wwPDB EM Validation Summary Report (i)

Mar 26, 2026 – 07:12 AM UTC

PDB ID	:	6L7O / pdb_00006l7o
EMDB ID	:	EMD-0849
Title	:	cryo-EM structure of cyanobacteria Fd-NDH-1L complex
Authors	:	Zhang, C.; Shuai, J.; Wu, J.; Lei, M.
Deposited on	:	2019-11-02
Resolution	:	3.20 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 (i) symbol.

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

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

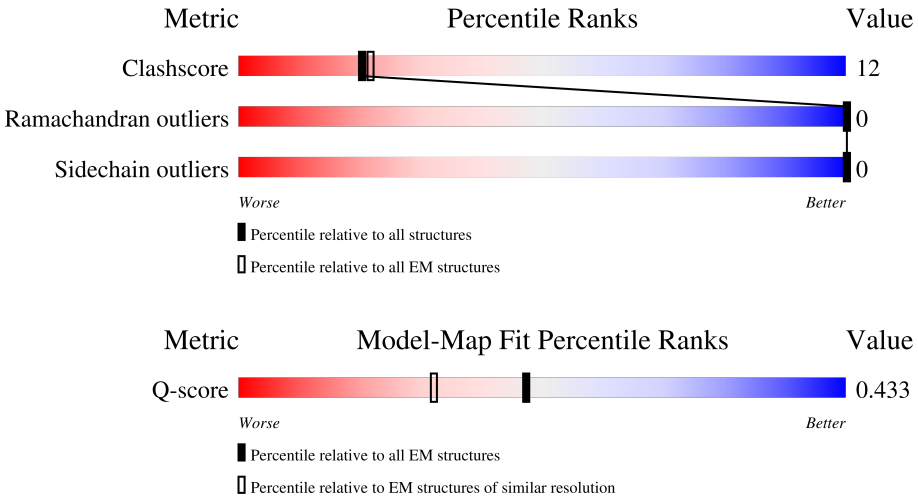
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.20 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

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	372	12% 81% 19%
2	B	515	79% 17%
3	C	132	10% 72% 20% 8%
4	D	529	5% 74% 21% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	101	76% 24%
6	F	656	16% 78% 21%
7	G	200	12% 78% 18%
8	H	394	16% 81% 19%
9	I	196	19% 76% 21%
10	J	168	12% 80% 13% 7%
11	K	237	6% 70% 16% 13%
12	L	76	16% 75% 21%
13	M	111	10% 89% 10%
14	N	150	11% 77% 21%
15	O	70	20% 84% 13%
16	P	44	11% 89% 5% 7%
17	Q	45	18% 78% 20%
18	R	98	77% 82% 17%
19	S	110	27% 45% 12% 44%
20	V	146	47% 50% 21% 29%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	AJP	A	405	X	-	-	-
24	AJP	A	406	X	-	-	-
24	AJP	A	407	X	-	-	-
24	AJP	A	408	X	-	-	-
24	AJP	A	409	X	-	-	-
24	AJP	B	606	X	-	-	-
24	AJP	B	607	X	-	-	-
24	AJP	B	608	X	-	-	-
24	AJP	B	609	X	-	-	-
24	AJP	B	610	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	AJP	B	611	X	-	-	-
24	AJP	B	612	X	-	-	-
24	AJP	B	613	X	-	-	-
24	AJP	B	614	X	-	-	-
24	AJP	B	615	X	-	-	-
24	AJP	B	616	X	-	X	-
24	AJP	B	617	X	-	-	-
24	AJP	C	201	X	-	-	-
24	AJP	C	202	X	-	-	-
24	AJP	D	603	X	-	-	-
24	AJP	D	604	X	-	-	-
24	AJP	D	605	X	-	-	-
24	AJP	D	606	X	-	-	-
24	AJP	D	607	X	-	-	-
24	AJP	D	608	X	-	-	-
24	AJP	D	609	X	-	-	-
24	AJP	D	610	X	-	-	-
24	AJP	D	611	X	-	-	-
24	AJP	D	612	X	-	-	-
24	AJP	D	613	X	-	-	-
24	AJP	D	614	X	-	-	-
24	AJP	E	201	X	-	-	-
24	AJP	F	706	X	-	-	-
24	AJP	F	707	X	-	-	-
24	AJP	F	708	X	-	-	-
24	AJP	F	709	X	-	-	-
24	AJP	F	710	X	-	-	-
24	AJP	F	711	X	-	-	-
24	AJP	F	712	X	-	-	-
24	AJP	F	713	X	-	-	-
24	AJP	F	714	X	-	-	-
24	AJP	F	715	X	-	-	-
24	AJP	F	716	X	-	-	-
24	AJP	F	717	X	-	-	-
24	AJP	F	718	X	-	-	-
24	AJP	G	301	X	-	-	-
24	AJP	G	302	X	-	-	-
24	AJP	G	303	X	-	-	-
24	AJP	G	304	X	-	-	-
24	AJP	G	305	X	-	-	-
24	AJP	G	306	X	-	-	-
24	AJP	G	307	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	AJP	Q	101	X	-	-	-
24	AJP	Q	102	X	-	-	-
24	AJP	Q	103	X	-	-	-
24	AJP	Q	104	X	-	-	-
24	AJP	Q	105	X	-	-	-
24	AJP	Q	106	X	-	-	-
24	AJP	Q	107	X	-	-	-
24	AJP	Q	108	X	-	-	-
27	SF4	K	301	-	-	X	-
28	FES	R	101	-	-	X	-

2 Entry composition (i)

There are 28 unique types of molecules in this entry. The entry contains 35037 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 NAD(P)H-quinone oxidoreductase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	371	2859	1919	444	486	10	0	0

- Molecule 2 is a protein called NAD(P)H-quinone oxidoreductase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	493	3732	2476	579	661	16	0	0

- Molecule 3 is a protein called NAD(P)H-quinone oxidoreductase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	121	978	669	150	155	4	0	0

- Molecule 4 is a protein called NAD(P)H-quinone oxidoreductase chain 4 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	504	3896	2613	606	656	21	0	0

- Molecule 5 is a protein called NAD(P)H-quinone oxidoreductase subunit 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	101	783	517	128	134	4	0	0

- Molecule 6 is a protein called NADH dehydrogenase subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	647	5004	3318	796	852	38	0	0

- Molecule 7 is a protein called NADH-quinone oxidoreductase subunit J.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	192	Total	C	N	O	S	0	0
			1463	974	229	256	4		

- Molecule 8 is a protein called NAD(P)H-quinone oxidoreductase subunit H.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	393	Total	C	N	O	S	0	0
			3177	2048	545	565	19		

- Molecule 9 is a protein called NAD(P)H-quinone oxidoreductase subunit I.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	190	Total	C	N	O	S	0	0
			1525	973	262	277	13		

- Molecule 10 is a protein called NAD(P)H-quinone oxidoreductase subunit J.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	156	Total	C	N	O	S	0	0
			1278	817	218	238	5		

- Molecule 11 is a protein called NAD(P)H-quinone oxidoreductase subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	206	Total	C	N	O	S	0	0
			1597	1024	276	284	13		

- Molecule 12 is a protein called NAD(P)H-quinone oxidoreductase subunit L.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	73	Total	C	N	O	S	0	0
			590	406	90	93	1		

- Molecule 13 is a protein called NAD(P)H-quinone oxidoreductase subunit M.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	110	Total	C	N	O	S	0	0
			879	548	160	169	2		

- Molecule 14 is a protein called NAD(P)H-quinone oxidoreductase subunit N.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	148	Total	C	N	O	S	0	0
			1165	758	201	205	1		

- Molecule 15 is a protein called NAD(P)H-quinone oxidoreductase subunit O.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	O	68	Total	C	N	O	0	0
			538	349	91	98		

- Molecule 16 is a protein called NAD(P)H-quinone oxidoreductase subunit P.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	41	Total	C	N	O	S	0	0
			321	212	52	55	2		

- Molecule 17 is a protein called NAD(P)H-quinone oxidoreductase subunit Q.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	44	Total	C	N	O	S	0	0
			332	221	53	56	2		

- Molecule 18 is a protein called Ferredoxin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	97	Total	C	N	O	S	0	0
			748	463	116	164	5		

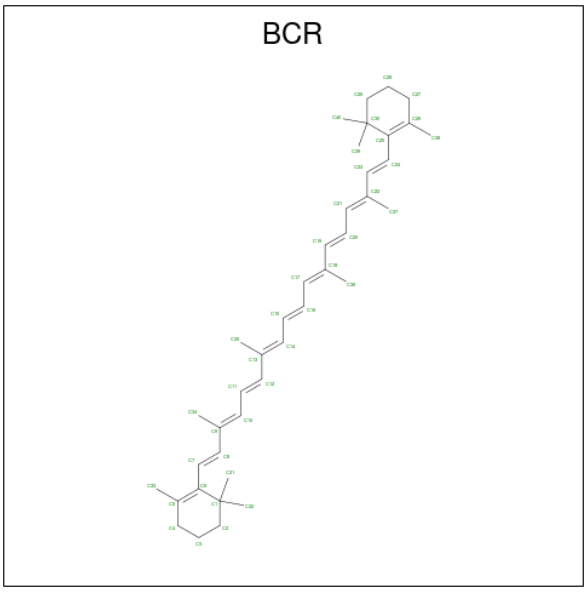
- Molecule 19 is a protein called Tlr0636 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	62	Total	C	N	O	S	0	0
			485	314	76	93	2		

- Molecule 20 is a protein called Tlr0472 protein.

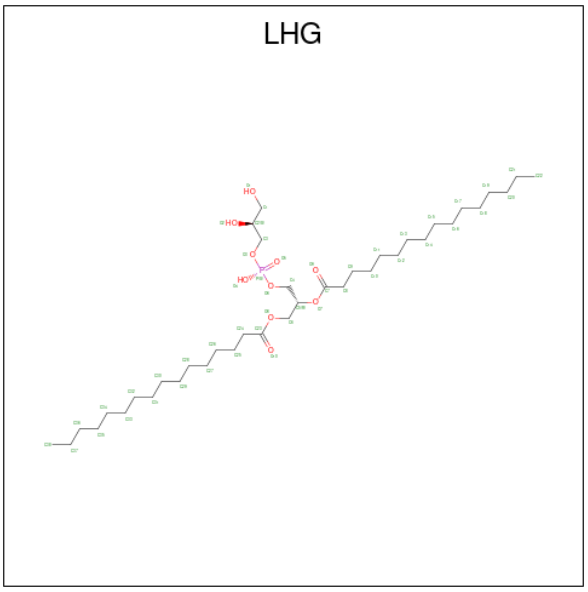
Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	103	Total	C	N	O	S	0	0
			797	517	133	143	4		

- Molecule 21 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



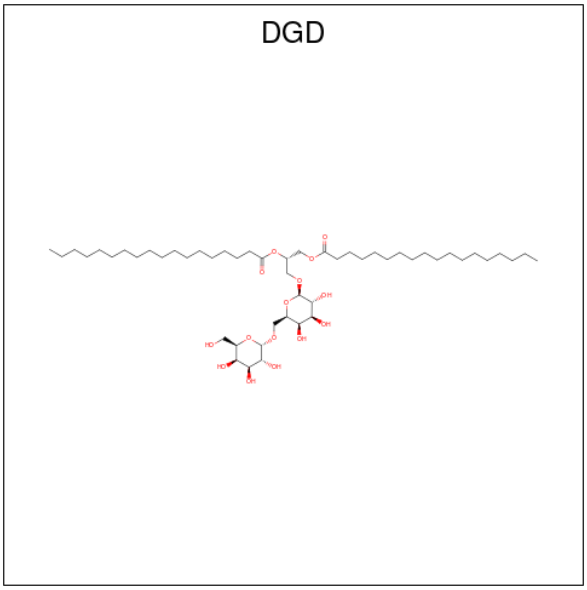
Mol	Chain	Residues	Atoms	AltConf
21	A	1	Total C 40 40	0
21	F	1	Total C 40 40	0
21	P	1	Total C 40 40	0

- Molecule 22 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



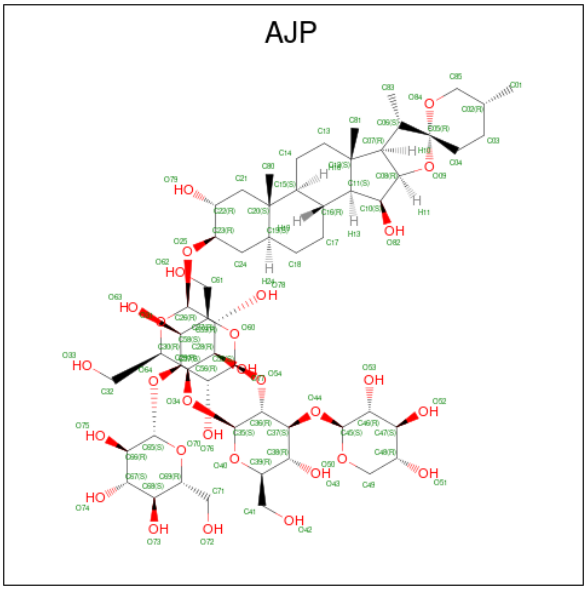
Mol	Chain	Residues	Atoms				AltConf
22	A	1	Total	C	O	P	0
			49	38	10	1	
22	B	1	Total	C	O	P	0
			49	38	10	1	
22	B	1	Total	C	O	P	0
			49	38	10	1	
22	B	1	Total	C	O	P	0
			49	38	10	1	
22	D	1	Total	C	O	P	0
			49	38	10	1	
22	D	1	Total	C	O	P	0
			49	38	10	1	
22	F	1	Total	C	O	P	0
			49	38	10	1	
22	F	1	Total	C	O	P	0
			49	38	10	1	
22	H	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 23 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			AltConf
23	A	1	Total	C	O	0
			66	51	15	
23	A	1	Total	C	O	0
			66	51	15	

- Molecule 24 is Digitonin (CCD ID: AJP) (formula: $C_{56}H_{92}O_{29}$).



Mol	Chain	Residues	Atoms	AltConf
24	A	1	Total C O 32 27 5	0
24	A	1	Total C O 32 27 5	0
24	A	1	Total C O 32 27 5	0
24	A	1	Total C O 32 27 5	0
24	A	1	Total C O 32 27 5	0
24	B	1	Total C O 32 27 5	0
24	B	1	Total C O 32 27 5	0
24	B	1	Total C O 32 27 5	0
24	B	1	Total C O 32 27 5	0
24	B	1	Total C O 32 27 5	0
24	B	1	Total C O 32 27 5	0
24	B	1	Total C O 32 27 5	0
24	B	1	Total C O 32 27 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
24	B	1	Total C O 32 27 5	0
24	B	1	Total C O 32 27 5	0
24	B	1	Total C O 32 27 5	0
24	B	1	Total C O 32 27 5	0
24	C	1	Total C O 32 27 5	0
24	C	1	Total C O 32 27 5	0
24	D	1	Total C O 32 27 5	0
24	D	1	Total C O 32 27 5	0
24	D	1	Total C O 32 27 5	0
24	D	1	Total C O 32 27 5	0
24	D	1	Total C O 32 27 5	0
24	D	1	Total C O 32 27 5	0
24	D	1	Total C O 32 27 5	0
24	D	1	Total C O 32 27 5	0
24	D	1	Total C O 32 27 5	0
24	D	1	Total C O 32 27 5	0
24	D	1	Total C O 32 27 5	0
24	D	1	Total C O 32 27 5	0
24	D	1	Total C O 32 27 5	0
24	E	1	Total C O 32 27 5	0
24	F	1	Total C O 32 27 5	0
24	F	1	Total C O 32 27 5	0

Continued on next page...

Continued from previous page...

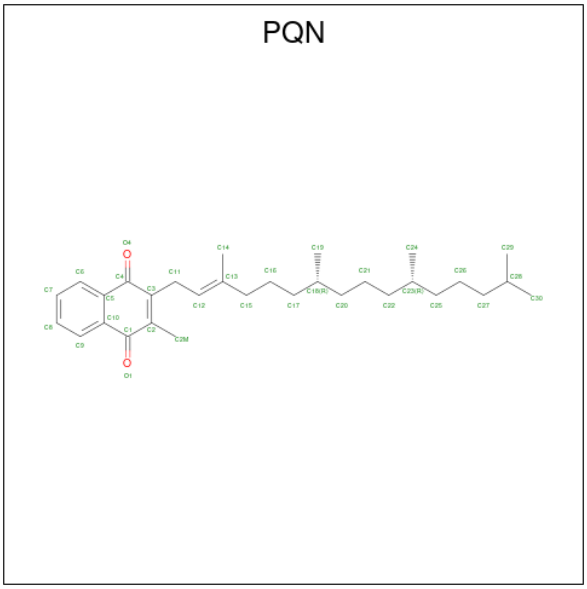
Mol	Chain	Residues	Atoms	AltConf
24	F	1	Total C O 32 27 5	0
24	F	1	Total C O 32 27 5	0
24	F	1	Total C O 32 27 5	0
24	F	1	Total C O 32 27 5	0
24	F	1	Total C O 32 27 5	0
24	F	1	Total C O 32 27 5	0
24	F	1	Total C O 32 27 5	0
24	F	1	Total C O 32 27 5	0
24	F	1	Total C O 32 27 5	0
24	F	1	Total C O 32 27 5	0
24	F	1	Total C O 32 27 5	0
24	G	1	Total C O 32 27 5	0
24	G	1	Total C O 32 27 5	0
24	G	1	Total C O 32 27 5	0
24	G	1	Total C O 32 27 5	0
24	G	1	Total C O 32 27 5	0
24	G	1	Total C O 32 27 5	0
24	G	1	Total C O 32 27 5	0
24	Q	1	Total C O 32 27 5	0
24	Q	1	Total C O 32 27 5	0
24	Q	1	Total C O 32 27 5	0

Continued on next page...

Continued from previous page...

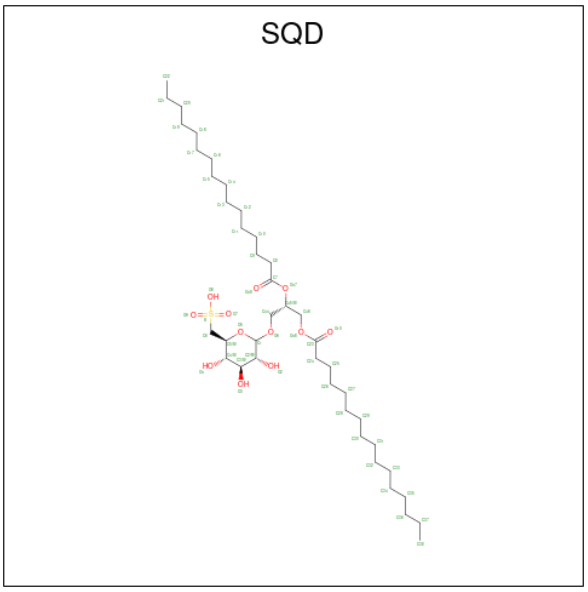
Mol	Chain	Residues	Atoms	AltConf
24	Q	1	Total C O 32 27 5	0
24	Q	1	Total C O 32 27 5	0
24	Q	1	Total C O 32 27 5	0
24	Q	1	Total C O 32 27 5	0
24	Q	1	Total C O 32 27 5	0

- Molecule 25 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



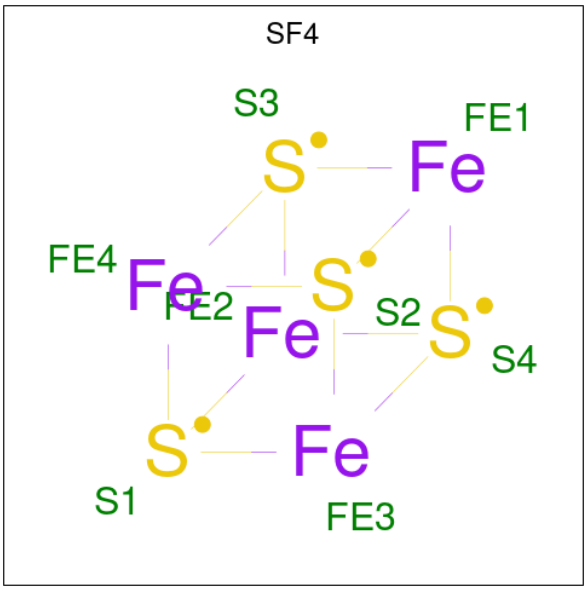
Mol	Chain	Residues	Atoms	AltConf
25	B	1	Total C O 33 31 2	0

- Molecule 26 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



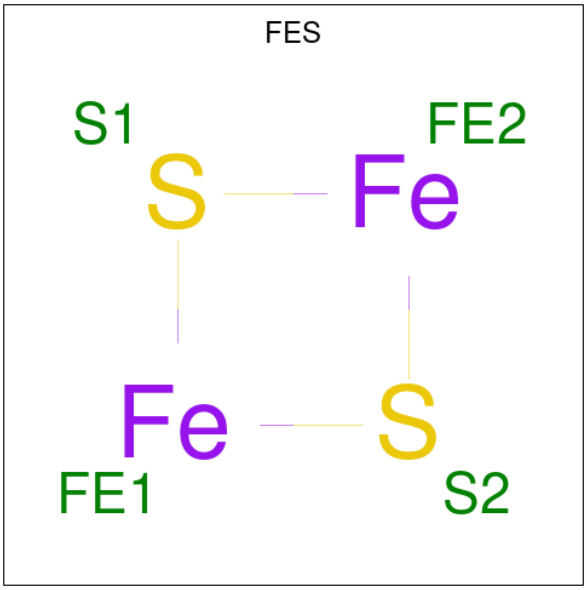
Mol	Chain	Residues	Atoms				AltConf
26	B	1	Total	C	O	S	0
			54	41	12	1	
26	F	1	Total	C	O	S	0
			54	41	12	1	
26	F	1	Total	C	O	S	0
			54	41	12	1	
26	L	1	Total	C	O	S	0
			54	41	12	1	

- Molecule 27 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	AltConf
27	I	1	Total Fe S 8 4 4	0
27	I	1	Total Fe S 8 4 4	0
27	K	1	Total Fe S 8 4 4	0

- Molecule 28 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



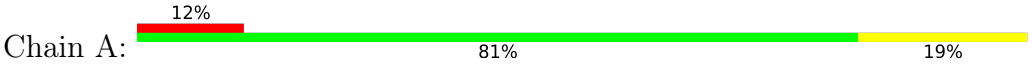
Mol	Chain	Residues	Atoms	AltConf
28	R	1	Total Fe S 4 2 2	0

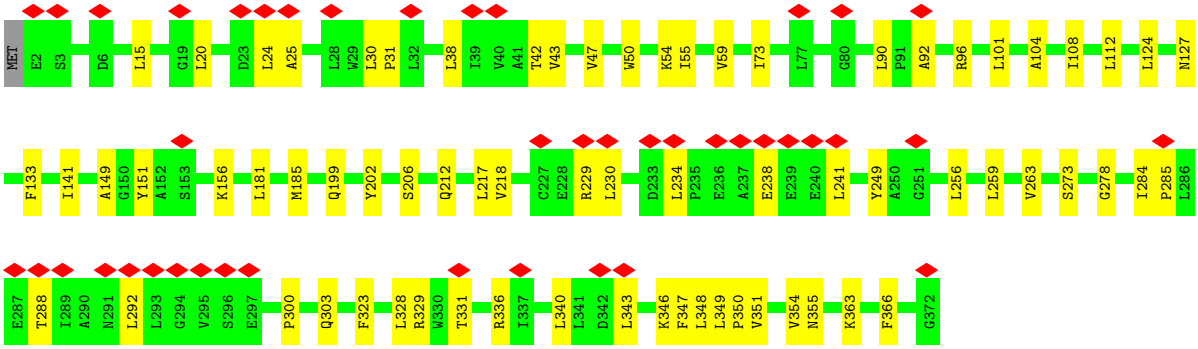
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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: NAD(P)H-quinone oxidoreductase subunit 1

