wwPDB EM Validation Summary Report ⓘ

Nov 28, 2022 – 11:30 PM JST

PDB ID	:	7VEB
EMDB ID	:	EMD-31945
Title	:	Phycocyanin rod structure of cyanobacterial phycobilisome
Authors	:	Kawakami, K.; Hamaguchi, T.; Hirose, Y.; Kosumi, D.; Miyata, M.; Kamiya, N.; Yonekura, K.
Deposited on	:	2021-09-08
Resolution	:	4.20 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 ⓘ symbol.

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

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

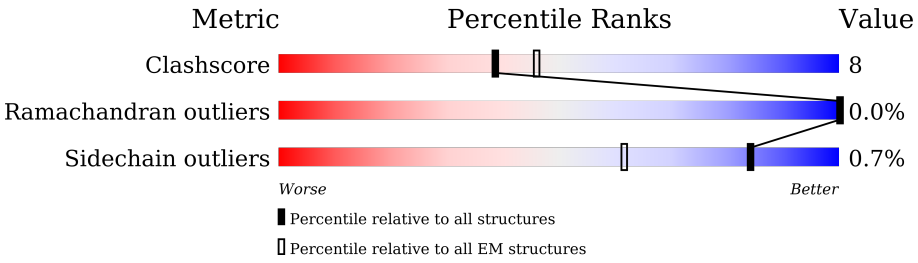
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance

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

The reported resolution of this entry is 4.20 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	A	162	88% 10%
1	C	162	84% 16%
1	E	162	83% 17%
1	G	162	88% 12%
1	I	162	89% 11%
1	K	162	86% 14%
1	M	162	89% 11%
1	O	162	86% 14%

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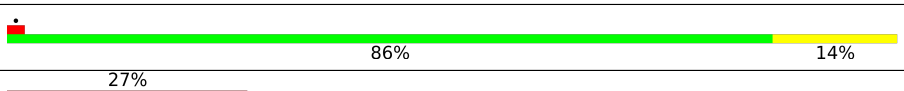
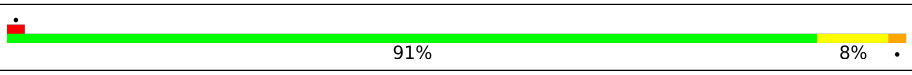
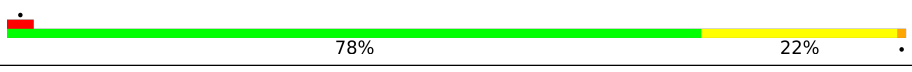
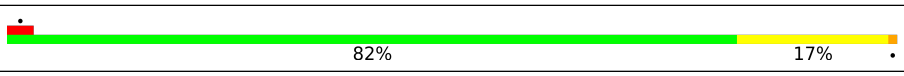
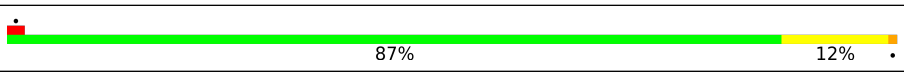
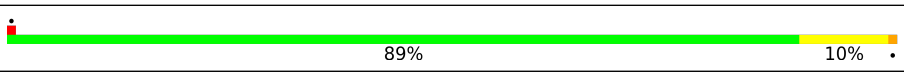
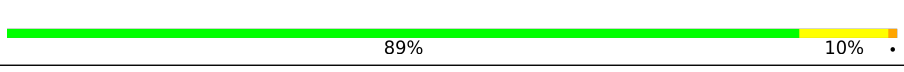
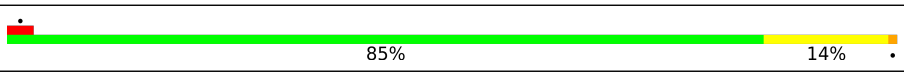
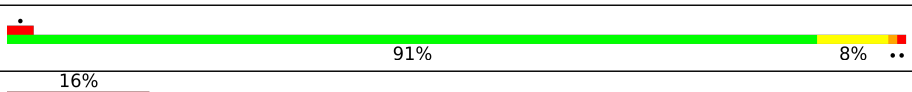
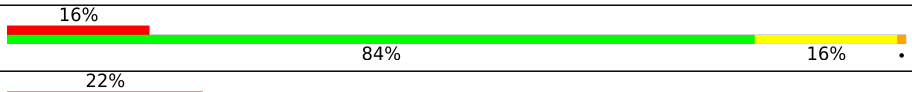
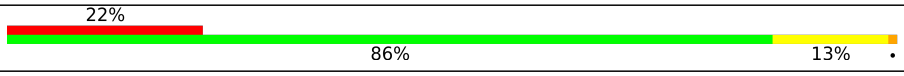
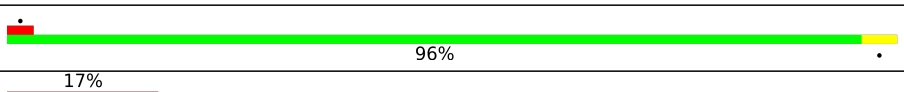
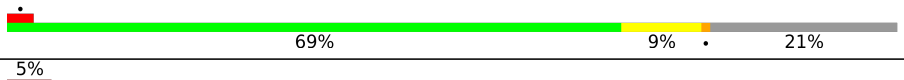
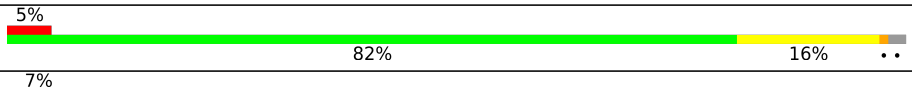
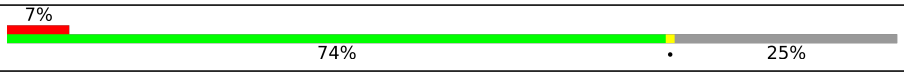
Mol	Chain	Length	Quality of chain
1	Q	162	
1	S	162	
1	U	162	
1	W	162	
2	B	172	
2	D	172	
2	F	172	
2	H	172	
2	J	172	
2	L	172	
2	N	172	
2	P	172	
2	R	172	
2	T	172	
2	V	172	
2	X	172	
3	Y	78	
4	Z	287	
5	a	246	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 35530 atoms, of which 0 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 C-phycocyanin alpha subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	162	Total	C	N	O	S	0	0
			1218	768	205	238	7		
1	C	162	Total	C	N	O	S	0	0
			1225	771	205	242	7		
1	E	162	Total	C	N	O	S	0	0
			1225	771	205	242	7		
1	G	162	Total	C	N	O	S	0	0
			1225	771	205	242	7		
1	I	162	Total	C	N	O	S	0	0
			1225	771	205	242	7		
1	K	162	Total	C	N	O	S	0	0
			1225	771	205	242	7		
1	M	162	Total	C	N	O	S	0	0
			1225	771	205	242	7		
1	O	162	Total	C	N	O	S	1	0
			1231	775	206	243	7		
1	Q	162	Total	C	N	O	S	0	0
			1225	771	205	242	7		
1	S	162	Total	C	N	O	S	0	0
			1205	762	202	234	7		
1	U	162	Total	C	N	O	S	0	0
			1225	771	205	242	7		
1	W	162	Total	C	N	O	S	0	0
			1222	770	205	240	7		

- Molecule 2 is a protein called C-phycocyanin beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	172	Total	C	N	O	S	0	0
			1274	789	228	249	8		
2	D	172	Total	C	N	O	S	0	0
			1271	788	228	247	8		
2	F	172	Total	C	N	O	S	0	0
			1274	789	228	249	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	172	Total	C	N	O	S	0	0
			1270	786	227	249	8		
2	J	172	Total	C	N	O	S	0	0
			1274	789	228	249	8		
2	L	172	Total	C	N	O	S	0	0
			1274	789	228	249	8		
2	N	172	Total	C	N	O	S	0	0
			1274	789	228	249	8		
2	P	172	Total	C	N	O	S	0	0
			1274	789	228	249	8		
2	R	172	Total	C	N	O	S	0	0
			1274	789	228	249	8		
2	T	172	Total	C	N	O	S	0	0
			1257	779	226	244	8		
2	V	172	Total	C	N	O	S	0	0
			1270	787	227	248	8		
2	X	172	Total	C	N	O	S	0	0
			1263	783	226	246	8		

- Molecule 3 is a protein called Phycobilisome 8.9 kDa linker polypeptide, phycocyanin-associated, rod.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Y	62	Total	C	N	O	S	0	0
			495	308	94	89	4		

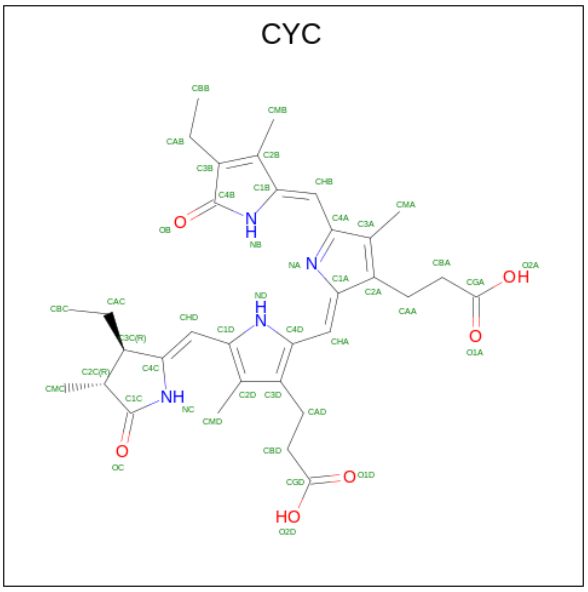
- Molecule 4 is a protein called Phycobilisome 32.1 kDa linker polypeptide, phycocyanin-associated, rod.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Z	282	Total	C	N	O	S	0	0
			2132	1339	382	409	2		

- Molecule 5 is a protein called Phycobilisome rod-core linker polypeptide CpcG2.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	a	185	Total	C	N	O	0	0
			1430	900	251	279		

- Molecule 6 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
6	A	1	Total	C	N	O	0
			43	33	4	6	
6	B	1	Total	C	N	O	0
			86	66	8	12	
6	B	1	Total	C	N	O	0
			86	66	8	12	
6	C	1	Total	C	N	O	0
			43	33	4	6	
6	D	1	Total	C	N	O	0
			86	66	8	12	
6	D	1	Total	C	N	O	0
			86	66	8	12	
6	E	1	Total	C	N	O	0
			43	33	4	6	
6	F	1	Total	C	N	O	0
			86	66	8	12	
6	F	1	Total	C	N	O	0
			86	66	8	12	
6	G	1	Total	C	N	O	0
			43	33	4	6	
6	H	1	Total	C	N	O	0
			86	66	8	12	
6	H	1	Total	C	N	O	0
			86	66	8	12	
6	I	1	Total	C	N	O	0
			43	33	4	6	
6	J	1	Total	C	N	O	0
			86	66	8	12	

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Mol	Chain	Residues	Atoms				AltConf
6	J	1	Total	C	N	O	0
			86	66	8	12	
6	K	1	Total	C	N	O	0
			43	33	4	6	
6	L	1	Total	C	N	O	0
			86	66	8	12	
6	L	1	Total	C	N	O	0
			86	66	8	12	
6	M	1	Total	C	N	O	0
			43	33	4	6	
6	N	1	Total	C	N	O	0
			86	66	8	12	
6	N	1	Total	C	N	O	0
			86	66	8	12	
6	O	1	Total	C	N	O	0
			43	33	4	6	
6	P	1	Total	C	N	O	0
			86	66	8	12	
6	P	1	Total	C	N	O	0
			86	66	8	12	
6	Q	1	Total	C	N	O	0
			43	33	4	6	
6	R	1	Total	C	N	O	0
			86	66	8	12	
6	R	1	Total	C	N	O	0
			86	66	8	12	
6	S	1	Total	C	N	O	0
			43	33	4	6	
6	T	1	Total	C	N	O	0
			86	66	8	12	
6	T	1	Total	C	N	O	0
			86	66	8	12	
6	U	1	Total	C	N	O	0
			43	33	4	6	
6	V	1	Total	C	N	O	0
			86	66	8	12	
6	V	1	Total	C	N	O	0
			86	66	8	12	
6	W	1	Total	C	N	O	0
			43	33	4	6	
6	X	1	Total	C	N	O	0
			86	66	8	12	

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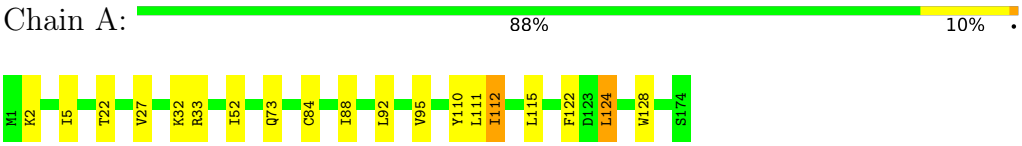
Mol	Chain	Residues	Atoms				AltConf
6	X	1	Total	C	N	O	0
			86	66	8	12	

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.

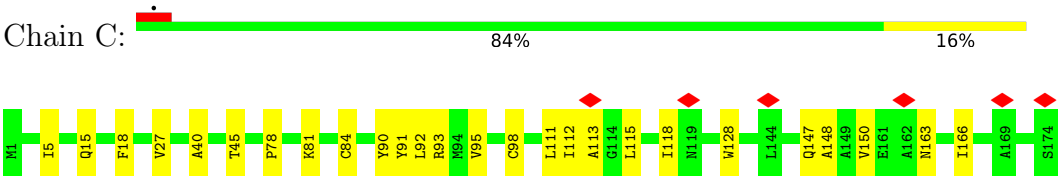
• Molecule 1: C-phycocyanin alpha subunit

Chain A:



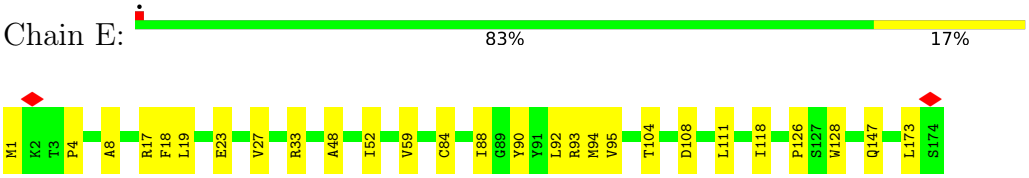
• Molecule 1: C-phycocyanin alpha subunit

Chain C:



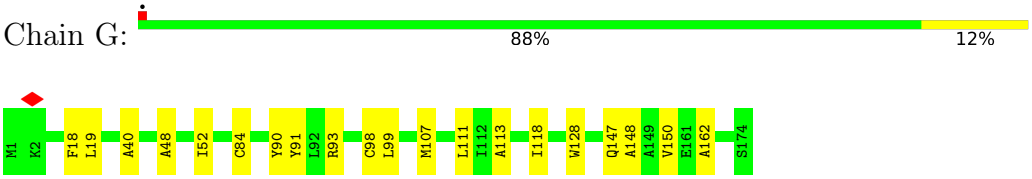
• Molecule 1: C-phycocyanin alpha subunit

Chain E:



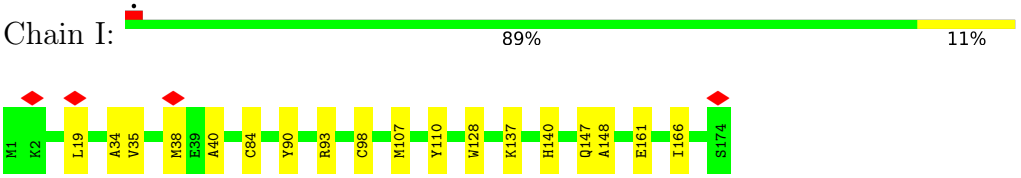
• Molecule 1: C-phycocyanin alpha subunit

Chain G:



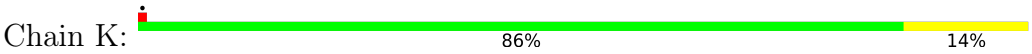
• Molecule 1: C-phycocyanin alpha subunit

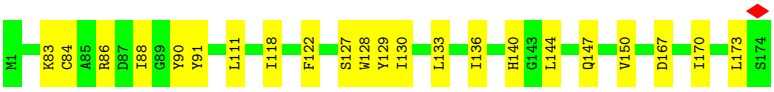
Chain I:



• Molecule 1: C-phycocyanin alpha subunit

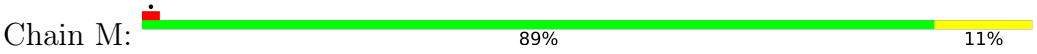
Chain K:

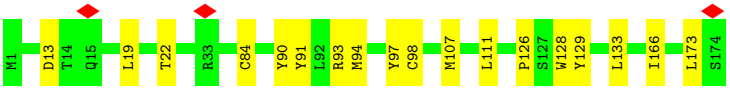




• Molecule 1: C-phycocyanin alpha subunit

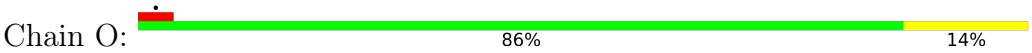
Chain M:

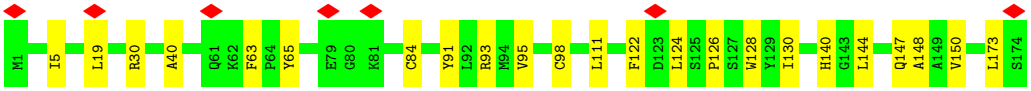




• Molecule 1: C-phycocyanin alpha subunit

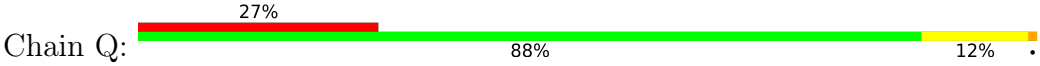
Chain O:

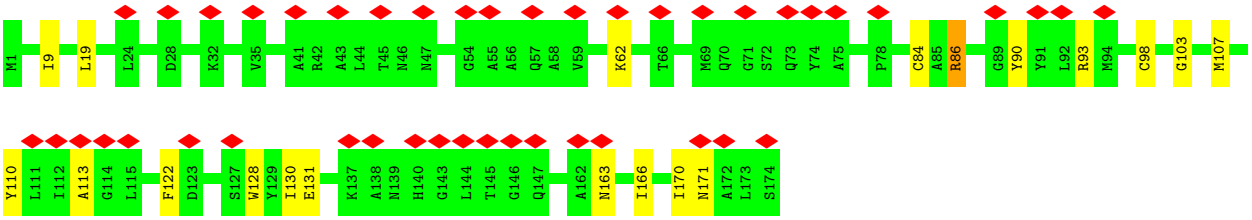




• Molecule 1: C-phycocyanin alpha subunit

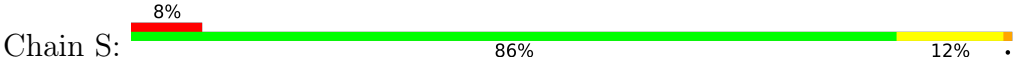
Chain Q:

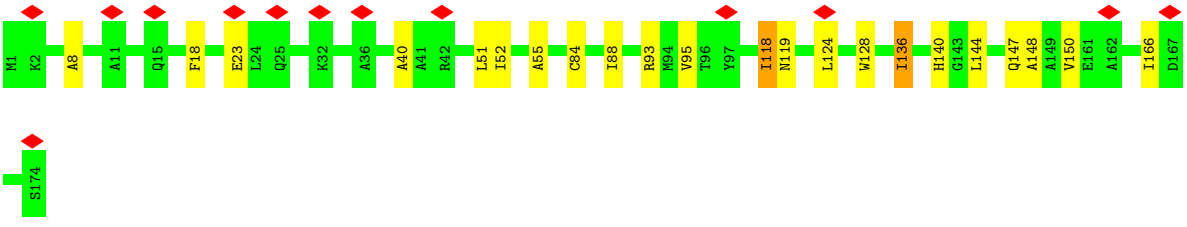




• Molecule 1: C-phycocyanin alpha subunit

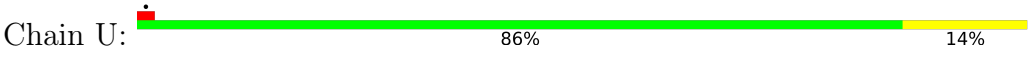
Chain S:

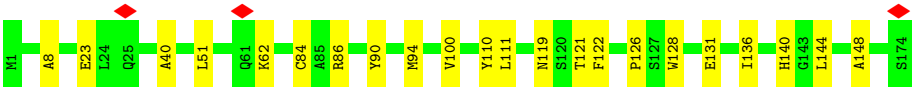




• Molecule 1: C-phycocyanin alpha subunit

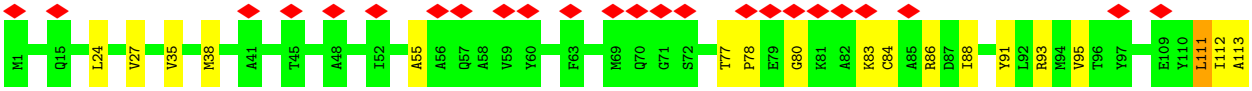
Chain U:

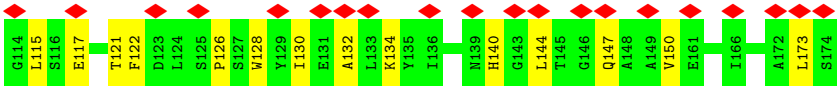




• Molecule 1: C-phycocyanin alpha subunit

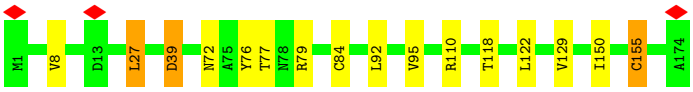
Chain W:





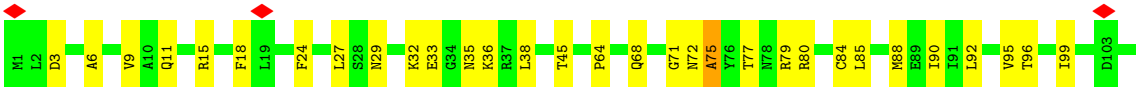
• Molecule 2: C-phycocyanin beta subunit

Chain B:



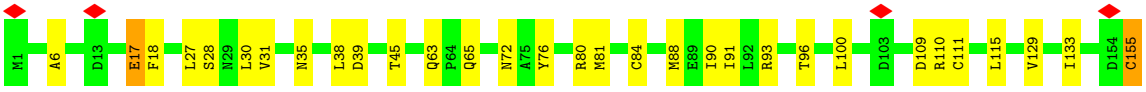
• Molecule 2: C-phycocyanin beta subunit

Chain D:



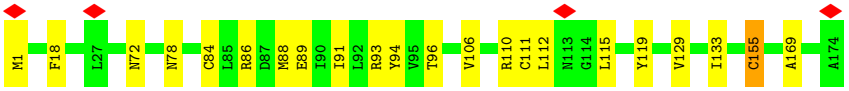
• Molecule 2: C-phycocyanin beta subunit

Chain F:



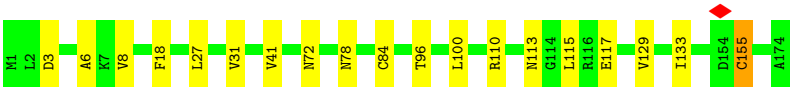
• Molecule 2: C-phycocyanin beta subunit

Chain H:



• Molecule 2: C-phycocyanin beta subunit

Chain J:

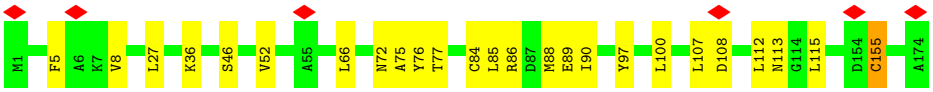


• Molecule 2: C-phycocyanin beta subunit

Chain L:

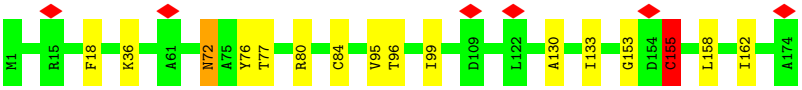
• Molecule 2: C-phycocyanin beta subunit

Chain N:



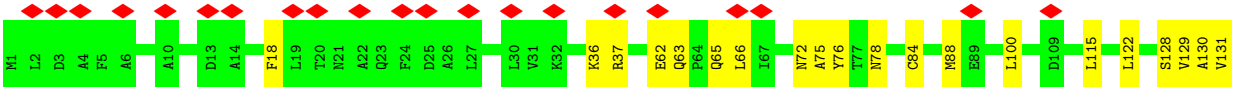
• Molecule 2: C-phycocyanin beta subunit

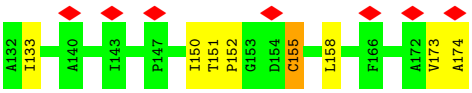
Chain P:



