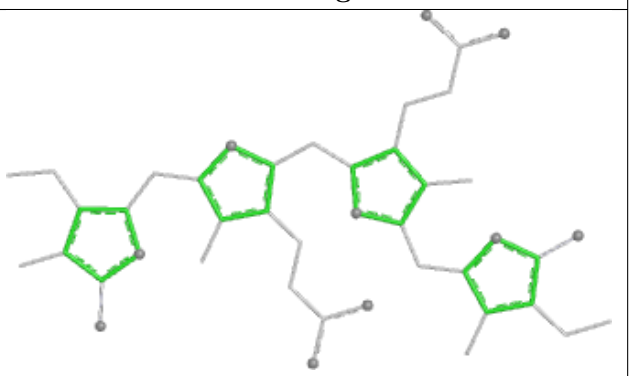
Bond lengths



Bond angles

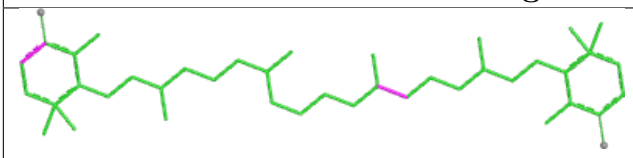


Torsions



Rings

Ligand 45D DI 400



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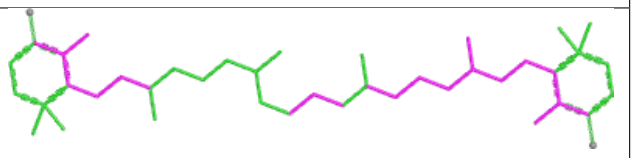
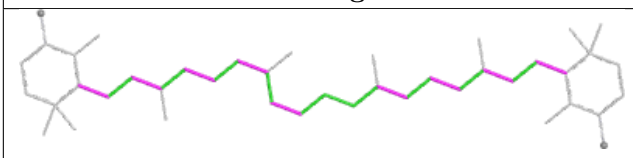
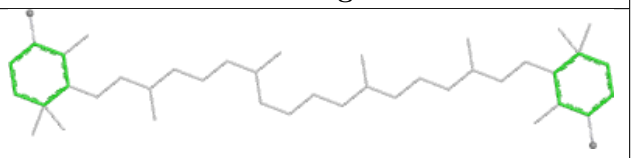