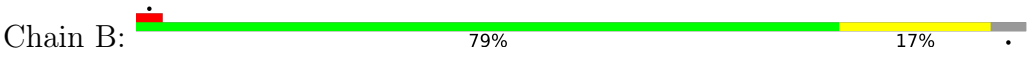
Chain A:

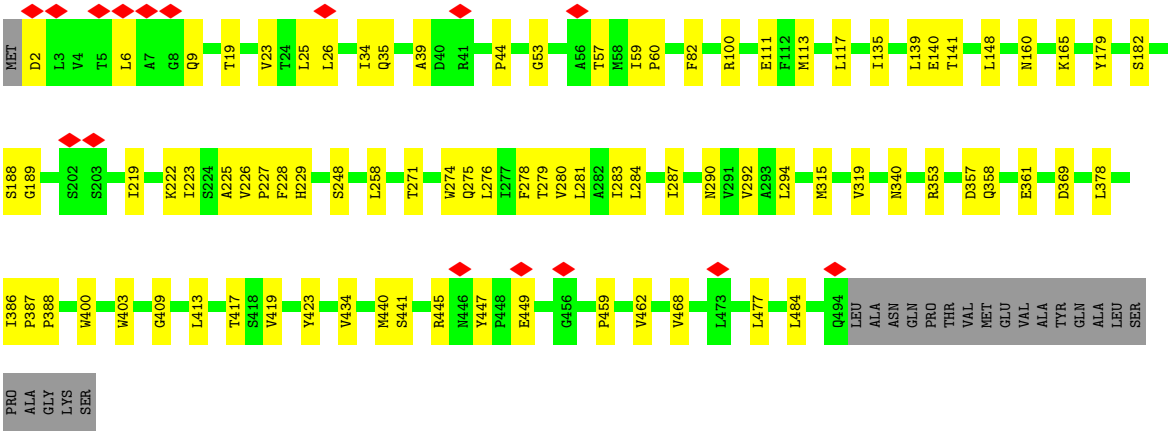




• Molecule 2: NAD(P)H-quinone oxidoreductase subunit 2

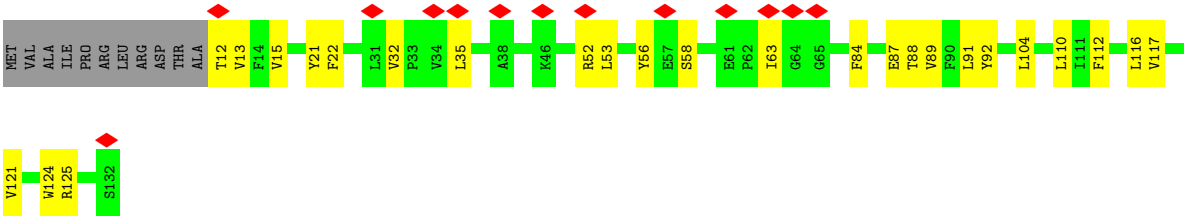
Chain B:





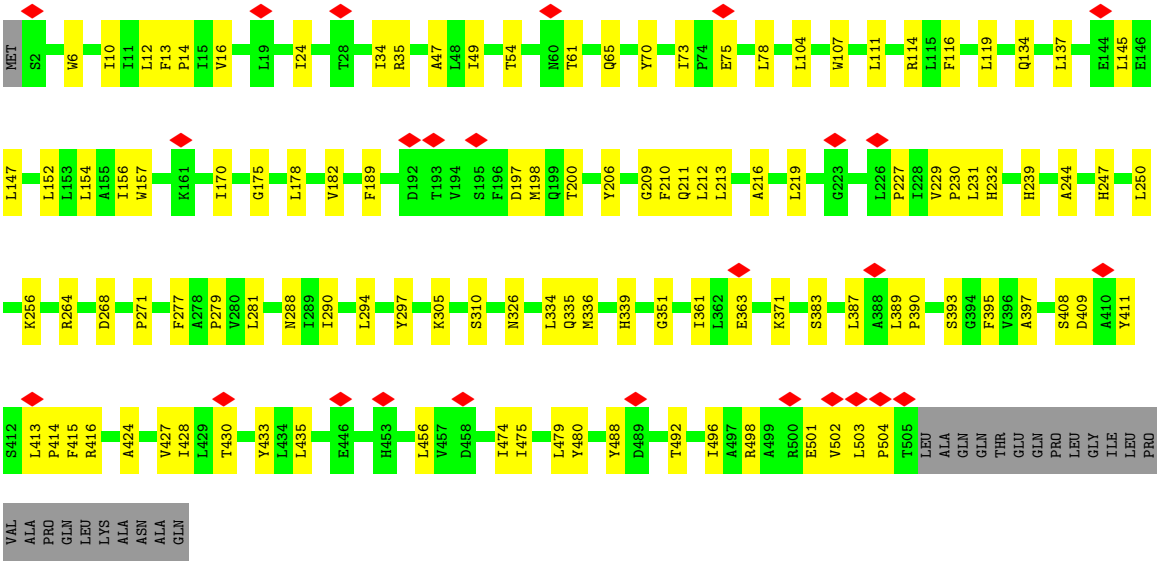
• Molecule 3: NAD(P)H-quinone oxidoreductase subunit 3

Chain C:



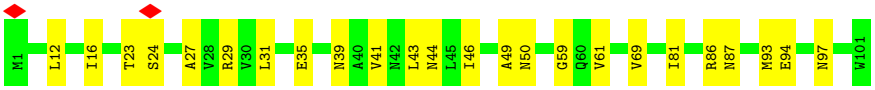
• Molecule 4: NAD(P)H-quinone oxidoreductase chain 4 1

Chain D:



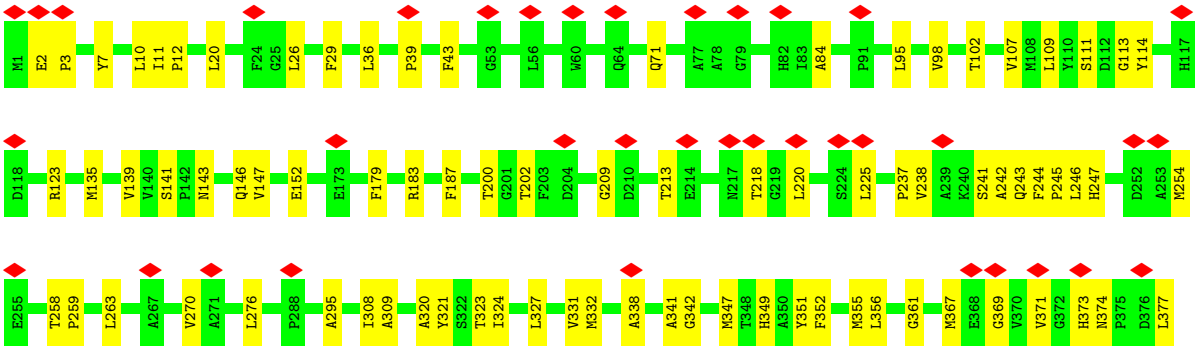
• Molecule 5: NAD(P)H-quinone oxidoreductase subunit 4L

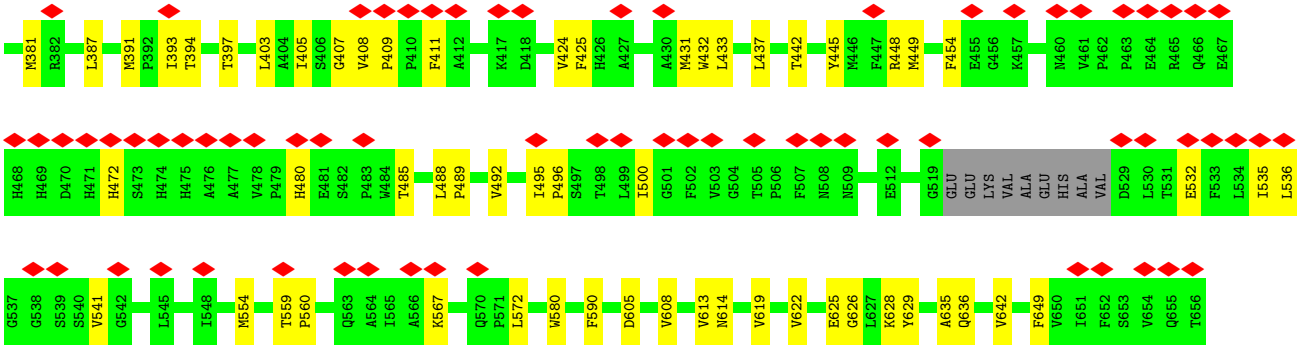
Chain E:



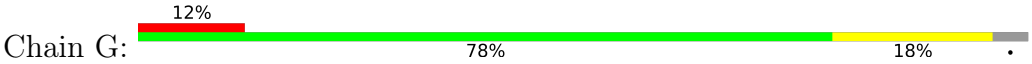
• Molecule 6: NADH dehydrogenase subunit 5

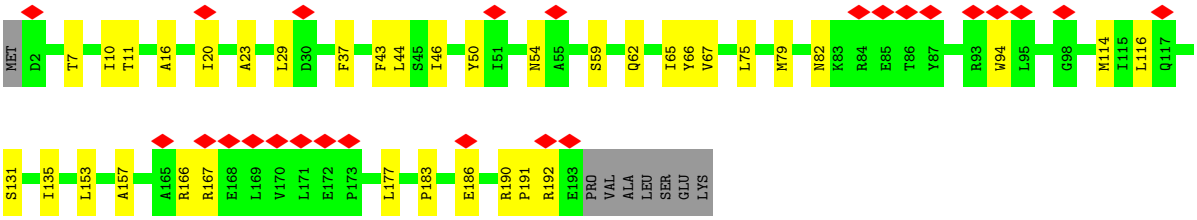
Chain F:



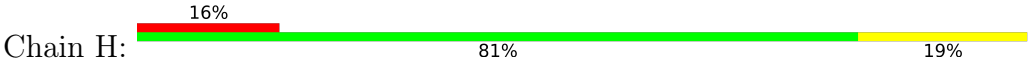


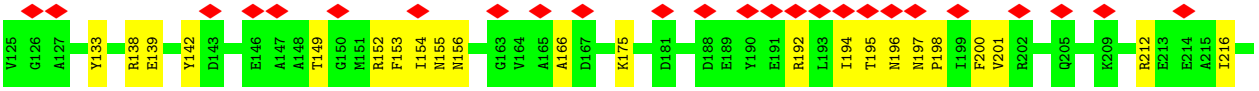
• Molecule 7: NADH-quinone oxidoreductase subunit J

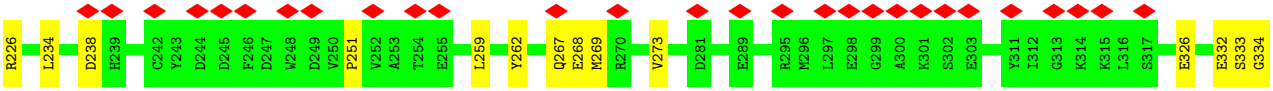


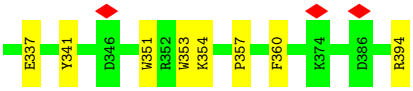


• Molecule 8: NAD(P)H-quinone oxidoreductase subunit H

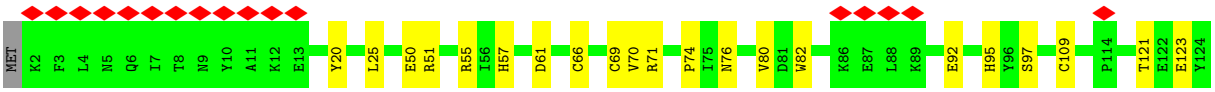


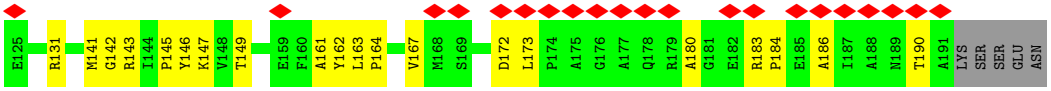




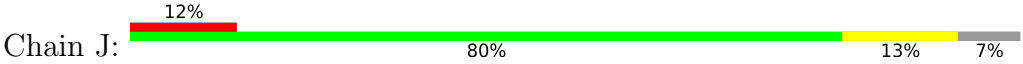


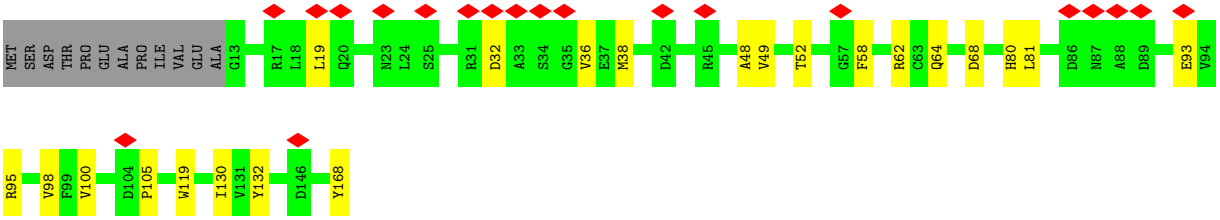
• Molecule 9: NAD(P)H-quinone oxidoreductase subunit I



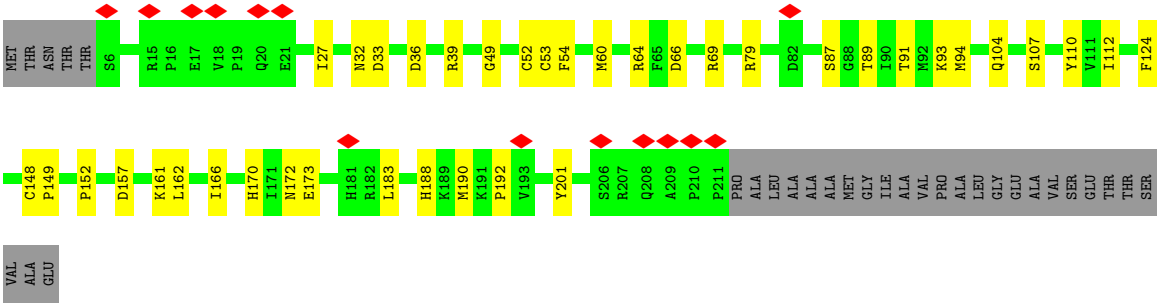


• Molecule 10: NAD(P)H-quinone oxidoreductase subunit J

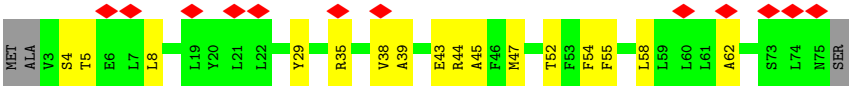




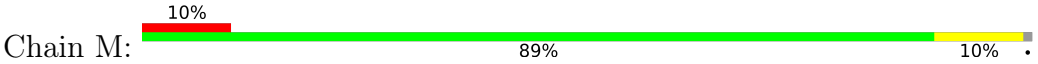
• Molecule 11: NAD(P)H-quinone oxidoreductase subunit K

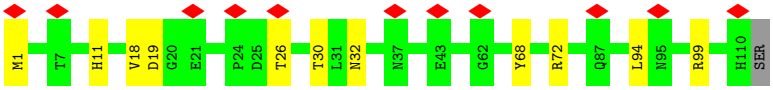


• Molecule 12: NAD(P)H-quinone oxidoreductase subunit L

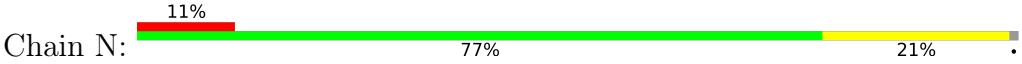


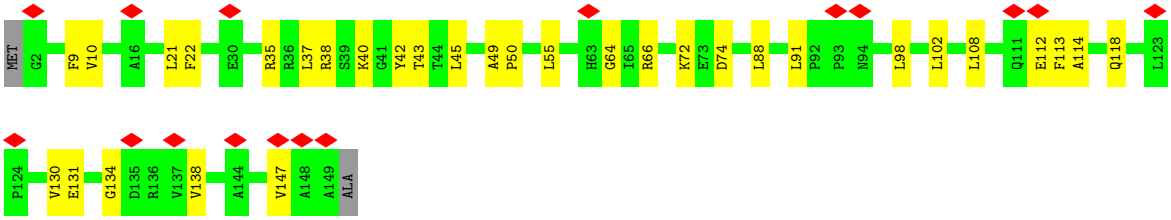
• Molecule 13: NAD(P)H-quinone oxidoreductase subunit M



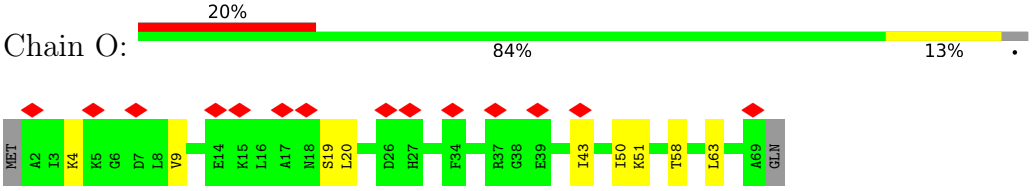


• Molecule 14: NAD(P)H-quinone oxidoreductase subunit N

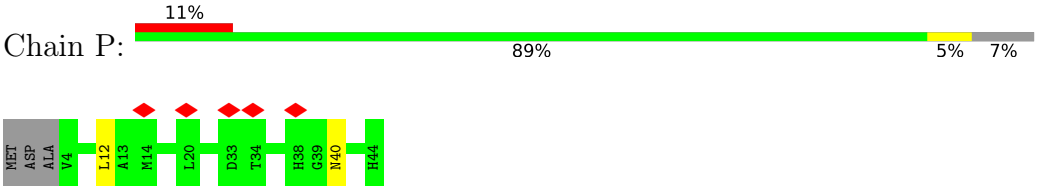




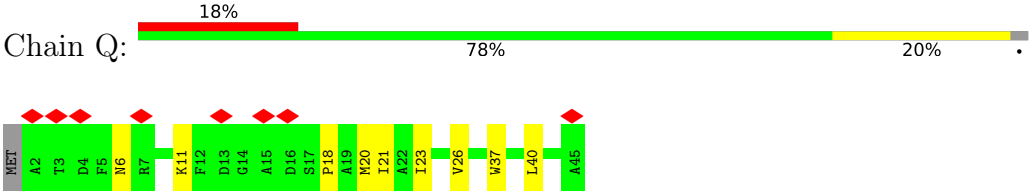
• Molecule 15: NAD(P)H-quinone oxidoreductase subunit O



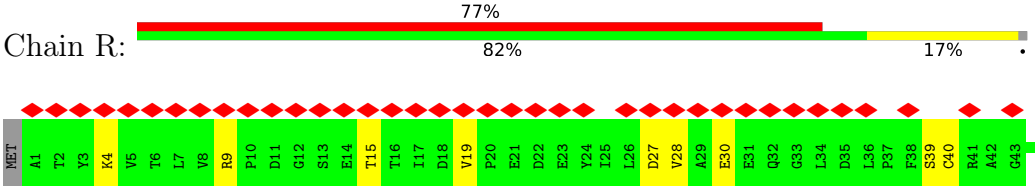
• Molecule 16: NAD(P)H-quinone oxidoreductase subunit P

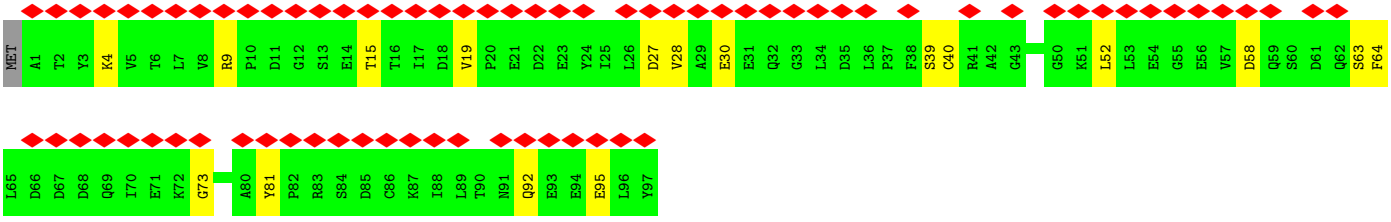


• Molecule 17: NAD(P)H-quinone oxidoreductase subunit Q

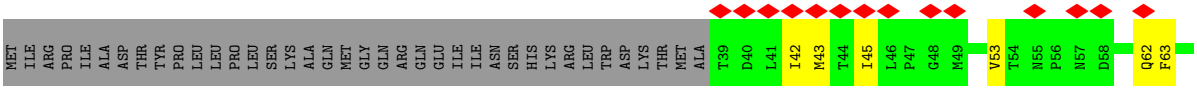


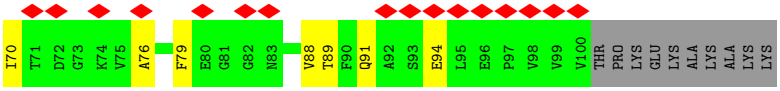
• Molecule 18: Ferredoxin-1



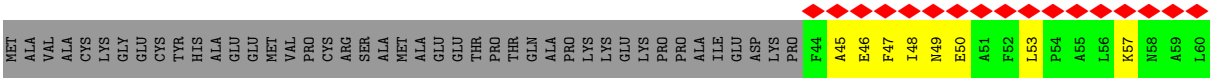


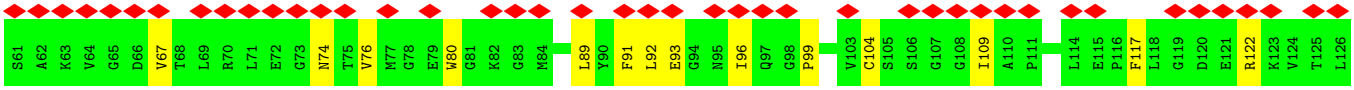
• Molecule 19: Tlr0636 protein

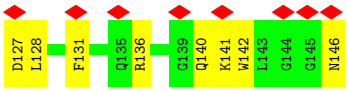




• Molecule 20: Tlr0472 protein







4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	338822	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.401	Depositor
Minimum map value	-0.167	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.038	Depositor
Map size (Å)	327.0, 327.0, 327.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.09, 1.09, 1.09	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DGD, SQD, AJP, FES, BCR, PQN, LHG, SF4

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	0.13	0/2932	0.36	0/4008
2	B	0.11	0/3818	0.30	0/5209
3	C	0.14	0/1008	0.38	0/1375
4	D	0.11	0/4003	0.32	0/5464
5	E	0.10	0/793	0.29	0/1077
6	F	0.11	0/5153	0.30	0/7020
7	G	0.10	0/1495	0.28	0/2050
8	H	0.11	0/3260	0.32	0/4417
9	I	0.11	0/1563	0.32	0/2119
10	J	0.10	0/1314	0.28	0/1789
11	K	0.14	0/1638	0.33	0/2230
12	L	0.12	0/610	0.34	0/835
13	M	0.08	0/895	0.27	0/1214
14	N	0.10	0/1197	0.29	0/1628
15	O	0.10	0/550	0.31	0/748
16	P	0.14	0/330	0.46	0/448
17	Q	0.09	0/341	0.29	0/464
18	R	0.11	0/758	0.32	0/1029
19	S	0.10	0/494	0.33	0/674
20	V	0.15	0/814	0.47	1/1097 (0.1%)
All	All	0.11	0/32966	0.32	1/44895 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	V	96	ILE	N-CA-C	-6.53	107.51	113.71

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	2859	0	2983	71	0
2	B	3732	0	3864	109	0
3	C	978	0	1008	43	0
4	D	3896	0	4041	129	0
5	E	783	0	837	20	0
6	F	5004	0	5033	128	0
7	G	1463	0	1546	52	0
8	H	3177	0	3155	58	0
9	I	1525	0	1500	33	0
10	J	1278	0	1233	15	0
11	K	1597	0	1628	35	0
12	L	590	0	602	12	0
13	M	879	0	860	9	0
14	N	1165	0	1176	28	0
15	O	538	0	549	7	0
16	P	321	0	317	2	0
17	Q	332	0	331	11	0
18	R	748	0	709	11	0
19	S	485	0	488	9	0
20	V	797	0	800	22	0
21	A	40	0	55	4	0
21	F	40	0	54	3	0
21	P	40	0	54	5	0
22	A	49	0	73	3	0
22	B	147	0	222	4	0
22	D	98	0	148	1	0
22	F	98	0	145	8	0
22	H	49	0	73	3	0
23	A	132	0	191	3	0
24	A	160	0	0	26	0
24	B	384	0	0	84	0
24	C	64	0	0	17	0
24	D	384	0	0	99	0
24	E	32	0	0	1	0
24	F	416	0	0	65	0
24	G	224	0	0	43	0
24	Q	256	0	0	22	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	B	33	0	44	0	0
26	B	54	0	78	3	0
26	F	108	0	156	6	0
26	L	54	0	77	1	0
27	I	16	0	0	1	0
27	K	8	0	0	3	0
28	R	4	0	0	2	0
All	All	35037	0	34030	841	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 12.