• Molecule 2: C-phycocyanin beta subunit

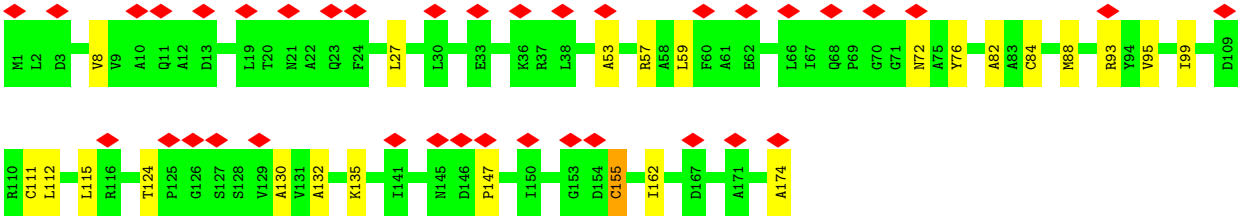
Chain R:





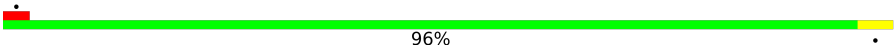
• Molecule 2: C-phycocyanin beta subunit

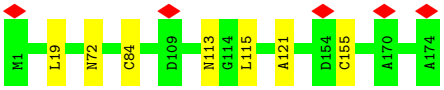
Chain T:



• Molecule 2: C-phycocyanin beta subunit

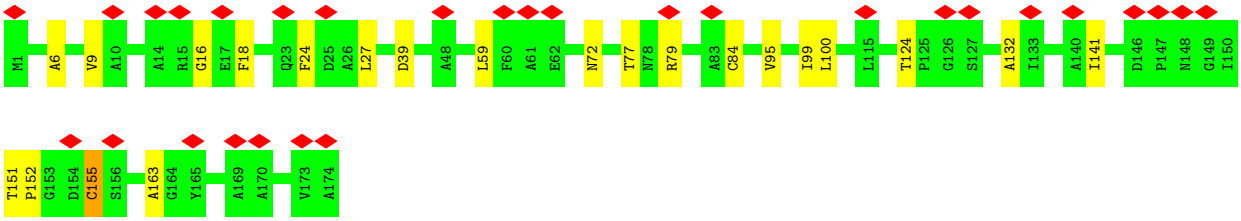
Chain V:





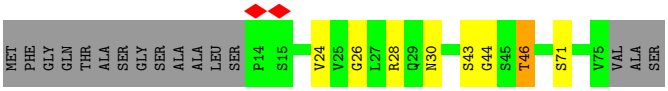
• Molecule 2: C-phycocyanin beta subunit

Chain X:



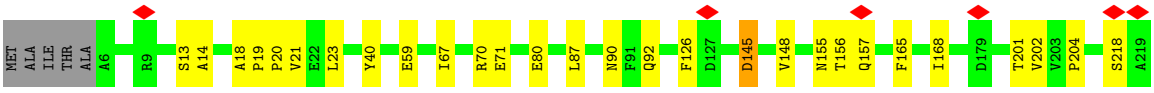
• Molecule 3: Phycobilisome 8.9 kDa linker polypeptide, phycocyanin-associated, rod

Chain Y:



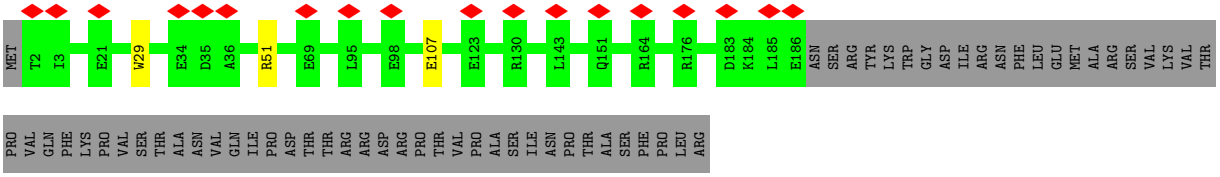
• Molecule 4: Phycobilisome 32.1 kDa linker polypeptide, phycocyanin-associated, rod

Chain Z:



• Molecule 5: Phycobilisome rod-core linker polypeptide CpcG2

Chain a:


MET T2 I3 E21 W29 E34 D35 A36 R51 E69 L95 E98 E107 E123 R130 L143 Q151 R164 R176 D183 K184 L185 E186 ASN SER ARG TYR LYS TRP GLY ASP ILE ARG ASN PHE LEU GLU MET ALA ARG SER VAL LYS VAL THR
PRO VAL GLN PHE LYS PRO VAL SER THR ALA ASN VAL GLN ILE PRO ASP THR THR ARG ARG ASP ARG PRO THR VAL PRO ALA SER ILE ASN PRO THR ALA SER PHE PRO LEU ARG

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	159537	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.150	Depositor
Minimum map value	-0.095	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0286	Depositor
Map size (Å)	297.6, 297.6, 297.6	wwPDB
Map dimensions	160, 160, 160	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.86, 1.86, 1.86	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.31	0/1240	0.48	0/1682
1	C	0.31	0/1247	0.50	0/1691
1	E	0.31	0/1247	0.47	0/1691
1	G	0.32	0/1247	0.48	0/1691
1	I	0.31	0/1247	0.47	0/1691
1	K	0.31	0/1247	0.49	0/1691
1	M	0.30	0/1247	0.47	0/1691
1	O	0.30	0/1256	0.48	0/1703
1	Q	0.30	0/1247	0.48	0/1691
1	S	0.29	0/1227	0.49	0/1666
1	U	0.29	0/1247	0.48	0/1691
1	W	0.30	0/1244	0.48	0/1687
2	B	0.31	0/1278	0.54	1/1729 (0.1%)
2	D	0.29	0/1275	0.54	0/1725
2	F	0.31	0/1278	0.53	1/1729 (0.1%)
2	H	0.33	0/1274	0.56	1/1725 (0.1%)
2	J	0.32	0/1278	0.52	1/1729 (0.1%)
2	L	0.34	0/1278	0.54	0/1729
2	N	0.33	0/1278	0.53	1/1729 (0.1%)
2	P	0.32	0/1278	0.54	1/1729 (0.1%)
2	R	0.40	1/1278 (0.1%)	0.55	1/1729 (0.1%)
2	T	0.35	1/1261 (0.1%)	0.54	1/1708 (0.1%)
2	V	0.33	0/1274	0.53	0/1724
2	X	0.28	0/1267	0.56	1/1716 (0.1%)
3	Y	0.28	0/503	0.61	0/675
4	Z	0.32	0/2177	0.55	0/2962
5	a	0.29	0/1461	0.50	0/1998
All	All	0.31	2/34381 (0.0%)	0.51	9/46602 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	155	CYS	CB-SG	9.84	1.99	1.82
2	T	155	CYS	CB-SG	6.11	1.92	1.82

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	X	155	CYS	CA-CB-SG	9.96	131.93	114.00
2	H	155	CYS	CA-CB-SG	8.95	130.10	114.00
2	R	155	CYS	CA-CB-SG	7.86	128.14	114.00
2	T	155	CYS	CA-CB-SG	6.51	125.71	114.00
2	F	155	CYS	CA-CB-SG	5.96	124.73	114.00

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	A	1218	0	1197	20	0
1	C	1225	0	1203	21	0
1	E	1225	0	1203	26	0
1	G	1225	0	1203	18	0
1	I	1225	0	1203	19	0
1	K	1225	0	1203	22	0
1	M	1225	0	1203	19	0
1	O	1231	0	1211	18	0
1	Q	1225	0	1203	18	0
1	S	1205	0	1180	20	0
1	U	1225	0	1203	19	0
1	W	1222	0	1201	26	0
2	B	1274	0	1277	20	0
2	D	1271	0	1275	36	0
2	F	1274	0	1277	29	0
2	H	1270	0	1266	22	0
2	J	1274	0	1277	18	0
2	L	1274	0	1277	20	0
2	N	1274	0	1277	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	P	1274	0	1277	20	0
2	R	1274	0	1277	22	0
2	T	1257	0	1247	20	0
2	V	1270	0	1271	11	0
2	X	1263	0	1258	22	0
3	Y	495	0	498	10	0
4	Z	2132	0	2016	29	0
5	a	1430	0	1309	0	0
6	A	43	0	38	7	0
6	B	86	0	75	17	0
6	C	43	0	37	5	0
6	D	86	0	76	19	0
6	E	43	0	38	11	0
6	F	86	0	76	18	0
6	G	43	0	38	7	0
6	H	86	0	76	13	0
6	I	43	0	37	10	0
6	J	86	0	76	14	0
6	K	43	0	38	13	0
6	L	86	0	76	16	0
6	M	43	0	38	9	0
6	N	86	0	76	17	0
6	O	43	0	38	7	0
6	P	86	0	76	12	0
6	Q	43	0	38	7	0
6	R	86	0	76	12	0
6	S	43	0	38	7	0
6	T	86	0	76	9	0
6	U	43	0	38	9	0
6	V	86	0	76	13	0
6	W	43	0	37	7	0
6	X	86	0	76	14	0
All	All	35530	0	34856	543	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 8.

The worst 5 of 543 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)
1:M:84:CYS:SG	6:M:201:CYC:HAC2	1.39	1.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:84:CYS:SG	6:Q:201:CYC:HAC2	1.39	1.61
1:A:84:CYS:SG	6:A:201:CYC:HAC2	1.40	1.61
1:C:84:CYS:SG	6:C:201:CYC:HAC2	1.36	1.60
1:K:84:CYS:SG	6:K:201:CYC:HAC2	1.44	1.58

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	A	160/162 (99%)	157 (98%)	2 (1%)	1 (1%)	25 64
1	C	160/162 (99%)	157 (98%)	3 (2%)	0	100 100
1	E	160/162 (99%)	157 (98%)	3 (2%)	0	100 100
1	G	160/162 (99%)	158 (99%)	2 (1%)	0	100 100
1	I	160/162 (99%)	157 (98%)	3 (2%)	0	100 100
1	K	160/162 (99%)	157 (98%)	3 (2%)	0	100 100
1	M	160/162 (99%)	157 (98%)	3 (2%)	0	100 100
1	O	161/162 (99%)	158 (98%)	3 (2%)	0	100 100
1	Q	160/162 (99%)	156 (98%)	4 (2%)	0	100 100
1	S	160/162 (99%)	156 (98%)	4 (2%)	0	100 100
1	U	160/162 (99%)	158 (99%)	2 (1%)	0	100 100
1	W	160/162 (99%)	156 (98%)	4 (2%)	0	100 100
2	B	169/172 (98%)	164 (97%)	5 (3%)	0	100 100
2	D	169/172 (98%)	162 (96%)	6 (4%)	1 (1%)	25 64
2	F	169/172 (98%)	164 (97%)	5 (3%)	0	100 100
2	H	169/172 (98%)	165 (98%)	4 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	J	169/172 (98%)	165 (98%)	4 (2%)	0	100	100
2	L	169/172 (98%)	165 (98%)	4 (2%)	0	100	100
2	N	169/172 (98%)	165 (98%)	4 (2%)	0	100	100
2	P	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
2	R	169/172 (98%)	165 (98%)	4 (2%)	0	100	100
2	T	169/172 (98%)	165 (98%)	4 (2%)	0	100	100
2	V	169/172 (98%)	166 (98%)	3 (2%)	0	100	100
2	X	169/172 (98%)	167 (99%)	2 (1%)	0	100	100
3	Y	60/78 (77%)	57 (95%)	3 (5%)	0	100	100
4	Z	280/287 (98%)	258 (92%)	22 (8%)	0	100	100
5	a	183/246 (74%)	173 (94%)	10 (6%)	0	100	100
All	All	4472/4619 (97%)	4349 (97%)	121 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	112	ILE
2	D	75	ALA

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	A	121/123 (98%)	120 (99%)	1 (1%)	81	89
1	C	123/123 (100%)	123 (100%)	0	100	100
1	E	123/123 (100%)	123 (100%)	0	100	100
1	G	123/123 (100%)	123 (100%)	0	100	100
1	I	123/123 (100%)	123 (100%)	0	100	100
1	K	123/123 (100%)	123 (100%)	0	100	100
1	M	123/123 (100%)	123 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	O	124/123 (101%)	122 (98%)	2 (2%)	62 79
1	Q	123/123 (100%)	122 (99%)	1 (1%)	81 89
1	S	118/123 (96%)	116 (98%)	2 (2%)	60 78
1	U	123/123 (100%)	123 (100%)	0	100 100
1	W	122/123 (99%)	121 (99%)	1 (1%)	81 89
2	B	127/127 (100%)	125 (98%)	2 (2%)	62 79
2	D	126/127 (99%)	126 (100%)	0	100 100
2	F	127/127 (100%)	126 (99%)	1 (1%)	81 89
2	H	126/127 (99%)	126 (100%)	0	100 100
2	J	127/127 (100%)	127 (100%)	0	100 100
2	L	127/127 (100%)	126 (99%)	1 (1%)	81 89
2	N	127/127 (100%)	127 (100%)	0	100 100
2	P	127/127 (100%)	126 (99%)	1 (1%)	81 89
2	R	127/127 (100%)	126 (99%)	1 (1%)	81 89
2	T	122/127 (96%)	122 (100%)	0	100 100
2	V	126/127 (99%)	126 (100%)	0	100 100
2	X	124/127 (98%)	124 (100%)	0	100 100
3	Y	54/66 (82%)	53 (98%)	1 (2%)	57 74
4	Z	212/238 (89%)	206 (97%)	6 (3%)	43 65
5	a	143/224 (64%)	140 (98%)	3 (2%)	53 71
All	All	3391/3528 (96%)	3368 (99%)	23 (1%)	84 90

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	Z	21	VAL
4	Z	233	GLU
4	Z	145	ASP
4	Z	242	VAL
1	O	111	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	35	ASN
1	O	140	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	MEN	R	72	2	7,8,9	1.17	1 (14%)	6,9,11	0.92	0
2	MEN	F	72	2	7,8,9	1.18	1 (14%)	6,9,11	1.65	2 (33%)
2	MEN	H	72	2	7,8,9	1.19	1 (14%)	6,9,11	1.29	1 (16%)
2	MEN	L	72	2	7,8,9	1.17	1 (14%)	6,9,11	1.10	0
2	MEN	N	72	2	7,8,9	1.23	1 (14%)	6,9,11	0.89	0
2	MEN	J	72	2	7,8,9	1.18	1 (14%)	6,9,11	1.15	1 (16%)
2	MEN	B	72	2	7,8,9	1.16	1 (14%)	6,9,11	1.38	2 (33%)
2	MEN	T	72	2	7,8,9	1.15	1 (14%)	6,9,11	1.04	1 (16%)
2	MEN	D	72	2	7,8,9	1.17	1 (14%)	6,9,11	1.09	1 (16%)
2	MEN	P	72	2	7,8,9	1.15	1 (14%)	6,9,11	1.31	2 (33%)
2	MEN	X	72	2	7,8,9	1.18	1 (14%)	6,9,11	1.18	1 (16%)
2	MEN	V	72	2	7,8,9	1.16	1 (14%)	6,9,11	1.66	2 (33%)

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
2	MEN	R	72	2	-	4/7/8/10	-
2	MEN	F	72	2	-	4/7/8/10	-
2	MEN	H	72	2	-	5/7/8/10	-
2	MEN	L	72	2	-	3/7/8/10	-
2	MEN	N	72	2	-	4/7/8/10	-
2	MEN	J	72	2	-	4/7/8/10	-
2	MEN	B	72	2	-	4/7/8/10	-
2	MEN	T	72	2	-	4/7/8/10	-
2	MEN	D	72	2	-	4/7/8/10	-
2	MEN	P	72	2	-	4/7/8/10	-
2	MEN	X	72	2	-	4/7/8/10	-
2	MEN	V	72	2	-	2/7/8/10	-

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	72	MEN	CE2-ND2	2.98	1.50	1.45
2	J	72	MEN	CE2-ND2	2.94	1.50	1.45
2	R	72	MEN	CE2-ND2	2.90	1.50	1.45
2	D	72	MEN	CE2-ND2	2.89	1.50	1.45
2	X	72	MEN	CE2-ND2	2.88	1.50	1.45

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	72	MEN	CA-CB-CG	-3.12	103.82	112.70
2	V	72	MEN	CA-CB-CG	-2.78	104.79	112.70
2	V	72	MEN	CB-CA-C	-2.70	106.41	111.47
2	B	72	MEN	CB-CA-C	-2.40	106.98	111.47
2	J	72	MEN	CB-CA-C	-2.32	107.12	111.47

There are no chirality outliers.

5 of 46 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	72	MEN	C-CA-CB-CG
2	F	72	MEN	C-CA-CB-CG
2	H	72	MEN	O-C-CA-CB
2	H	72	MEN	C-CA-CB-CG
2	J	72	MEN	C-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	P	72	MEN	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

36 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	$\#\|Z\| > 2$
6	CYC	R	202	-	42,46,46	2.09	13 (30%)	50,67,67	3.66	27 (54%)
6	CYC	Q	201	-	42,46,46	2.13	12 (28%)	50,67,67	4.88	20 (40%)
6	CYC	X	201	-	42,46,46	2.17	13 (30%)	50,67,67	3.58	24 (48%)
6	CYC	U	201	-	42,46,46	2.13	13 (30%)	50,67,67	3.28	19 (38%)
6	CYC	C	201	-	42,46,46	2.09	12 (28%)	50,67,67	3.42	22 (44%)
6	CYC	P	202	-	42,46,46	2.13	14 (33%)	50,67,67	3.49	23 (46%)
6	CYC	S	201	-	42,46,46	2.12	12 (28%)	50,67,67	3.40	20 (40%)
6	CYC	F	201	-	42,46,46	2.12	11 (26%)	50,67,67	3.57	26 (52%)
6	CYC	X	202	-	42,46,46	2.06	12 (28%)	50,67,67	3.61	24 (48%)
6	CYC	M	201	-	42,46,46	2.15	13 (30%)	50,67,67	3.33	21 (42%)
6	CYC	J	201	-	42,46,46	2.19	12 (28%)	50,67,67	3.37	23 (46%)
6	CYC	R	201	-	42,46,46	2.15	12 (28%)	50,67,67	3.39	22 (44%)
6	CYC	L	201	-	42,46,46	2.13	12 (28%)	50,67,67	3.37	20 (40%)
6	CYC	P	201	-	42,46,46	2.13	12 (28%)	50,67,67	3.40	23 (46%)
6	CYC	E	201	-	42,46,46	2.18	13 (30%)	50,67,67	3.33	20 (40%)
6	CYC	V	201	-	42,46,46	2.14	11 (26%)	50,67,67	3.27	19 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	CYC	D	202	-	42,46,46	2.22	15 (35%)	50,67,67	3.44	23 (46%)
6	CYC	A	201	-	42,46,46	2.08	12 (28%)	50,67,67	3.48	21 (42%)
6	CYC	L	202	-	42,46,46	2.10	13 (30%)	50,67,67	3.43	24 (48%)
6	CYC	B	201	-	42,46,46	2.09	13 (30%)	50,67,67	3.42	20 (40%)
6	CYC	I	201	-	42,46,46	2.13	13 (30%)	50,67,67	3.26	22 (44%)
6	CYC	N	202	-	42,46,46	2.09	12 (28%)	50,67,67	3.41	23 (46%)
6	CYC	B	202	-	42,46,46	2.19	12 (28%)	50,67,67	3.48	29 (58%)
6	CYC	W	201	-	42,46,46	2.15	14 (33%)	50,67,67	3.39	24 (48%)
6	CYC	H	201	-	42,46,46	2.22	11 (26%)	50,67,67	3.44	23 (46%)
6	CYC	F	202	-	42,46,46	2.20	15 (35%)	50,67,67	3.42	20 (40%)
6	CYC	T	202	-	42,46,46	2.10	13 (30%)	50,67,67	3.42	22 (44%)
6	CYC	J	202	-	42,46,46	2.19	13 (30%)	50,67,67	3.39	28 (56%)
6	CYC	T	201	-	42,46,46	2.20	11 (26%)	50,67,67	3.52	23 (46%)
6	CYC	H	202	-	42,46,46	2.06	13 (30%)	50,67,67	3.57	25 (50%)
6	CYC	G	201	-	42,46,46	2.15	11 (26%)	50,67,67	3.52	23 (46%)
6	CYC	O	201	-	42,46,46	2.11	12 (28%)	50,67,67	3.44	22 (44%)
6	CYC	N	201	-	42,46,46	2.22	11 (26%)	50,67,67	3.41	23 (46%)
6	CYC	K	201	-	42,46,46	2.12	13 (30%)	50,67,67	3.36	21 (42%)
6	CYC	V	202	-	42,46,46	2.17	13 (30%)	50,67,67	3.26	24 (48%)
6	CYC	D	201	-	42,46,46	2.13	12 (28%)	50,67,67	3.45	23 (46%)

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
6	CYC	R	202	-	-	9/25/74/74	0/4/4/4
6	CYC	Q	201	-	-	9/25/74/74	0/4/4/4
6	CYC	X	201	-	-	15/25/74/74	0/4/4/4
6	CYC	U	201	-	-	9/25/74/74	0/4/4/4
6	CYC	C	201	-	-	11/25/74/74	0/4/4/4
6	CYC	P	202	-	-	12/25/74/74	0/4/4/4
6	CYC	S	201	-	-	8/25/74/74	0/4/4/4
6	CYC	F	201	-	-	12/25/74/74	0/4/4/4
6	CYC	X	202	-	-	13/25/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	CYC	M	201	-	-	8/25/74/74	0/4/4/4
6	CYC	J	201	-	-	12/25/74/74	0/4/4/4
6	CYC	R	201	-	-	13/25/74/74	0/4/4/4
6	CYC	L	201	-	-	11/25/74/74	0/4/4/4
6	CYC	P	201	-	-	11/25/74/74	0/4/4/4
6	CYC	E	201	-	-	8/25/74/74	0/4/4/4
6	CYC	V	201	-	-	10/25/74/74	0/4/4/4
6	CYC	D	202	-	-	18/25/74/74	0/4/4/4
6	CYC	A	201	-	-	11/25/74/74	0/4/4/4
6	CYC	L	202	-	-	14/25/74/74	0/4/4/4
6	CYC	B	201	-	-	7/25/74/74	0/4/4/4
6	CYC	I	201	-	-	10/25/74/74	0/4/4/4
6	CYC	N	202	-	-	9/25/74/74	0/4/4/4
6	CYC	B	202	-	-	10/25/74/74	0/4/4/4
6	CYC	W	201	-	-	10/25/74/74	0/4/4/4
6	CYC	H	201	-	-	8/25/74/74	0/4/4/4
6	CYC	F	202	-	-	16/25/74/74	0/4/4/4
6	CYC	T	202	-	-	13/25/74/74	0/4/4/4
6	CYC	J	202	-	-	14/25/74/74	0/4/4/4
6	CYC	T	201	-	-	13/25/74/74	0/4/4/4
6	CYC	H	202	-	-	17/25/74/74	0/4/4/4
6	CYC	G	201	-	-	10/25/74/74	0/4/4/4
6	CYC	O	201	-	-	6/25/74/74	0/4/4/4
6	CYC	N	201	-	-	11/25/74/74	0/4/4/4
6	CYC	K	201	-	-	11/25/74/74	0/4/4/4
6	CYC	V	202	-	-	9/25/74/74	0/4/4/4
6	CYC	D	201	-	-	10/25/74/74	0/4/4/4

The worst 5 of 449 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	N	201	CYC	C1C-NC	-7.07	1.28	1.37
6	T	201	CYC	OB-C4B	6.93	1.36	1.23
6	Q	201	CYC	OB-C4B	6.93	1.36	1.23
6	X	201	CYC	OB-C4B	6.92	1.36	1.23
6	V	201	CYC	OB-C4B	6.88	1.36	1.23

The worst 5 of 816 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	Q	201	CYC	O1A-CGA-CBA	-15.17	74.34	123.08
6	Q	201	CYC	O2A-CGA-O1A	-15.07	85.75	123.30
6	Q	201	CYC	O2A-CGA-CBA	14.33	160.09	114.03
6	X	202	CYC	C3B-C4B-NB	13.54	117.72	106.78
6	R	202	CYC	C3B-C4B-NB	13.39	117.59	106.78

There are no chirality outliers.

5 of 398 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	201	CYC	NA-C4A-CHB-C1B
6	A	201	CYC	C3A-C4A-CHB-C1B
6	A	201	CYC	NC-C4C-CHD-C1D
6	A	201	CYC	ND-C1D-CHD-C4C
6	A	201	CYC	C2D-C1D-CHD-C4C

There are no ring outliers.