Bond angles

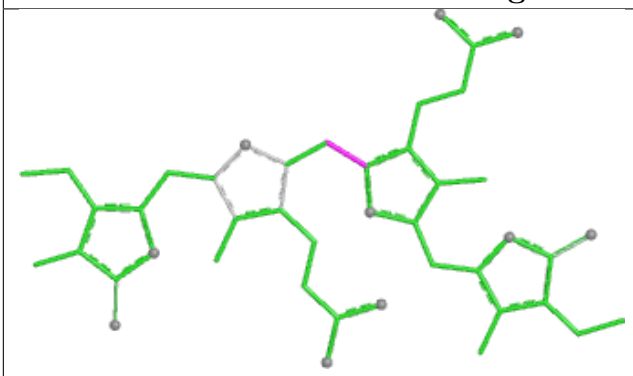


Torsions

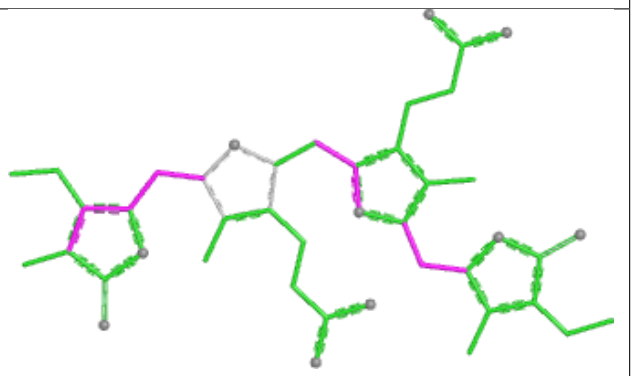


Rings

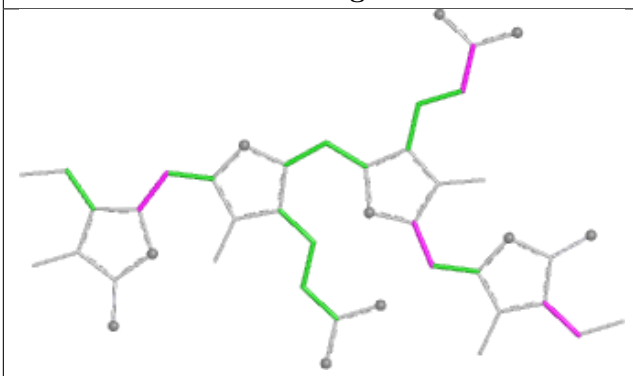
Ligand CYC AA 200



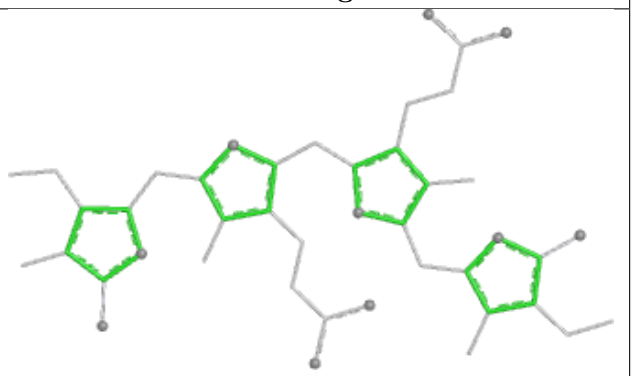
Bond lengths



Bond angles

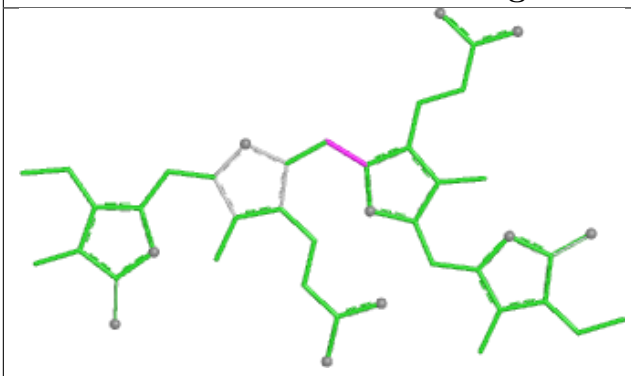


Torsions

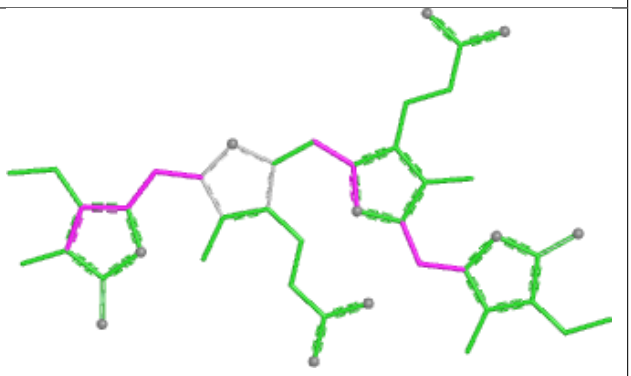


Rings

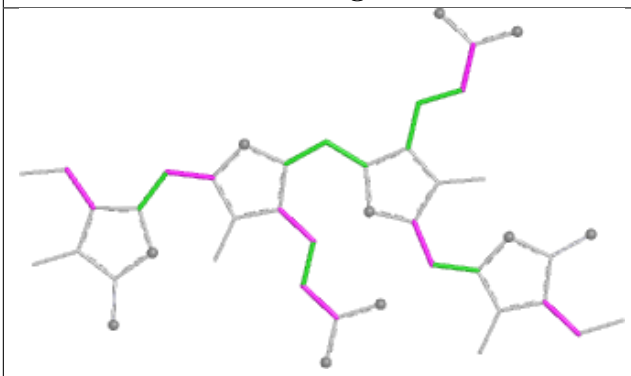
Ligand CYC CD 200



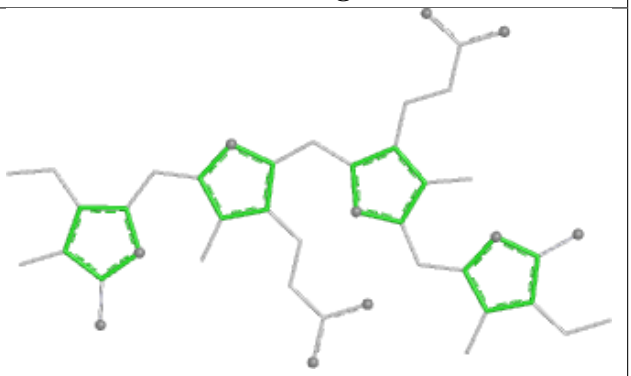
Bond lengths



Bond angles

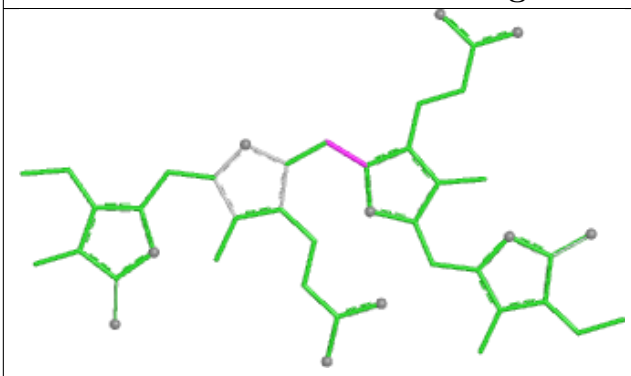


Torsions

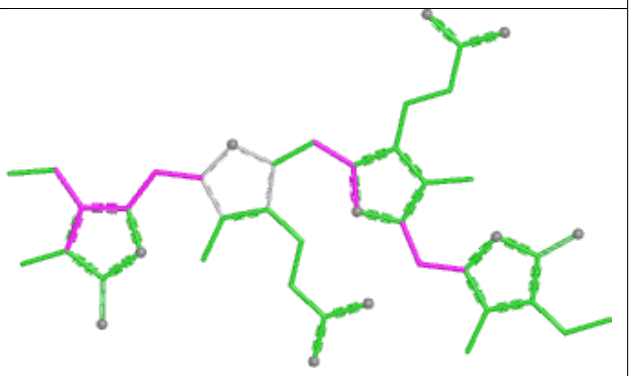


Rings

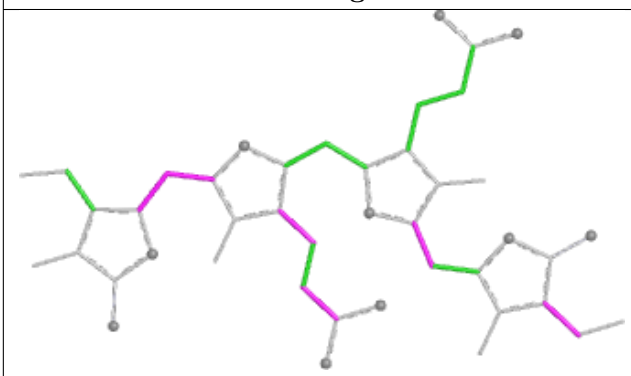
Ligand CYC DB 200



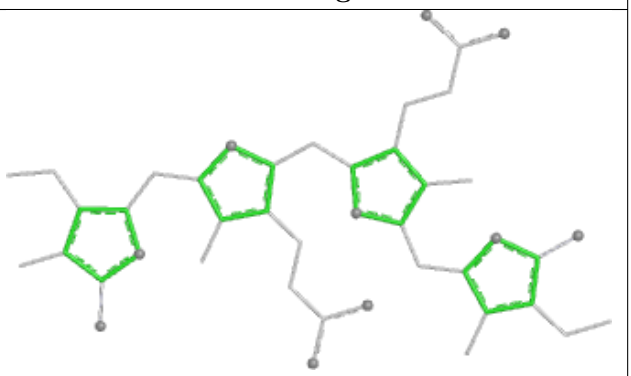
Bond lengths



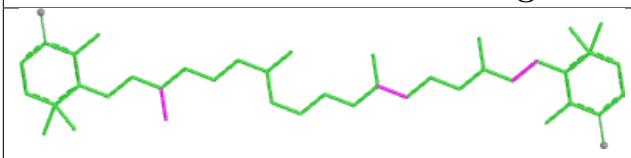
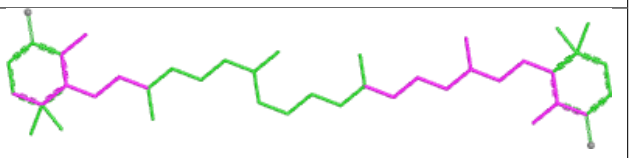
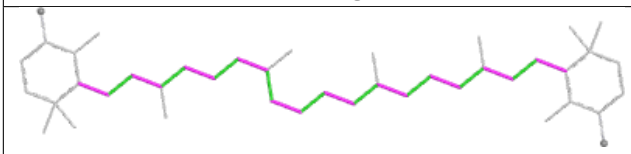
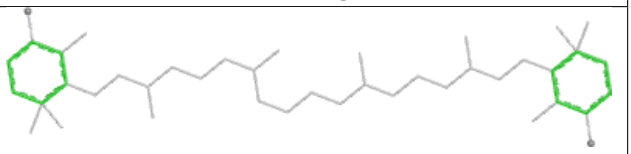
Bond angles

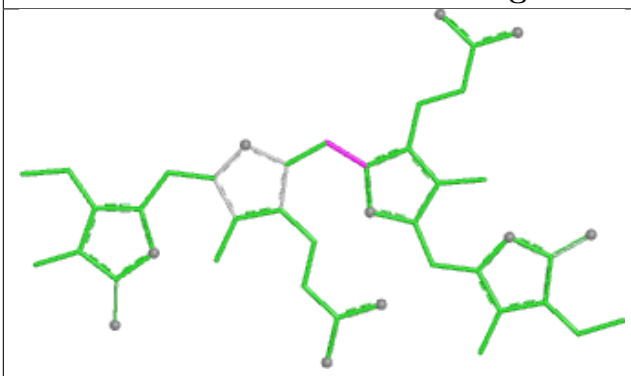
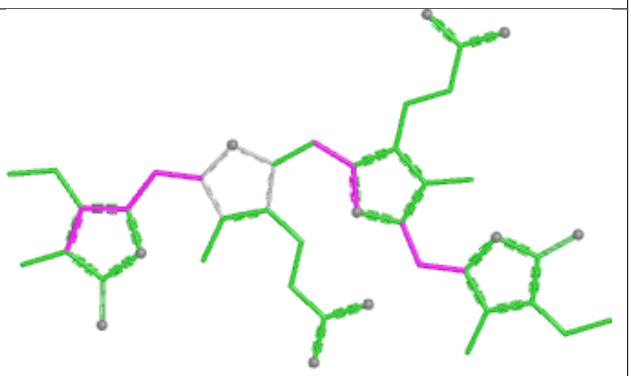
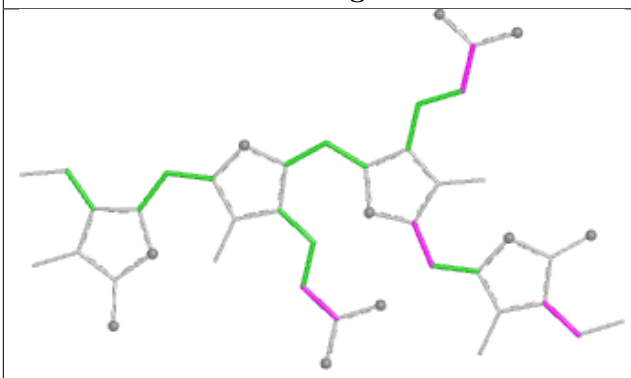
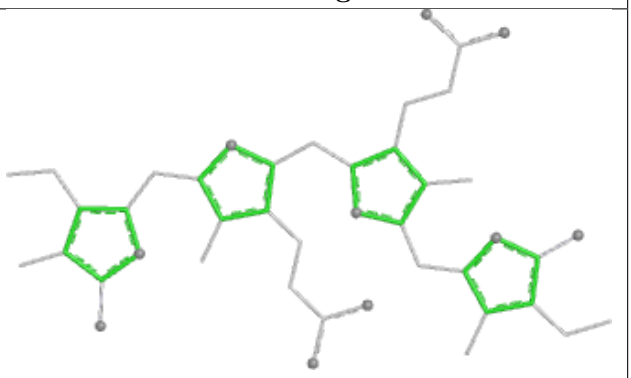