The worst 5 of 841 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)
4:D:413:LEU:HD21	24:D:608:AJP:C80	1.23	1.64
2:B:484:LEU:HD11	24:B:606:AJP:C13	1.27	1.60
2:B:287:ILE:CD1	24:B:616:AJP:C83	1.75	1.59
7:G:7:THR:HG22	24:G:302:AJP:C83	1.18	1.56
6:F:39:PRO:HB3	24:F:714:AJP:C83	1.23	1.55

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	369/372 (99%)	342 (93%)	27 (7%)	0	100	100
2	B	491/515 (95%)	472 (96%)	19 (4%)	0	100	100
3	C	119/132 (90%)	115 (97%)	4 (3%)	0	100	100
4	D	502/529 (95%)	477 (95%)	25 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
6	F	643/656 (98%)	613 (95%)	30 (5%)	0	100	100
7	G	190/200 (95%)	183 (96%)	7 (4%)	0	100	100
8	H	391/394 (99%)	359 (92%)	32 (8%)	0	100	100
9	I	188/196 (96%)	177 (94%)	11 (6%)	0	100	100
10	J	154/168 (92%)	147 (96%)	7 (4%)	0	100	100
11	K	204/237 (86%)	193 (95%)	11 (5%)	0	100	100
12	L	71/76 (93%)	65 (92%)	6 (8%)	0	100	100
13	M	108/111 (97%)	100 (93%)	8 (7%)	0	100	100
14	N	146/150 (97%)	140 (96%)	6 (4%)	0	100	100
15	O	66/70 (94%)	61 (92%)	5 (8%)	0	100	100
16	P	39/44 (89%)	37 (95%)	2 (5%)	0	100	100
17	Q	42/45 (93%)	42 (100%)	0	0	100	100
18	R	95/98 (97%)	95 (100%)	0	0	100	100
19	S	60/110 (54%)	58 (97%)	2 (3%)	0	100	100
20	V	101/146 (69%)	93 (92%)	8 (8%)	0	100	100
All	All	4078/4350 (94%)	3863 (95%)	215 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	300/302 (99%)	300 (100%)	0	100	100
2	B	396/413 (96%)	396 (100%)	0	100	100
3	C	100/109 (92%)	100 (100%)	0	100	100
4	D	404/424 (95%)	404 (100%)	0	100	100
5	E	82/82 (100%)	82 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	519/527 (98%)	519 (100%)	0	100	100
7	G	159/166 (96%)	159 (100%)	0	100	100
8	H	337/338 (100%)	337 (100%)	0	100	100
9	I	166/172 (96%)	166 (100%)	0	100	100
10	J	138/148 (93%)	138 (100%)	0	100	100
11	K	175/196 (89%)	175 (100%)	0	100	100
12	L	61/63 (97%)	61 (100%)	0	100	100
13	M	95/96 (99%)	95 (100%)	0	100	100
14	N	119/120 (99%)	119 (100%)	0	100	100
15	O	57/59 (97%)	57 (100%)	0	100	100
16	P	35/37 (95%)	35 (100%)	0	100	100
17	Q	31/32 (97%)	31 (100%)	0	100	100
18	R	85/86 (99%)	85 (100%)	0	100	100
19	S	55/97 (57%)	55 (100%)	0	100	100
20	V	83/118 (70%)	83 (100%)	0	100	100
All	All	3397/3585 (95%)	3397 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 49 such sidechains are listed below:

Mol	Chain	Res	Type
9	I	95	HIS
11	K	170	HIS
9	I	116	ASN
11	K	20	GLN
13	M	23	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)

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

83 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	$\#\|Z\| > 2$
24	AJP	D	604	-	37,37,95	1.57	8 (21%)	58,62,149	2.33	21 (36%)
24	AJP	F	713	-	37,37,95	1.42	7 (18%)	58,62,149	2.16	18 (31%)
24	AJP	D	606	-	37,37,95	1.41	6 (16%)	58,62,149	2.07	18 (31%)
22	LHG	A	402	-	48,48,48	0.63	1 (2%)	51,54,54	1.28	6 (11%)
22	LHG	F	703	-	48,48,48	0.59	1 (2%)	51,54,54	1.26	6 (11%)
24	AJP	Q	108	-	37,37,95	1.28	7 (18%)	58,62,149	2.07	16 (27%)
24	AJP	B	609	-	37,37,95	1.32	7 (18%)	58,62,149	2.17	16 (27%)
24	AJP	G	305	-	37,37,95	1.32	8 (21%)	58,62,149	2.01	18 (31%)
24	AJP	F	706	-	37,37,95	1.35	7 (18%)	58,62,149	1.97	20 (34%)
24	AJP	G	304	-	37,37,95	1.40	8 (21%)	58,62,149	2.05	18 (31%)
22	LHG	B	602	-	48,48,48	0.62	2 (4%)	51,54,54	1.28	6 (11%)
24	AJP	F	717	-	37,37,95	1.31	8 (21%)	58,62,149	2.14	17 (29%)
24	AJP	G	307	-	37,37,95	1.29	6 (16%)	58,62,149	1.96	16 (27%)
24	AJP	A	406	-	37,37,95	1.31	3 (8%)	58,62,149	2.08	20 (34%)
24	AJP	B	606	-	37,37,95	1.54	7 (18%)	58,62,149	2.21	19 (32%)
22	LHG	D	602	-	48,48,48	0.63	2 (4%)	51,54,54	1.29	6 (11%)
24	AJP	B	615	-	37,37,95	1.22	7 (18%)	58,62,149	1.95	16 (27%)
24	AJP	G	302	-	37,37,95	1.33	8 (21%)	58,62,149	2.08	19 (32%)
24	AJP	D	614	-	37,37,95	1.30	7 (18%)	58,62,149	2.05	17 (29%)
24	AJP	Q	101	-	37,37,95	1.28	7 (18%)	58,62,149	2.01	15 (25%)
24	AJP	F	712	-	37,37,95	1.19	4 (10%)	58,62,149	1.95	16 (27%)
24	AJP	B	616	-	37,37,95	1.38	7 (18%)	58,62,149	2.13	17 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	BCR	P	101	-	41,41,41	1.13	2 (4%)	56,56,56	1.24	6 (10%)
24	AJP	F	711	-	37,37,95	1.35	7 (18%)	58,62,149	1.97	18 (31%)
27	SF4	K	301	11	0,12,12	-	-	-		
26	SQD	F	704	-	52,54,54	0.95	3 (5%)	62,65,65	1.43	9 (14%)
24	AJP	D	611	-	37,37,95	1.29	7 (18%)	58,62,149	2.15	16 (27%)
22	LHG	B	603	-	48,48,48	0.62	1 (2%)	51,54,54	1.27	6 (11%)
24	AJP	Q	104	-	37,37,95	1.32	7 (18%)	58,62,149	1.99	18 (31%)
24	AJP	A	409	-	37,37,95	1.26	7 (18%)	58,62,149	2.04	18 (31%)
27	SF4	I	202	9	0,12,12	-	-	-		
24	AJP	D	608	-	37,37,95	1.35	7 (18%)	58,62,149	2.14	18 (31%)
24	AJP	D	605	-	37,37,95	1.30	7 (18%)	58,62,149	2.00	18 (31%)
24	AJP	B	614	-	37,37,95	1.22	6 (16%)	58,62,149	1.92	15 (25%)
24	AJP	C	201	-	37,37,95	1.34	8 (21%)	58,62,149	1.94	16 (27%)
21	BCR	A	401	-	41,41,41	1.12	2 (4%)	56,56,56	1.26	5 (8%)
24	AJP	Q	102	-	37,37,95	1.53	8 (21%)	58,62,149	2.21	18 (31%)
24	AJP	B	612	-	37,37,95	1.33	7 (18%)	58,62,149	2.08	18 (31%)
24	AJP	G	303	-	37,37,95	1.34	9 (24%)	58,62,149	2.19	17 (29%)
26	SQD	F	705	-	52,54,54	0.96	3 (5%)	62,65,65	1.43	9 (14%)
24	AJP	D	610	-	37,37,95	1.48	7 (18%)	58,62,149	2.18	21 (36%)
24	AJP	D	607	-	37,37,95	1.30	7 (18%)	58,62,149	2.03	18 (31%)
24	AJP	F	710	-	37,37,95	1.39	6 (16%)	58,62,149	2.19	20 (34%)
24	AJP	B	611	-	37,37,95	1.50	9 (24%)	58,62,149	2.30	18 (31%)
24	AJP	Q	103	-	37,37,95	1.35	7 (18%)	58,62,149	2.11	17 (29%)
24	AJP	D	613	-	37,37,95	1.26	5 (13%)	58,62,149	2.12	18 (31%)
25	PQN	B	601	-	34,34,34	2.86	9 (26%)	43,45,45	1.99	6 (13%)
24	AJP	B	608	-	37,37,95	1.19	7 (18%)	58,62,149	1.94	16 (27%)
26	SQD	L	101	-	52,54,54	0.96	3 (5%)	62,65,65	1.45	10 (16%)
24	AJP	F	714	-	37,37,95	1.43	9 (24%)	58,62,149	2.07	17 (29%)
24	AJP	Q	107	-	37,37,95	1.29	7 (18%)	58,62,149	2.02	17 (29%)
24	AJP	F	709	-	37,37,95	1.35	7 (18%)	58,62,149	2.01	20 (34%)
24	AJP	F	707	-	37,37,95	1.44	8 (21%)	58,62,149	1.99	17 (29%)
24	AJP	F	708	-	37,37,95	1.38	7 (18%)	58,62,149	2.06	21 (36%)
21	BCR	F	701	-	41,41,41	1.09	2 (4%)	56,56,56	1.26	6 (10%)
24	AJP	A	405	-	37,37,95	1.39	7 (18%)	58,62,149	2.02	17 (29%)
24	AJP	F	716	-	37,37,95	1.60	8 (21%)	58,62,149	2.10	22 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	AJP	D	603	-	37,37,95	1.61	8 (21%)	58,62,149	2.10	22 (37%)
24	AJP	B	610	-	37,37,95	1.33	8 (21%)	58,62,149	2.01	17 (29%)
24	AJP	B	613	-	37,37,95	1.38	7 (18%)	58,62,149	2.04	19 (32%)
24	AJP	B	607	-	37,37,95	1.32	8 (21%)	58,62,149	1.96	16 (27%)
22	LHG	B	604	-	48,48,48	0.61	1 (2%)	51,54,54	1.27	6 (11%)
24	AJP	B	617	-	37,37,95	1.22	7 (18%)	58,62,149	2.00	17 (29%)
24	AJP	A	407	-	37,37,95	1.31	6 (16%)	58,62,149	2.16	16 (27%)
26	SQD	B	605	-	52,54,54	0.96	2 (3%)	62,65,65	1.42	9 (14%)
24	AJP	E	201	-	37,37,95	1.35	7 (18%)	58,62,149	2.08	18 (31%)
22	LHG	D	601	-	48,48,48	0.63	2 (4%)	51,54,54	1.28	6 (11%)
24	AJP	A	408	-	37,37,95	1.38	8 (21%)	58,62,149	2.08	20 (34%)
22	LHG	F	702	-	48,48,48	0.62	1 (2%)	51,54,54	1.28	6 (11%)
24	AJP	G	301	-	37,37,95	1.57	7 (18%)	58,62,149	2.13	20 (34%)
24	AJP	D	612	-	37,37,95	1.30	6 (16%)	58,62,149	2.07	17 (29%)
24	AJP	G	306	-	37,37,95	1.46	7 (18%)	58,62,149	2.07	19 (32%)
22	LHG	H	401	-	48,48,48	0.58	0	51,54,54	1.27	6 (11%)
24	AJP	F	715	-	37,37,95	1.21	7 (18%)	58,62,149	1.93	16 (27%)
24	AJP	D	609	-	37,37,95	1.40	8 (21%)	58,62,149	2.02	13 (22%)
24	AJP	Q	105	-	37,37,95	1.21	6 (16%)	58,62,149	2.00	16 (27%)
23	DGD	A	403	-	67,67,67	0.84	2 (2%)	81,81,81	1.41	12 (14%)
27	SF4	I	201	9	0,12,12	-	-	-		
24	AJP	Q	106	-	37,37,95	1.15	6 (16%)	58,62,149	2.02	17 (29%)
23	DGD	A	404	-	67,67,67	0.85	2 (2%)	81,81,81	1.42	11 (13%)
28	FES	R	101	18	0,4,4	-	-	-		
24	AJP	F	718	-	37,37,95	1.21	5 (13%)	58,62,149	2.04	17 (29%)
24	AJP	C	202	-	37,37,95	1.43	9 (24%)	58,62,149	2.02	16 (27%)

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
24	AJP	D	604	-	12/12/14/38	-	0/6/6/11
24	AJP	F	713	-	12/12/14/38	-	0/6/6/11
24	AJP	D	606	-	12/12/14/38	-	0/6/6/11

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	LHG	A	402	-	-	20/53/53/53	-
22	LHG	F	703	-	-	24/53/53/53	-
24	AJP	Q	108	-	12/12/14/38	-	0/6/6/11
24	AJP	B	609	-	12/12/14/38	-	0/6/6/11
24	AJP	G	305	-	12/12/14/38	-	0/6/6/11
24	AJP	F	706	-	12/12/14/38	-	0/6/6/11
24	AJP	G	304	-	12/12/14/38	-	0/6/6/11
22	LHG	B	602	-	-	27/53/53/53	-
24	AJP	F	717	-	12/12/14/38	-	0/6/6/11
24	AJP	G	307	-	12/12/14/38	-	0/6/6/11
24	AJP	A	406	-	12/12/14/38	-	0/6/6/11
24	AJP	B	606	-	12/12/14/38	-	0/6/6/11
22	LHG	D	602	-	-	19/53/53/53	-
24	AJP	B	615	-	12/12/14/38	-	0/6/6/11
24	AJP	G	302	-	12/12/14/38	-	0/6/6/11
24	AJP	D	614	-	12/12/14/38	-	0/6/6/11
24	AJP	Q	101	-	12/12/14/38	-	0/6/6/11
24	AJP	F	712	-	12/12/14/38	-	0/6/6/11
24	AJP	B	616	-	12/12/14/38	-	0/6/6/11
24	AJP	F	711	-	12/12/14/38	-	0/6/6/11
21	BCR	P	101	-	-	13/29/63/63	0/2/2/2
27	SF4	K	301	11	-	-	0/6/5/5
26	SQD	F	704	-	-	20/49/69/69	0/1/1/1
24	AJP	D	611	-	12/12/14/38	-	0/6/6/11
22	LHG	B	603	-	-	21/53/53/53	-
24	AJP	Q	104	-	12/12/14/38	-	0/6/6/11
24	AJP	A	409	-	12/12/14/38	-	0/6/6/11
27	SF4	I	202	9	-	-	0/6/5/5
24	AJP	D	608	-	12/12/14/38	-	0/6/6/11
24	AJP	D	605	-	12/12/14/38	-	0/6/6/11
24	AJP	B	614	-	12/12/14/38	-	0/6/6/11
24	AJP	C	201	-	12/12/14/38	-	0/6/6/11
21	BCR	A	401	-	-	10/29/63/63	0/2/2/2
24	AJP	Q	102	-	12/12/14/38	-	0/6/6/11

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	AJP	B	612	-	12/12/14/38	-	0/6/6/11
24	AJP	G	303	-	12/12/14/38	-	0/6/6/11
26	SQD	F	705	-	-	16/49/69/69	0/1/1/1
24	AJP	D	610	-	12/12/14/38	-	0/6/6/11
24	AJP	D	607	-	12/12/14/38	-	0/6/6/11
24	AJP	F	710	-	12/12/14/38	-	0/6/6/11
24	AJP	B	611	-	12/12/14/38	-	0/6/6/11
24	AJP	Q	103	-	12/12/14/38	-	0/6/6/11
24	AJP	D	613	-	12/12/14/38	-	0/6/6/11
25	PQN	B	601	-	-	7/23/43/43	0/2/2/2
24	AJP	B	608	-	12/12/14/38	-	0/6/6/11
26	SQD	L	101	-	-	17/49/69/69	0/1/1/1
24	AJP	F	714	-	12/12/14/38	-	0/6/6/11
24	AJP	Q	107	-	12/12/14/38	-	0/6/6/11
24	AJP	F	709	-	12/12/14/38	-	0/6/6/11
24	AJP	F	707	-	12/12/14/38	-	0/6/6/11
24	AJP	F	708	-	12/12/14/38	-	0/6/6/11
21	BCR	F	701	-	-	11/29/63/63	0/2/2/2
24	AJP	A	405	-	12/12/14/38	-	0/6/6/11
24	AJP	F	716	-	12/12/14/38	-	0/6/6/11
24	AJP	D	603	-	12/12/14/38	-	0/6/6/11
24	AJP	B	610	-	12/12/14/38	-	0/6/6/11
24	AJP	B	613	-	12/12/14/38	-	0/6/6/11
24	AJP	B	607	-	12/12/14/38	-	0/6/6/11
24	AJP	B	617	-	12/12/14/38	-	0/6/6/11
22	LHG	B	604	-	-	25/53/53/53	-
24	AJP	A	407	-	12/12/14/38	-	0/6/6/11
26	SQD	B	605	-	-	14/49/69/69	0/1/1/1
24	AJP	E	201	-	12/12/14/38	-	0/6/6/11
22	LHG	D	601	-	-	18/53/53/53	-
24	AJP	A	408	-	12/12/14/38	-	0/6/6/11
22	LHG	F	702	-	-	24/53/53/53	-
24	AJP	G	301	-	12/12/14/38	-	0/6/6/11
24	AJP	D	612	-	12/12/14/38	-	0/6/6/11

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	AJP	G	306	-	12/12/14/38	-	0/6/6/11
22	LHG	H	401	-	-	22/53/53/53	-
24	AJP	F	715	-	12/12/14/38	-	0/6/6/11
24	AJP	D	609	-	12/12/14/38	-	0/6/6/11
24	AJP	Q	105	-	12/12/14/38	-	0/6/6/11
23	DGD	A	403	-	-	18/55/95/95	0/2/2/2
27	SF4	I	201	9	-	-	0/6/5/5
24	AJP	Q	106	-	12/12/14/38	-	0/6/6/11
23	DGD	A	404	-	-	19/55/95/95	0/2/2/2
28	FES	R	101	18	-	-	0/1/1/1
24	AJP	F	718	-	12/12/14/38	-	0/6/6/11
24	AJP	C	202	-	12/12/14/38	-	0/6/6/11

The worst 5 of 464 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	601	PQN	C12-C13	8.55	1.52	1.33
25	B	601	PQN	O4-C4	8.28	1.40	1.23
25	B	601	PQN	O1-C1	8.21	1.40	1.23
24	B	606	AJP	C16-C11	-3.99	1.48	1.54
25	B	601	PQN	C2-C1	-3.76	1.39	1.47

The worst 5 of 1199 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	601	PQN	C11-C12-C13	-8.07	112.93	126.83
24	B	611	AJP	C20-C15-C16	-7.59	104.72	112.43
24	B	606	AJP	C19-C24-C23	-7.29	105.73	114.40
24	D	604	AJP	C20-C15-C16	-7.23	105.08	112.43
24	F	717	AJP	C20-C15-C16	-7.21	105.11	112.43

5 of 720 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	A	405	AJP	C10
24	A	405	AJP	C02
24	A	405	AJP	C07
24	A	405	AJP	C12
24	A	405	AJP	C15

5 of 345 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	F	701	BCR	C21-C22-C23-C24
21	P	101	BCR	C20-C21-C22-C23
22	A	402	LHG	O1-C1-C2-C3
22	A	402	LHG	C2-C3-O3-P
22	A	402	LHG	C3-O3-P-O5

There are no ring outliers.

79 monomers are involved in 391 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	D	604	AJP	9	0
24	F	713	AJP	2	0
24	D	606	AJP	6	0
22	A	402	LHG	3	0
22	F	703	LHG	7	0
24	Q	108	AJP	1	0
24	B	609	AJP	3	0
24	G	305	AJP	10	0
24	F	706	AJP	2	0
24	G	304	AJP	6	0
24	F	717	AJP	1	0
24	G	307	AJP	3	0
24	A	406	AJP	2	0
24	B	606	AJP	19	0
24	B	615	AJP	7	0
24	G	302	AJP	6	0
24	D	614	AJP	4	0
24	Q	101	AJP	3	0
24	F	712	AJP	11	0
24	B	616	AJP	23	0
21	P	101	BCR	5	0
24	F	711	AJP	8	0
27	K	301	SF4	3	0
26	F	704	SQD	5	0
24	D	611	AJP	7	0
22	B	603	LHG	2	0
24	Q	104	AJP	1	0
24	A	409	AJP	9	0
27	I	202	SF4	1	0
24	D	608	AJP	13	0
24	D	605	AJP	6	0

Continued on next page...

Continued from previous page...