36 monomers are involved in 273 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	R	202	CYC	5	0
6	Q	201	CYC	7	0
6	X	201	CYC	7	0
6	U	201	CYC	9	0
6	C	201	CYC	5	0
6	P	202	CYC	6	0
6	S	201	CYC	7	0
6	F	201	CYC	10	0
6	X	202	CYC	7	0
6	M	201	CYC	9	0
6	J	201	CYC	7	0
6	R	201	CYC	7	0
6	L	201	CYC	9	0
6	P	201	CYC	6	0
6	E	201	CYC	11	0
6	V	201	CYC	6	0
6	D	202	CYC	10	0
6	A	201	CYC	7	0
6	L	202	CYC	7	0
6	B	201	CYC	5	0
6	I	201	CYC	10	0

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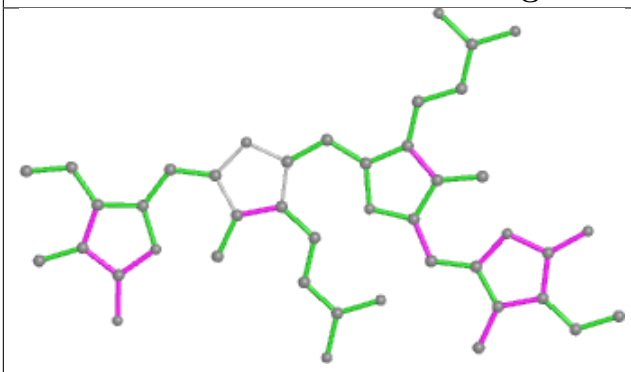
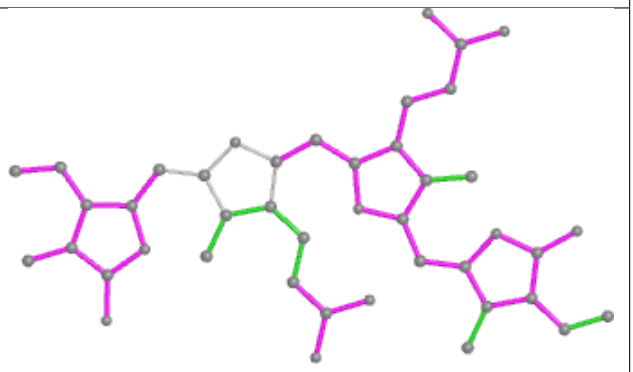
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	N	202	CYC	6	0
6	B	202	CYC	12	0
6	W	201	CYC	7	0
6	H	201	CYC	9	0
6	F	202	CYC	8	0
6	T	202	CYC	3	0
6	J	202	CYC	7	0
6	T	201	CYC	6	0
6	H	202	CYC	4	0
6	G	201	CYC	7	0
6	O	201	CYC	7	0
6	N	201	CYC	11	0
6	K	201	CYC	13	0
6	V	202	CYC	7	0
6	D	201	CYC	9	0

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.

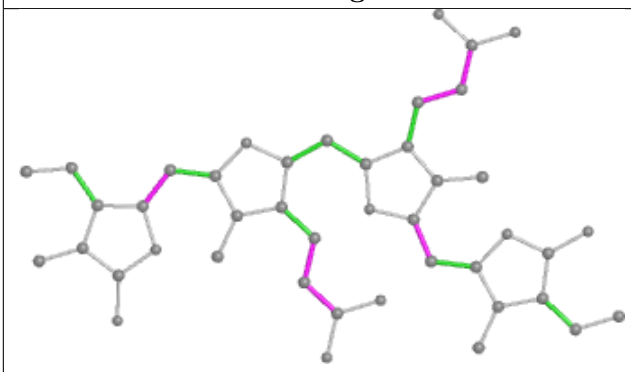
Ligand CYC R 202



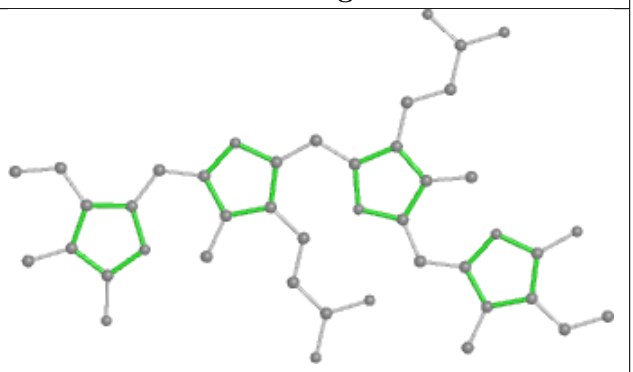
Bond lengths



Bond angles

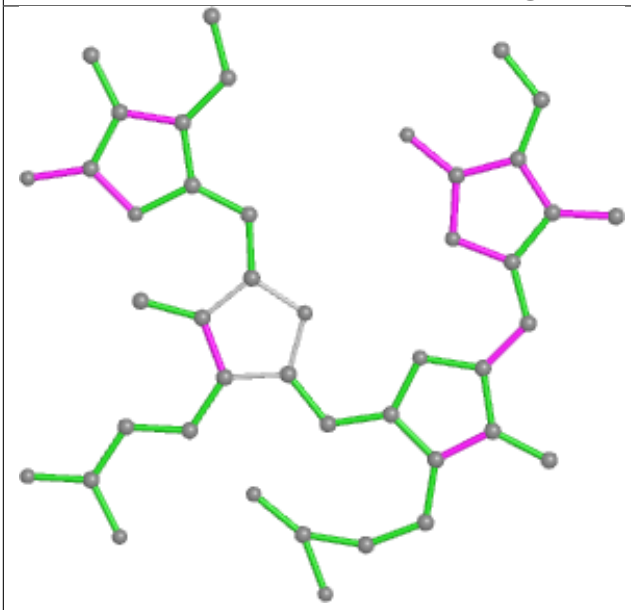


Torsions

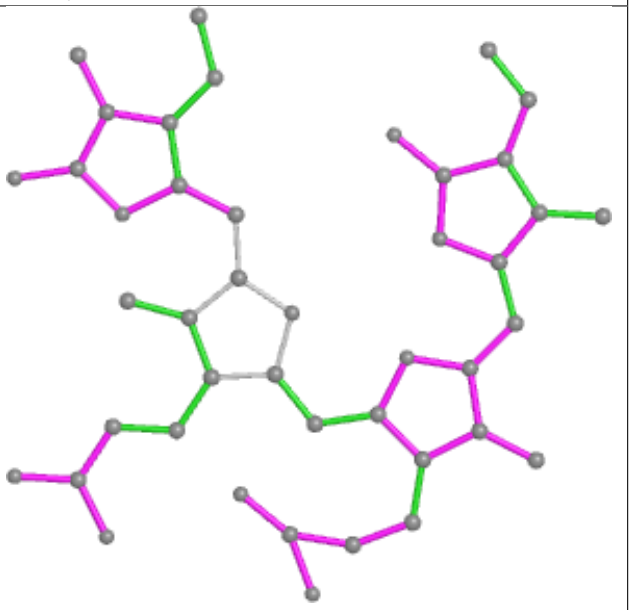


Rings

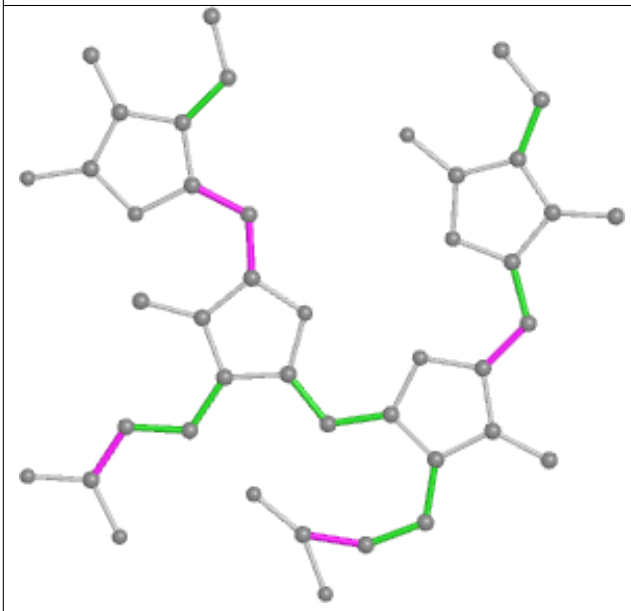
Ligand CYC Q 201



Bond lengths



Bond angles



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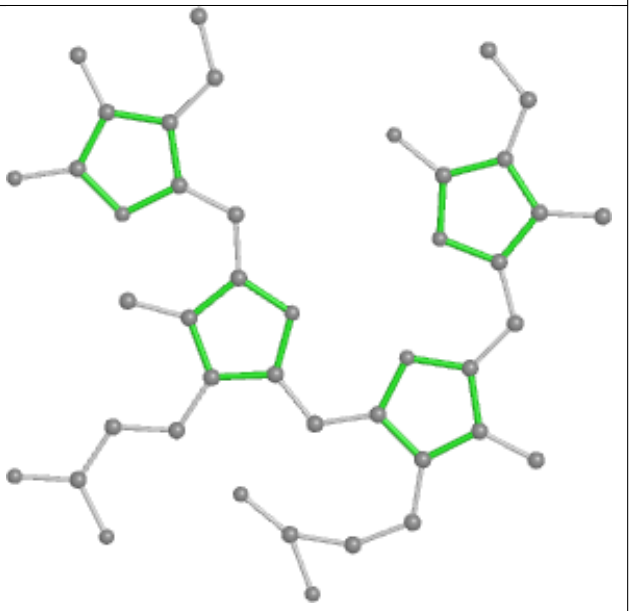
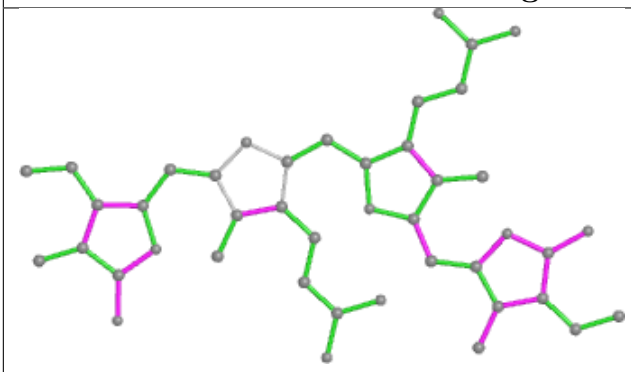
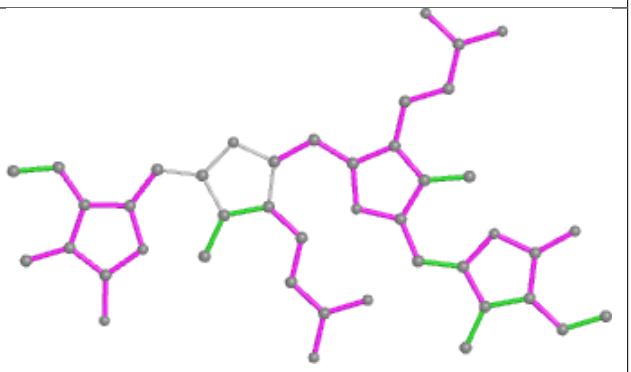


Rings

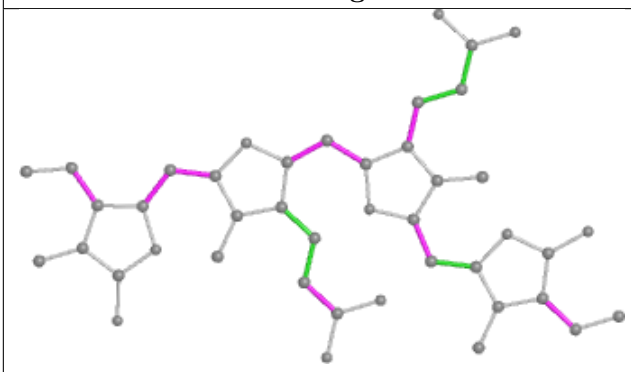
Ligand CYC X 201



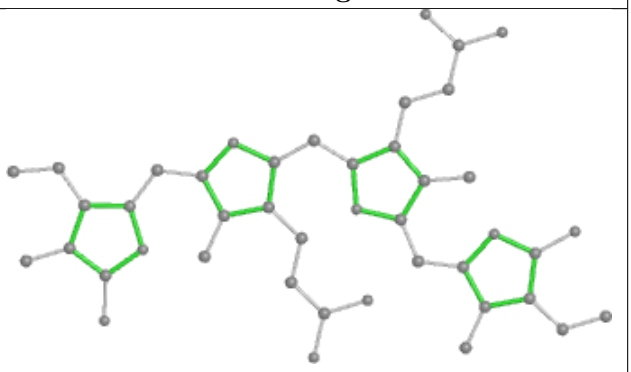
Bond lengths



Bond angles

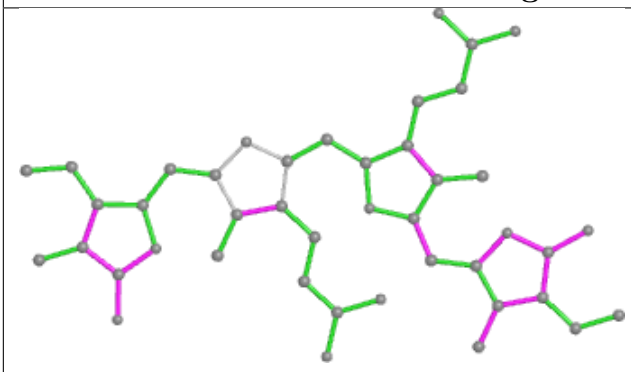


Torsions

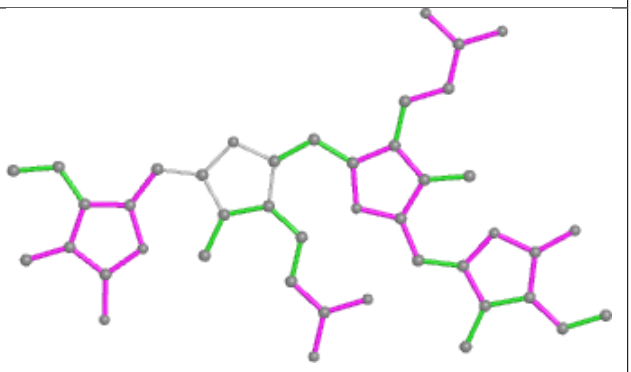


Rings

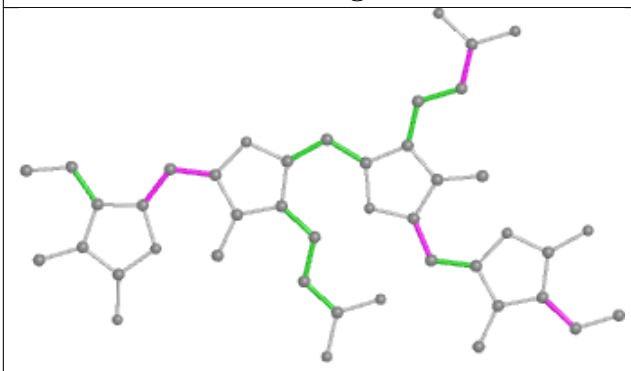
Ligand CYC U 201



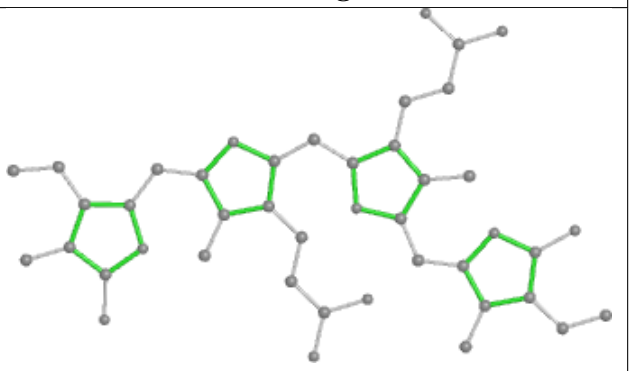
Bond lengths



Bond angles

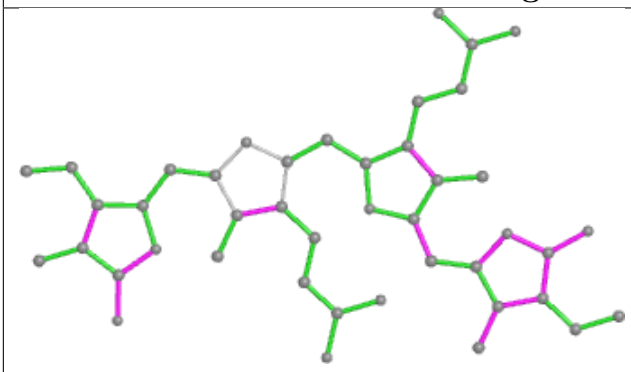


Torsions

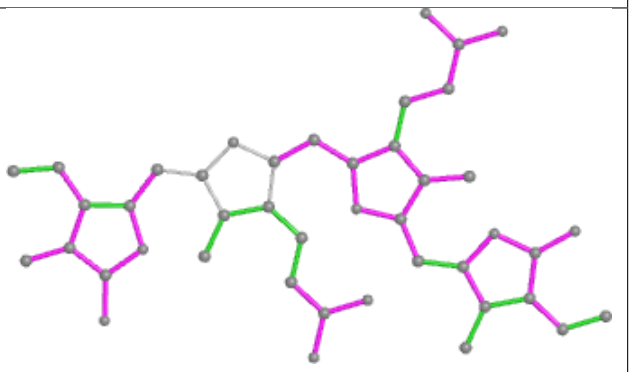


Rings

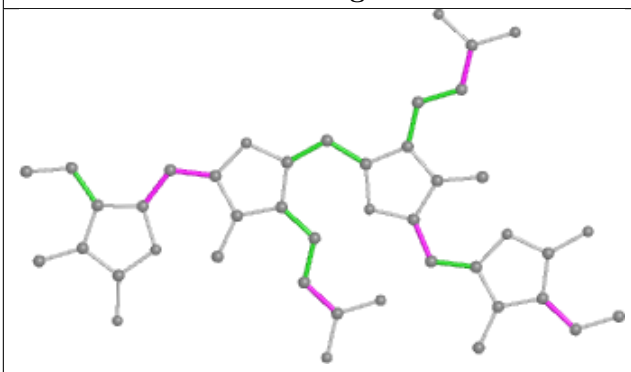
Ligand CYC C 201



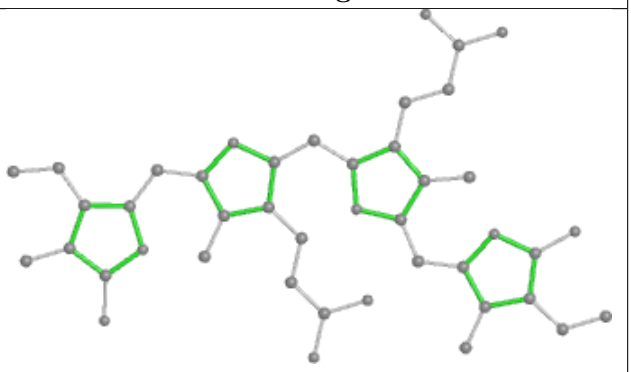
Bond lengths



Bond angles

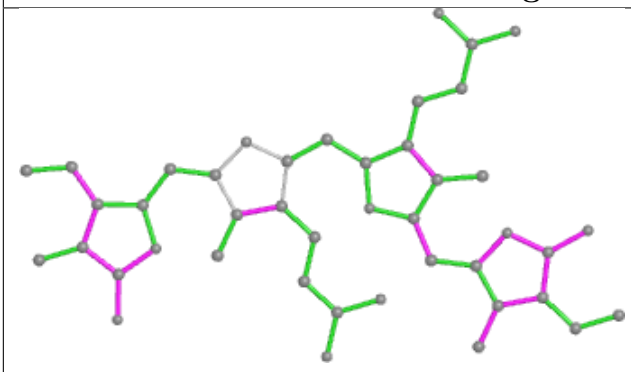


Torsions



Rings

Ligand CYC P 202



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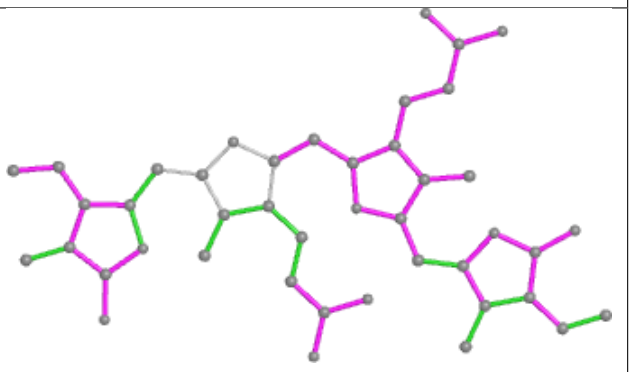

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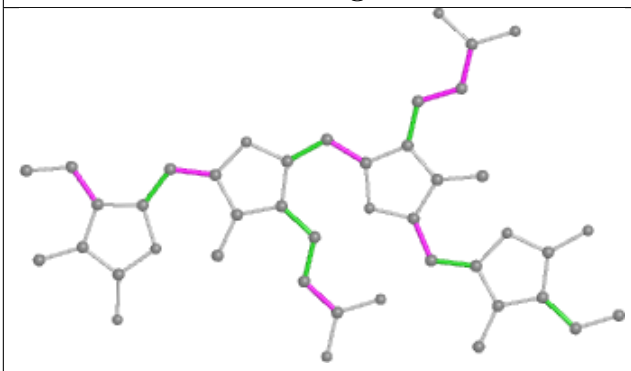

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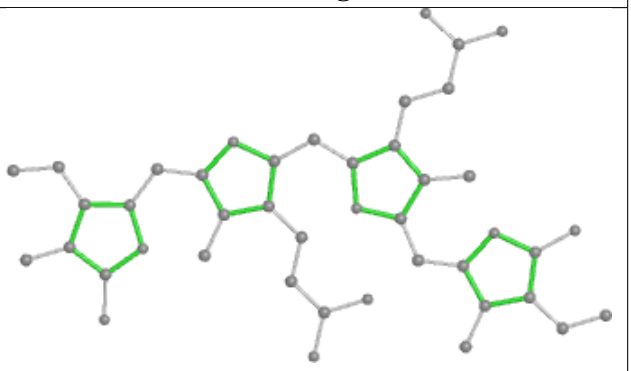
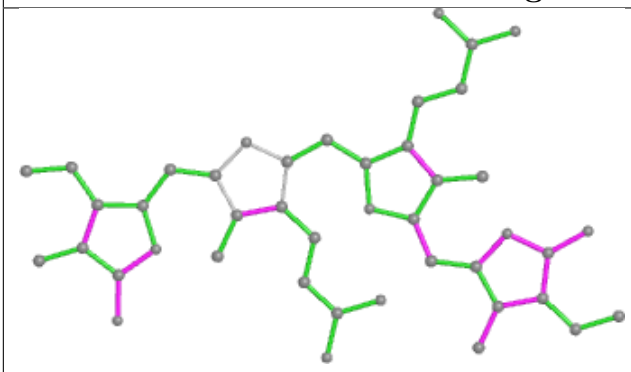
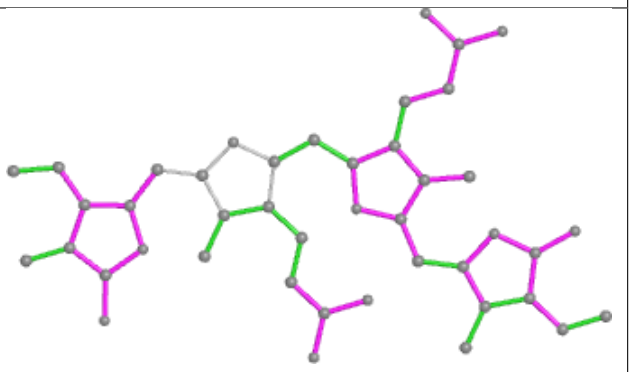