Torsions

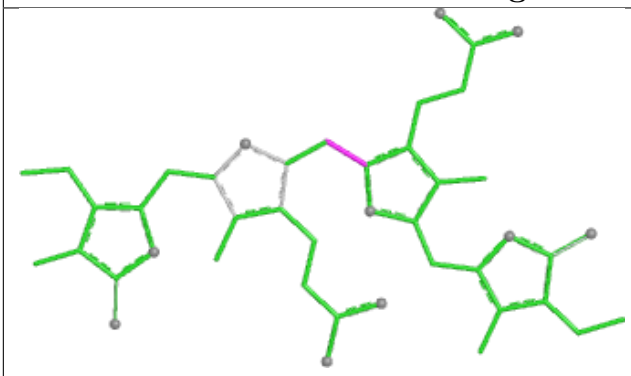


Rings

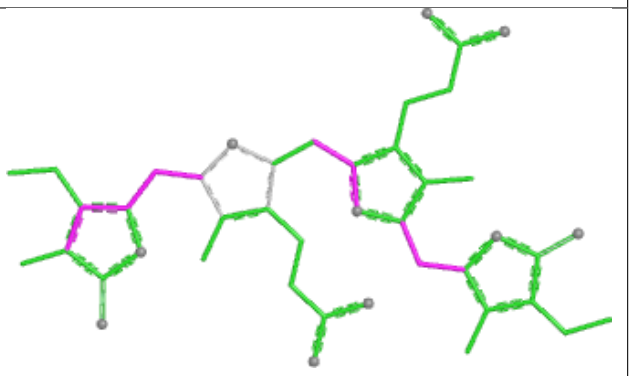
Ligand 45D EA 400	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CYC AP 200	
 Bond lengths	 Bond angles
 Torsions	 Rings

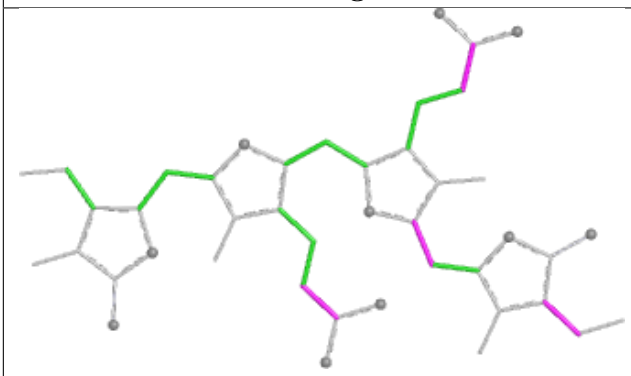
Ligand CYC BX 200



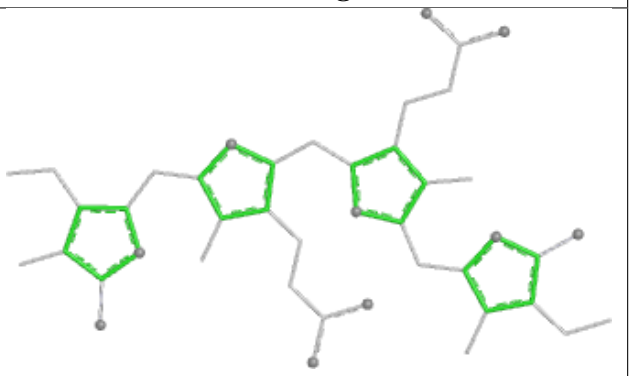
Bond lengths



Bond angles

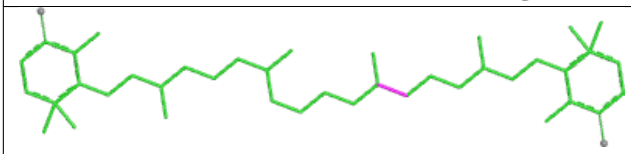


Torsions

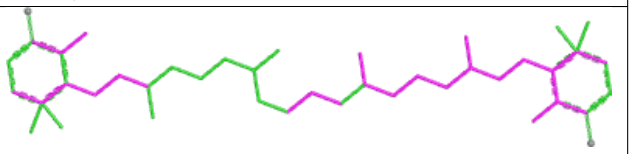


Rings

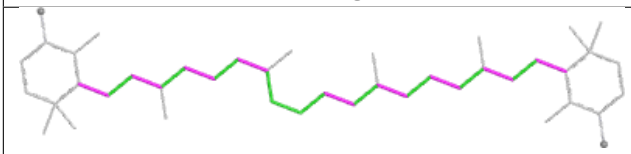
Ligand 45D CQ 400



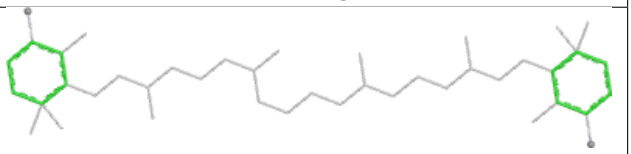
Bond lengths



Bond angles

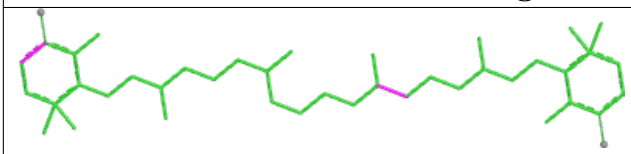


Torsions

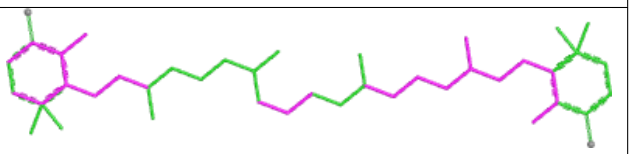


Rings

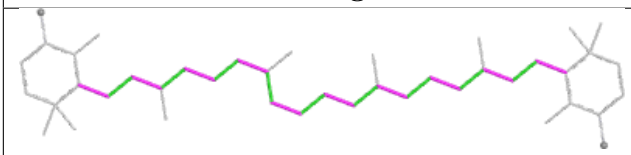
Ligand 45D BH 400



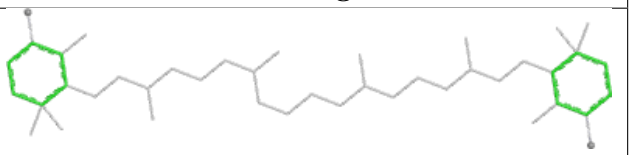
Bond lengths



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.

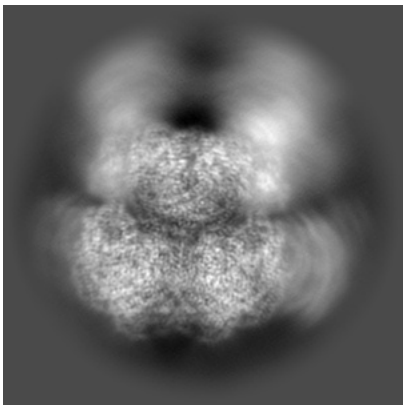
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-25030. These allow visual inspection of the internal detail of the map and identification of artifacts.