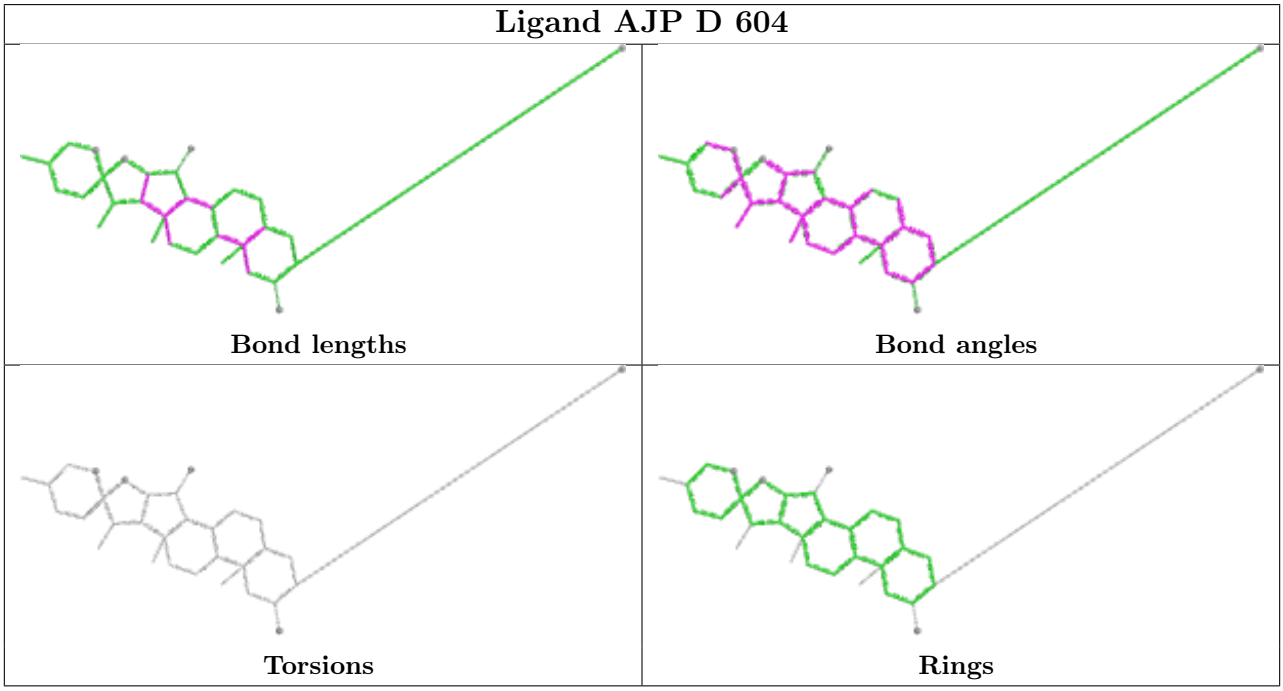
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	B	614	AJP	9	0
24	C	201	AJP	5	0
21	A	401	BCR	4	0
24	Q	102	AJP	7	0
24	B	612	AJP	2	0
24	G	303	AJP	5	0
26	F	705	SQD	1	0
24	D	610	AJP	10	0
24	D	607	AJP	6	0
24	F	710	AJP	5	0
24	B	611	AJP	5	0
24	Q	103	AJP	1	0
24	D	613	AJP	18	0
24	B	608	AJP	4	0
26	L	101	SQD	1	0
24	F	714	AJP	8	0
24	Q	107	AJP	5	0
24	F	709	AJP	2	0
24	F	707	AJP	11	0
24	F	708	AJP	4	0
21	F	701	BCR	3	0
24	A	405	AJP	1	0
24	F	716	AJP	3	0
24	D	603	AJP	4	0
24	B	610	AJP	2	0
24	B	613	AJP	1	0
24	B	607	AJP	5	0
22	B	604	LHG	2	0
24	B	617	AJP	8	0
24	A	407	AJP	10	0
26	B	605	SQD	3	0
24	E	201	AJP	1	0
22	D	601	LHG	1	0
24	A	408	AJP	6	0
22	F	702	LHG	1	0
24	G	301	AJP	10	0
24	D	612	AJP	11	0
24	G	306	AJP	6	0
22	H	401	LHG	3	0
24	F	715	AJP	2	0
24	D	609	AJP	9	0
24	Q	105	AJP	2	0

Continued on next page...

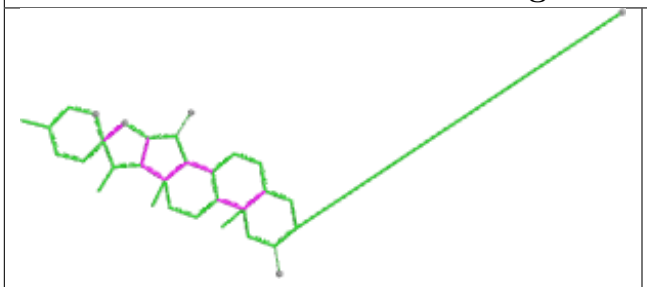
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	A	403	DGD	1	0
24	Q	106	AJP	5	0
23	A	404	DGD	2	0
28	R	101	FES	2	0
24	F	718	AJP	12	0
24	C	202	AJP	12	0

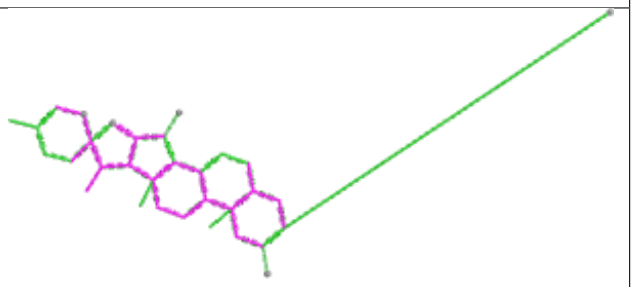
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