Rings

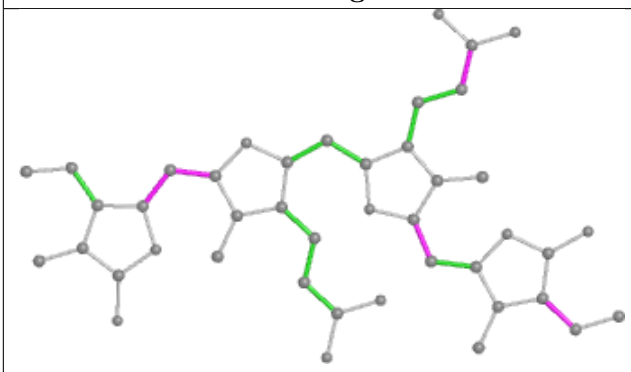
Ligand CYC S 201



Bond lengths



Bond angles



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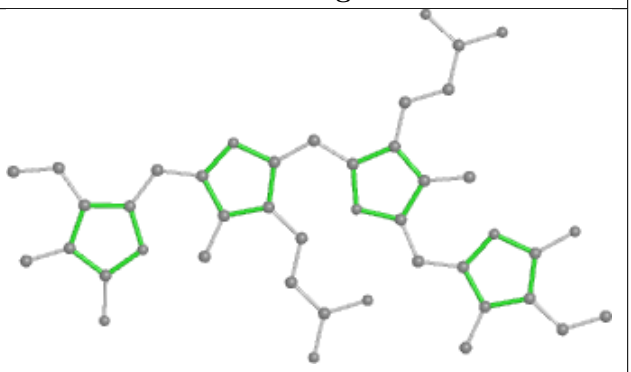
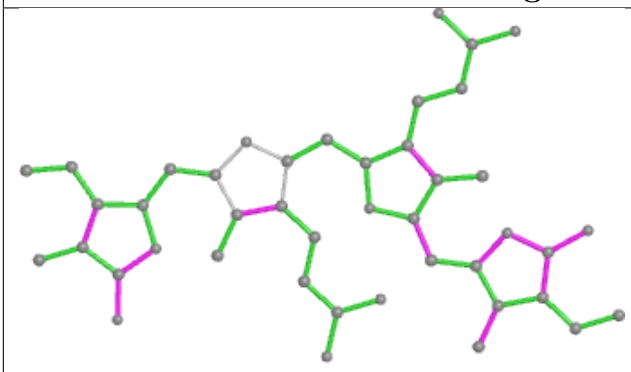


Rings

Ligand CYC F 201



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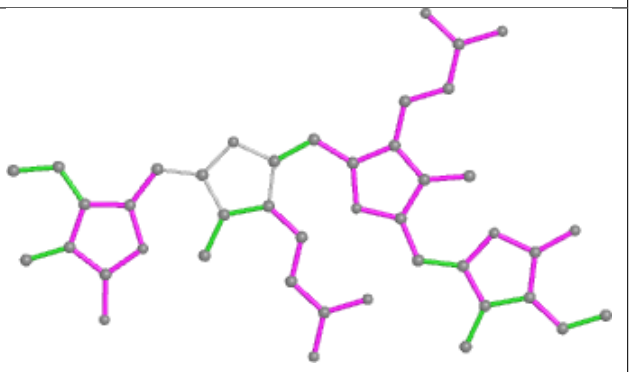
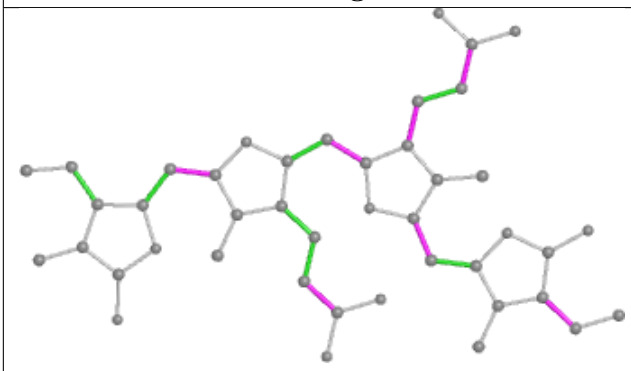


Bond angles



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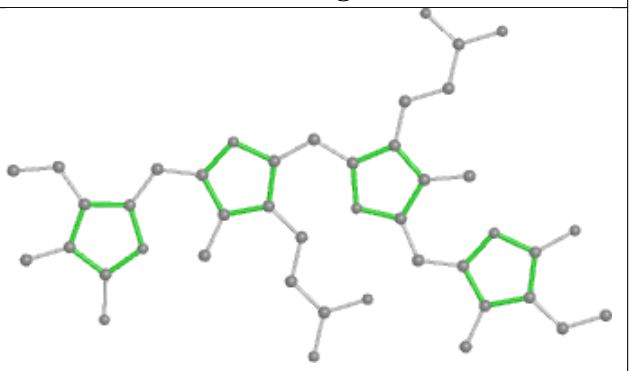
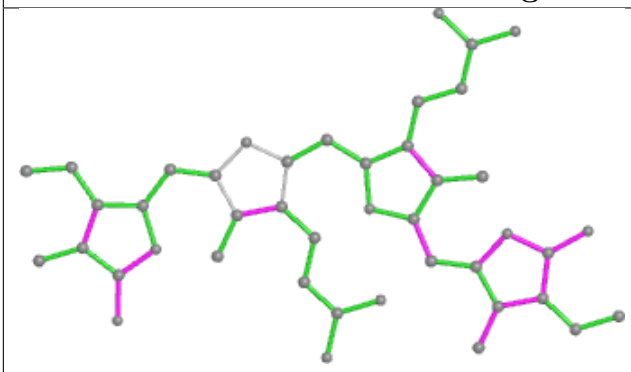
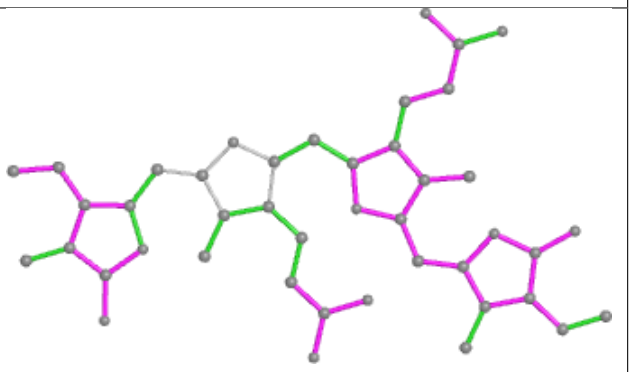


Rings

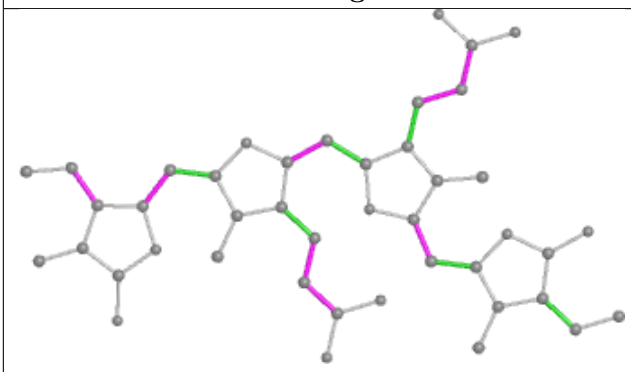
Ligand CYC X 202



Bond lengths



Bond angles



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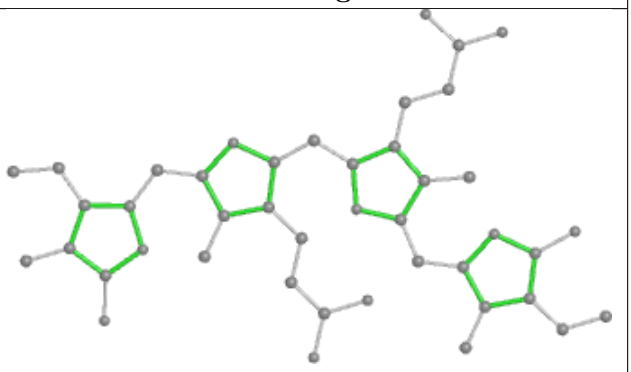
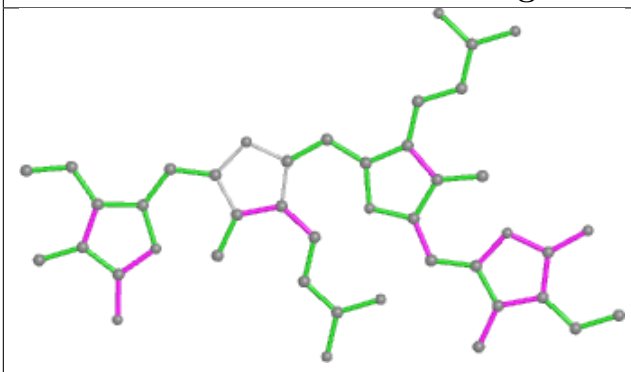


Rings

Ligand CYC M 201



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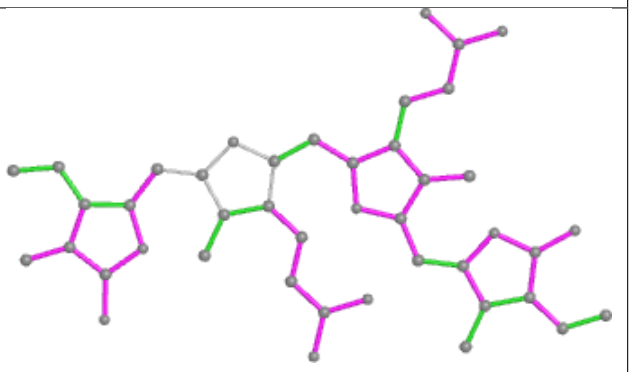
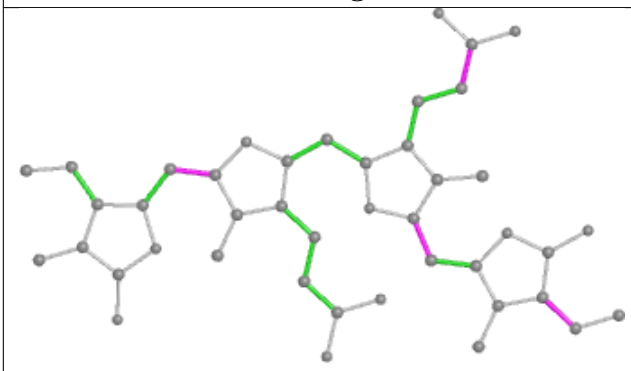


Bond angles



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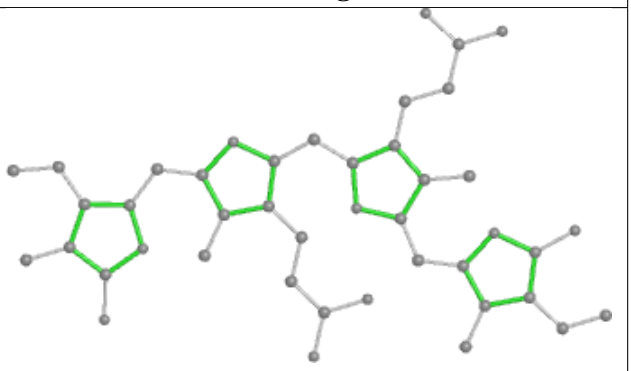

Rings

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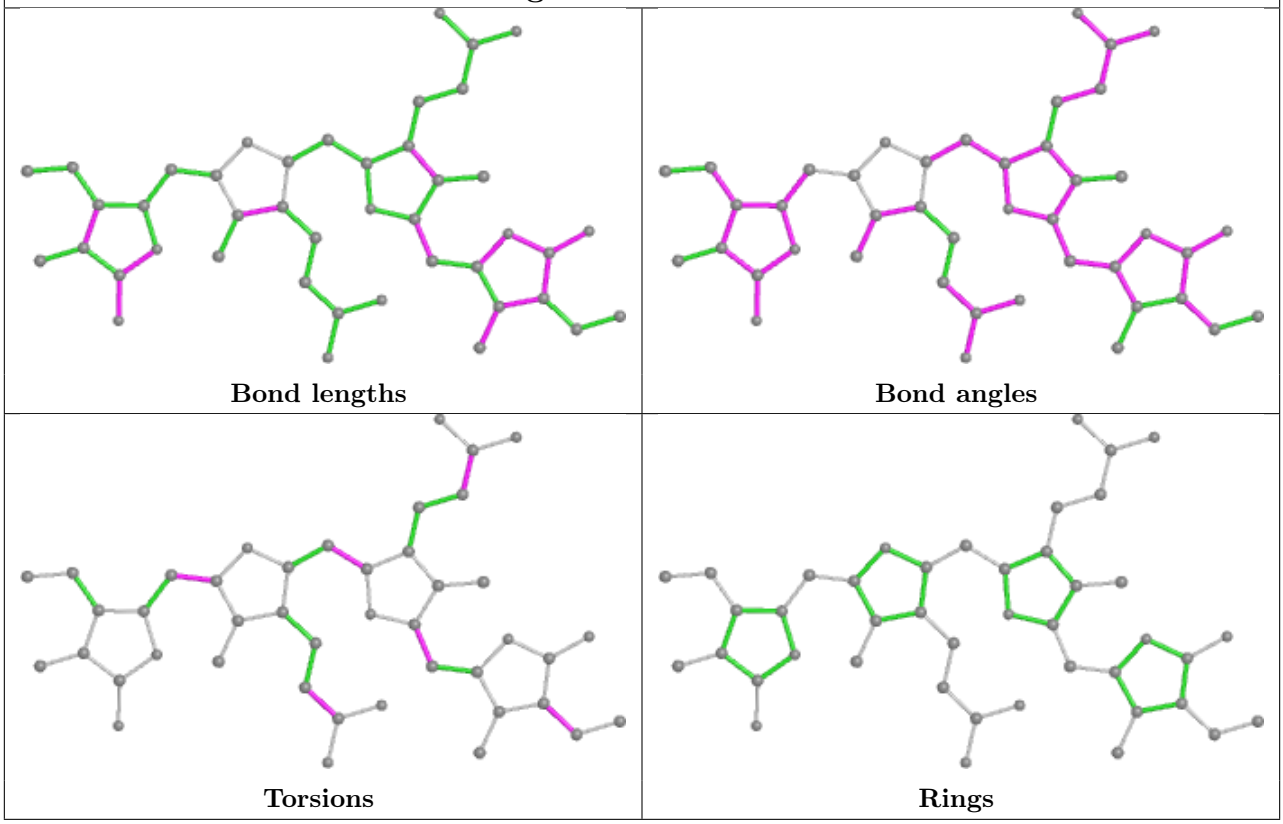
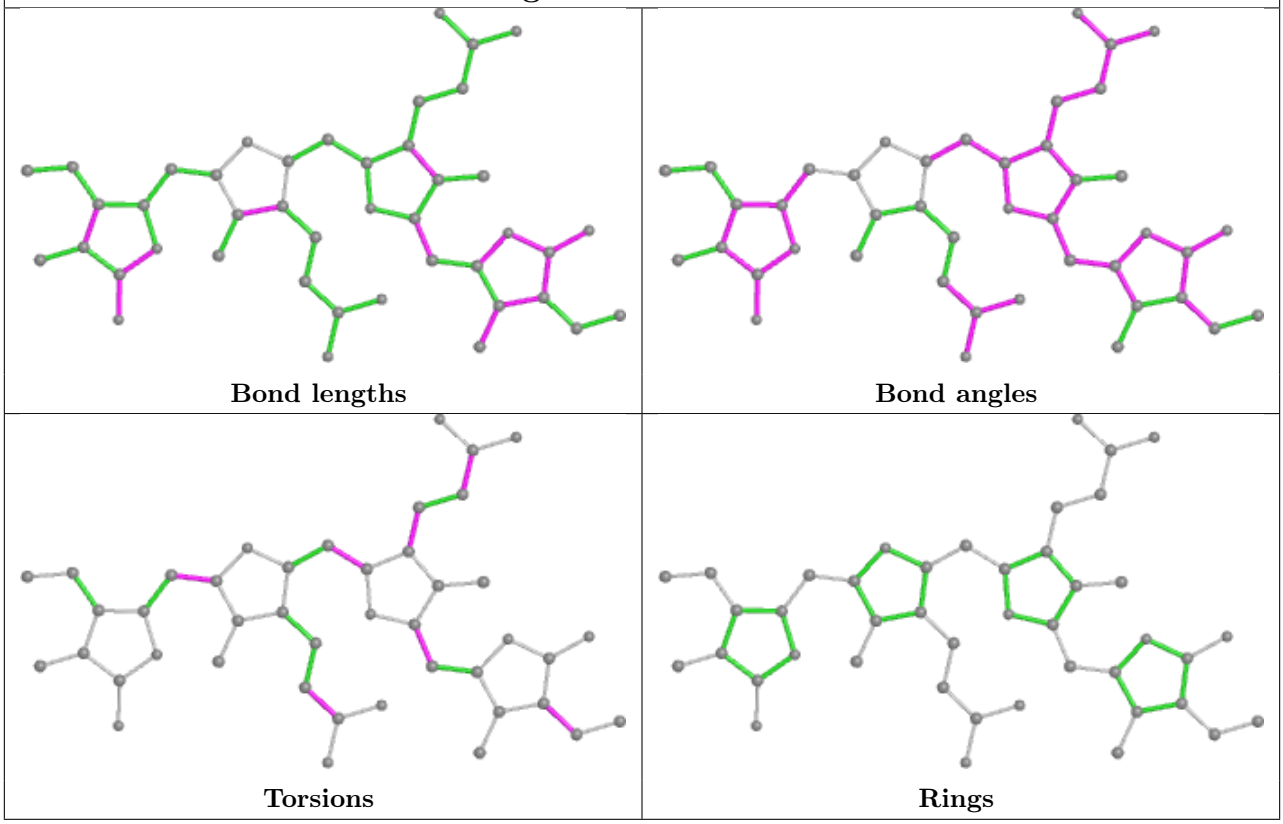
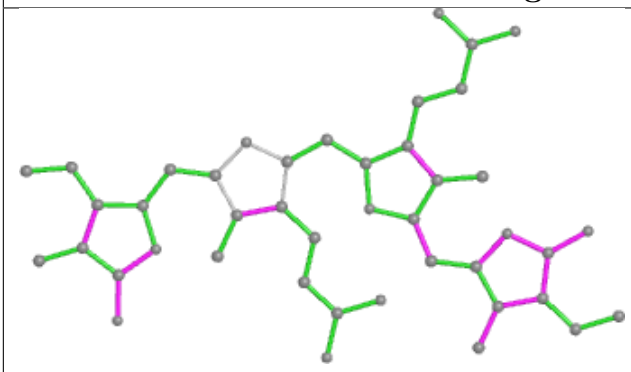


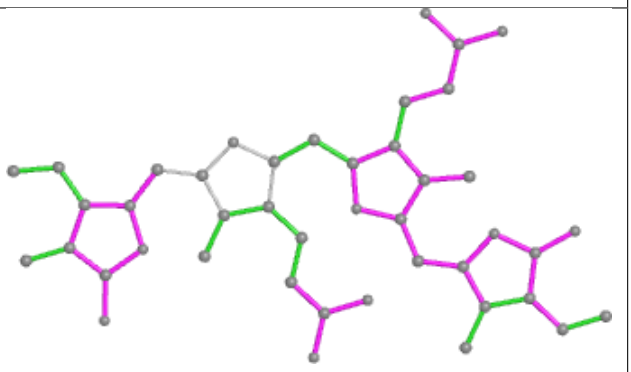
Ligand CYC R 201



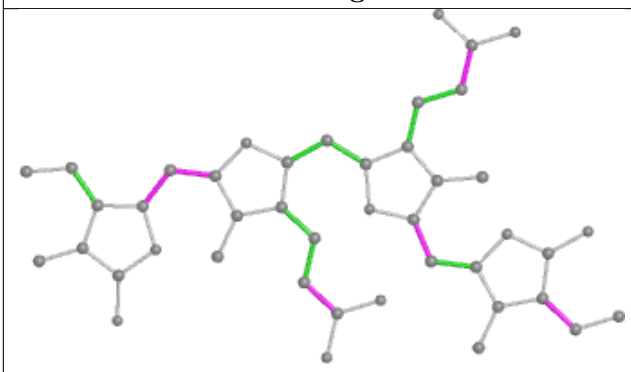
Ligand CYC L 201



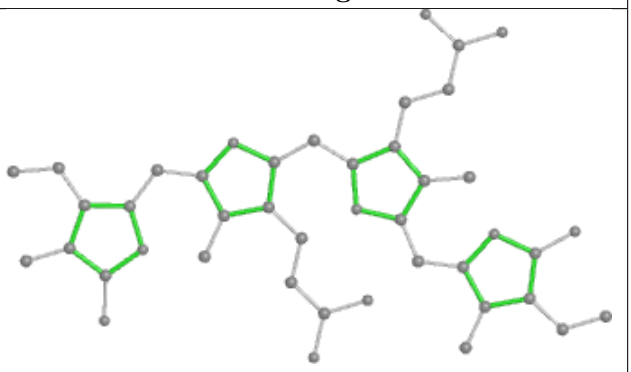
Bond lengths



Bond angles

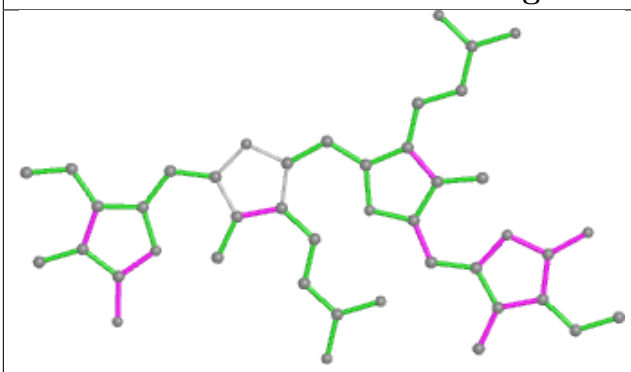


Torsions



Rings

Ligand CYC P 201



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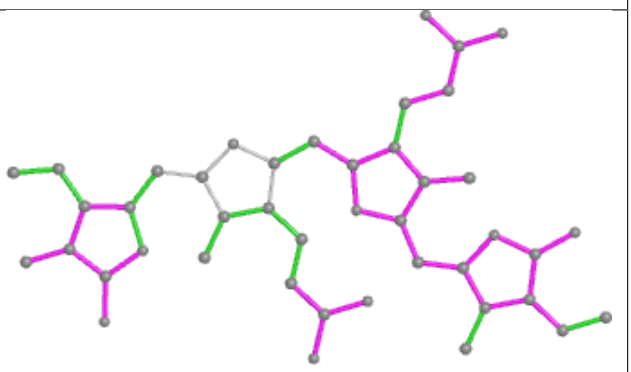
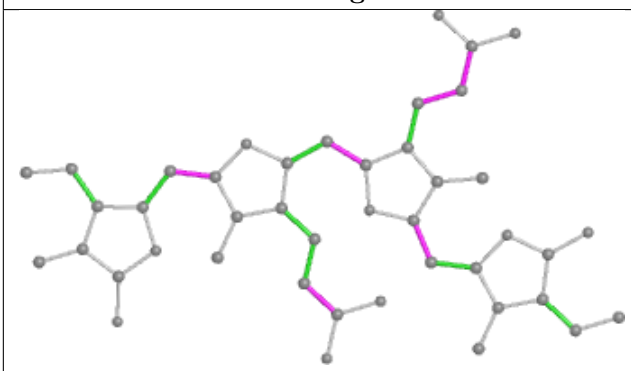
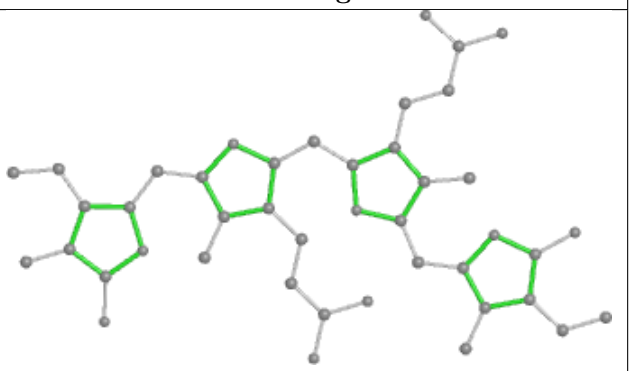