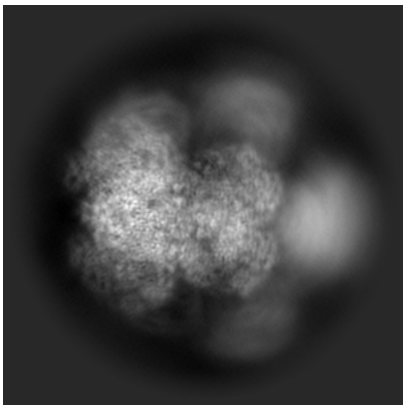
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

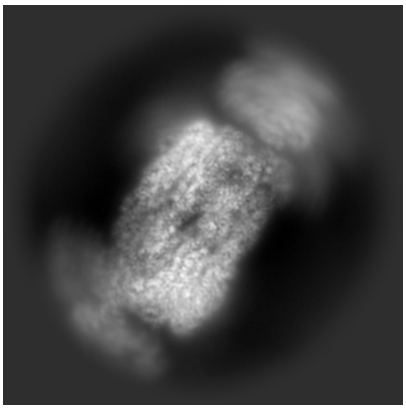
6.1.1 Primary map



X

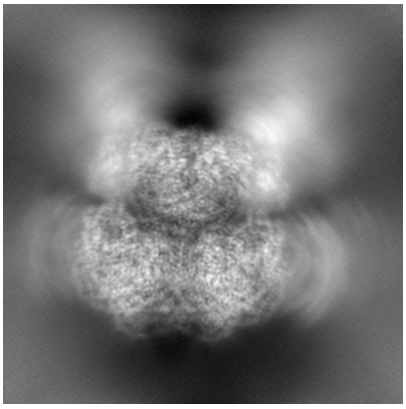


Y

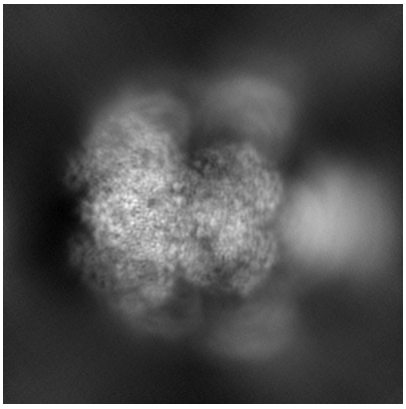


Z

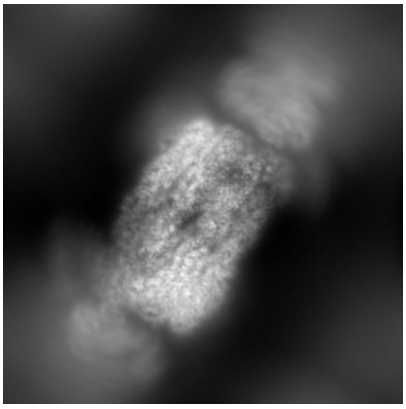
6.1.2 Raw map



X



Y

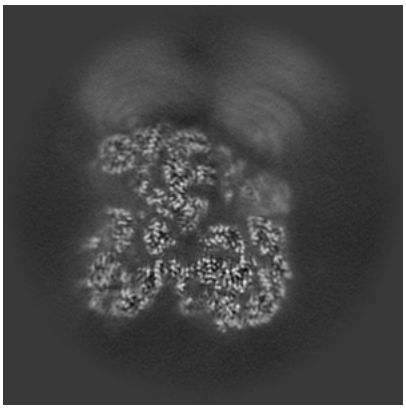


Z

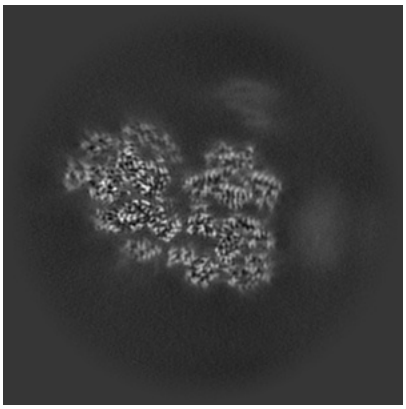
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

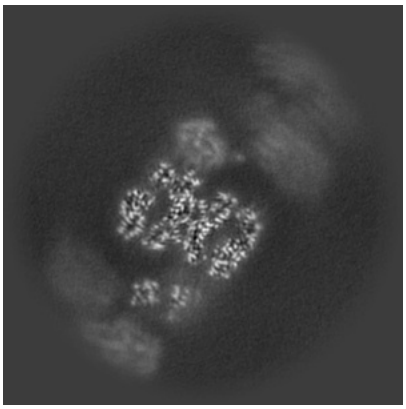
6.2.1 Primary map



X Index: 180

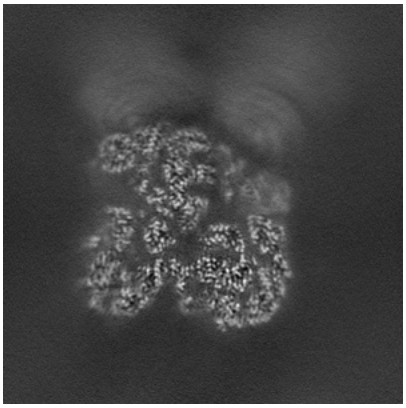


Y Index: 180

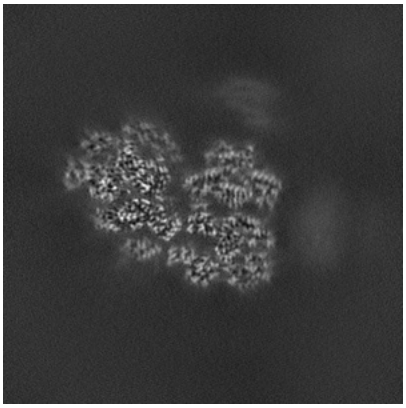


Z Index: 180

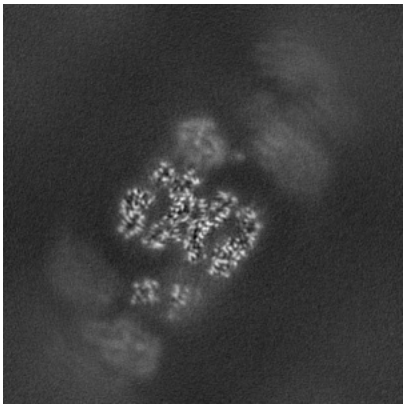
6.2.2 Raw map



X Index: 180



Y Index: 180

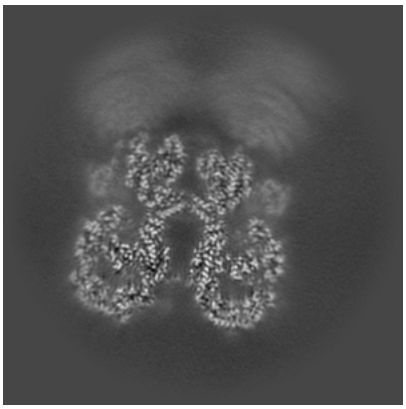


Z Index: 180

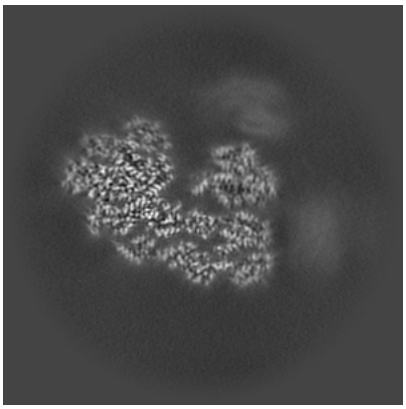
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