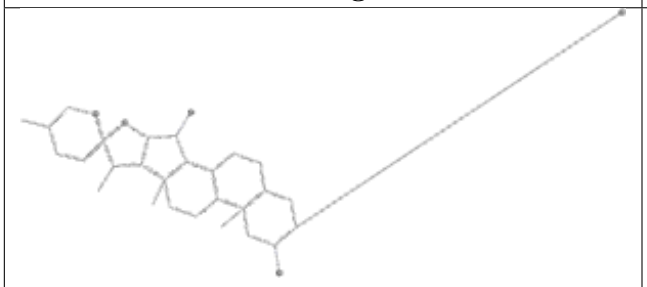
Ligand AJP F 713



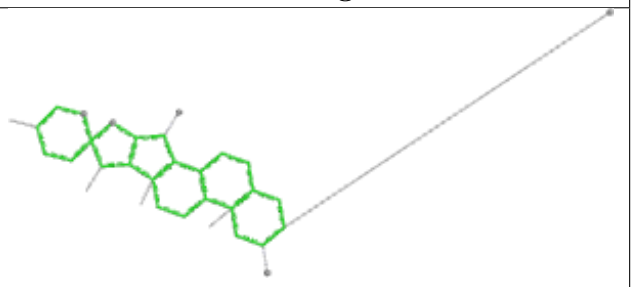
Bond lengths



Bond angles

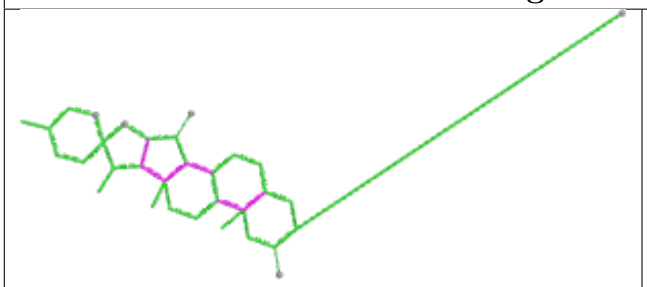


Torsions

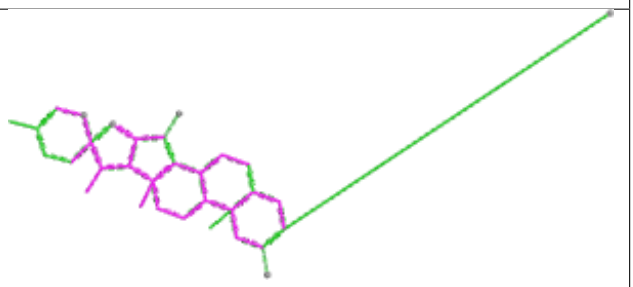


Rings

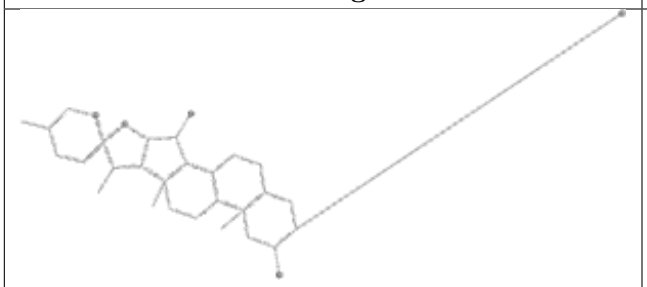
Ligand AJP D 606



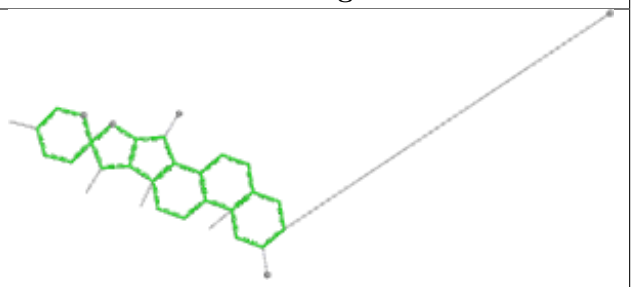
Bond lengths



Bond angles

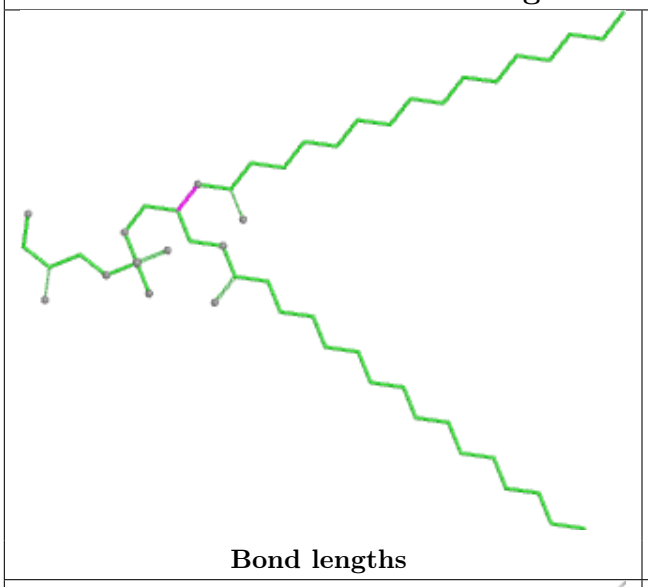


Torsions

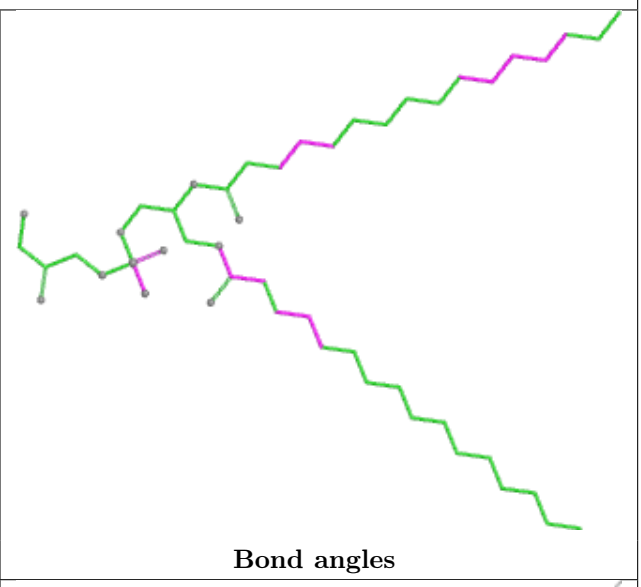


Rings

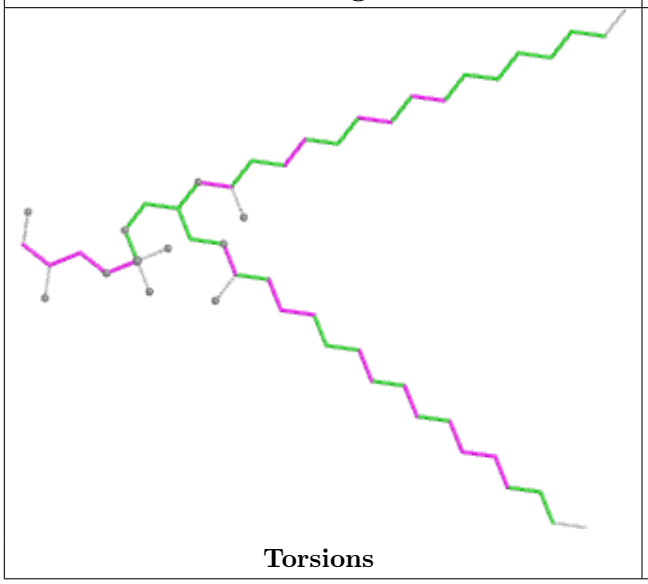
Ligand LHG A 402



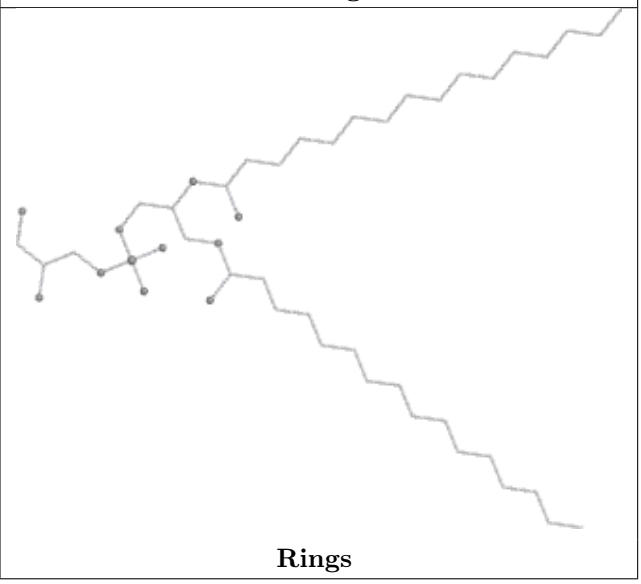
Bond lengths



Bond angles

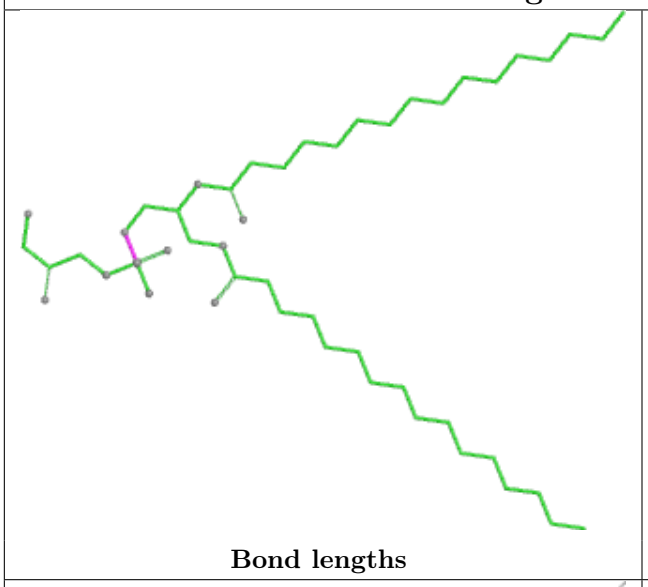


Torsions

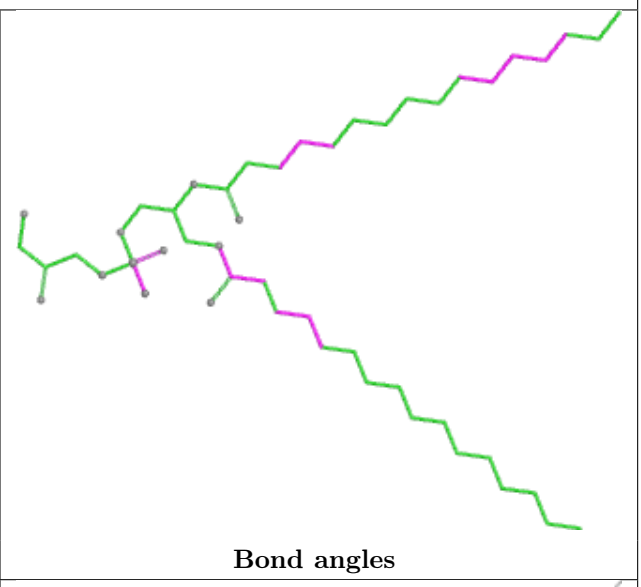


Rings

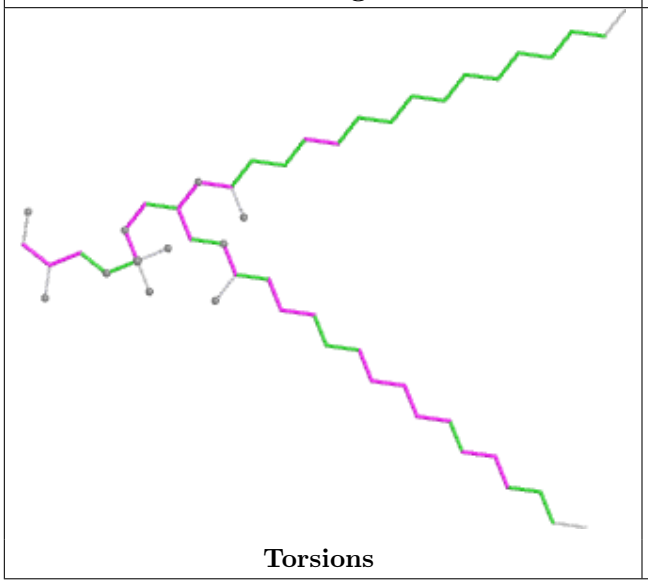
Ligand LHG F 703



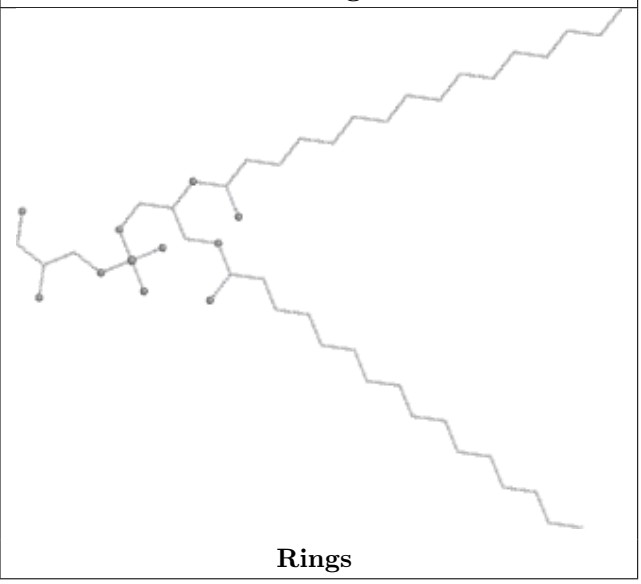
Bond lengths



Bond angles

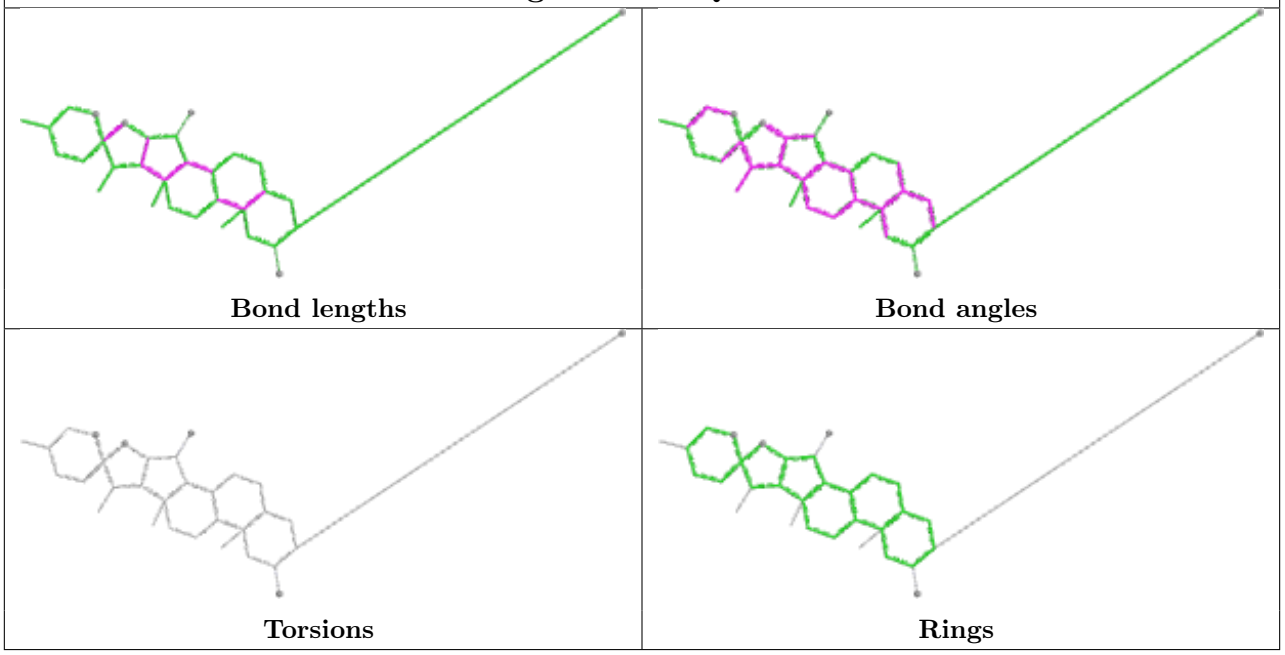


Torsions

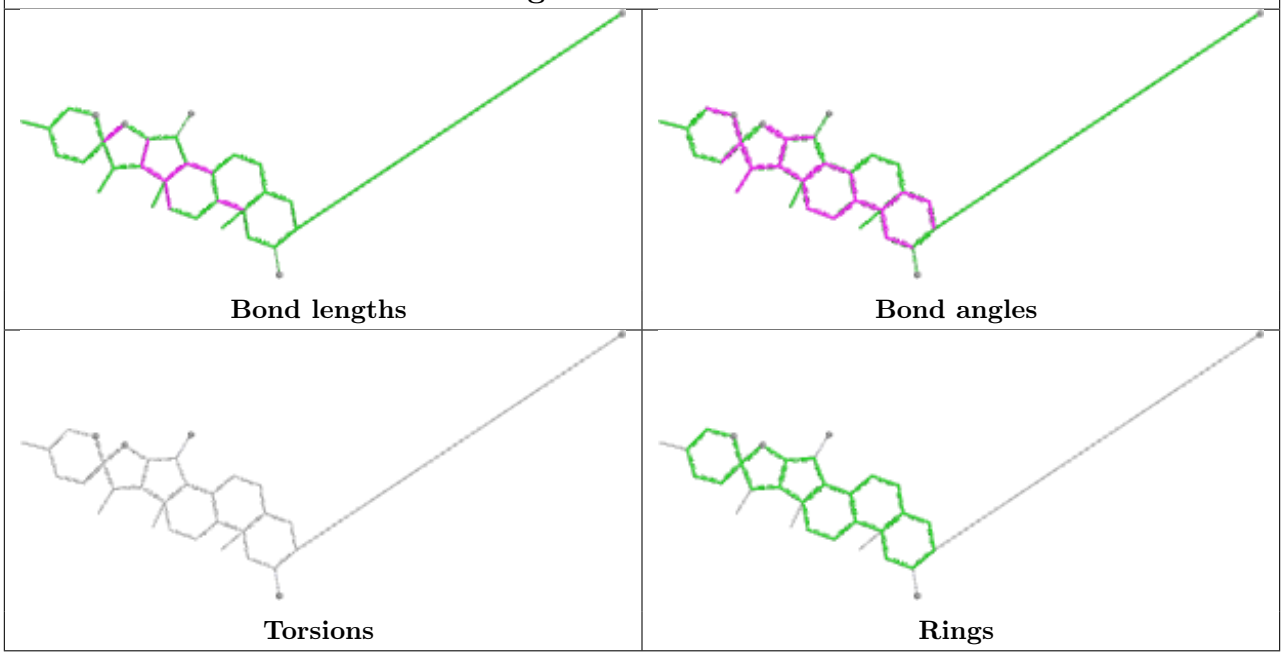


Rings

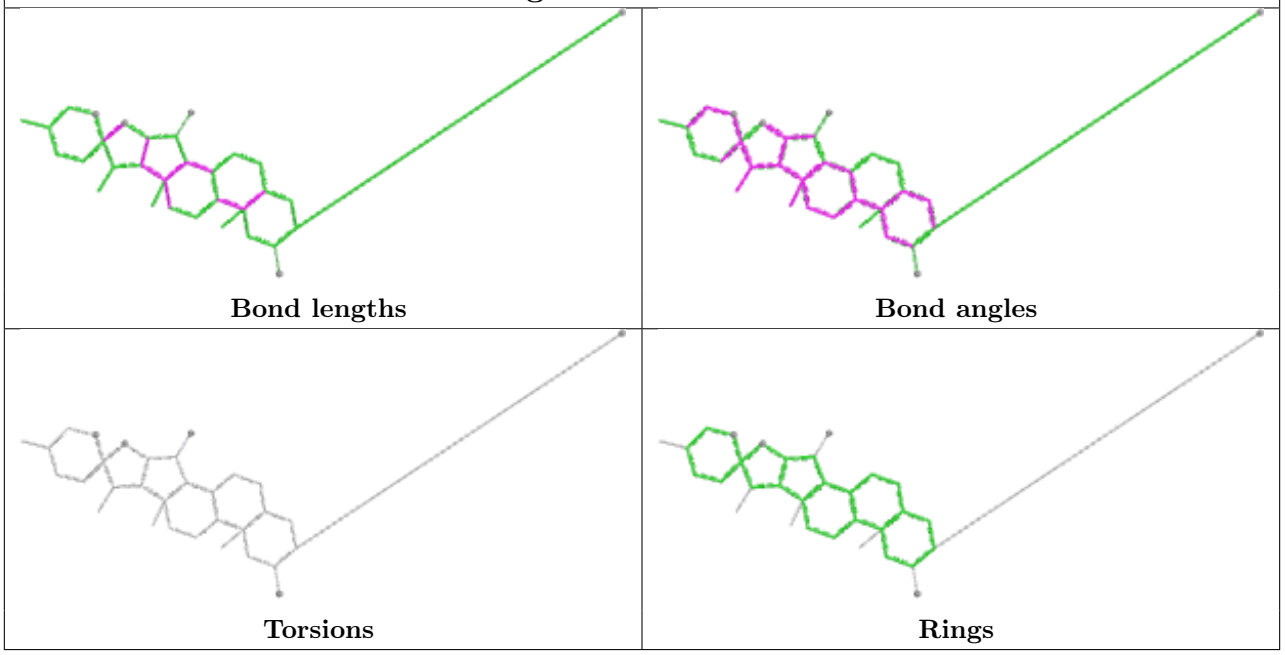
Ligand AJP Q 108



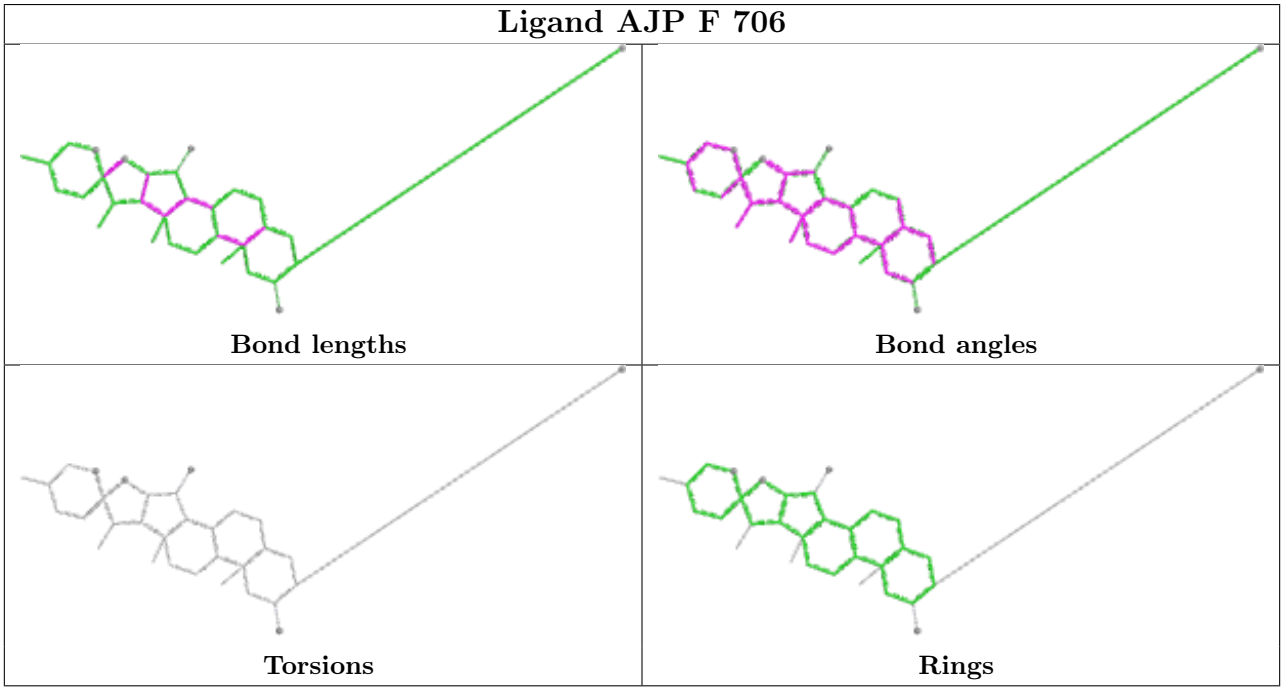
Ligand AJP B 609



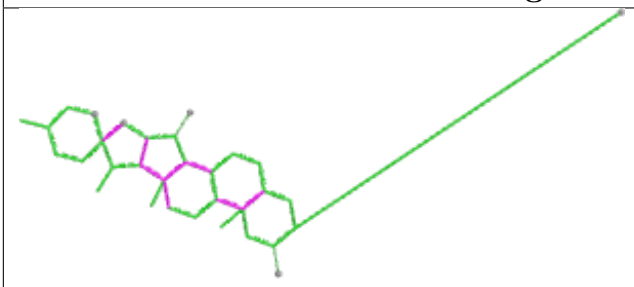
Ligand AJP G 305



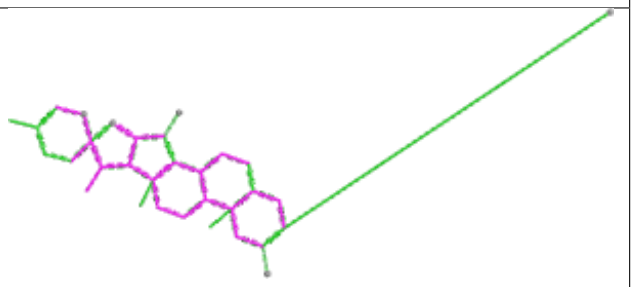
Ligand AJP F 706



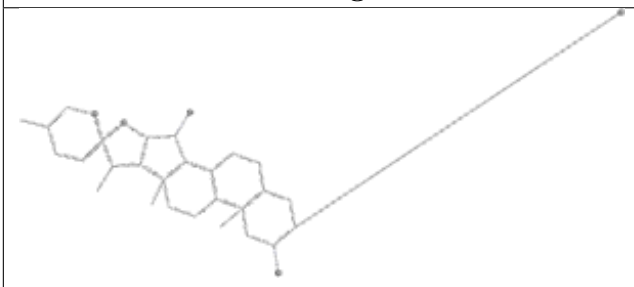
Ligand AJP G 304



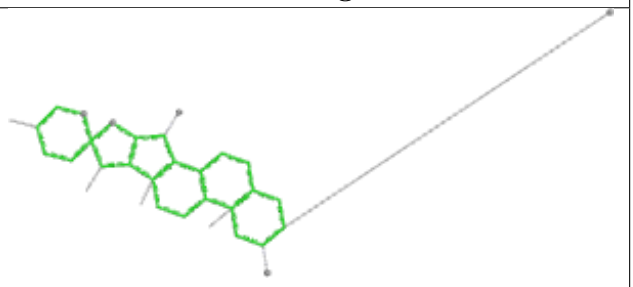
Bond lengths



Bond angles

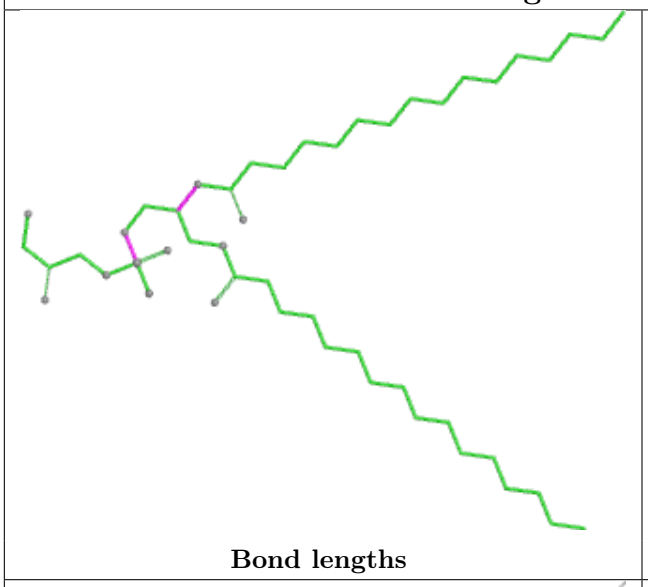


Torsions

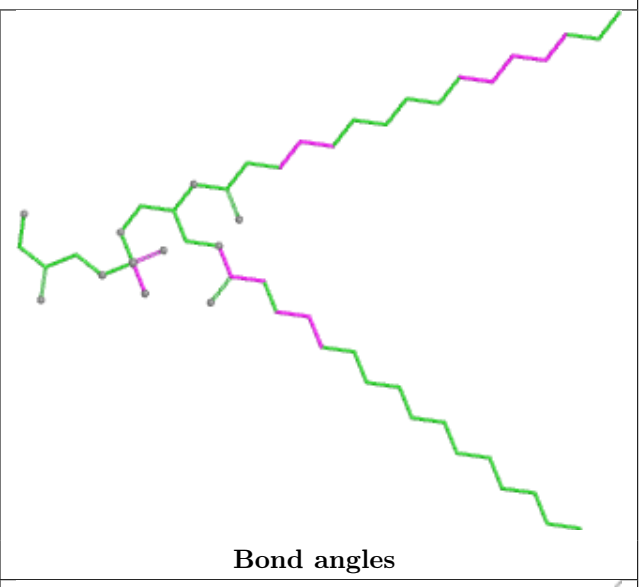


Rings

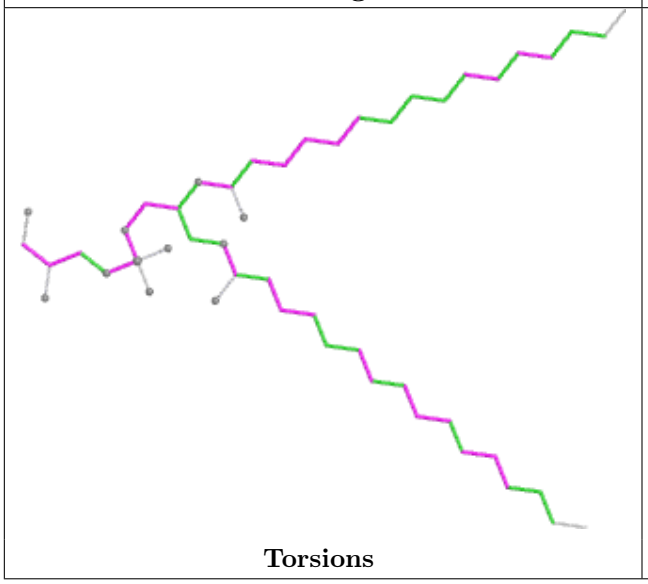
Ligand LHG B 602



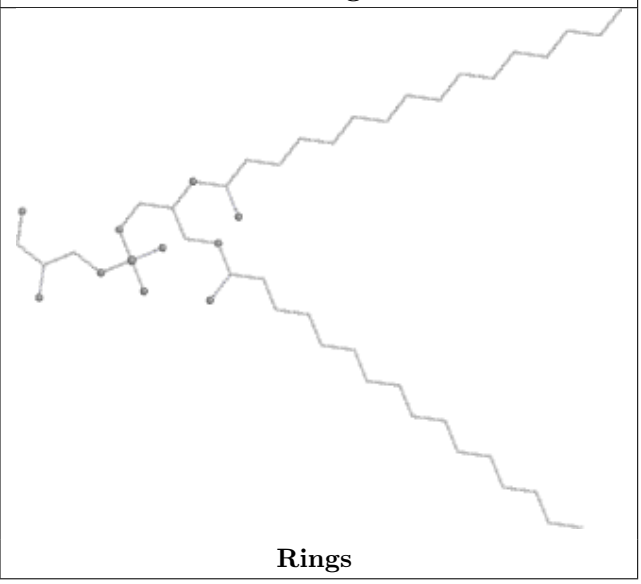
Bond lengths



Bond angles

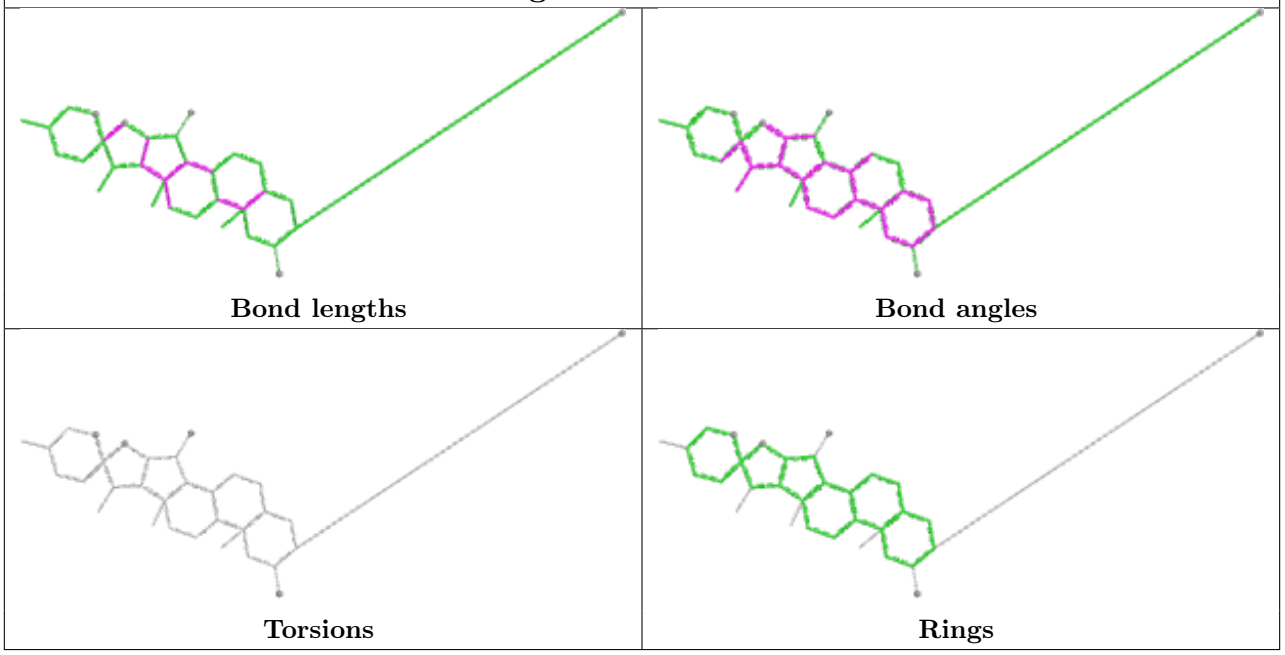


Torsions

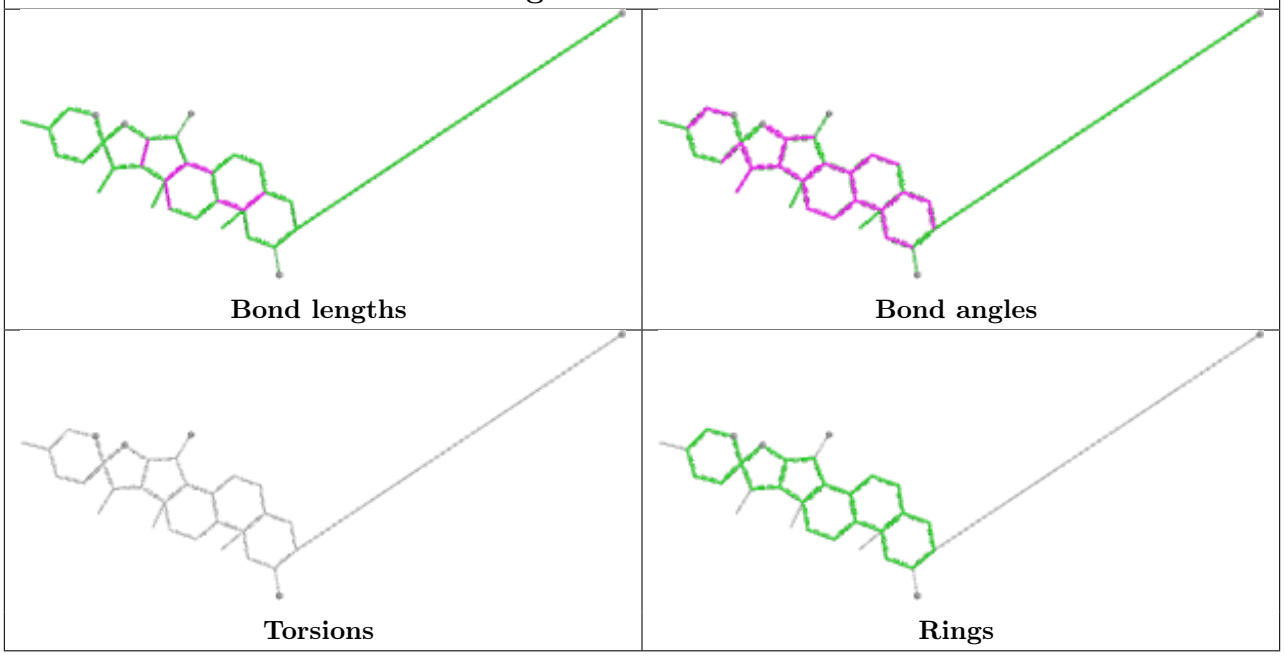


Rings

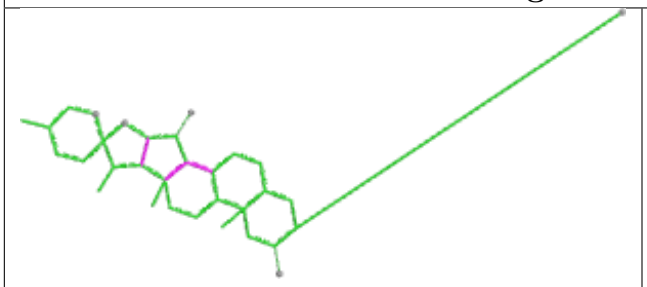
Ligand AJP F 717



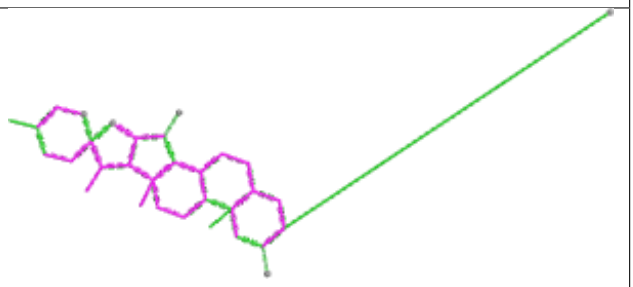
Ligand AJP G 307



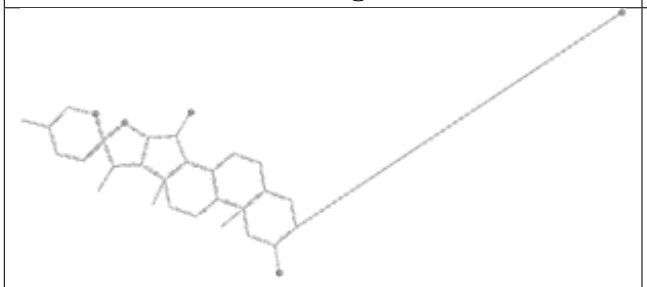
Ligand AJP A 406



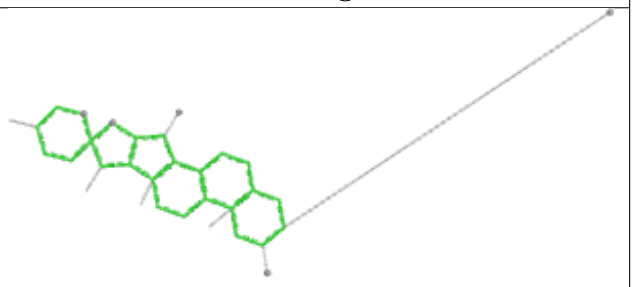