Bond angles

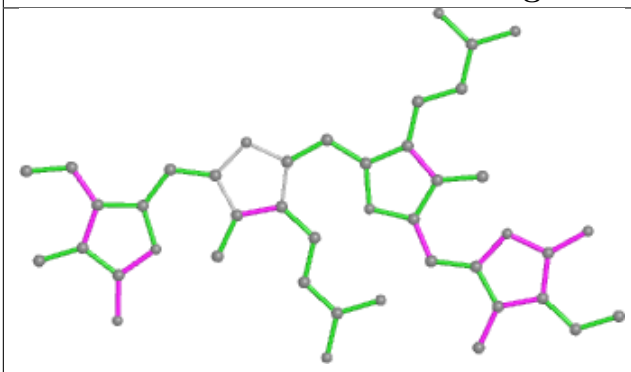


Torsions

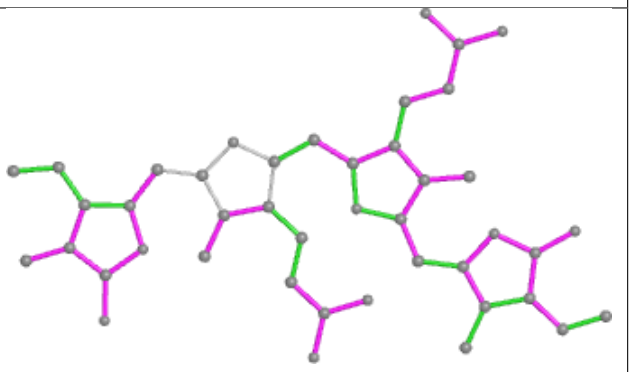


Rings

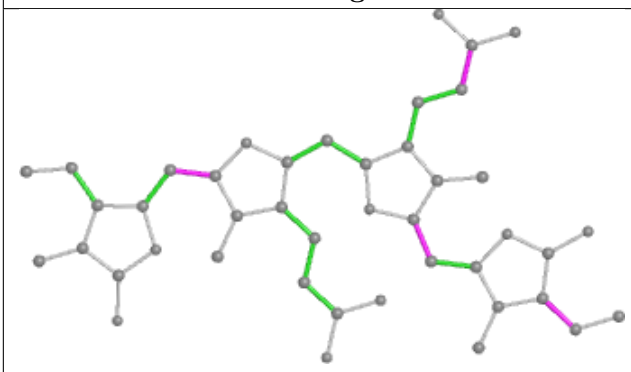
Ligand CYC E 201



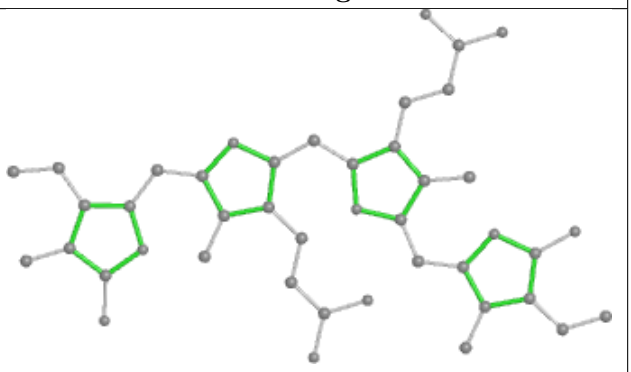
Bond lengths



Bond angles

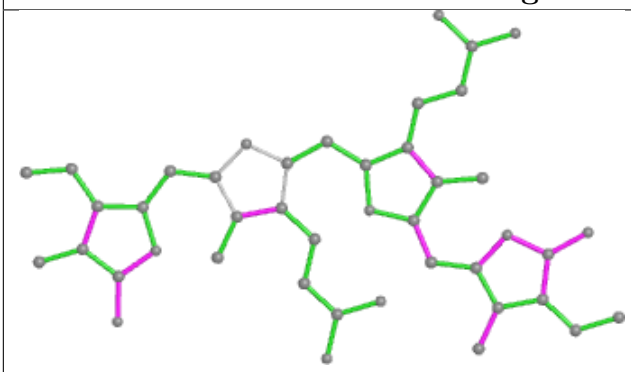


Torsions

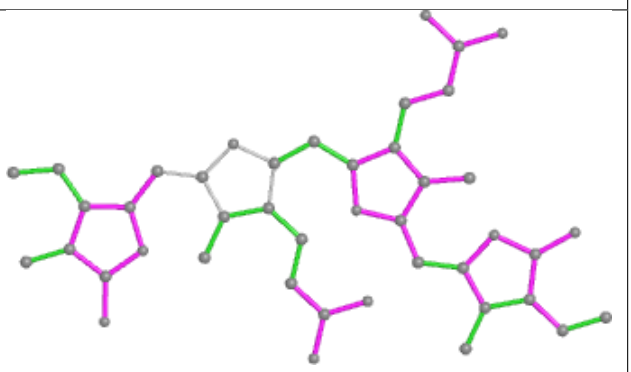


Rings

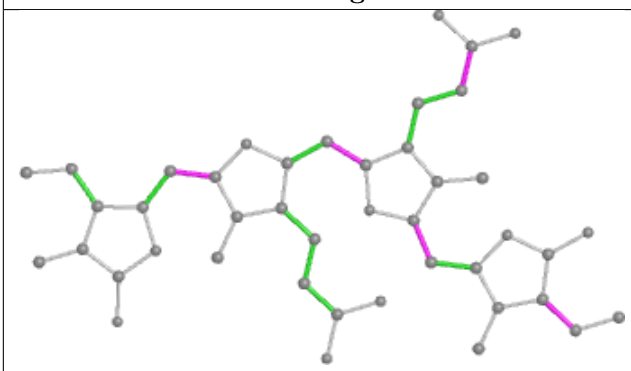
Ligand CYC V 201



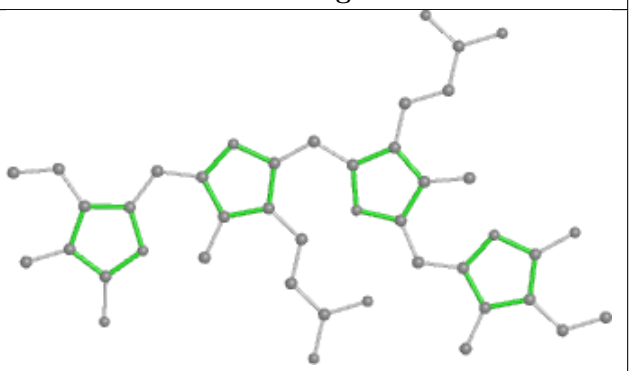
Bond lengths



Bond angles

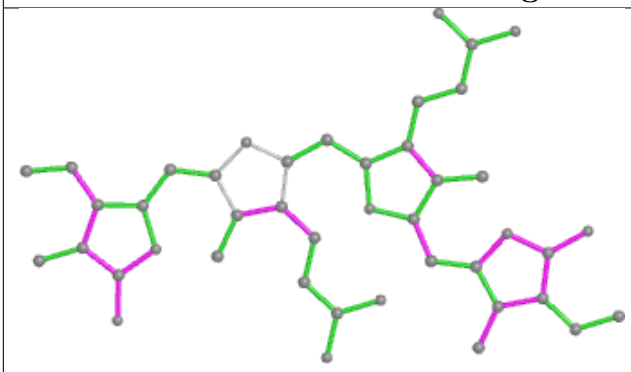


Torsions



Rings

Ligand CYC D 202



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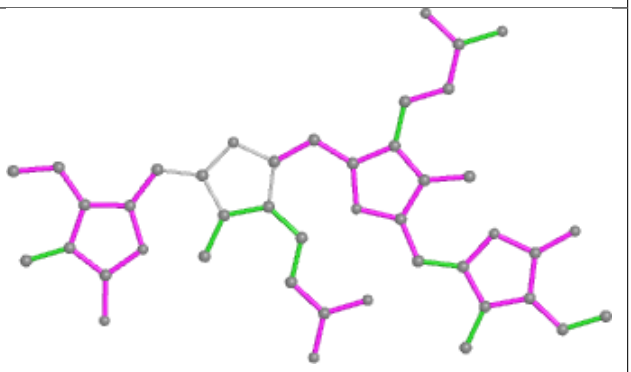
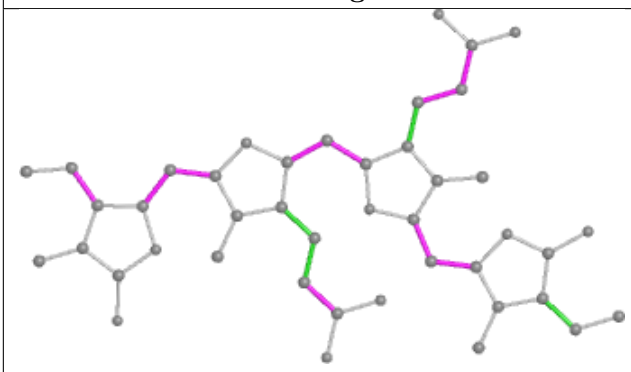
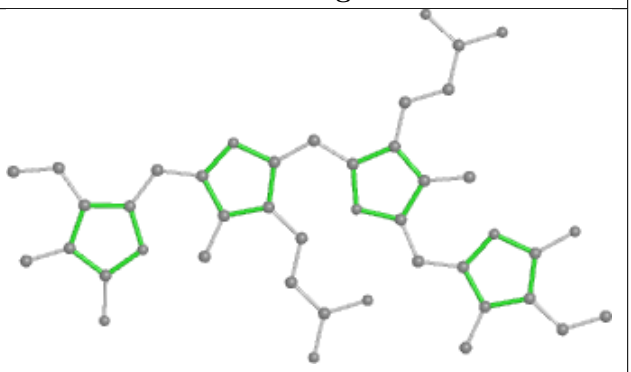


Bond angles

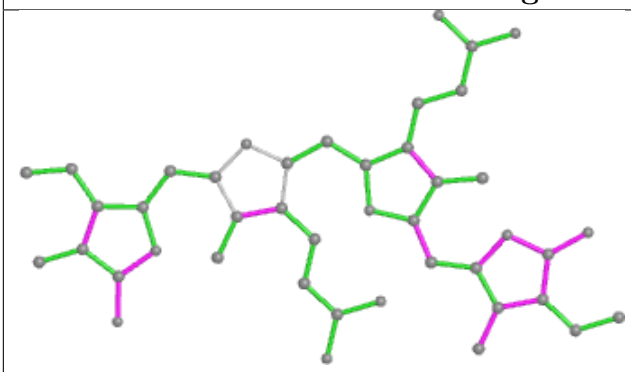


Torsions



Rings

Ligand CYC A 201



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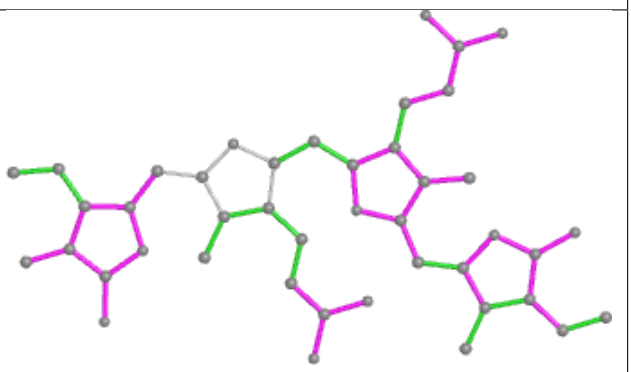
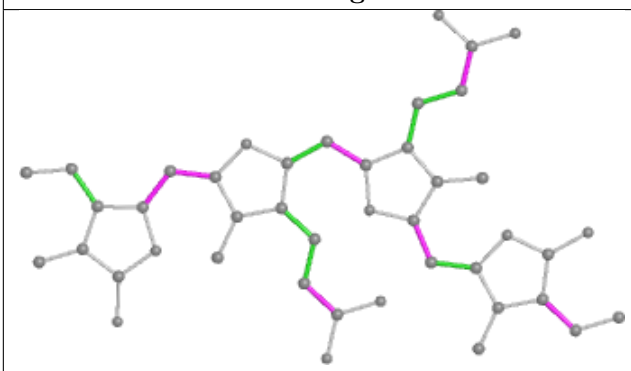


Bond angles



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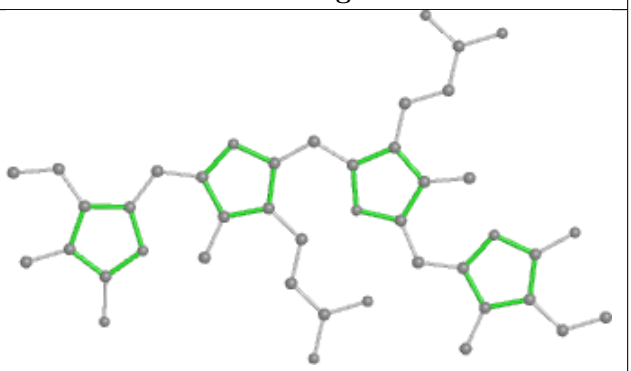
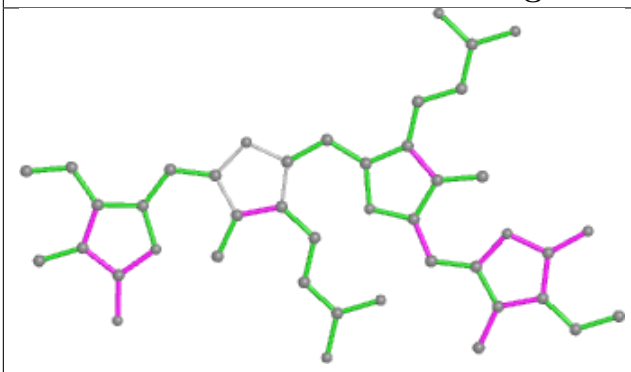
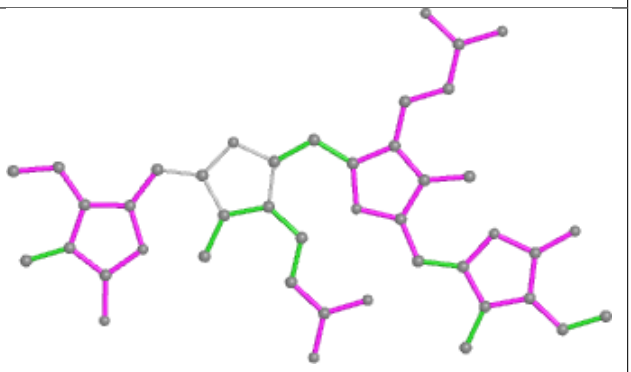


Rings

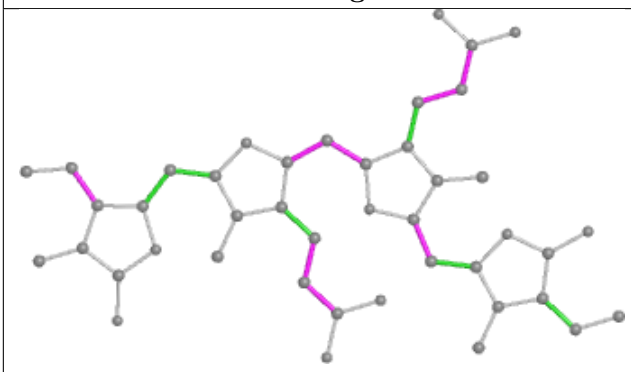
Ligand CYC L 202



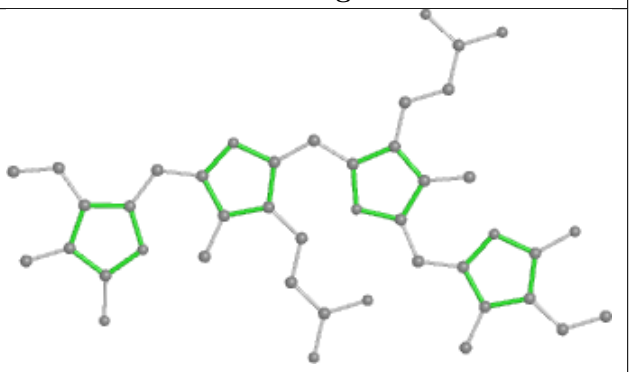
Bond lengths



Bond angles

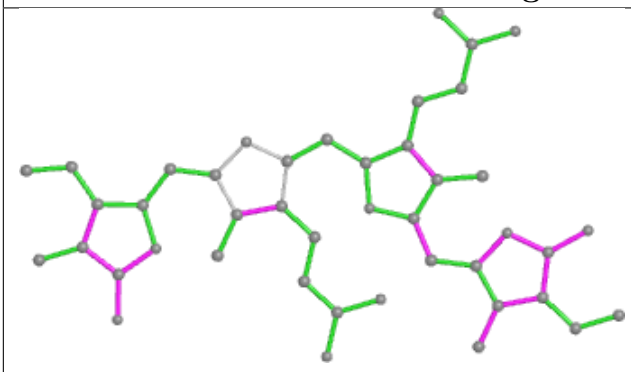


Torsions

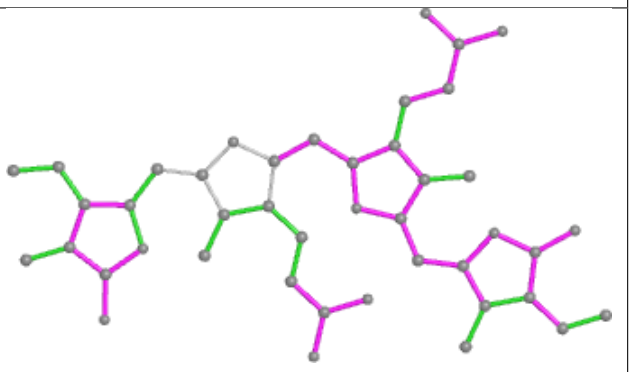


Rings

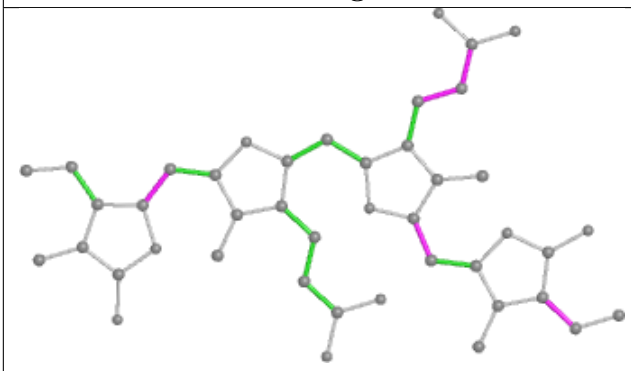
Ligand CYC B 201



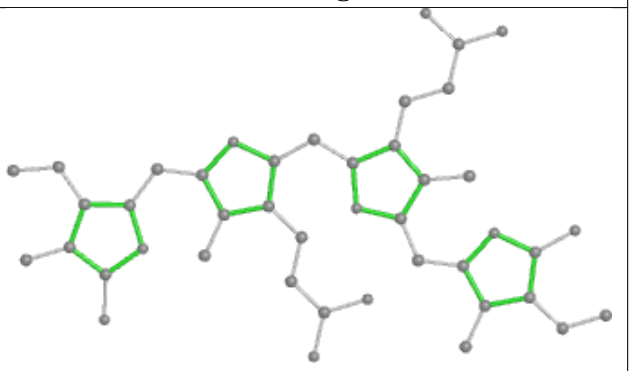
Bond lengths



Bond angles

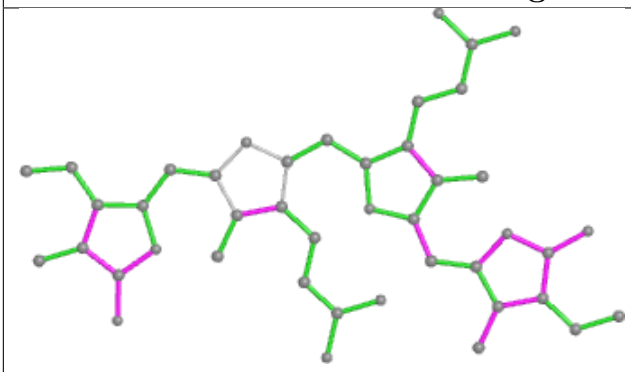


Torsions

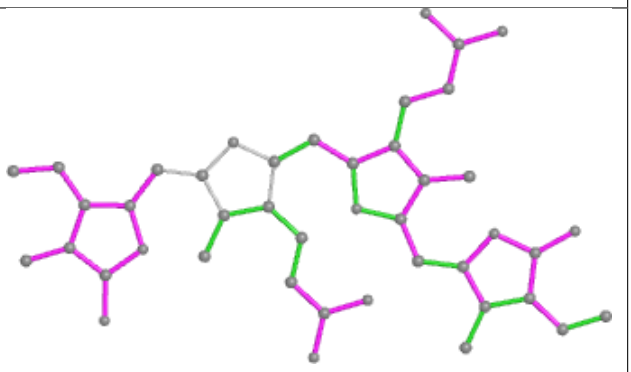


Rings

Ligand CYC I 201



Bond lengths



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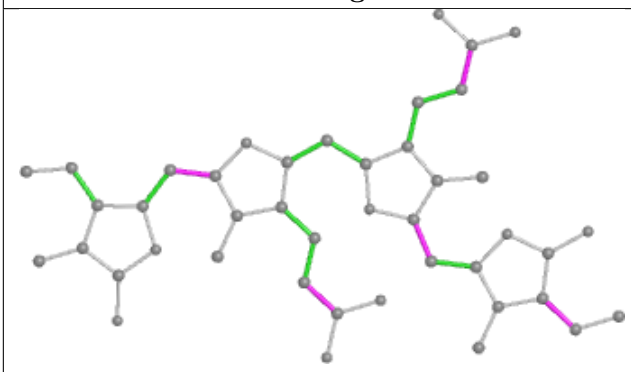
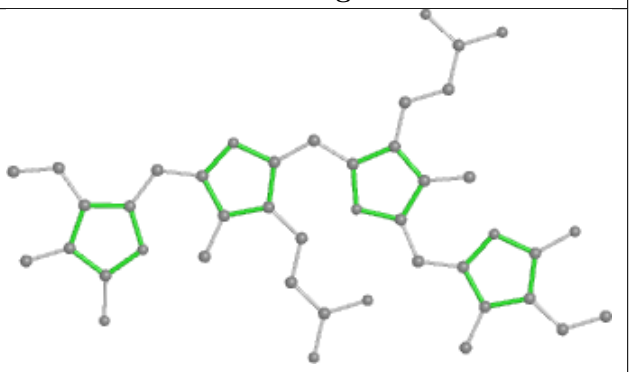
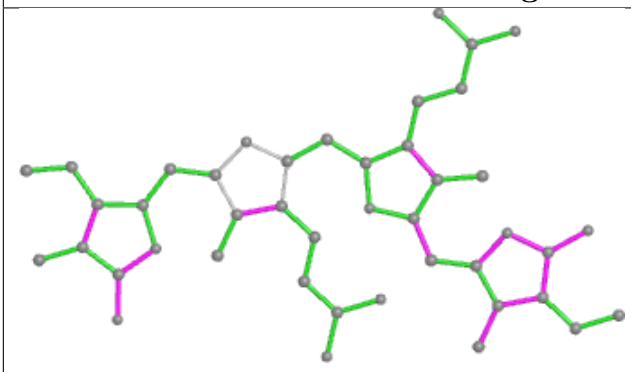


Torsions



Rings

Ligand CYC N 202



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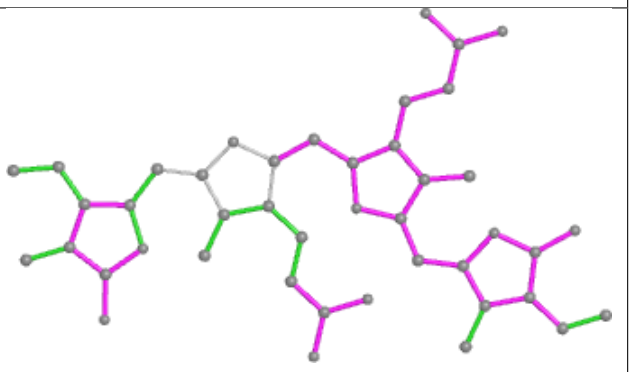

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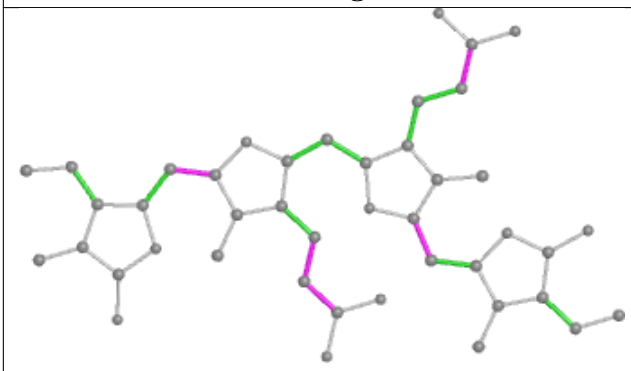

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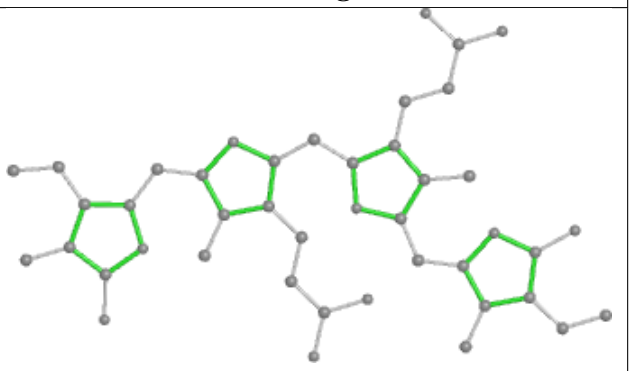
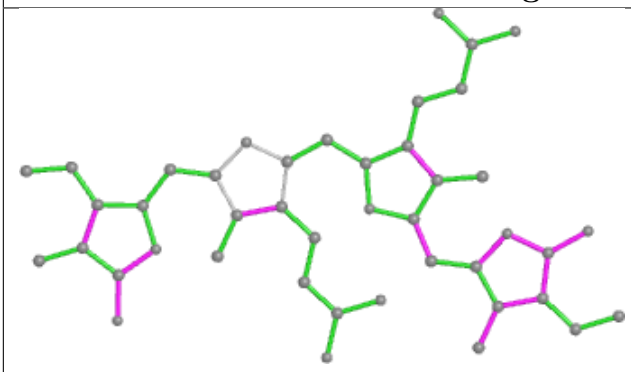