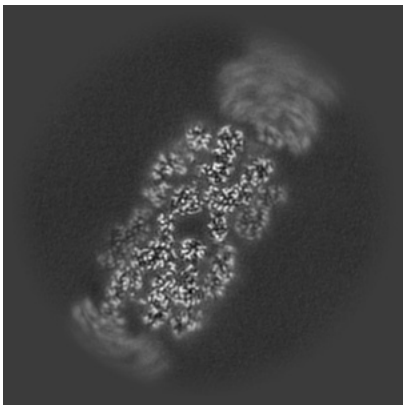
6.3.1 Primary map



X Index: 168

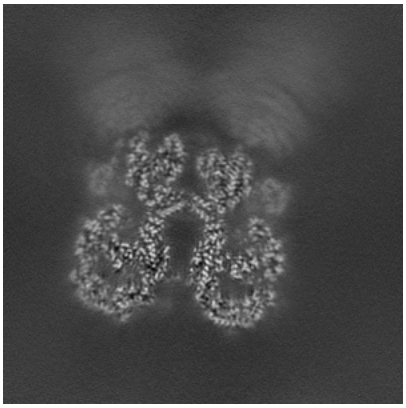


Y Index: 186

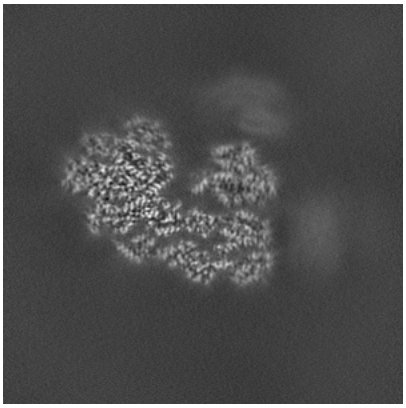


Z Index: 139

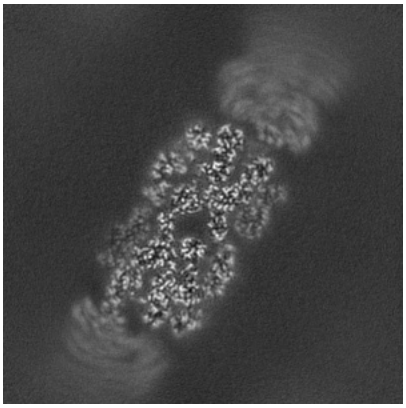
6.3.2 Raw map



X Index: 168



Y Index: 186

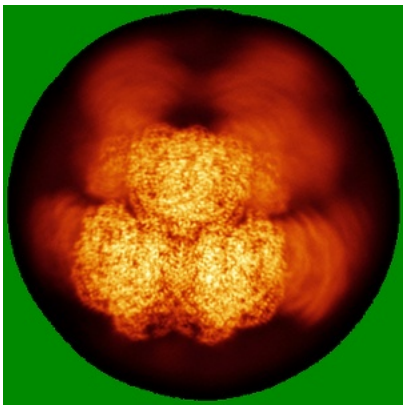


Z Index: 139

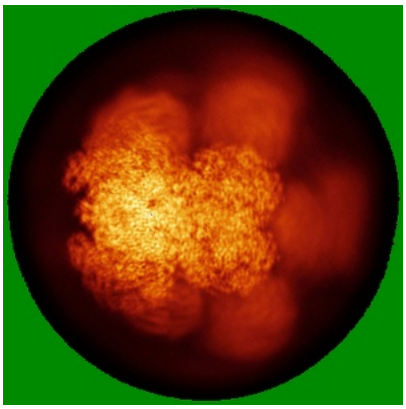
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

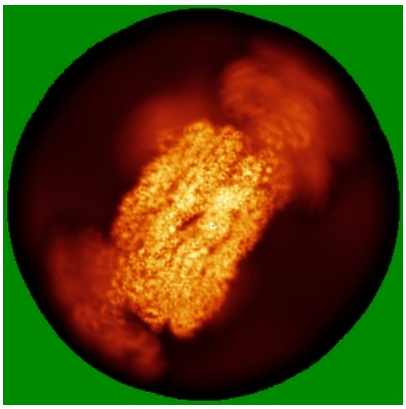
6.4.1 Primary map



X

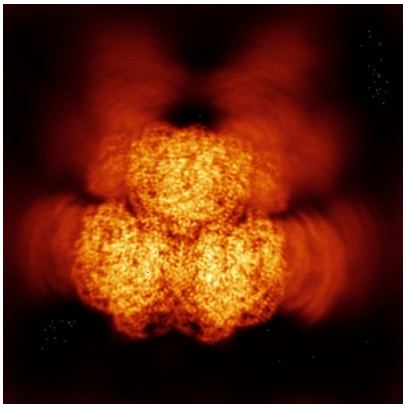


Y

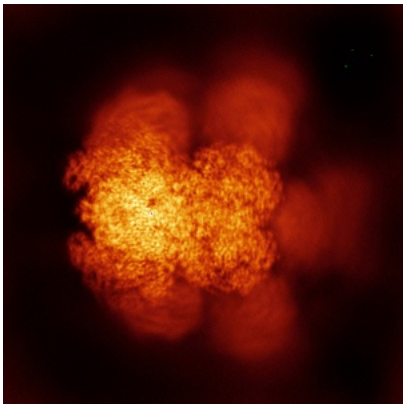


Z

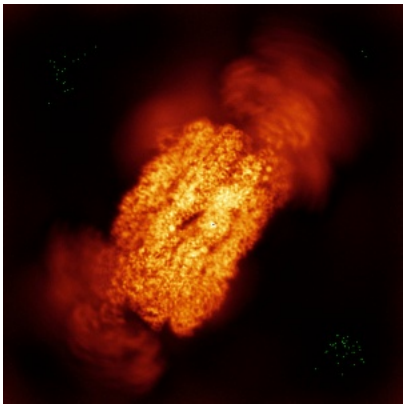
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.437. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

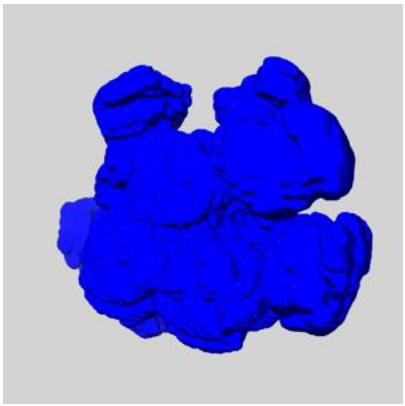
6.6 Mask visualisation

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

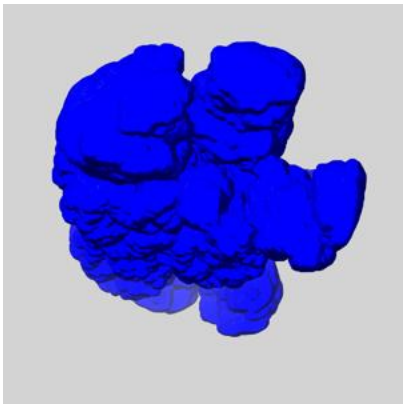
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