Bond lengths



Bond angles

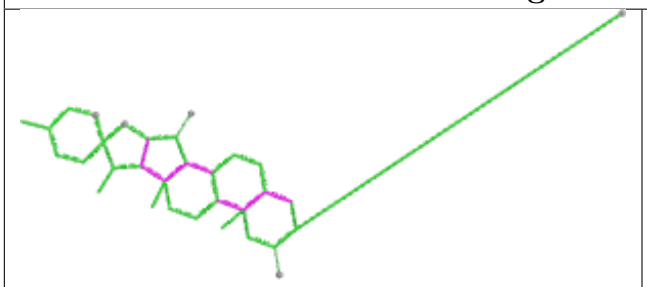


Torsions

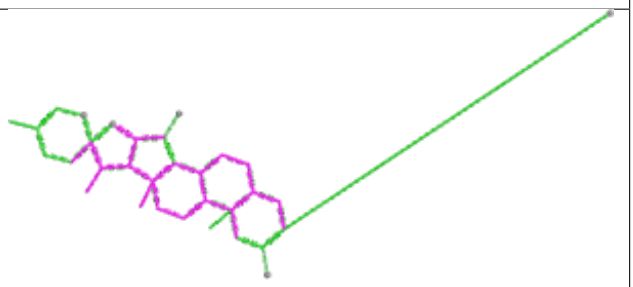


Rings

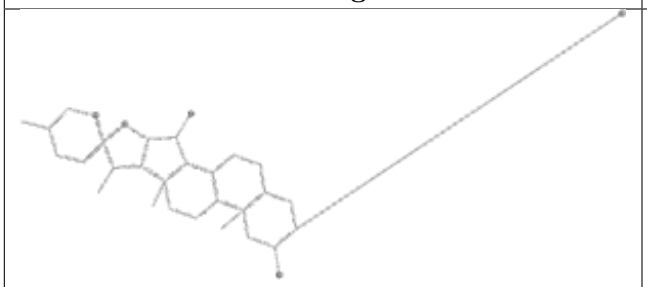
Ligand AJP B 606



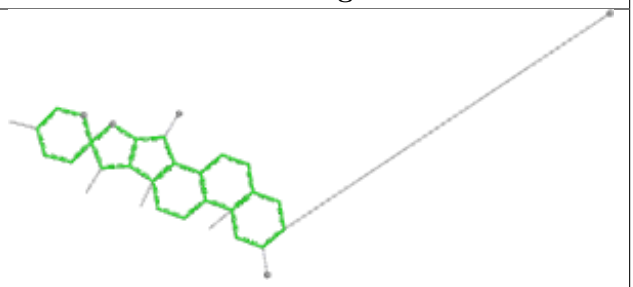
Bond lengths



Bond angles

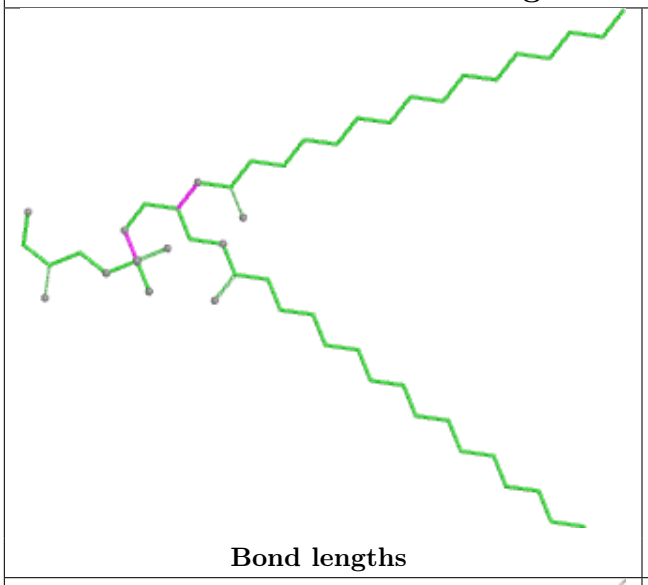


Torsions

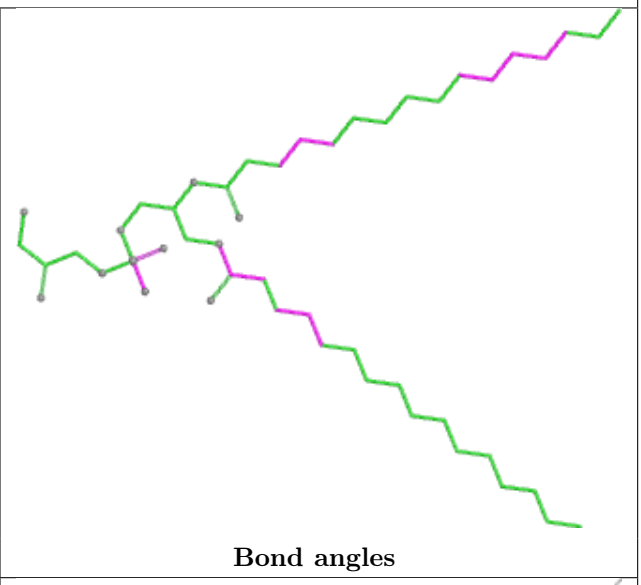


Rings

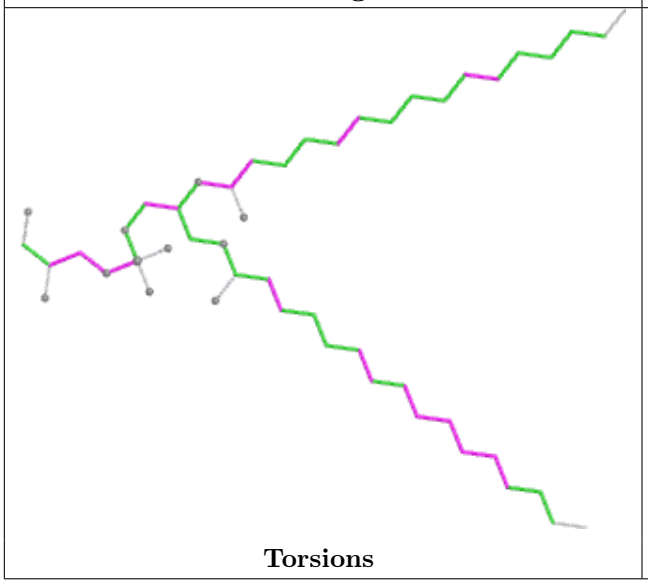
Ligand LHG D 602



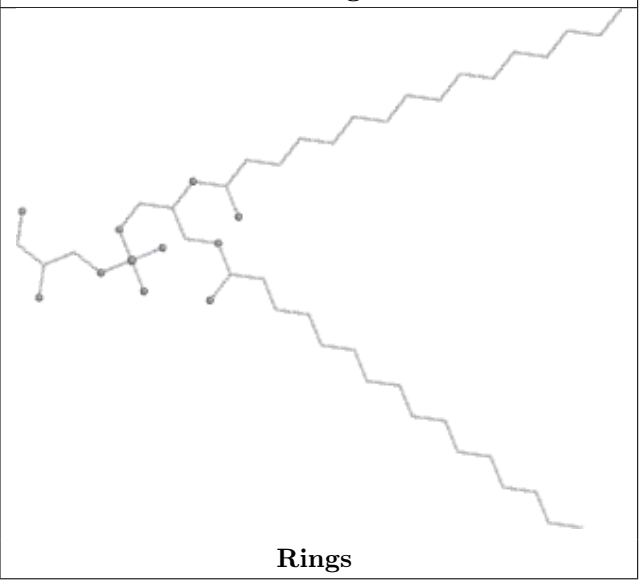
Bond lengths



Bond angles

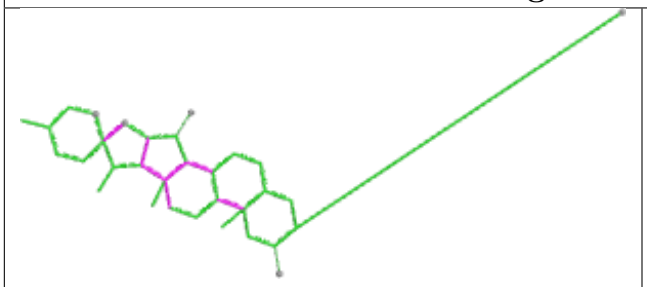


Torsions

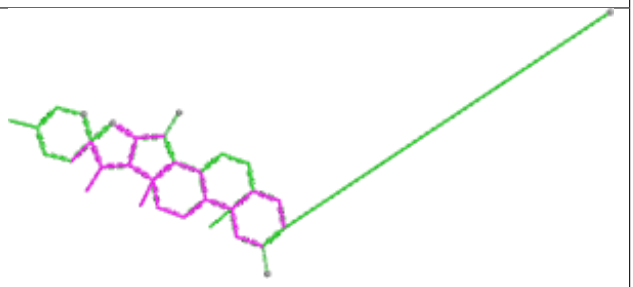


Rings

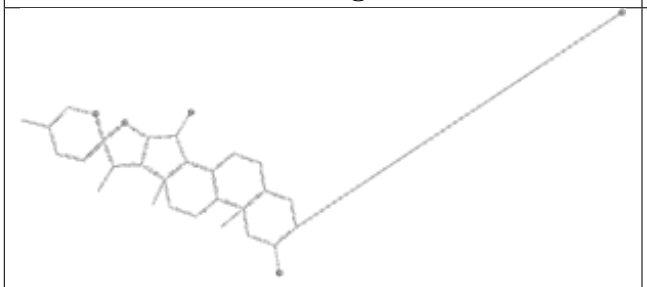
Ligand AJP B 615



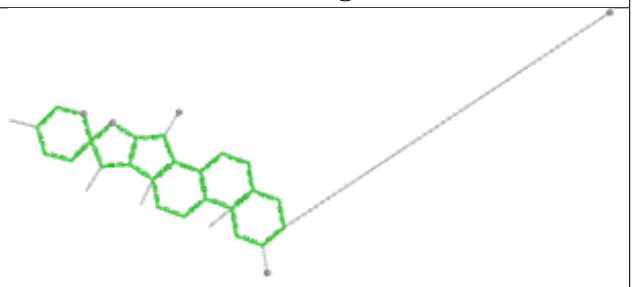
Bond lengths



Bond angles

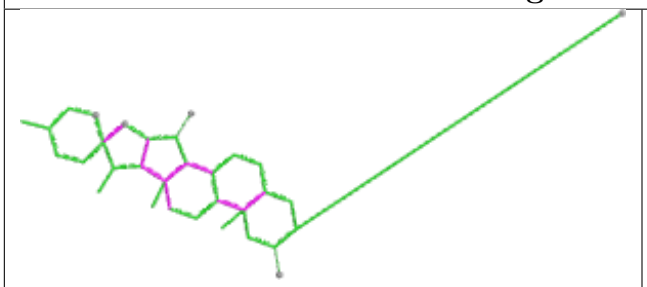


Torsions

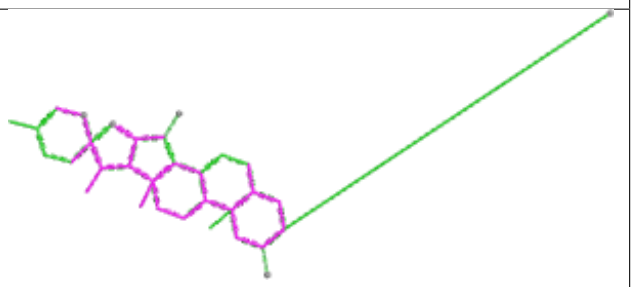


Rings

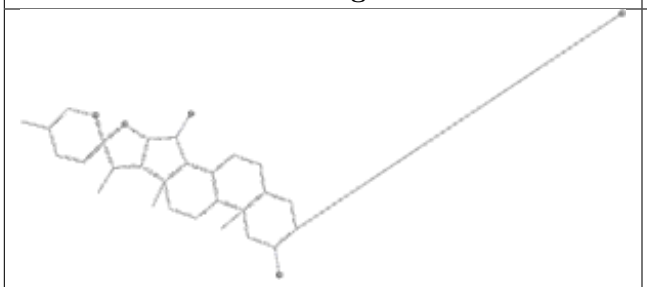
Ligand AJP G 302



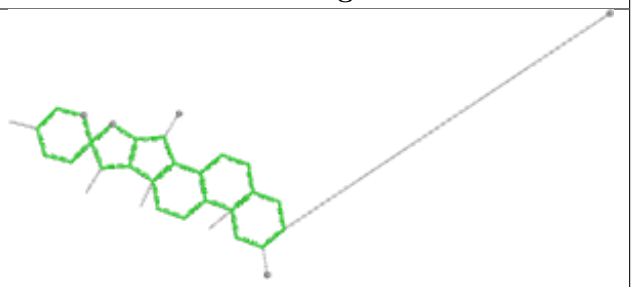
Bond lengths



Bond angles

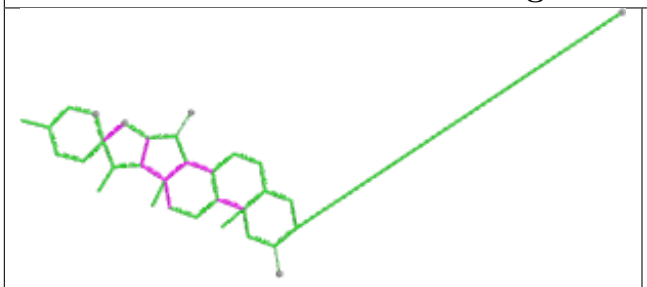


Torsions

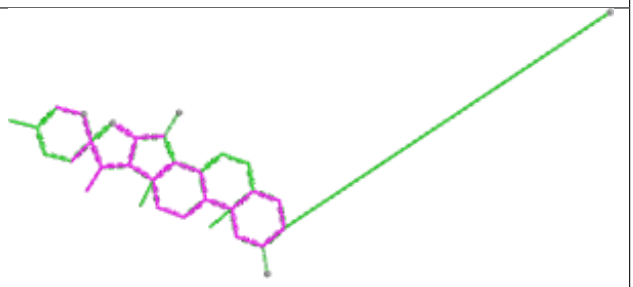


Rings

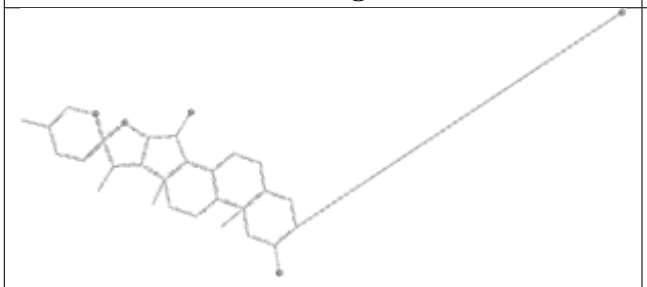
Ligand AJP D 614



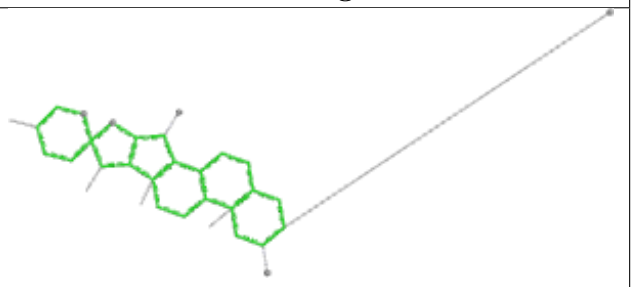
Bond lengths



Bond angles

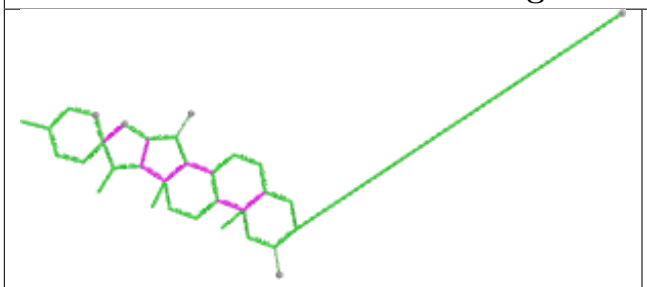


Torsions

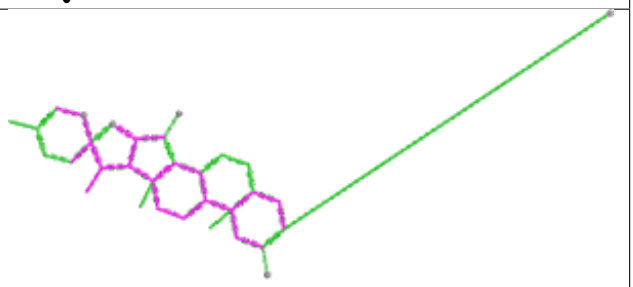


Rings

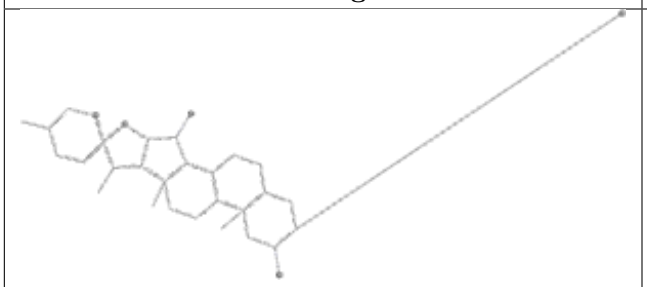
Ligand AJP Q 101



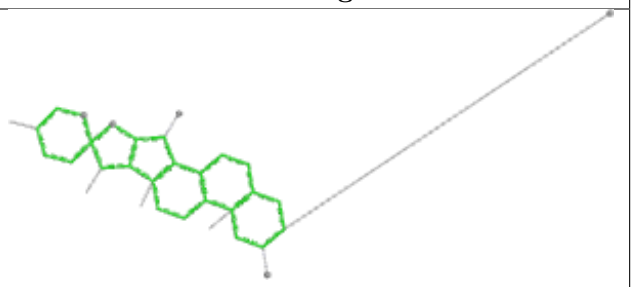
Bond lengths



Bond angles

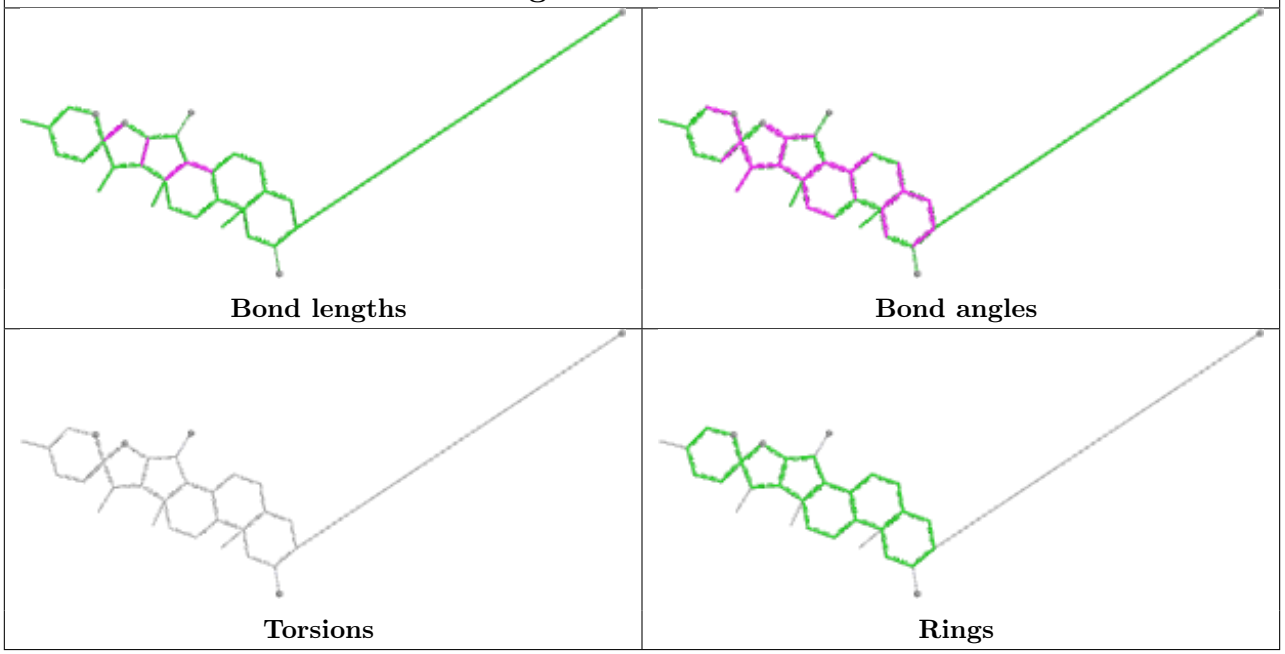


Torsions

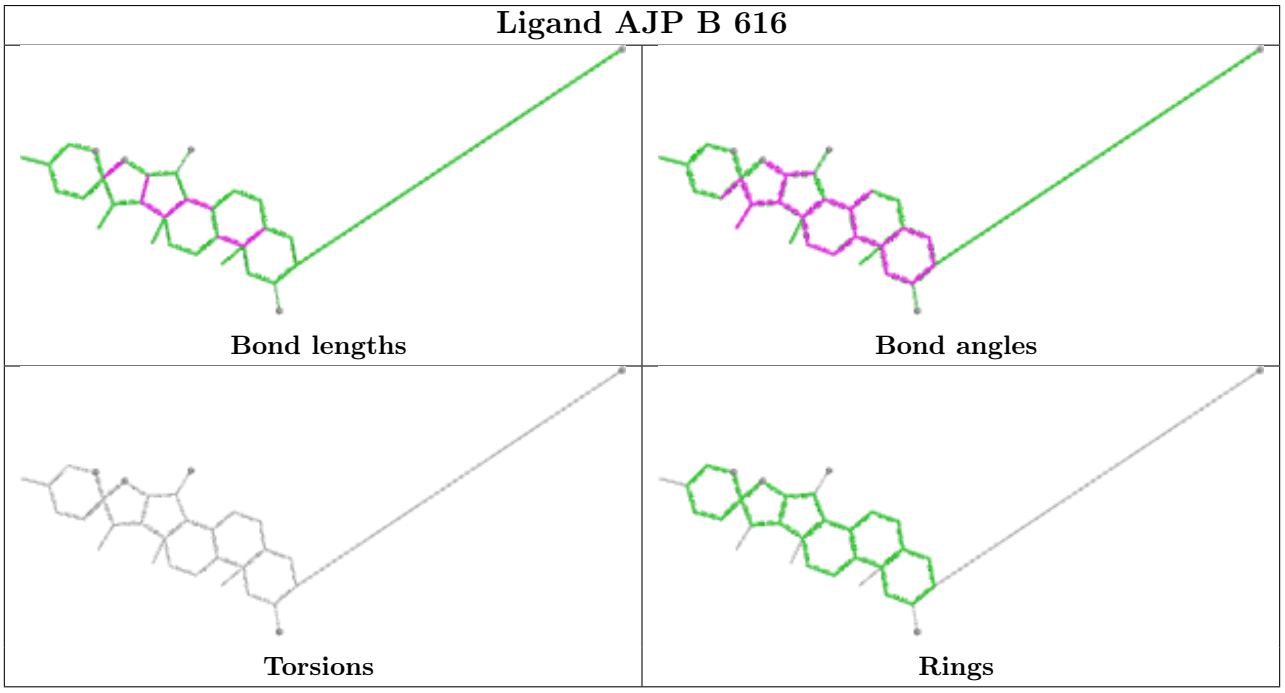


Rings

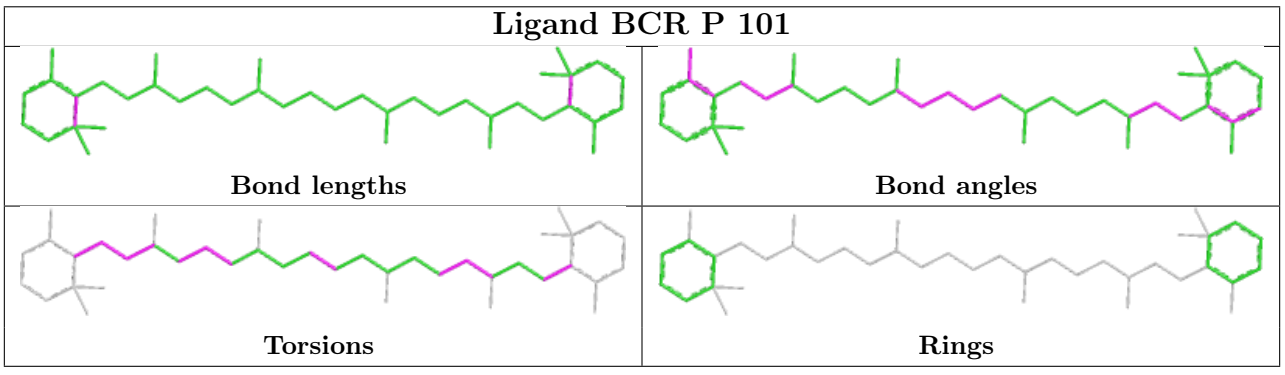
Ligand AJP F 712



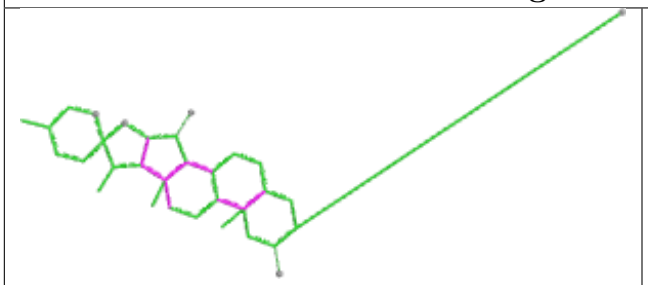
Ligand AJP B 616



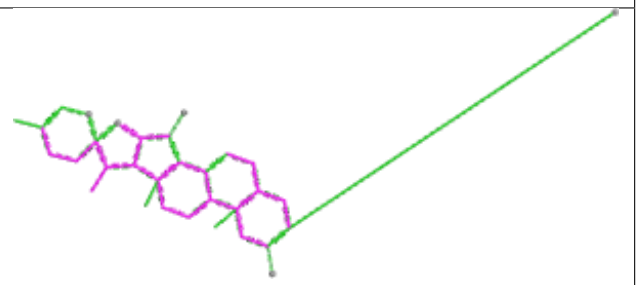
Ligand BCR P 101



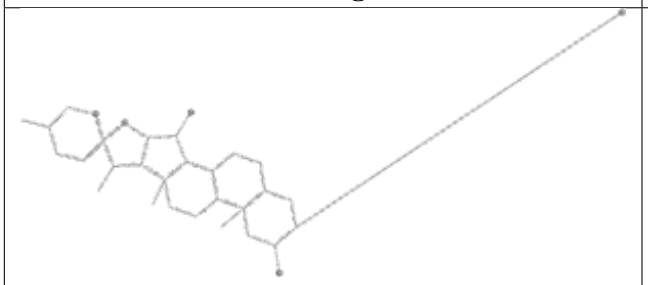
Ligand AJP F 711



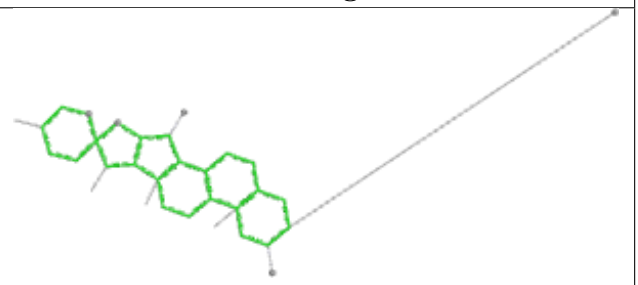
Bond lengths



Bond angles