Rings

Ligand CYC B 202



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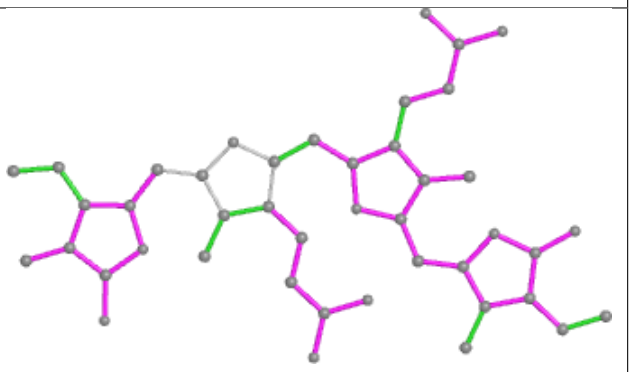

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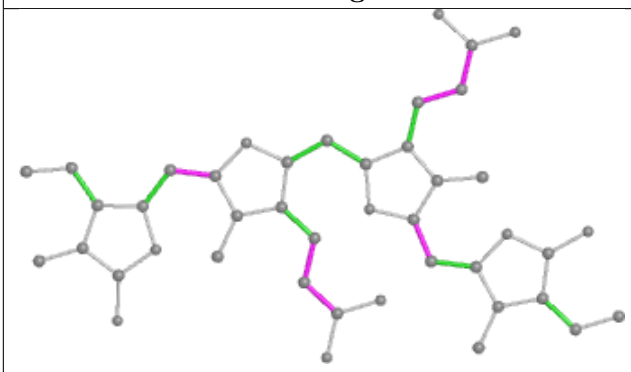

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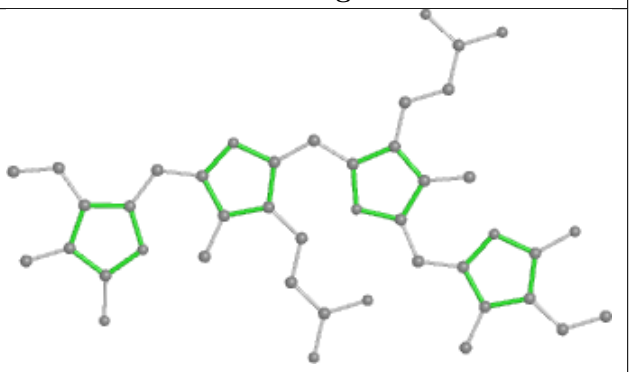

Rings

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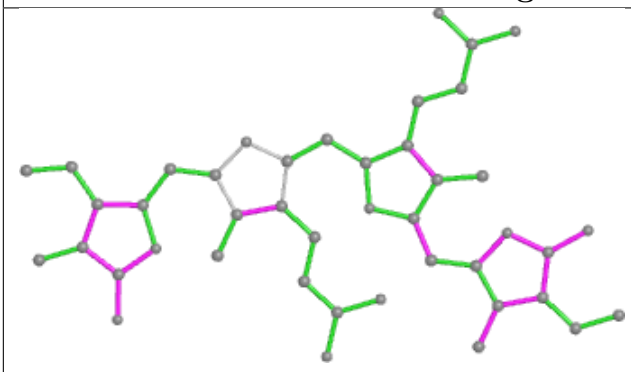

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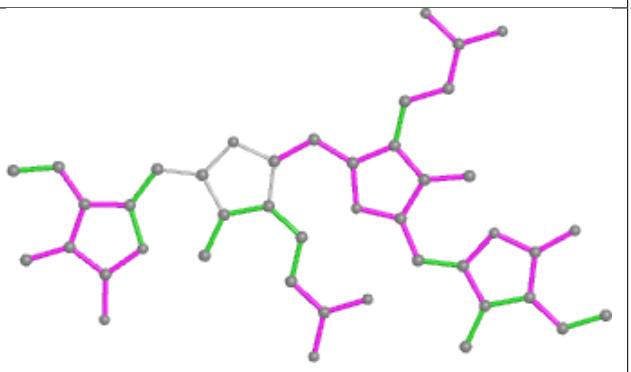

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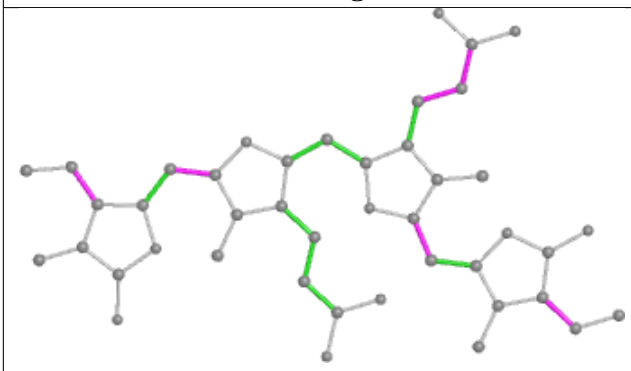

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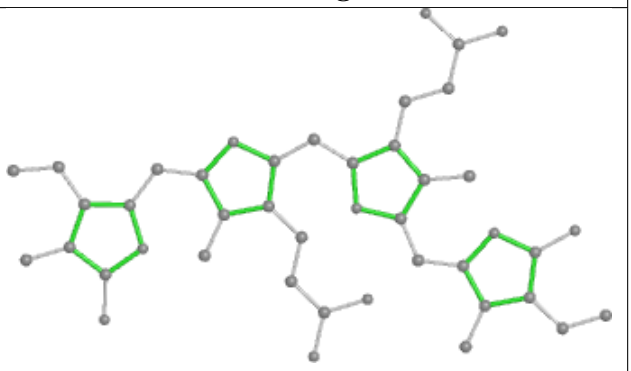

Rings

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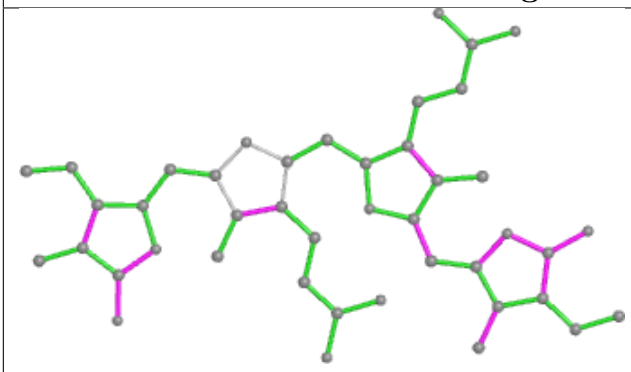

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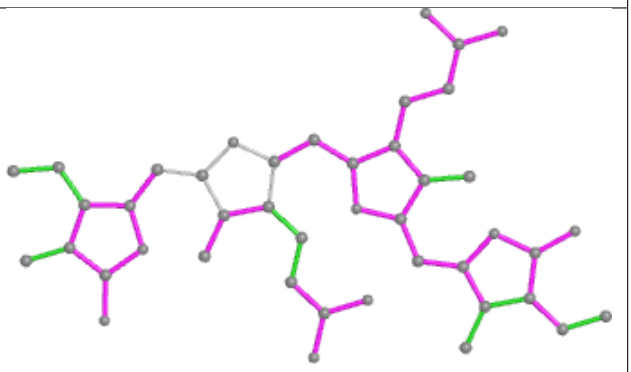

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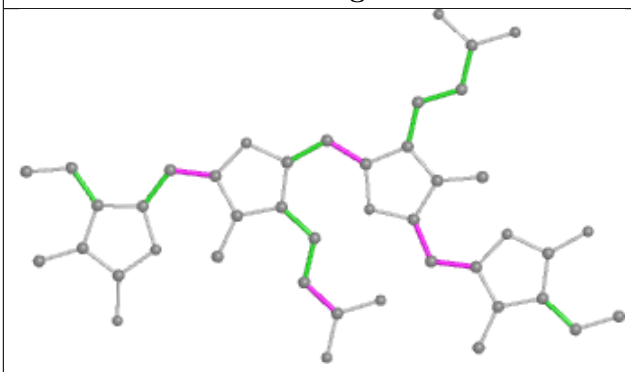

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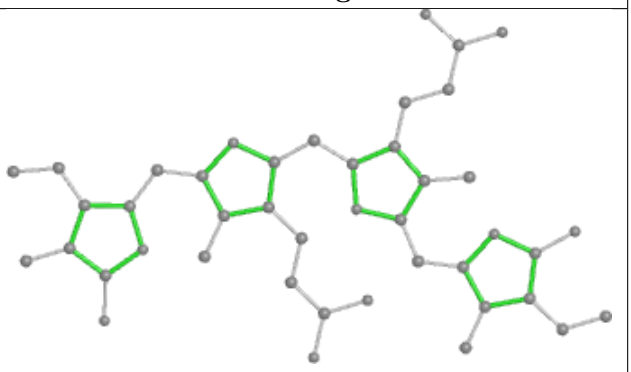
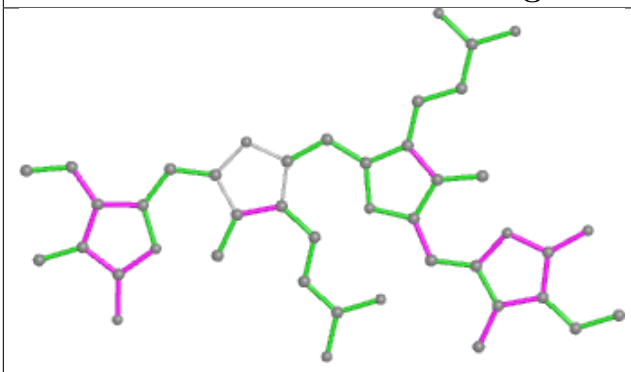


Rings

Ligand CYC F 202



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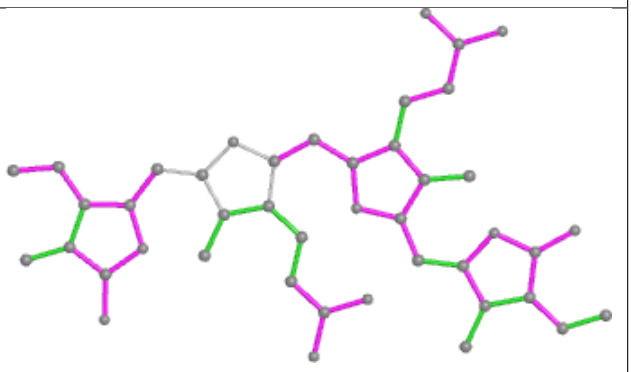

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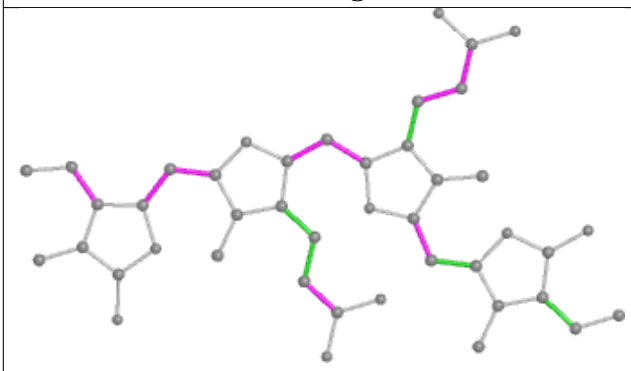

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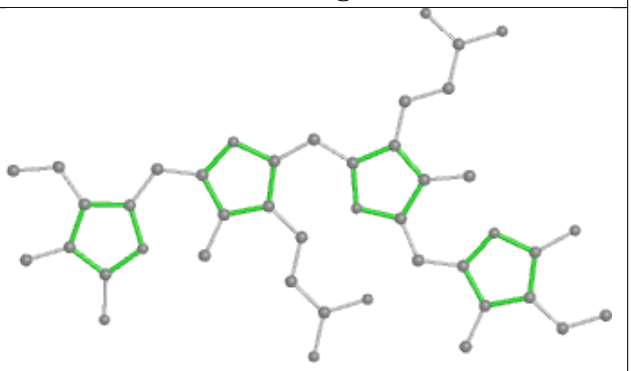
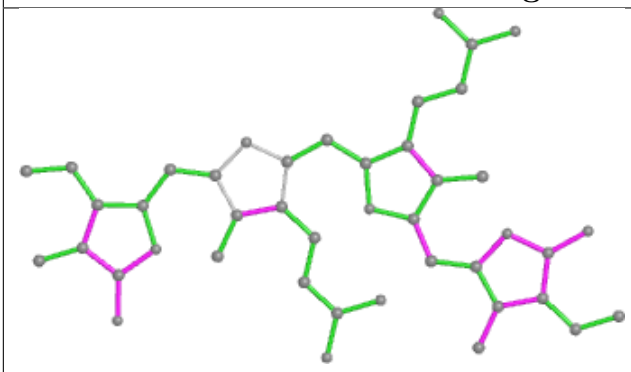


Rings

Ligand CYC T 202



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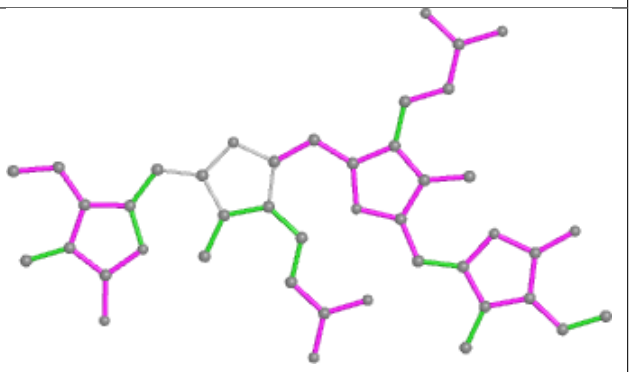

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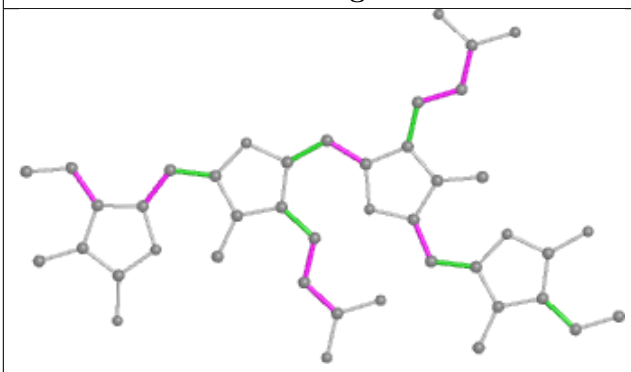

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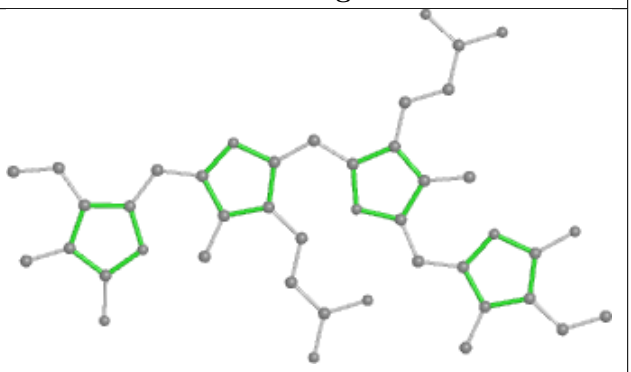
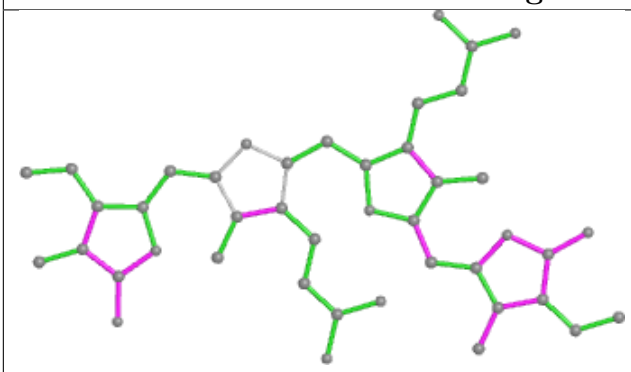


Rings

Ligand CYC J 202



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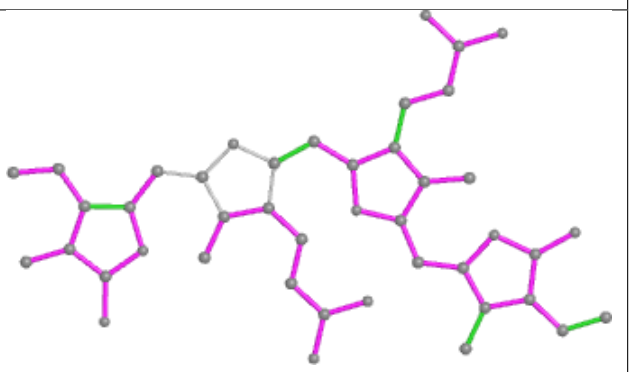

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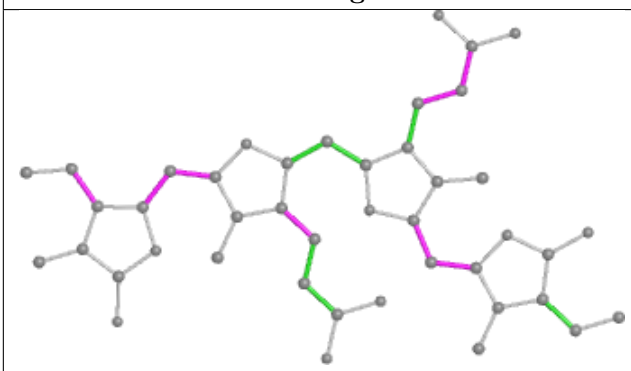

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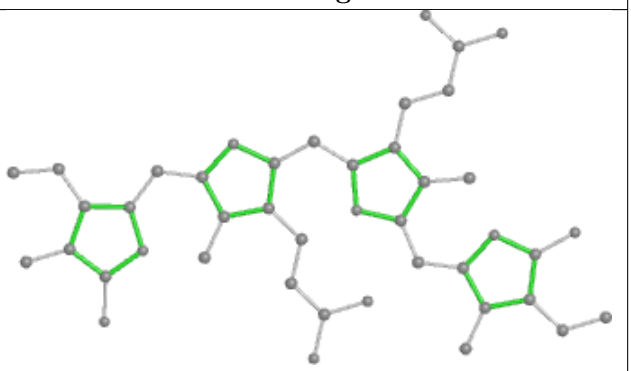
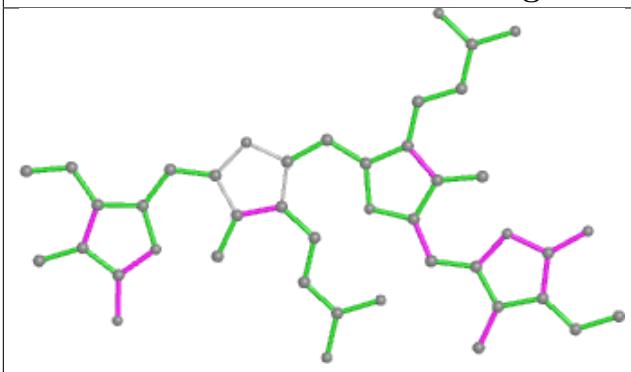


Rings

Ligand CYC T 201



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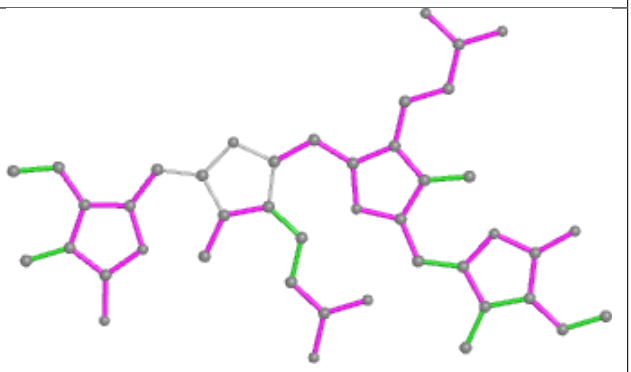

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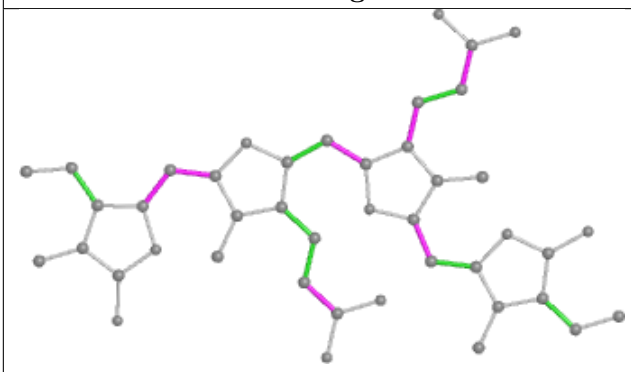

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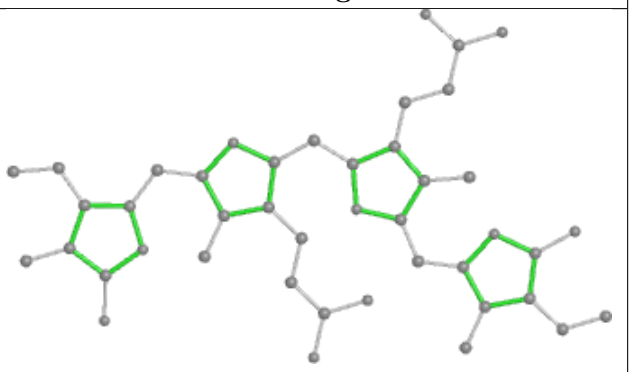
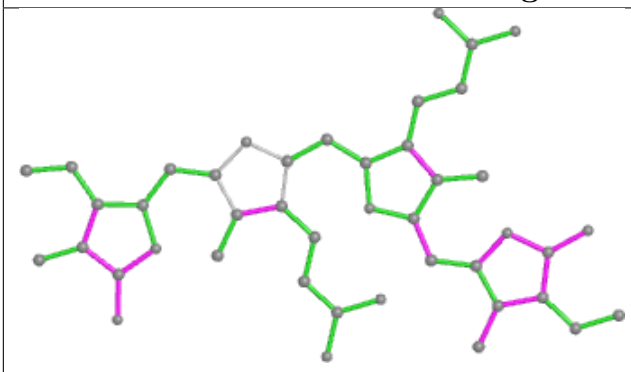


Rings

Ligand CYC H 202



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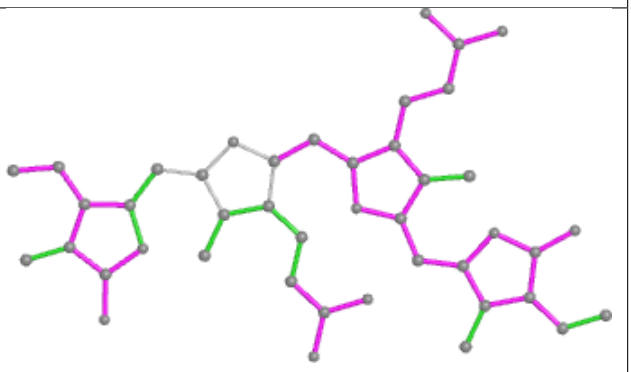

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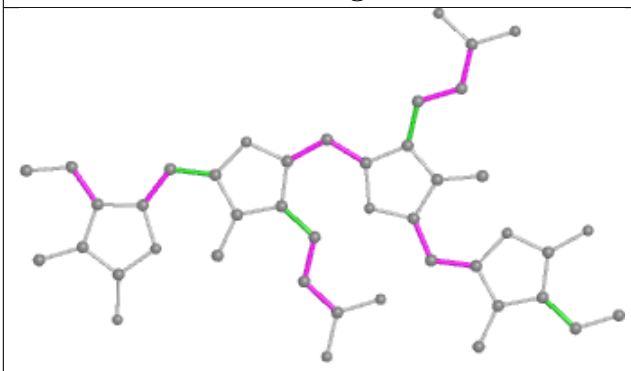