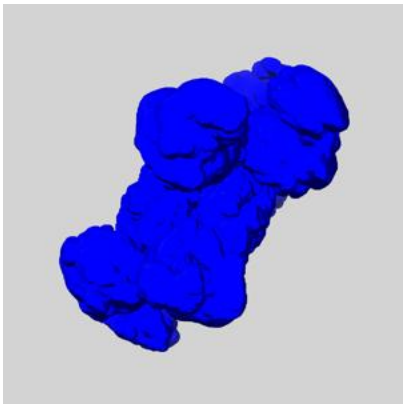
6.6.1 emd_25030_msk_1.map



X



Y

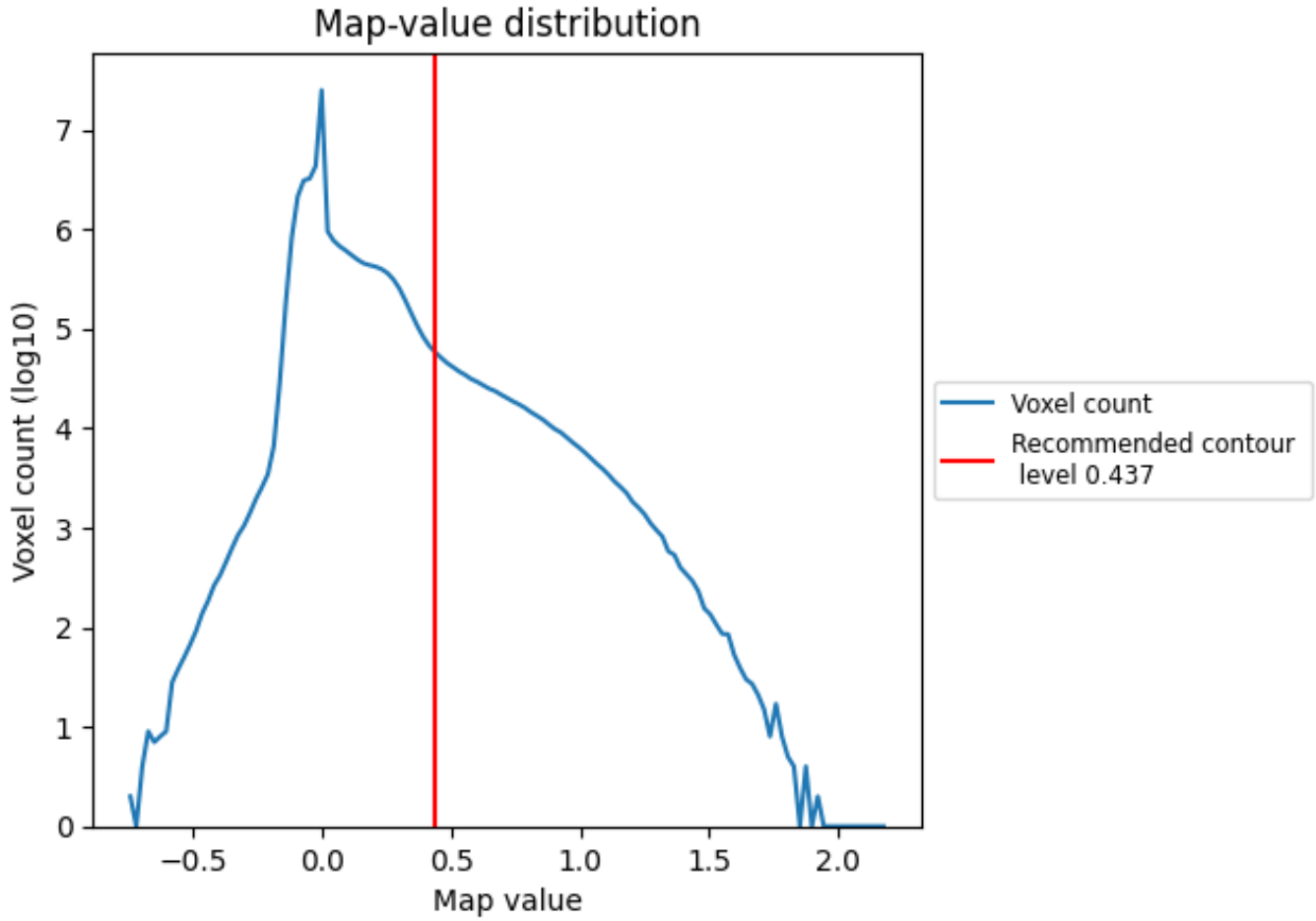


Z

7 Map analysis

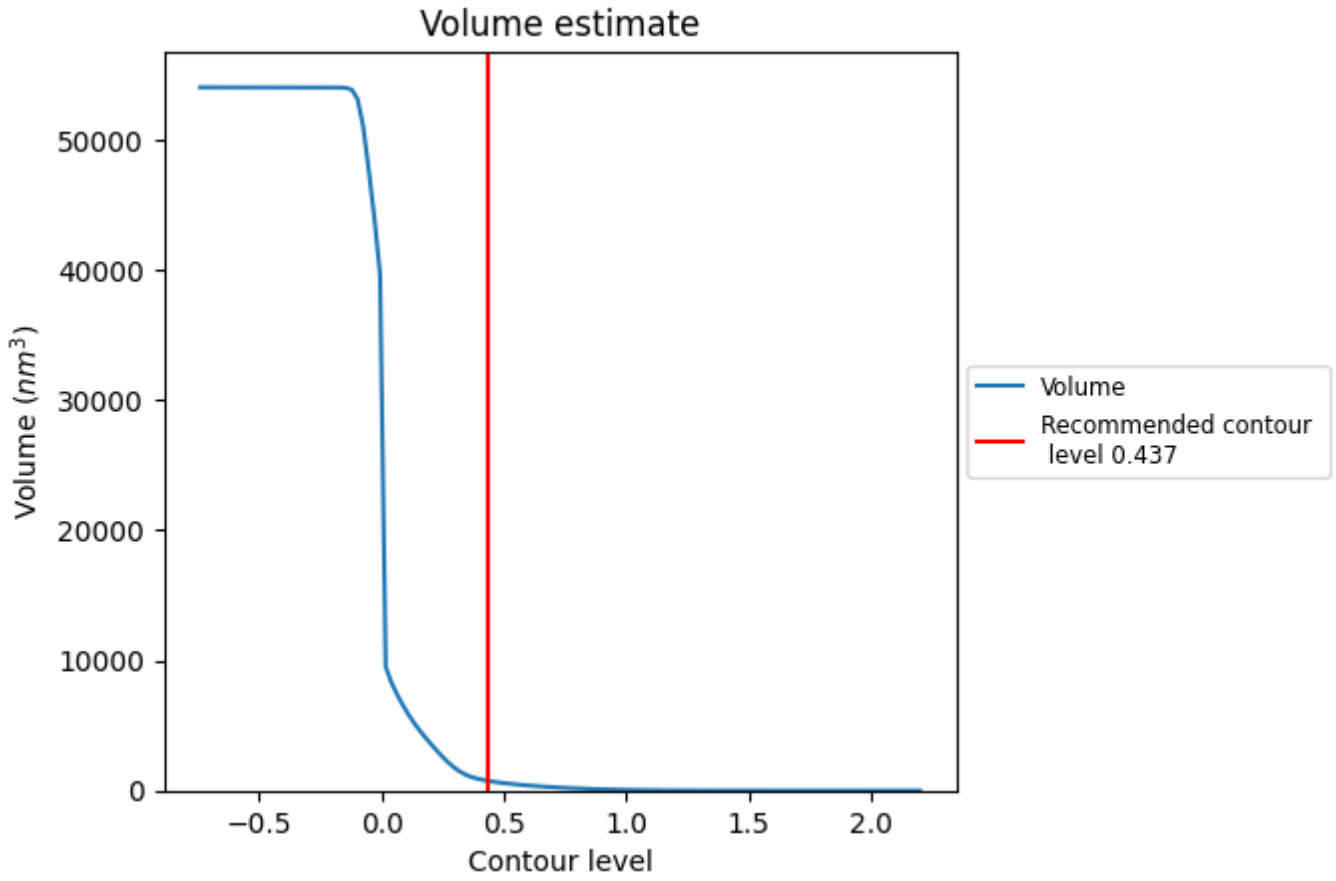
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

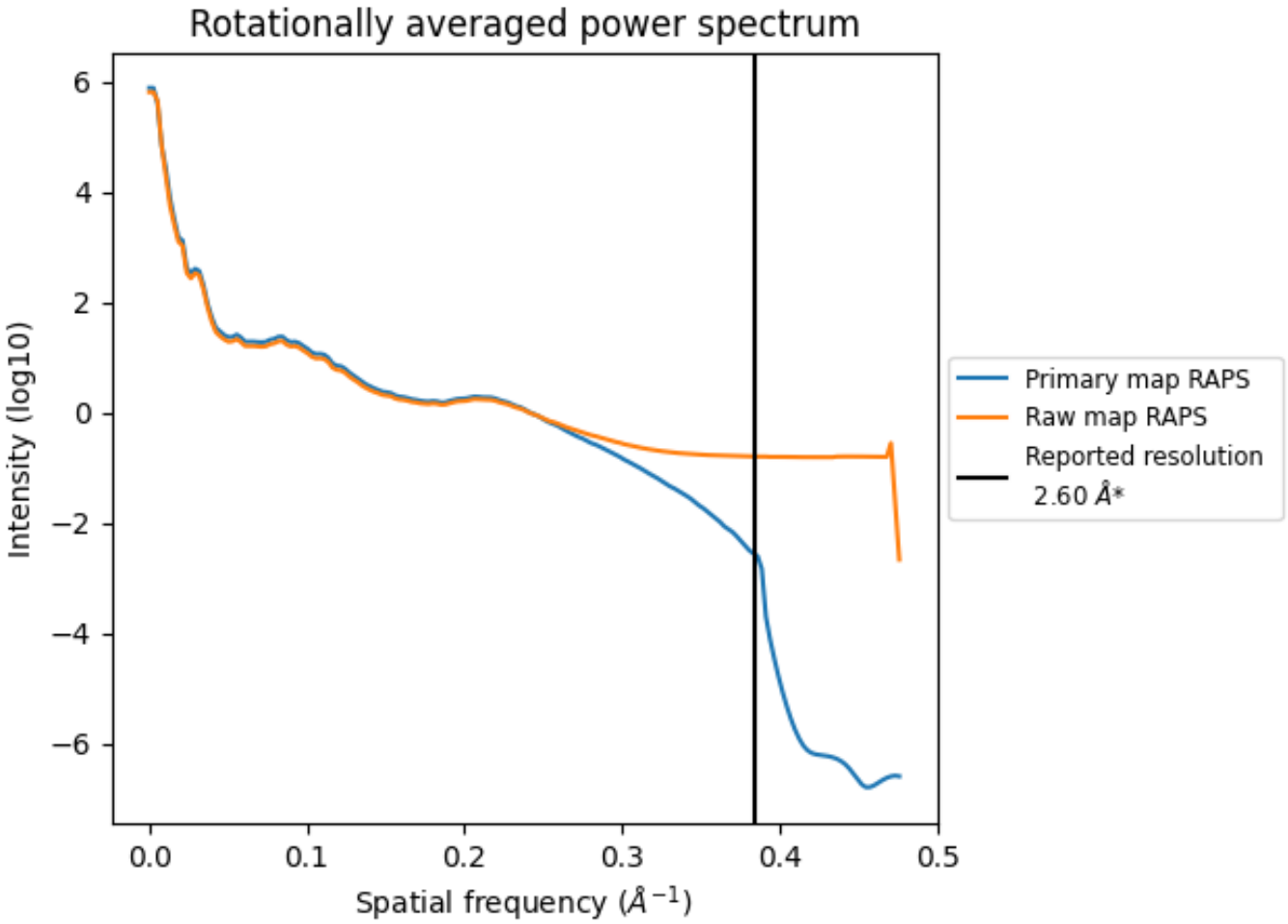
7.2 Volume estimate (i)