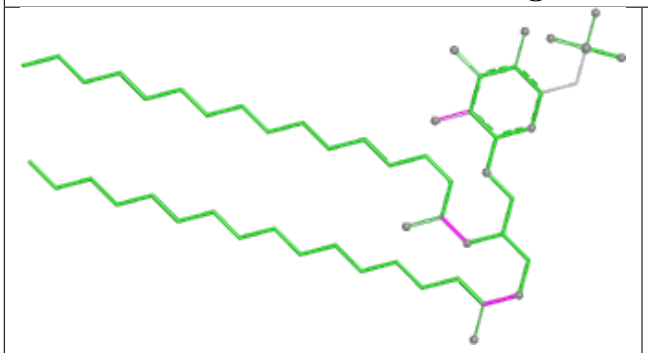


Torsions

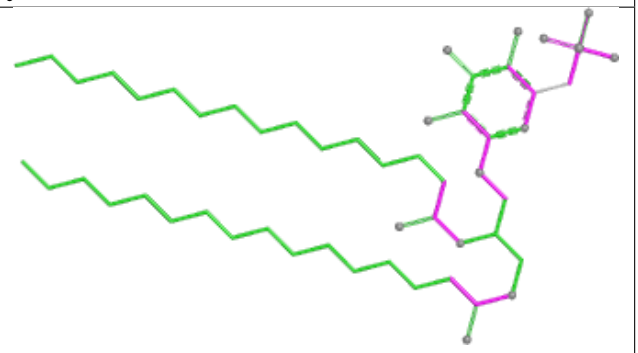


Rings

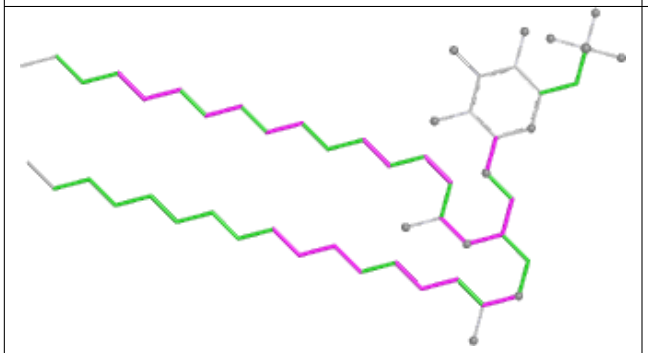
Ligand SQD F 704



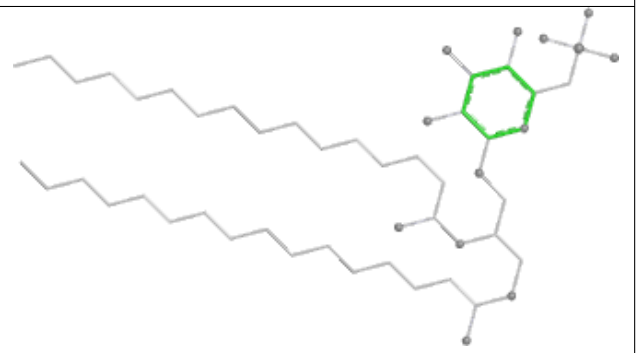
Bond lengths



Bond angles

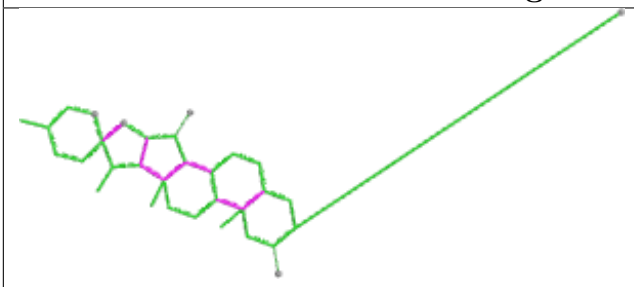


Torsions

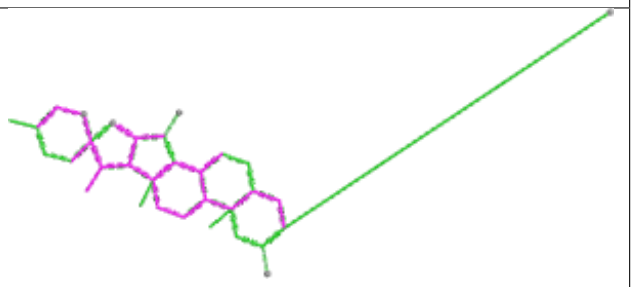


Rings

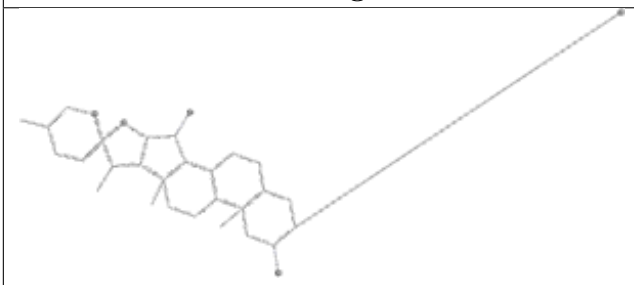
Ligand AJP D 611



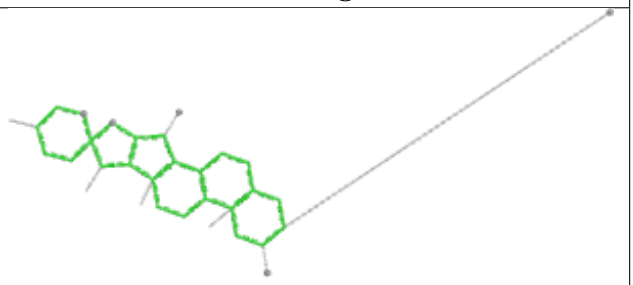
Bond lengths



Bond angles

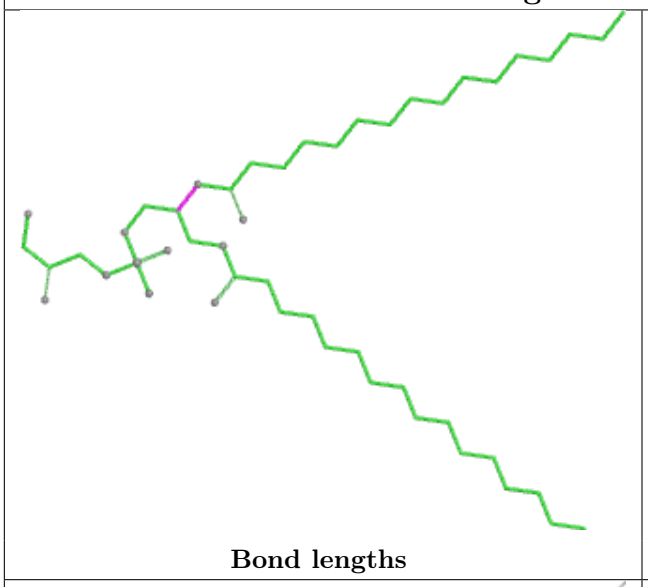


Torsions

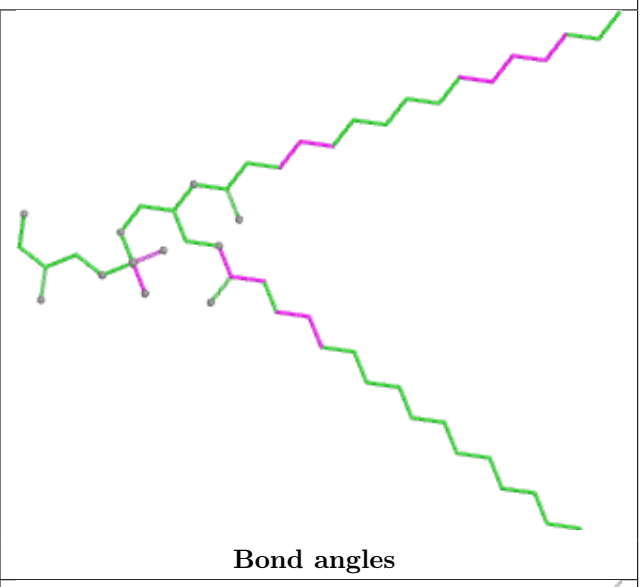


Rings

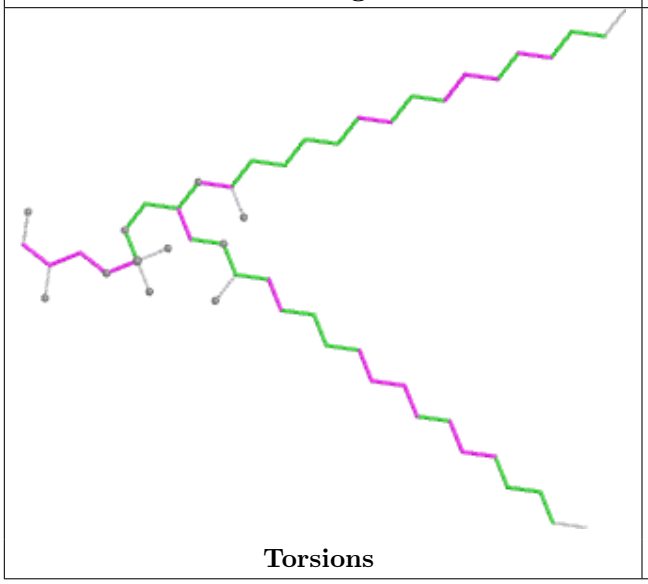
Ligand LHG B 603



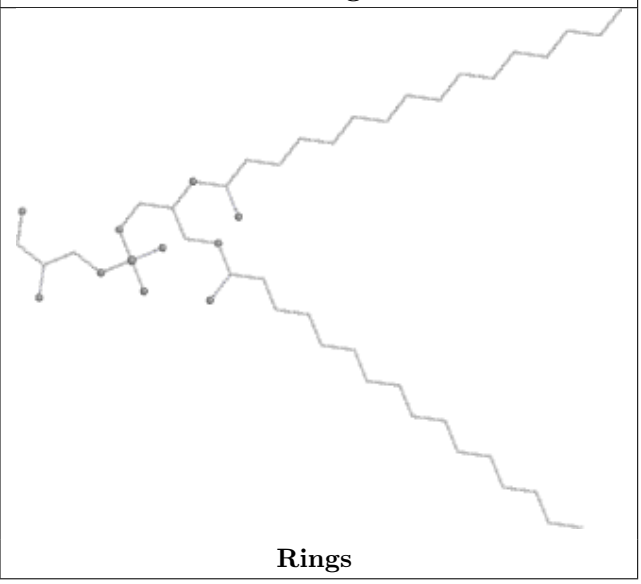
Bond lengths



Bond angles

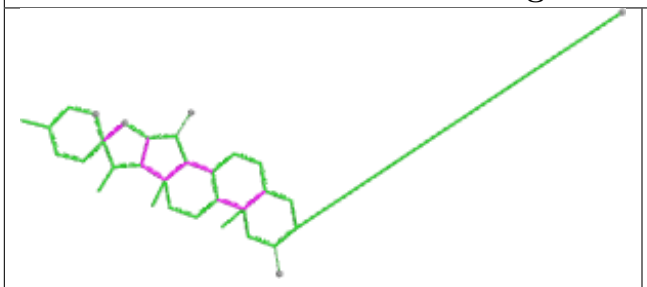


Torsions

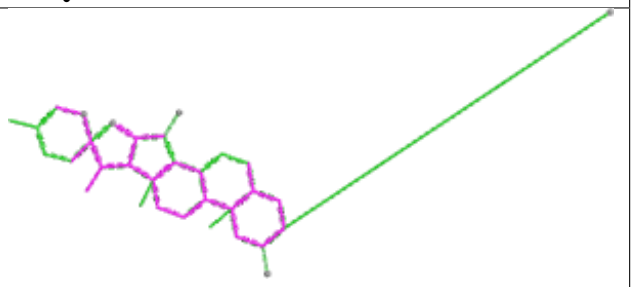


Rings

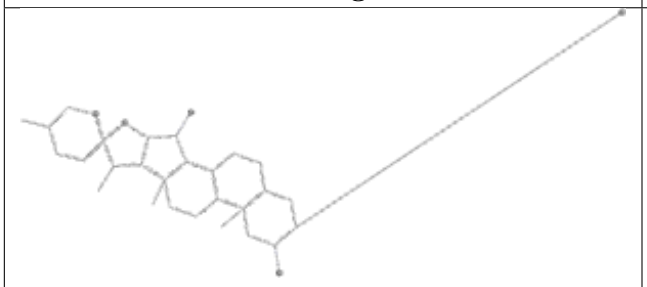
Ligand AJP Q 104



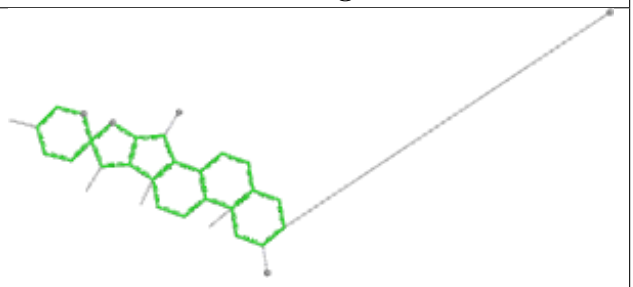
Bond lengths



Bond angles

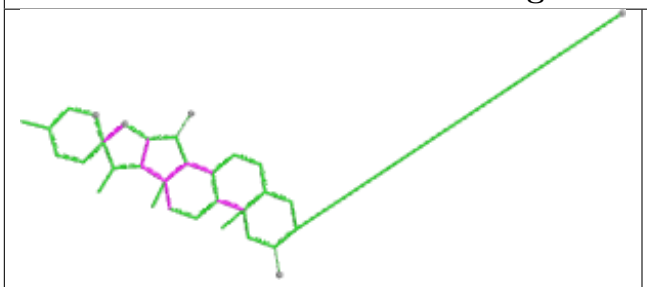


Torsions

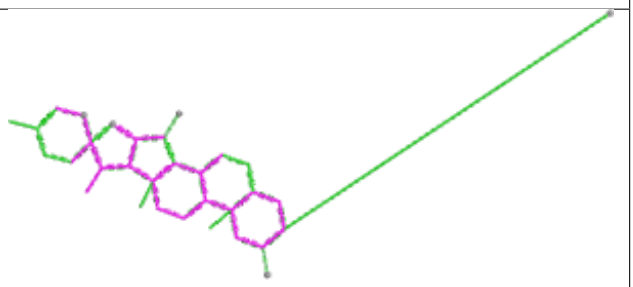


Rings

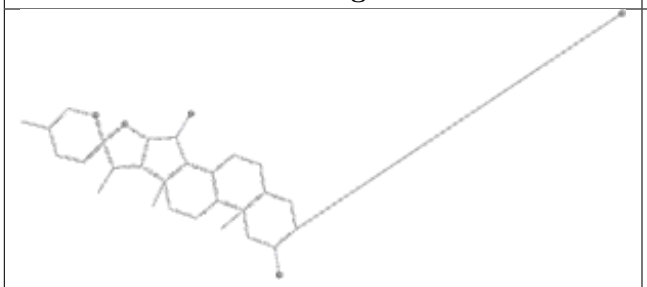
Ligand AJP A 409



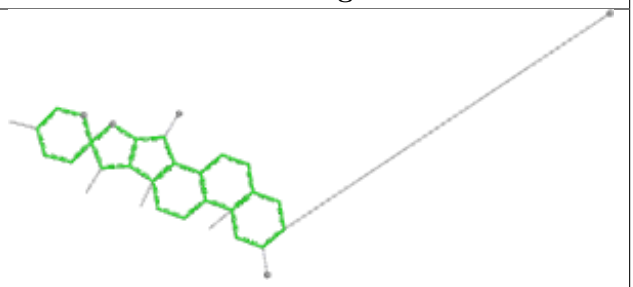
Bond lengths



Bond angles

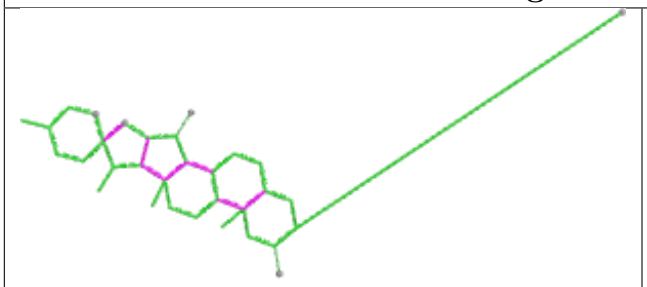


Torsions

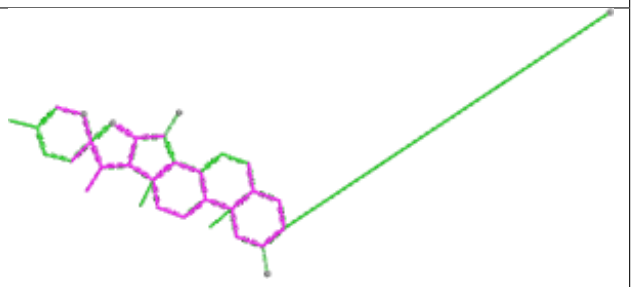


Rings

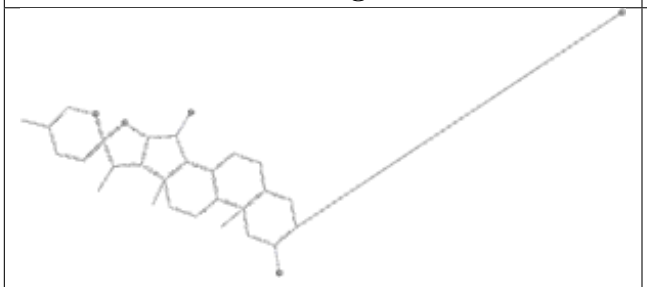
Ligand AJP D 608



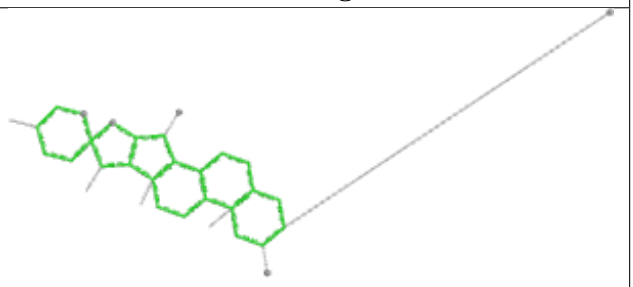
Bond lengths



Bond angles

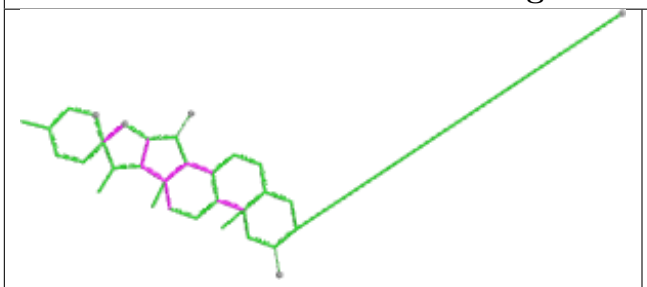


Torsions

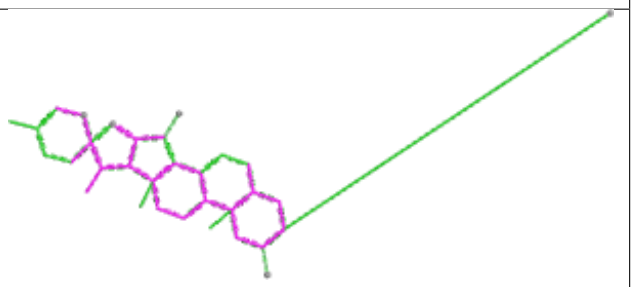


Rings

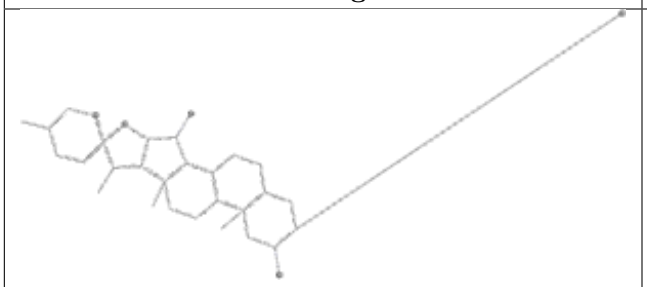
Ligand AJP D 605



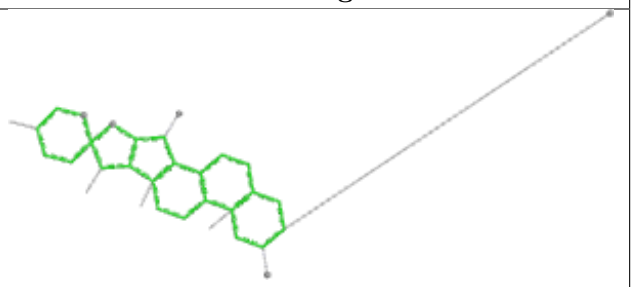
Bond lengths



Bond angles

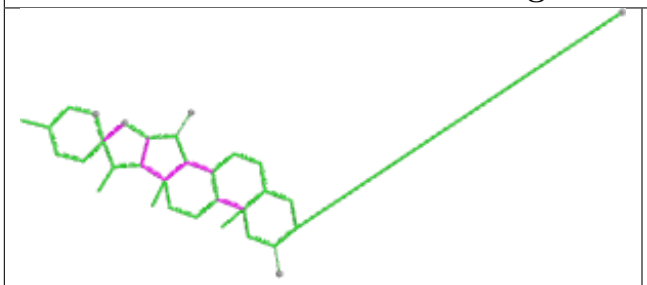


Torsions

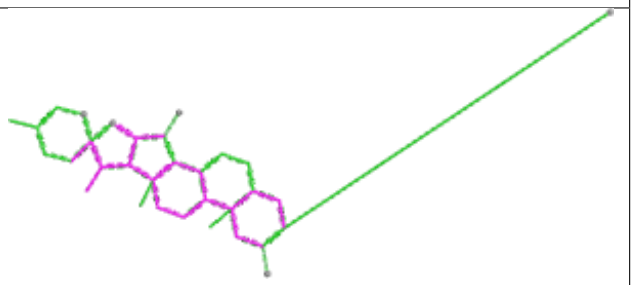


Rings

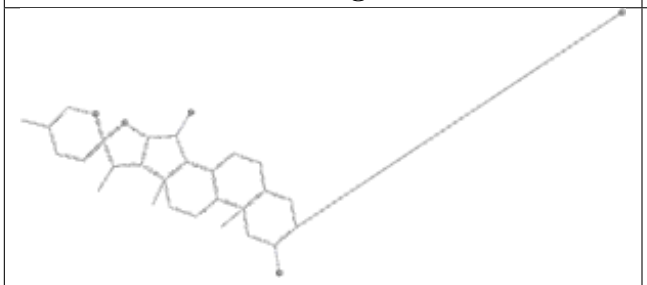
Ligand AJP B 614



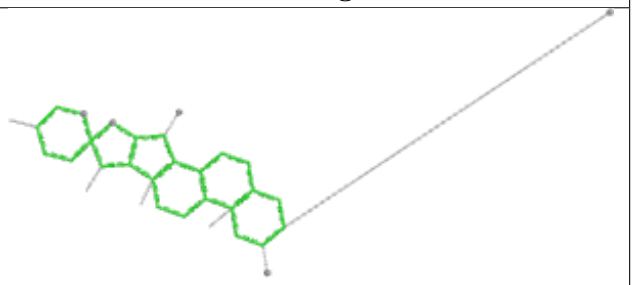
Bond lengths



Bond angles