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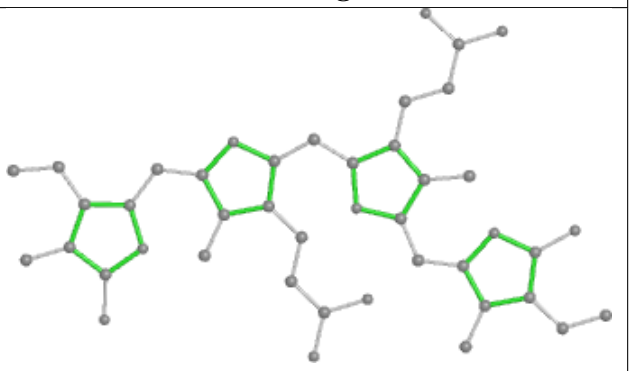
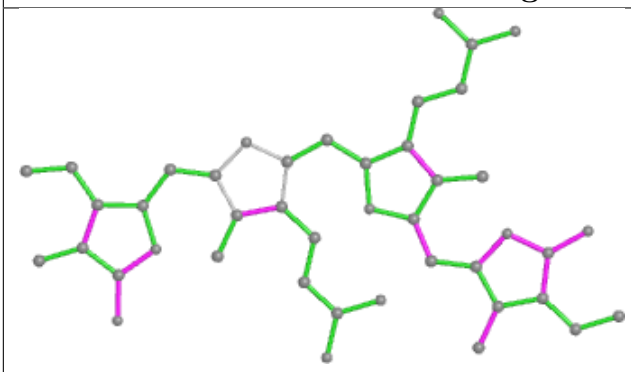


Rings

Ligand CYC G 201



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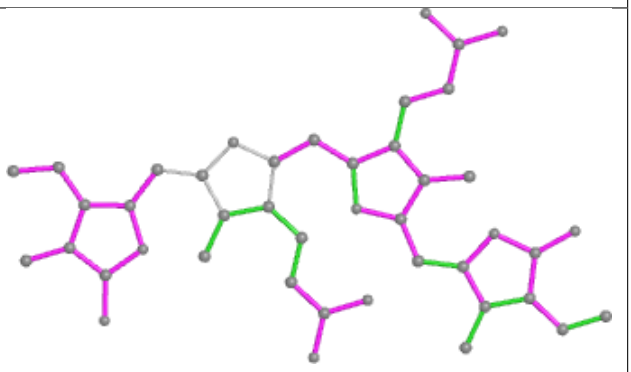

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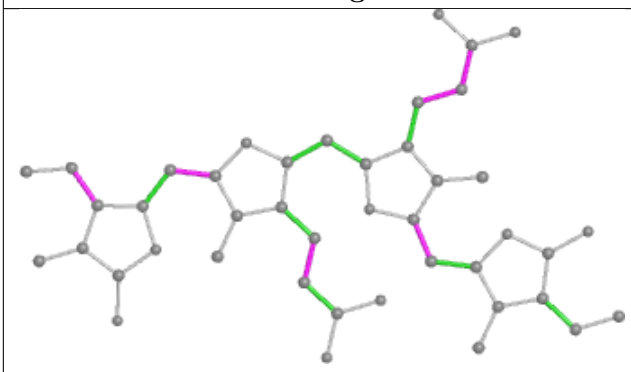

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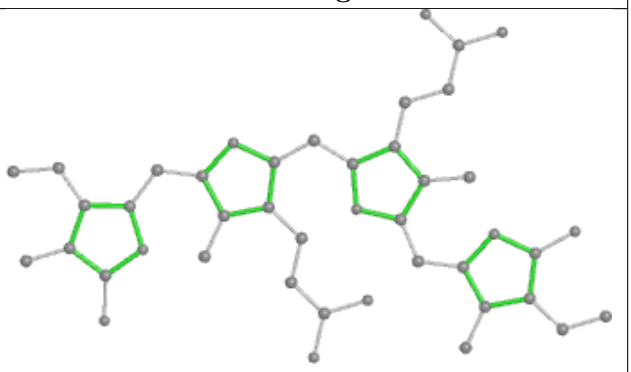

Rings

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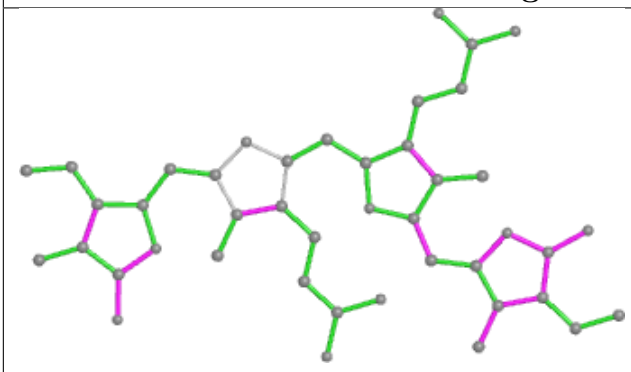

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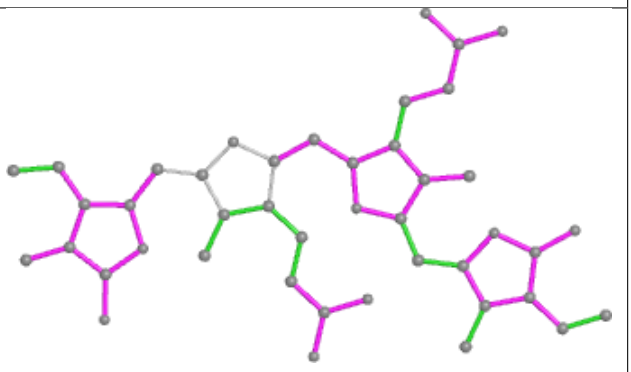

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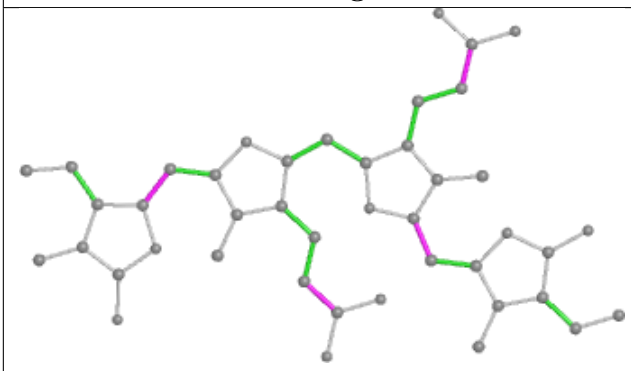

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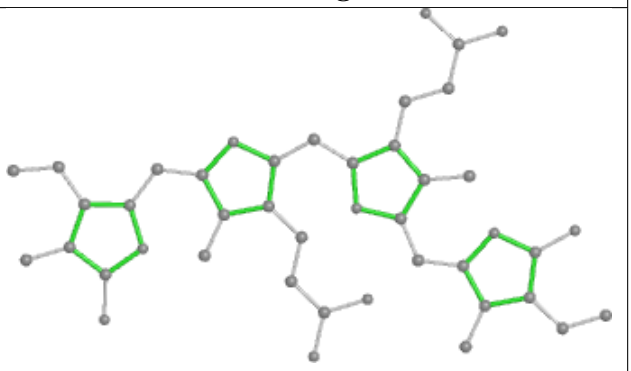
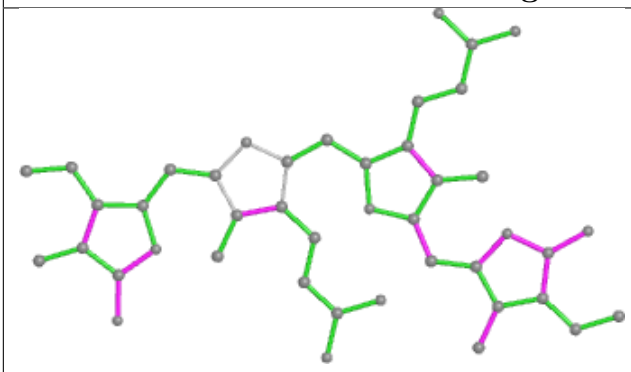


Rings

Ligand CYC N 201



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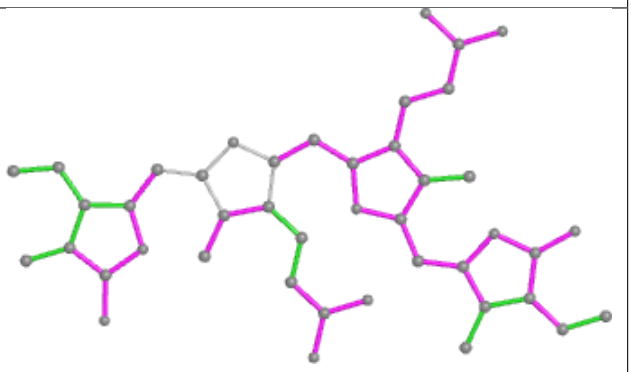

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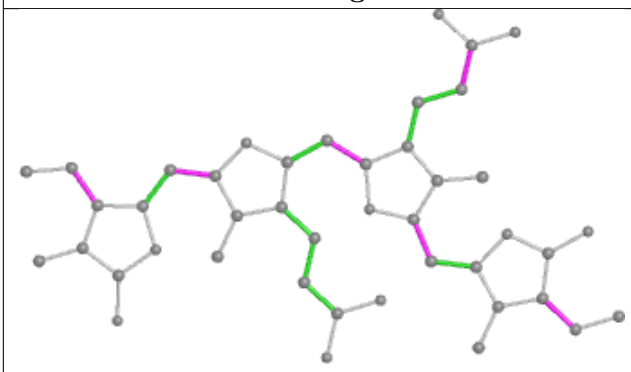

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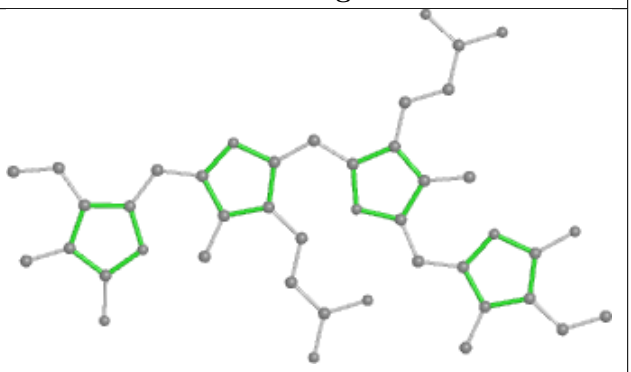
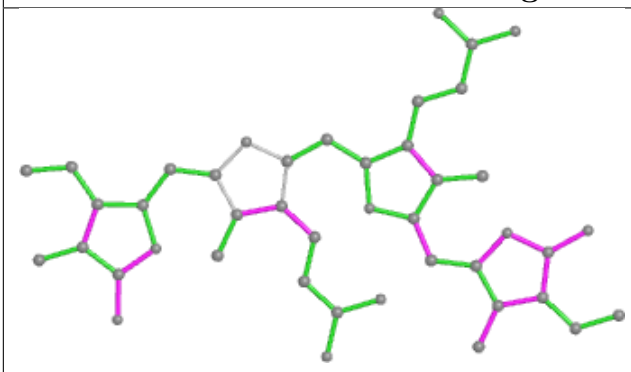


Rings

Ligand CYC K 201



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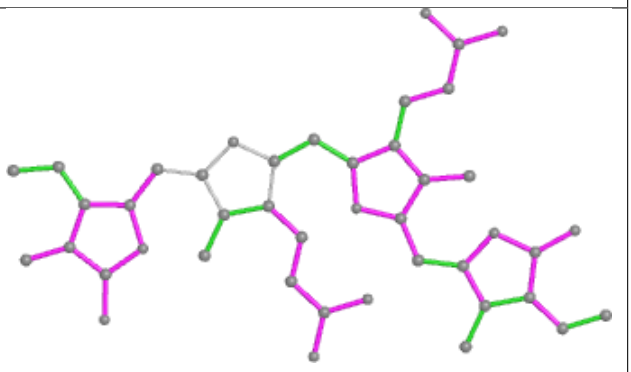
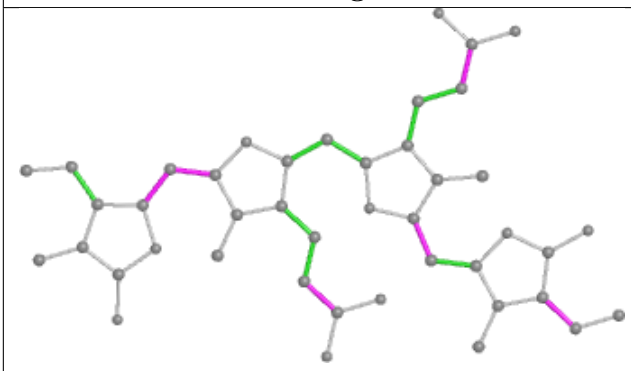


Bond angles



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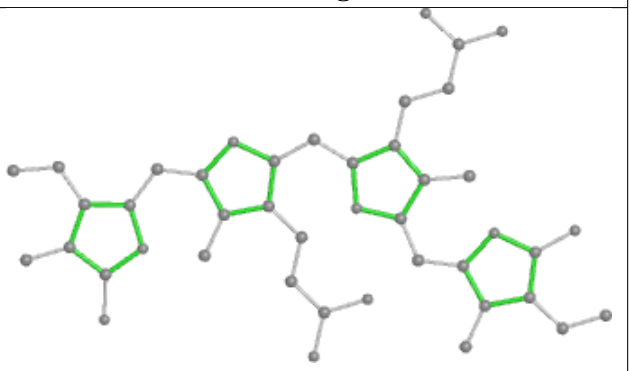
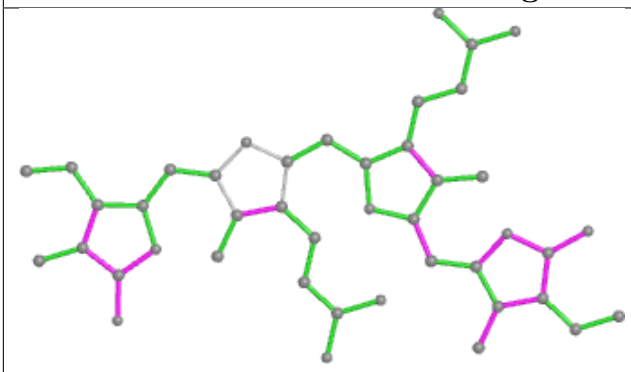


Rings

Ligand CYC V 202



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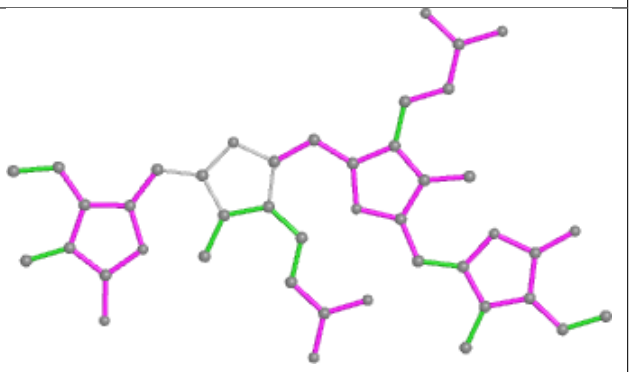
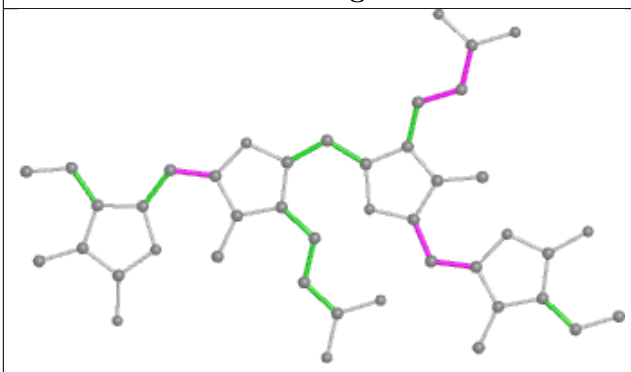
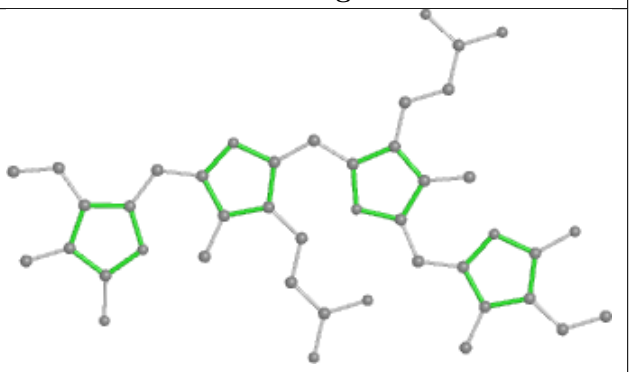


Bond angles

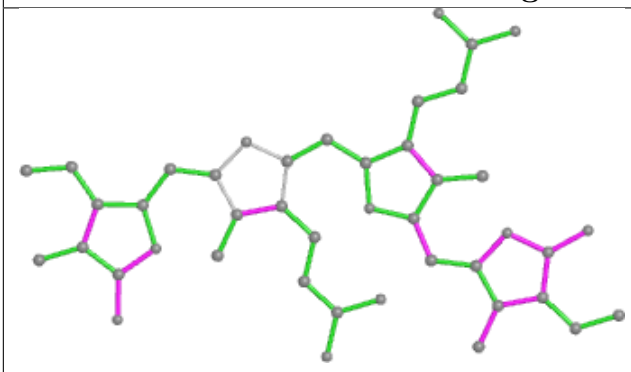


Torsions

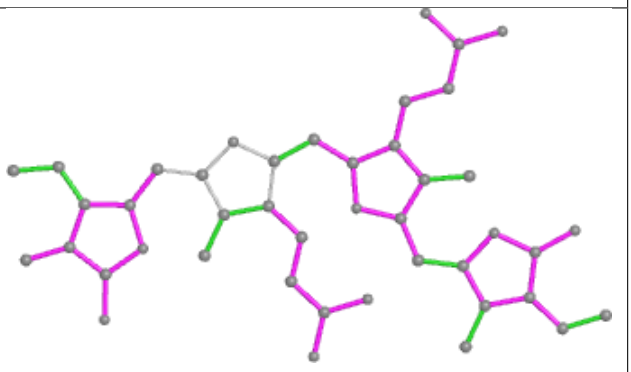


Rings

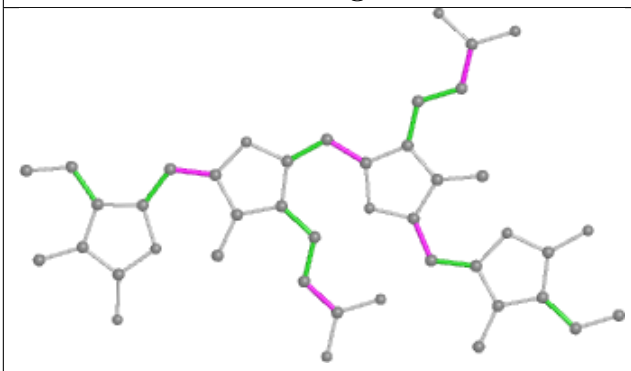
Ligand CYC D 201



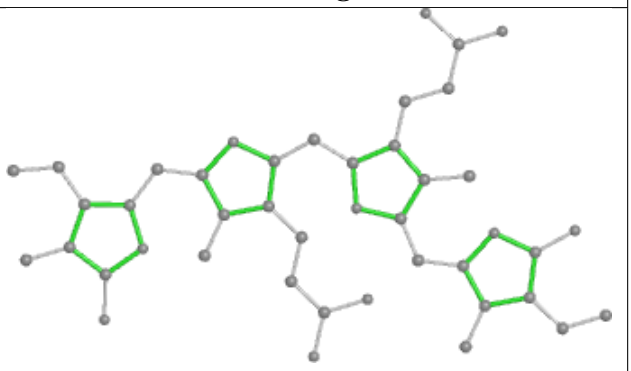
Bond lengths



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

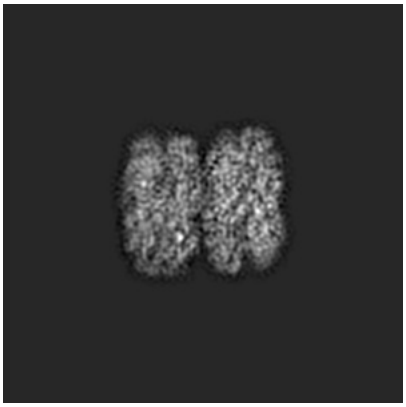
This section contains visualisations of the EMDB entry EMD-31945. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

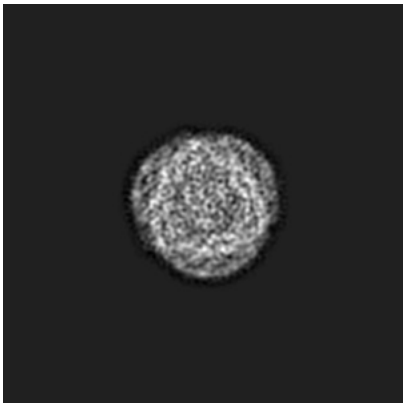
6.1 Orthogonal projections

6.1.1 Primary map

X



Y

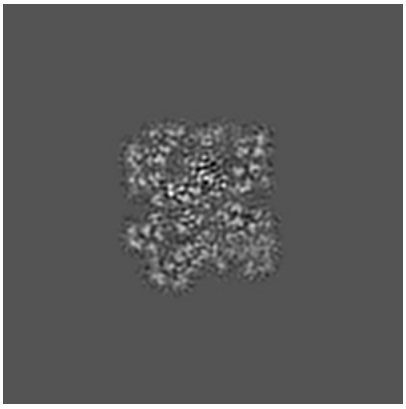


Z

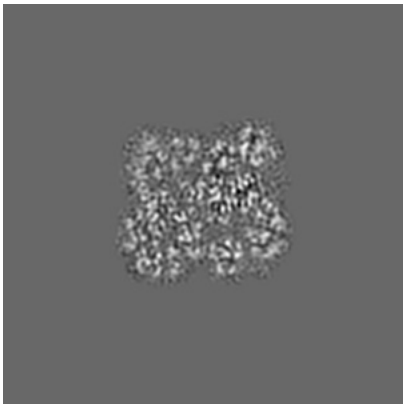
The images above show the map projected in three orthogonal directions.