The volume at the recommended contour level is 737 nm^3; this corresponds to an approximate mass of 666 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

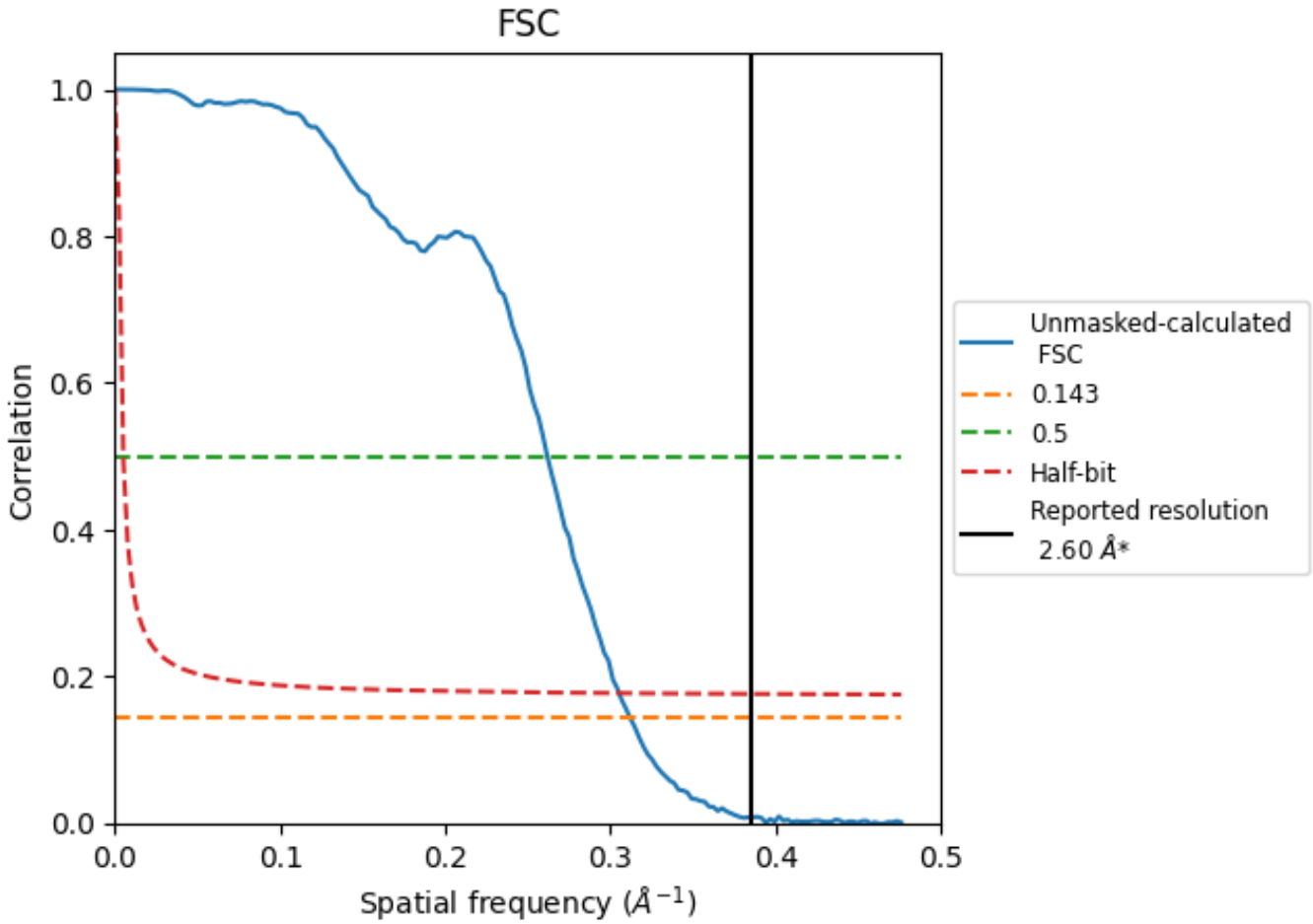


*Reported resolution corresponds to spatial frequency of 0.385 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.385 Å^{-1}

8.2 Resolution estimates (i)

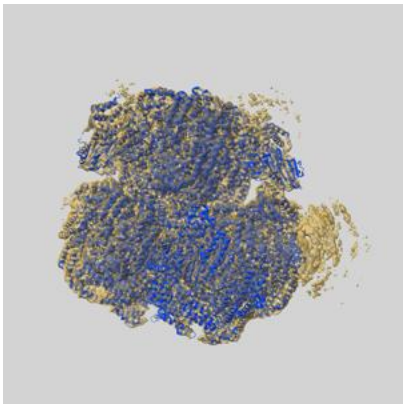
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.21	3.82	3.28

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.21 differs from the reported value 2.6 by more than 10 %

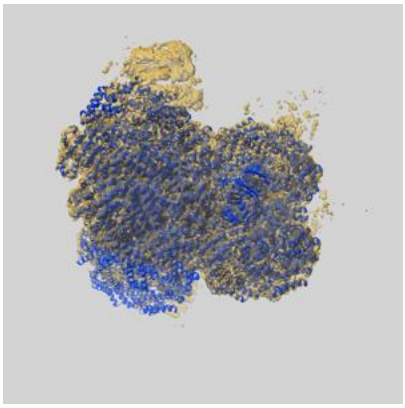
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-25030 and PDB model 7SC9. Per-residue inclusion information can be found in section 3 on page 18.

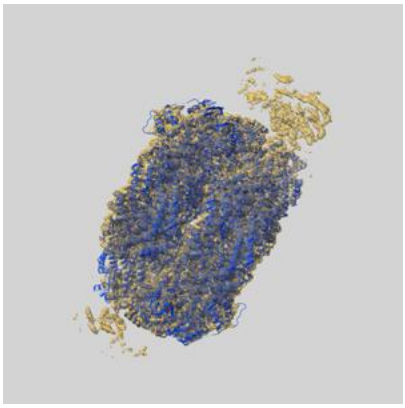
9.1 Map-model overlay



X



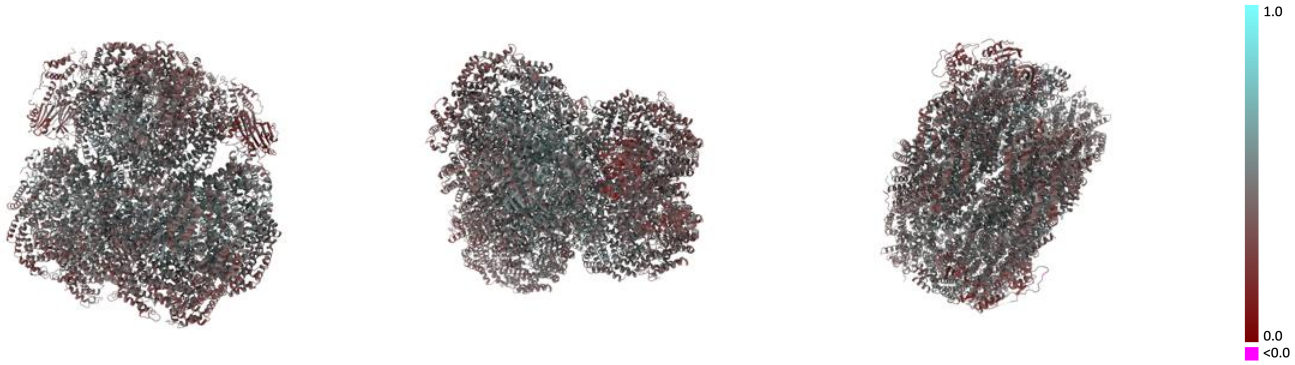
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.437 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