6.2 Central slices

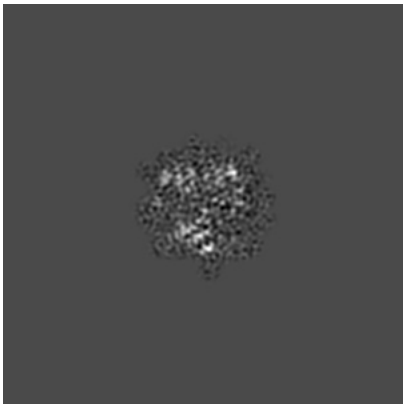
6.2.1 Primary map



X Index: 80



Y Index: 80

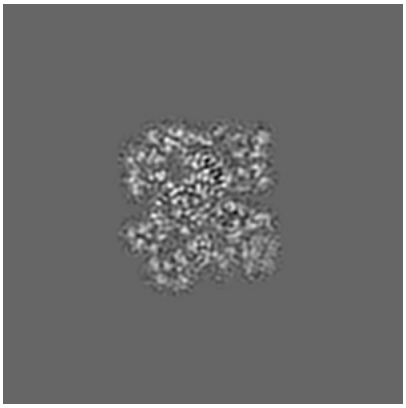


Z Index: 80

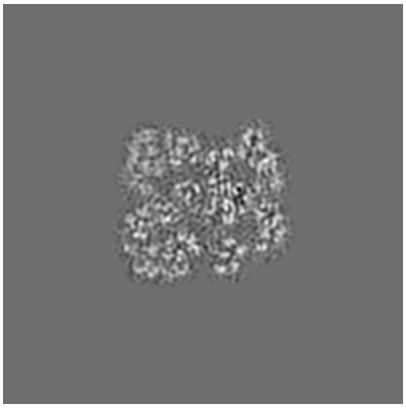
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

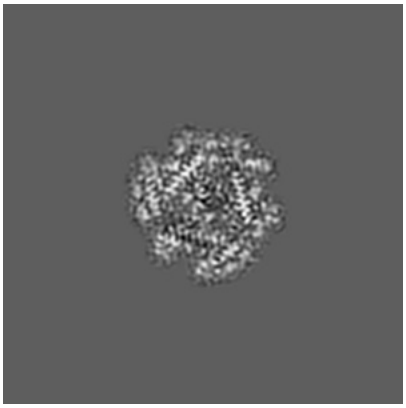
6.3.1 Primary map



X Index: 81



Y Index: 83



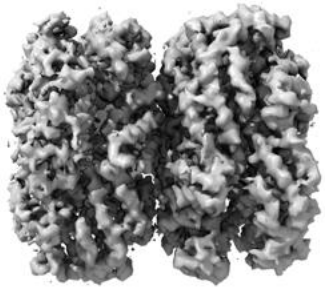
Z Index: 88

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

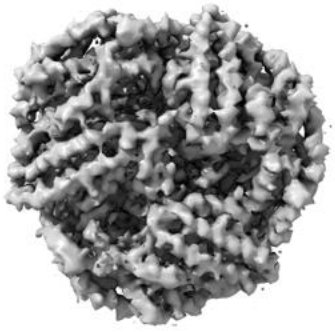
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0286. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

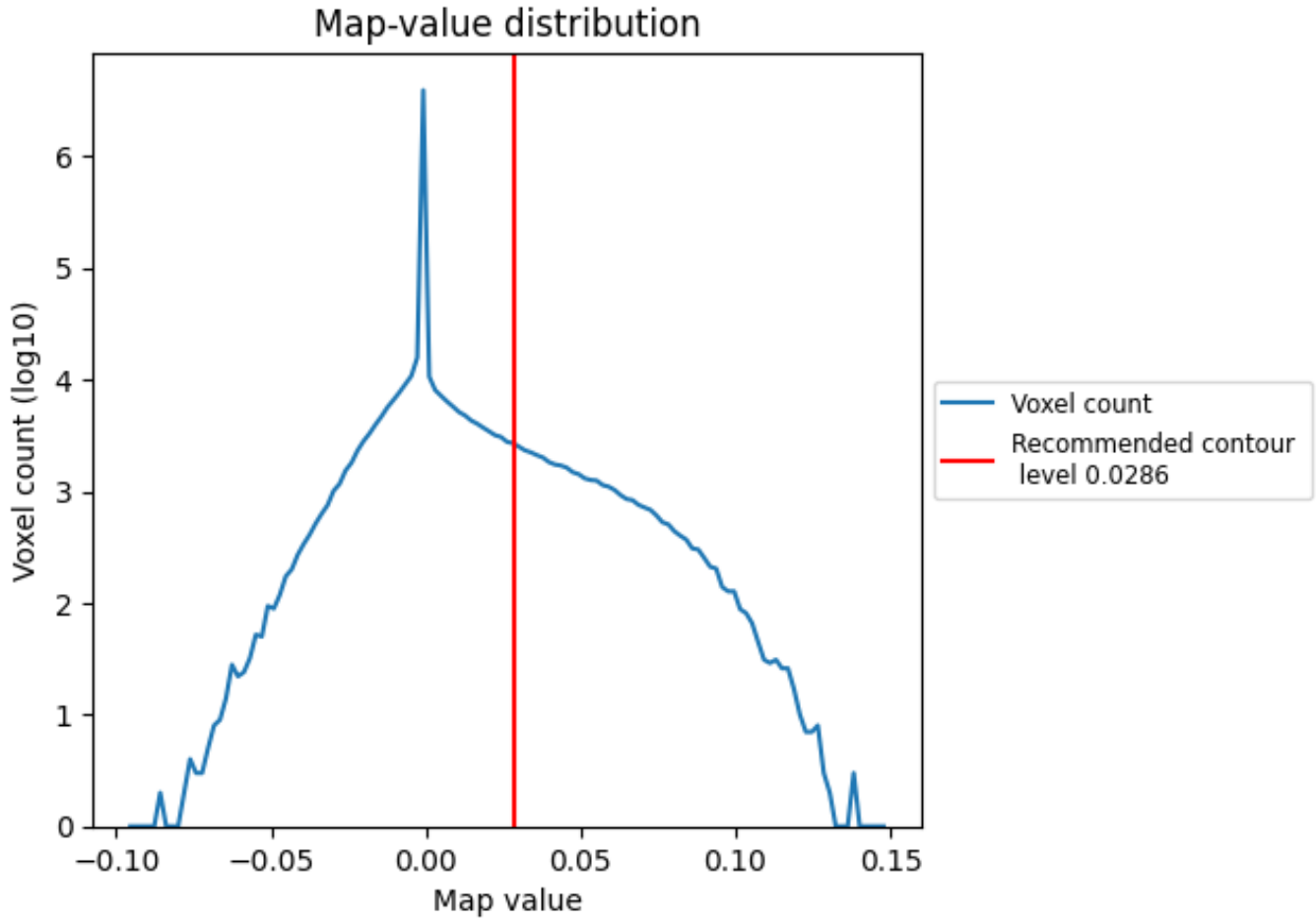
6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

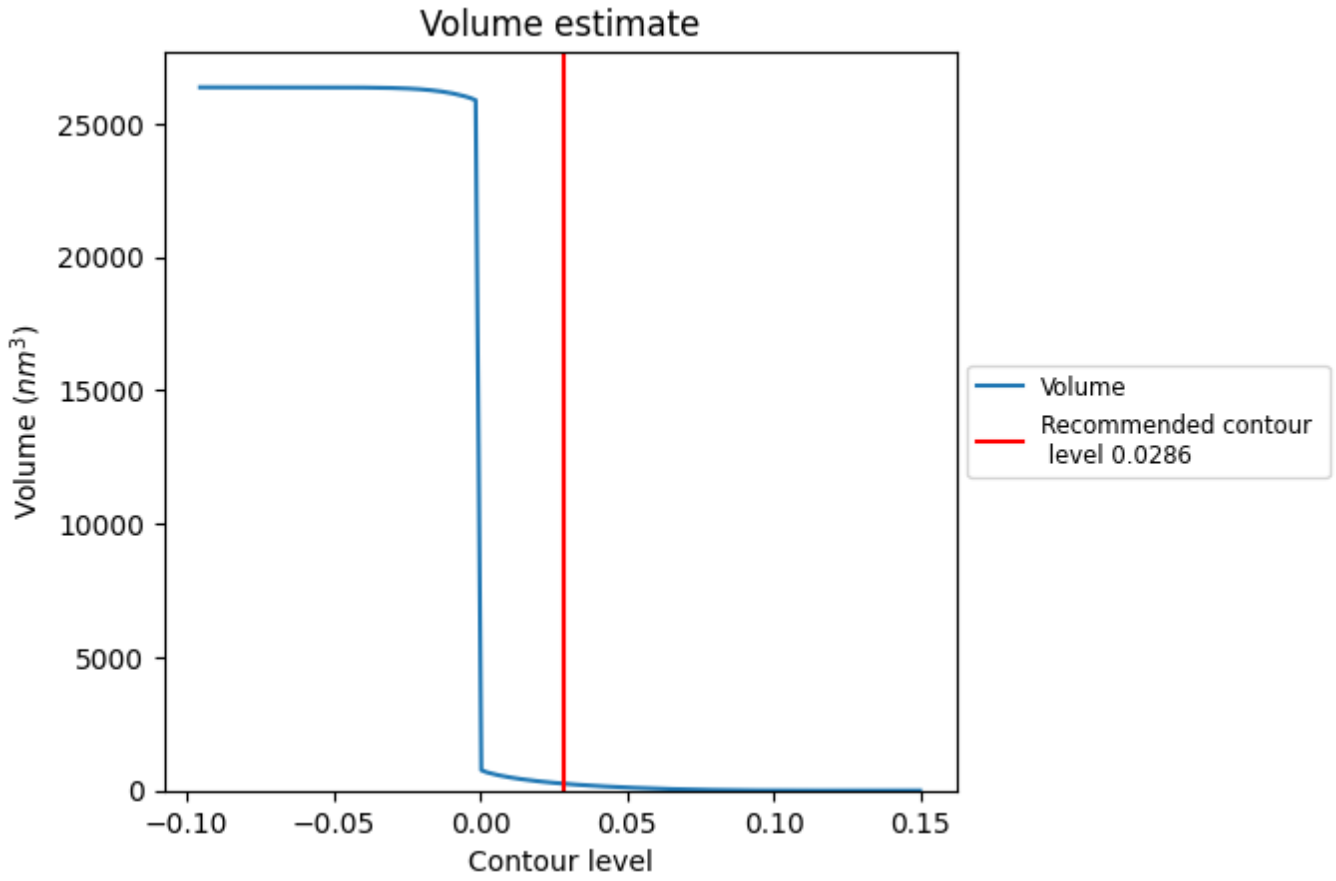
This section contains the results of statistical analysis of the map.

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.

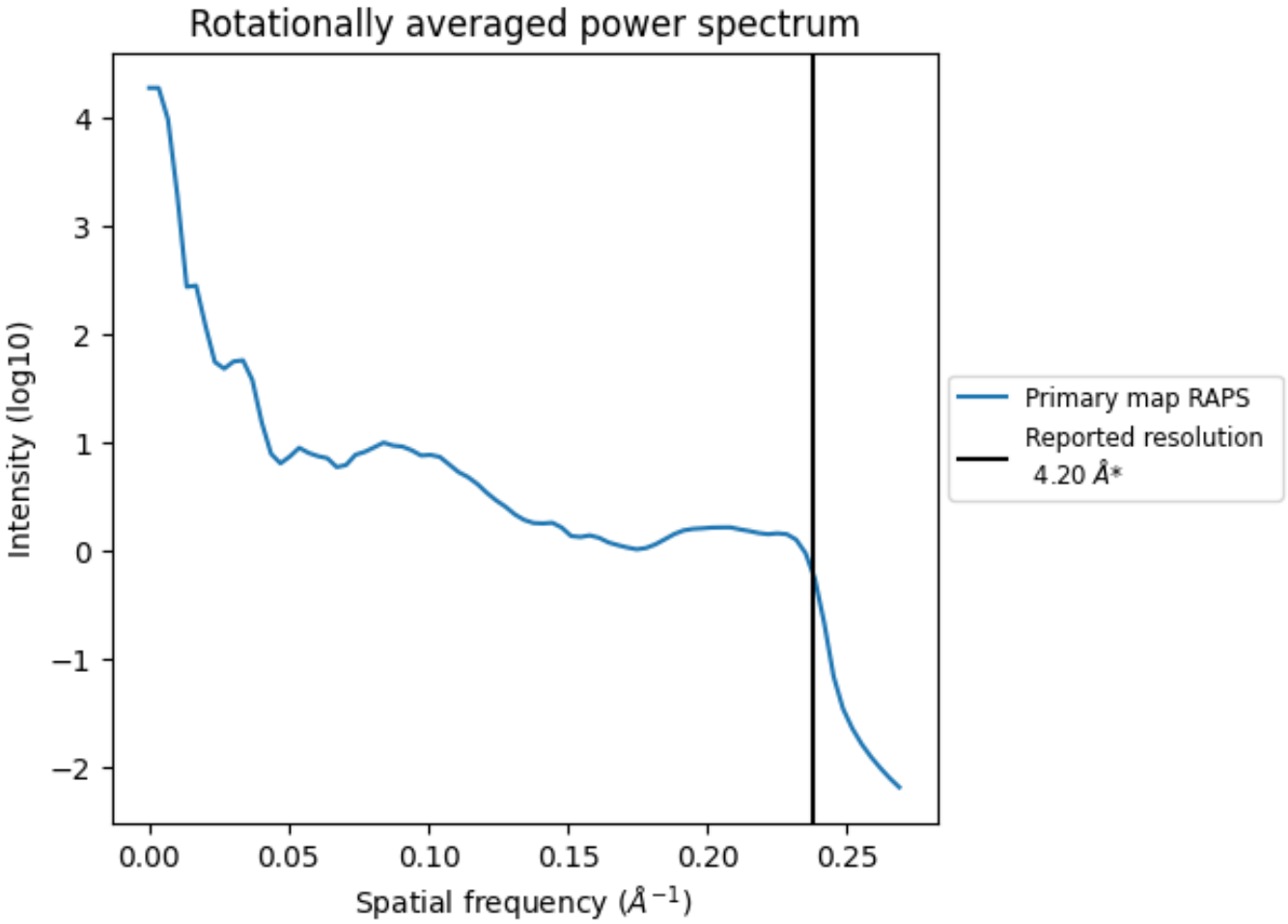
7.2 Volume estimate (i)



The volume at the recommended contour level is 257 nm^3; this corresponds to an approximate mass of 232 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)

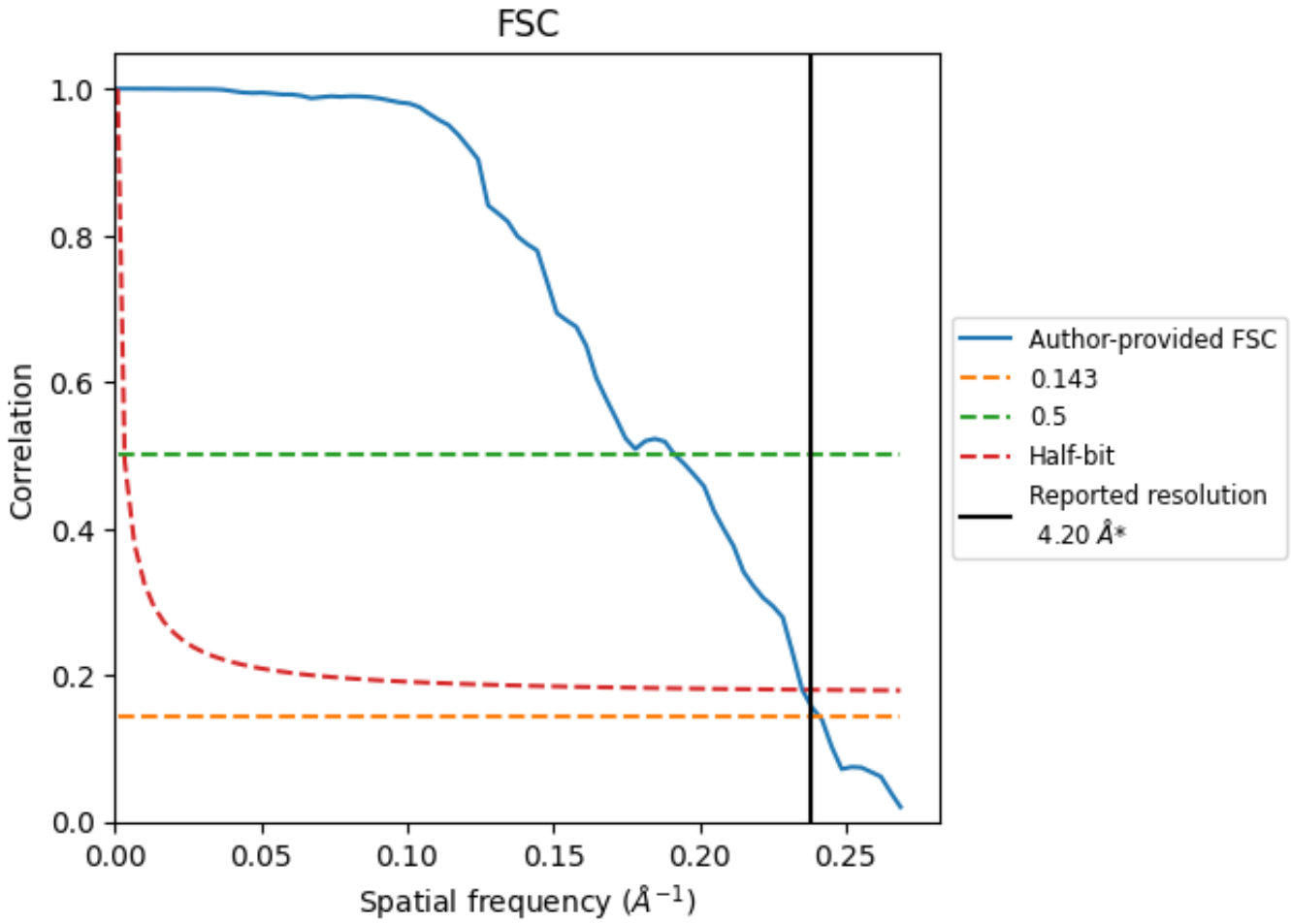


*Reported resolution corresponds to spatial frequency of 0.238 Å^{-1}

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 0.238 Å^{-1}

8.2 Resolution estimates (i)

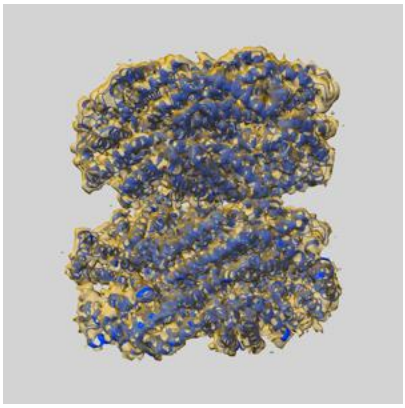
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.15	5.22	4.25
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

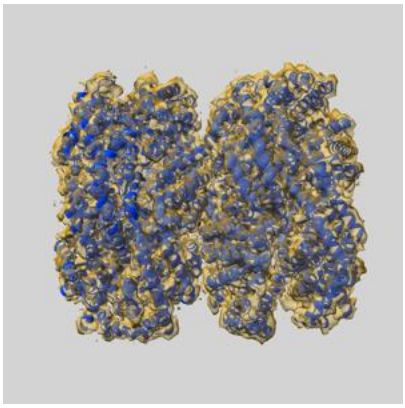
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-31945 and PDB model 7VEB. Per-residue inclusion information can be found in section 3 on page 9.

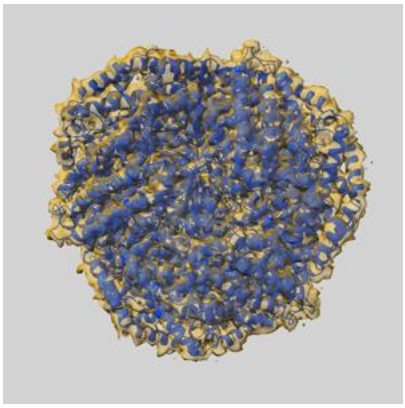
9.1 Map-model overlay



X



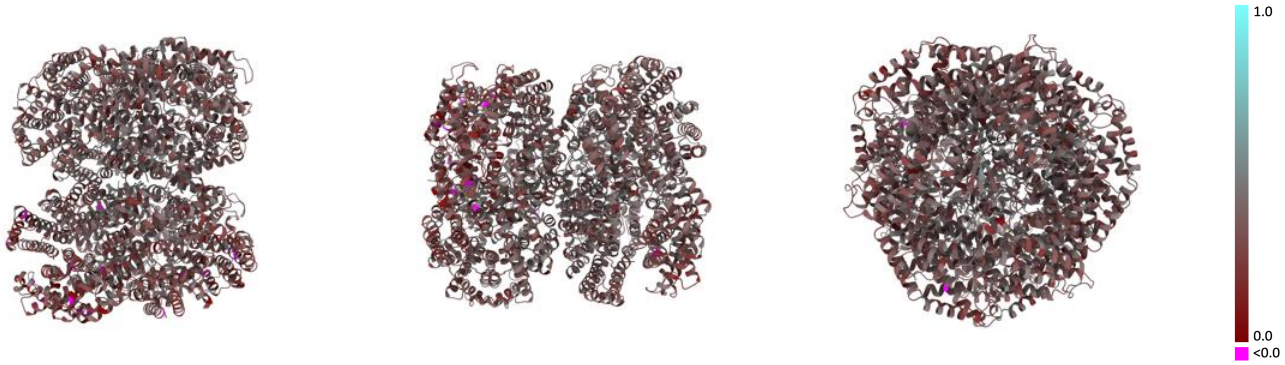
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0286 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.

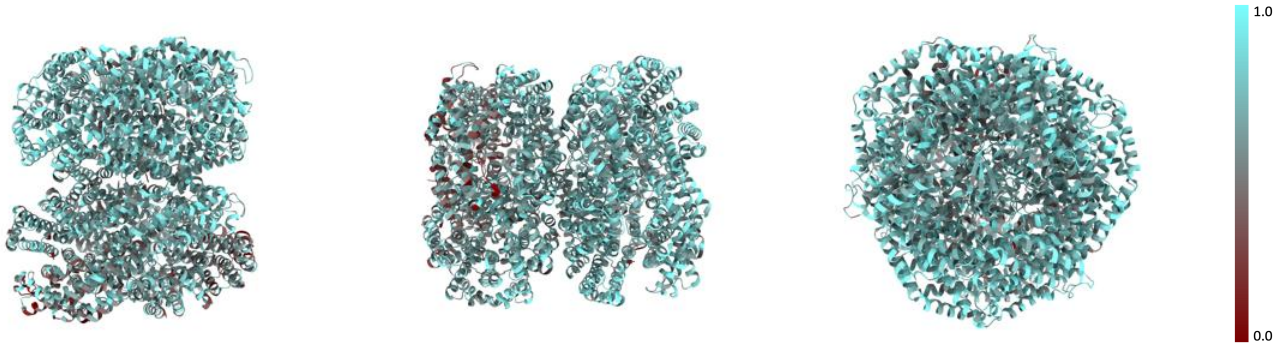
9.2 Q-score mapped to coordinate model



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.

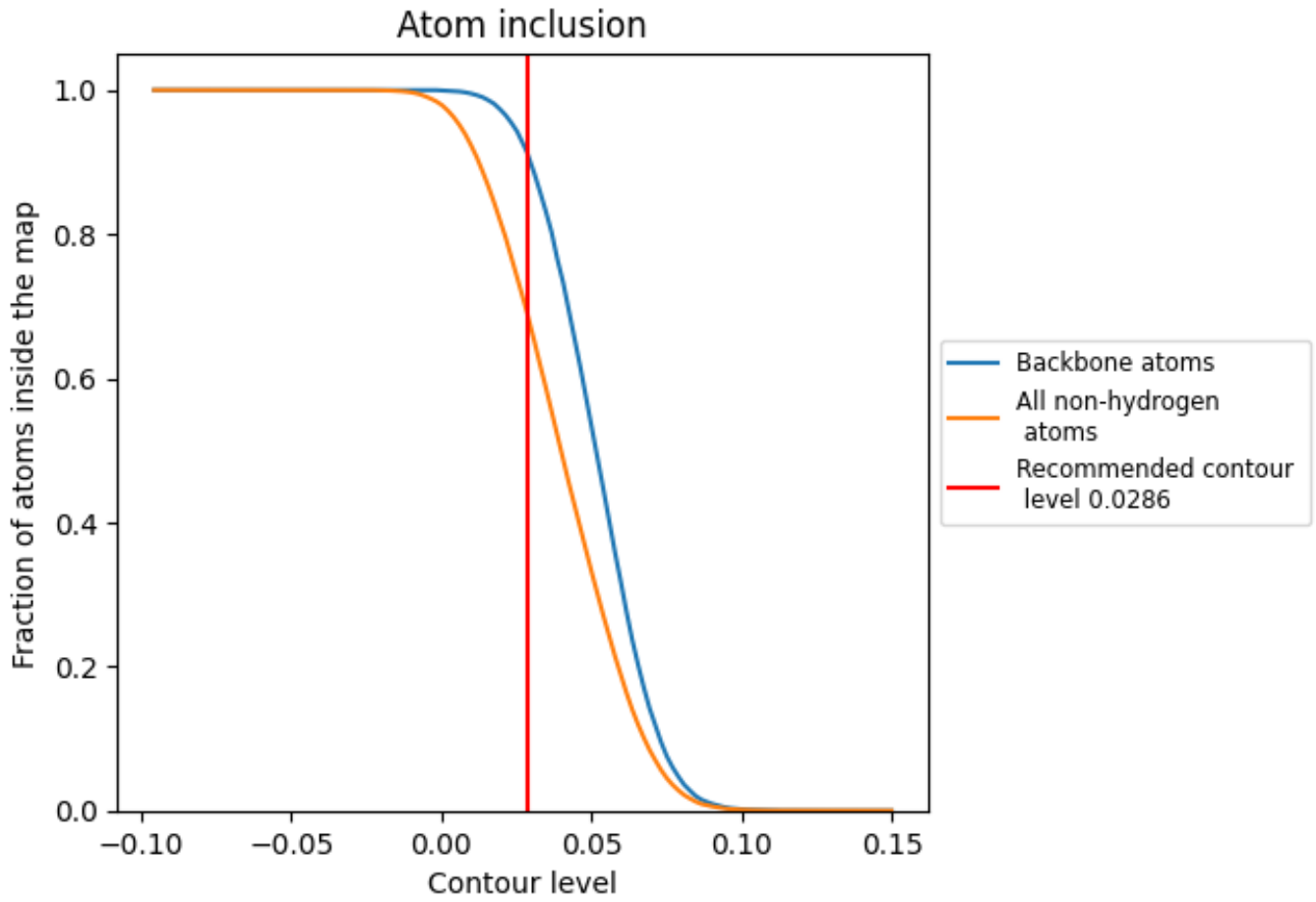
9.3 Atom inclusion mapped to coordinate model



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 (0.0286).

9.4 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 69% 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 (0.0286) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6912	0.3430
A	0.7277	0.3550
B	0.7491	0.3500
C	0.7099	0.3290
D	0.7545	0.3620
E	0.7575	0.3590
F	0.7370	0.3740
G	0.7486	0.3570
H	0.7256	0.3620
I	0.7373	0.3490
J	0.7325	0.3470
K	0.7510	0.3520
L	0.7257	0.3680
M	0.7115	0.3570
N	0.6993	0.3590
O	0.6841	0.3100
P	0.6933	0.3580
Q	0.5496	0.2860
R	0.6179	0.3000
S	0.6280	0.3290
T	0.5763	0.2900
U	0.7099	0.3370
V	0.6992	0.3520
W	0.5436	0.2680
X	0.6049	0.3020
Y	0.7011	0.4010
Z	0.7228	0.3980
a	0.6499	0.3430