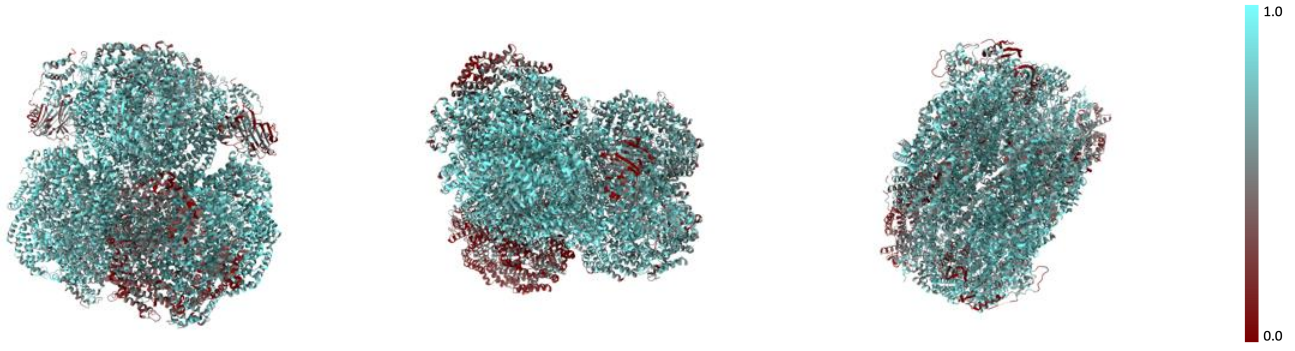
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

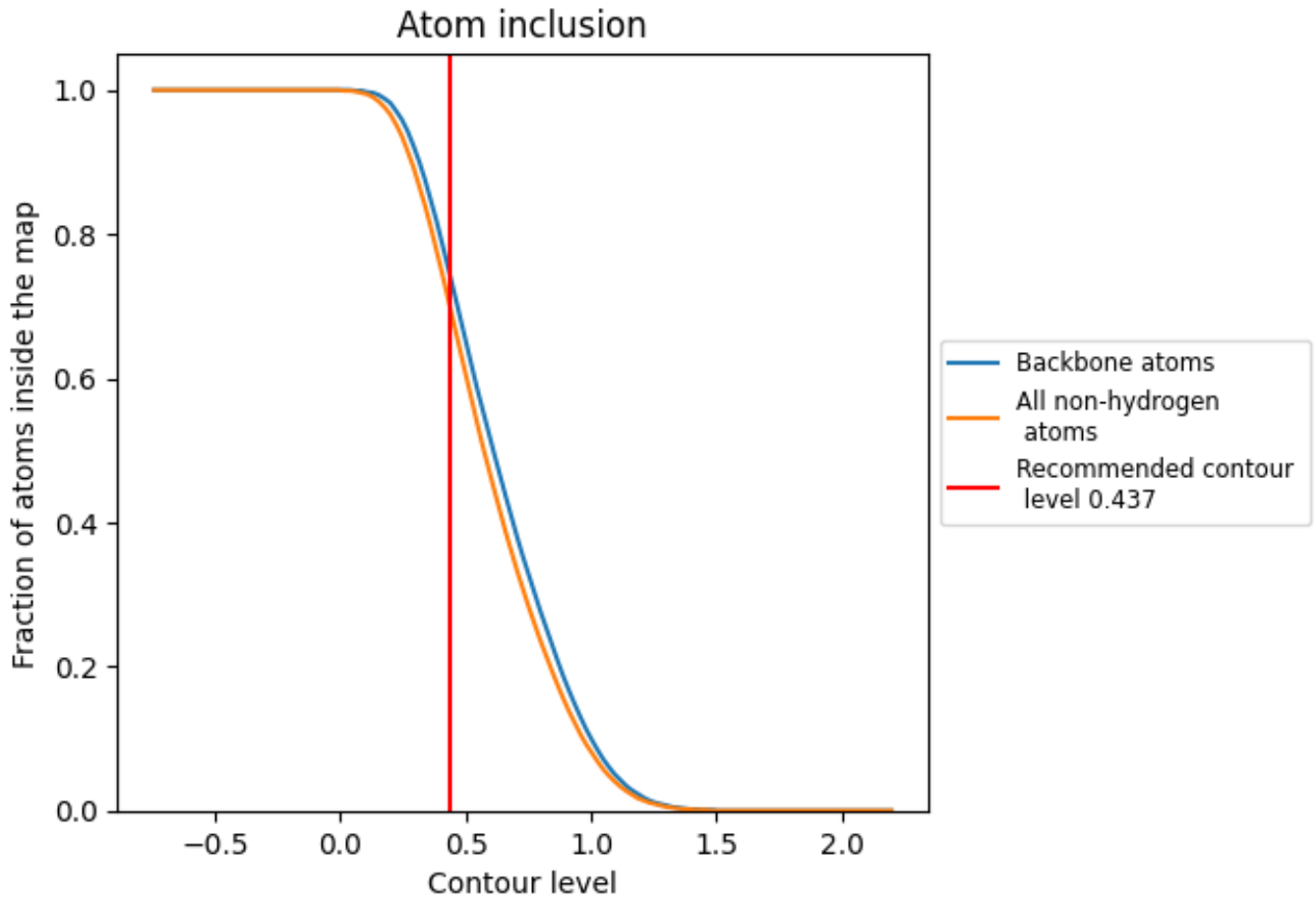
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.437).

9.4 Atom inclusion (i)



At the recommended contour level, 74% of all backbone atoms, 70% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.437) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7000	0.4490
AA	0.1520	0.4250
AB	0.1360	0.4150
AC	0.1510	0.3650
AD	0.1330	0.3650
AE	0.1950	0.3820
AF	0.1110	0.4160
AH	0.7940	0.4590
AI	0.8780	0.5300
AJ	0.8590	0.5140
AK	0.8170	0.4500
AL	0.8520	0.4480
AN	0.8150	0.4280
AO	0.8740	0.5150
AP	0.8640	0.5240
AQ	0.8760	0.5290
AR	0.8240	0.4710
AS	0.8470	0.4560
AU	0.7730	0.4120
AV	0.7770	0.3790
AW	0.8360	0.4240
AX	0.8320	0.4630
AY	0.8430	0.4670
AZ	0.7550	0.4430
BA	0.2260	0.4480
BB	0.6910	0.4870
BD	0.8150	0.4770
BF	0.7100	0.4110
BG	0.7790	0.4650
BH	0.4920	0.3840
BI	0.3540	0.4400
BJ	0.3880	0.4340
BK	0.3630	0.3980
BL	0.3660	0.3950
BM	0.4280	0.4030

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Chain	Atom inclusion	Q-score
BN	0.3660	0.4290
BP	0.8290	0.4820
BQ	0.8910	0.5340
BR	0.8610	0.5150
BS	0.8450	0.4730
BT	0.8600	0.4790
BV	0.8430	0.4430
BW	0.8770	0.5250
BX	0.8760	0.5350
BY	0.8810	0.5450
BZ	0.8640	0.5050
CA	0.8620	0.4900
CC	0.7390	0.4680
CD	0.7860	0.4440
CE	0.8190	0.4310
CF	0.8330	0.4530
CG	0.8620	0.4790
CH	0.8350	0.4820
CJ	0.4930	0.4900
CK	0.7020	0.5160
CM	0.8370	0.4890
CO	0.7360	0.4290
CP	0.7950	0.4820
CQ	0.5480	0.3920
CR	0.7290	0.3970
CS	0.7170	0.4240
CT	0.6720	0.4280
CU	0.7300	0.4660
CV	0.8490	0.4910
CW	0.8240	0.4460
CY	0.6870	0.4010
CZ	0.6930	0.4120
DA	0.8000	0.4400
DB	0.8350	0.4930
DC	0.8360	0.5030
DD	0.7940	0.4570
DF	0.8370	0.5040
DG	0.4650	0.3670
DH	0.6460	0.4310
DI	0.4850	0.3140
DJ	0.7160	0.4080
DK	0.6920	0.4030

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Chain	Atom inclusion	Q-score
DL	0.7080	0.3920
DM	0.7990	0.4600
DN	0.8510	0.4840
DO	0.8420	0.4730
DQ	0.6830	0.3800
DR	0.7130	0.4220
DS	0.8300	0.4720
DT	0.8240	0.4920
DU	0.8310	0.4930
DV	0.7550	0.4100
DX	0.8290	0.5090
DY	0.4460	0.4080
DZ	0.6390	0.4060
EA	0.5100	0.3400