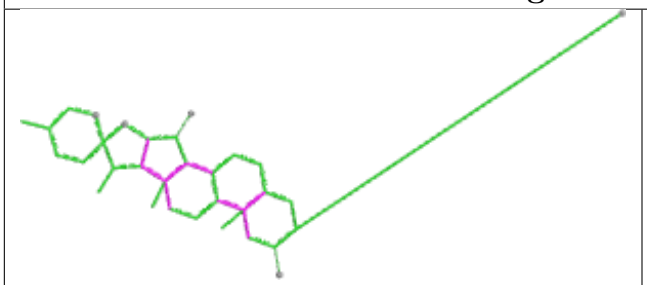


Torsions

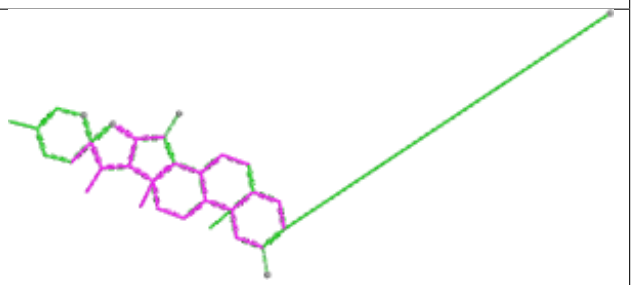


Rings

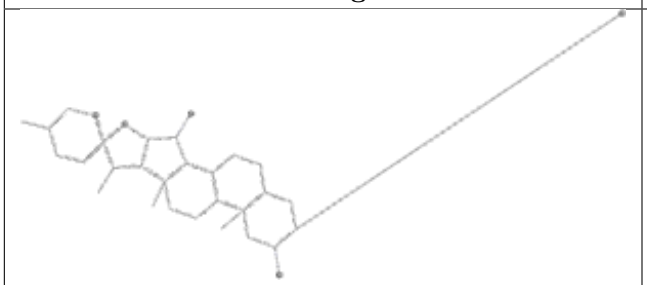
Ligand AJP C 201



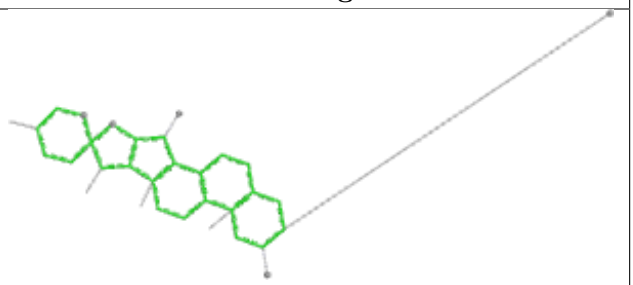
Bond lengths



Bond angles



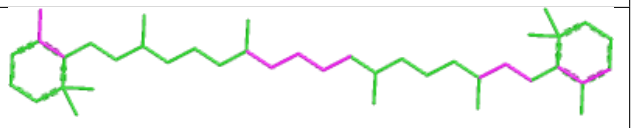
Torsions



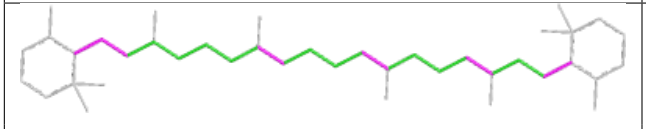
Rings

Ligand BCR A 401

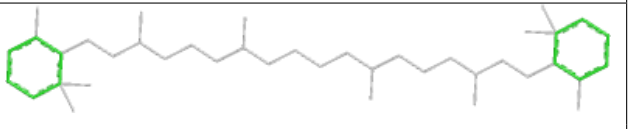
Bond lengths



Bond angles

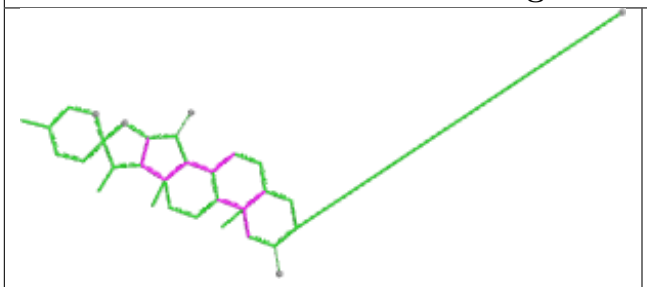


Torsions

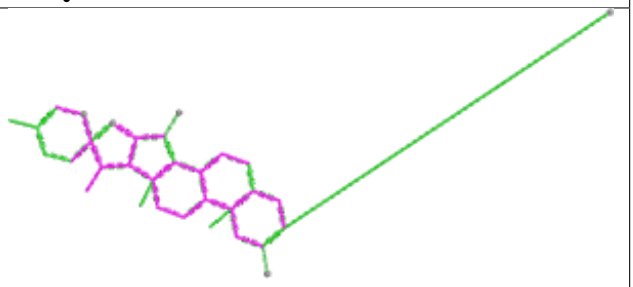


Rings

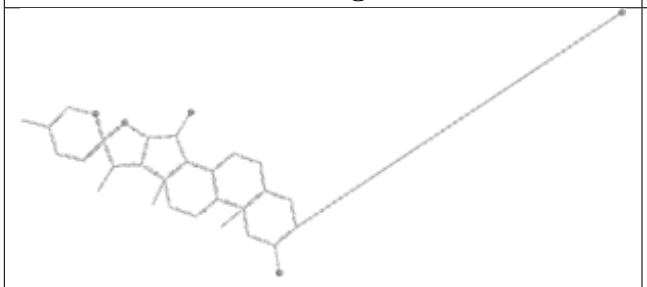
Ligand AJP Q 102



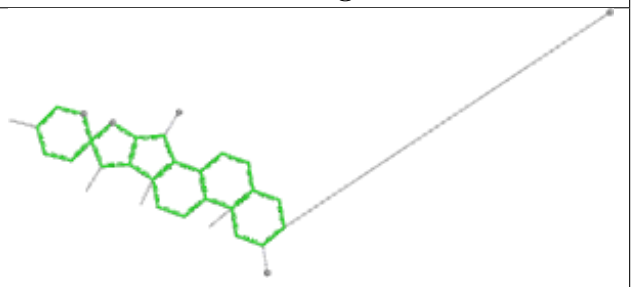
Bond lengths



Bond angles

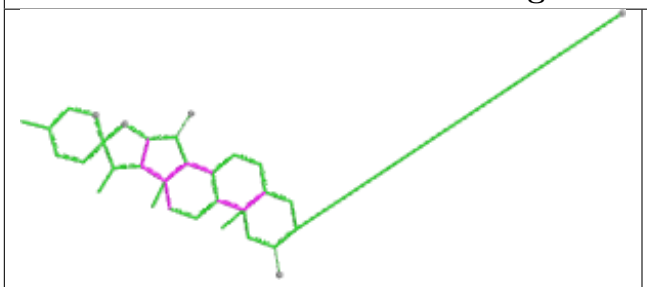


Torsions

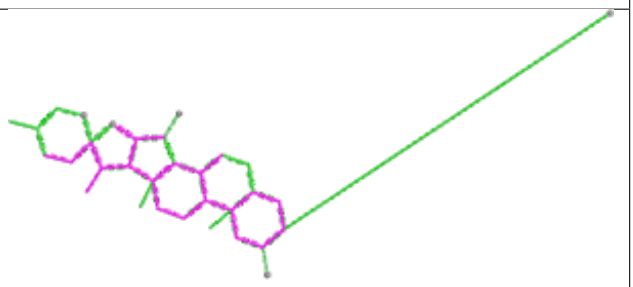


Rings

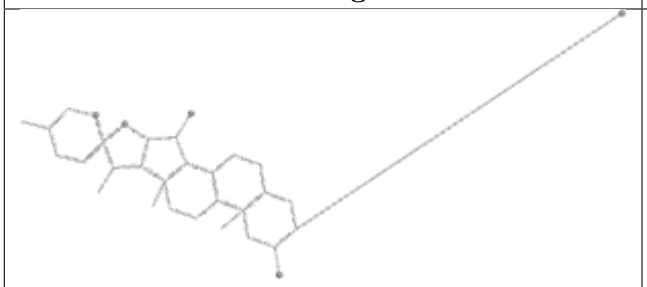
Ligand AJP B 612



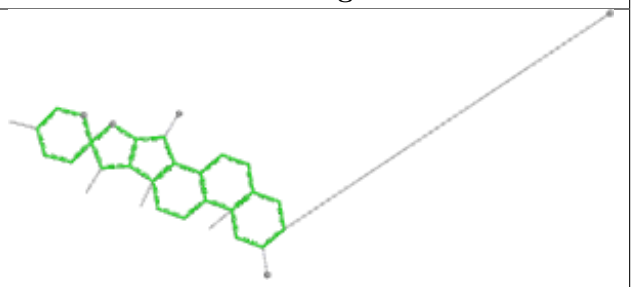
Bond lengths



Bond angles

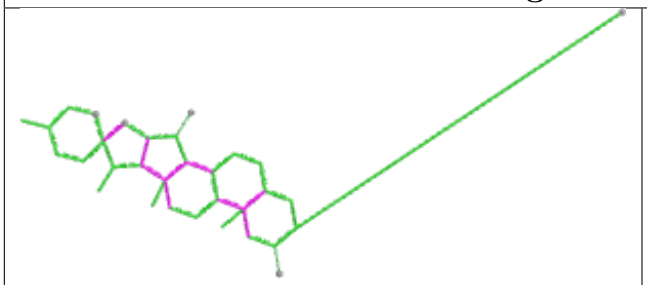


Torsions

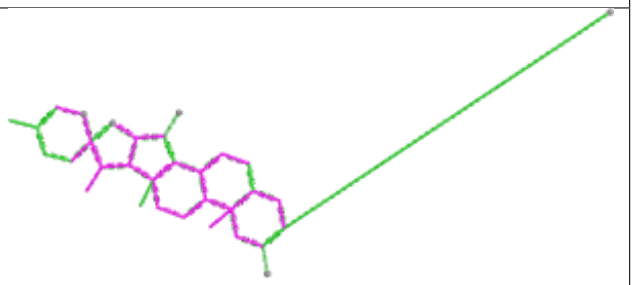


Rings

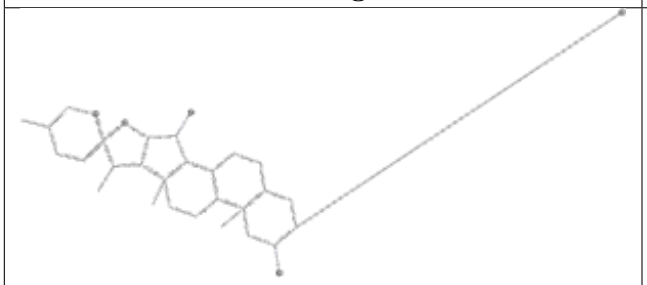
Ligand AJP G 303



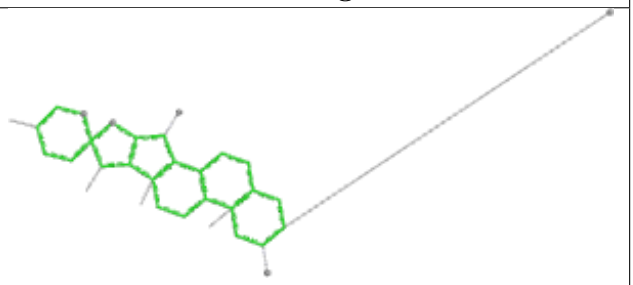
Bond lengths



Bond angles

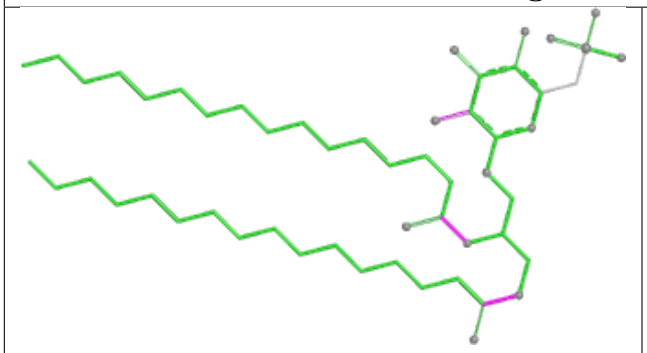


Torsions

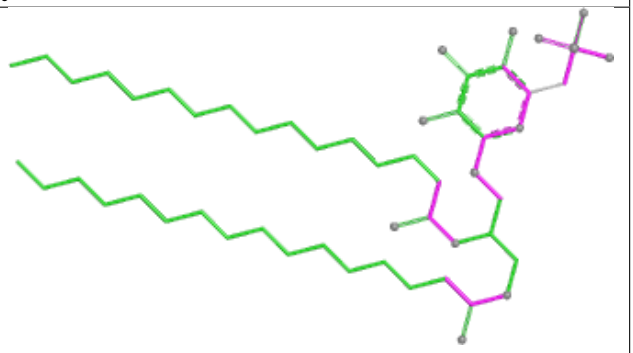


Rings

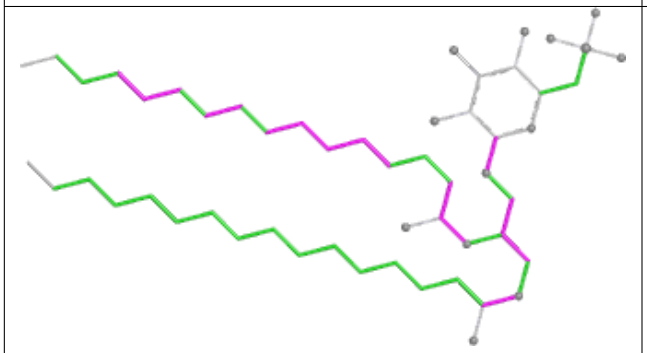
Ligand SQD F 705



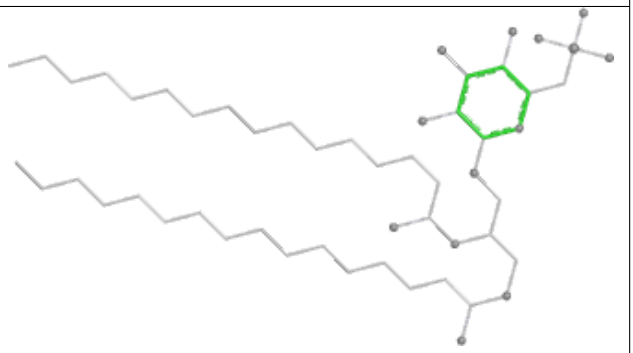
Bond lengths



Bond angles

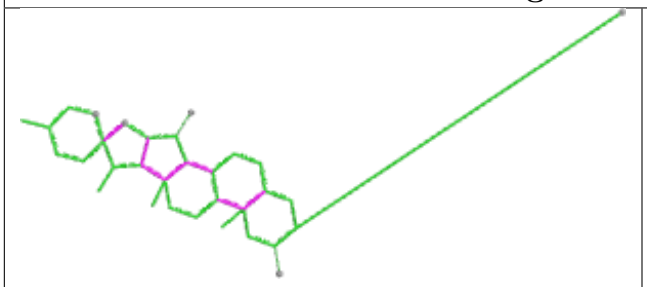


Torsions

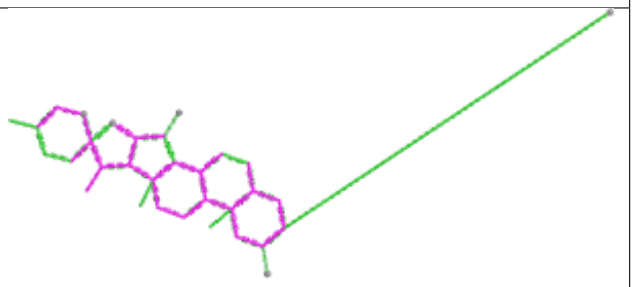


Rings

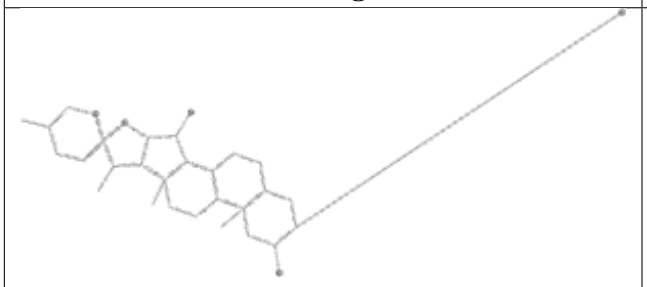
Ligand AJP D 610



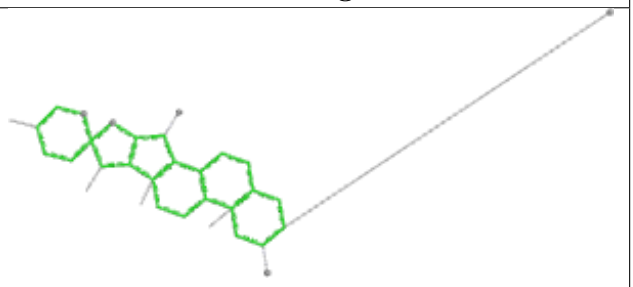
Bond lengths



Bond angles

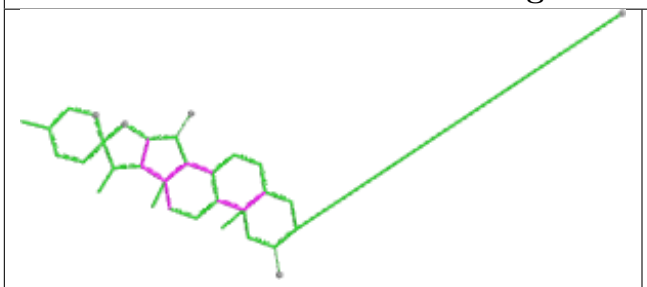


Torsions

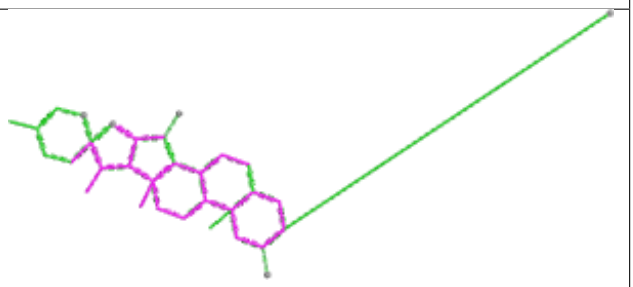


Rings

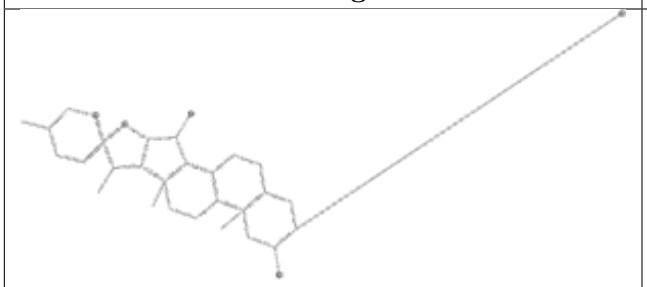
Ligand AJP D 607



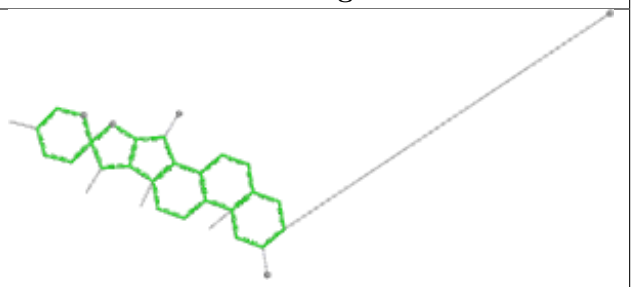
Bond lengths



Bond angles

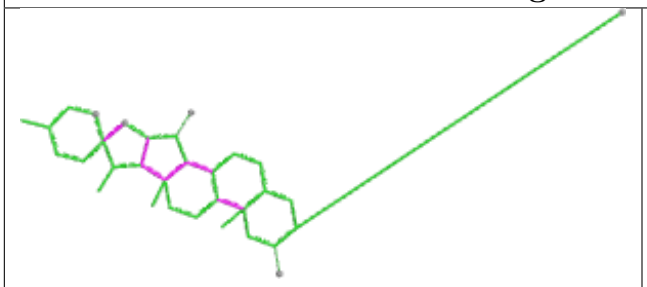


Torsions

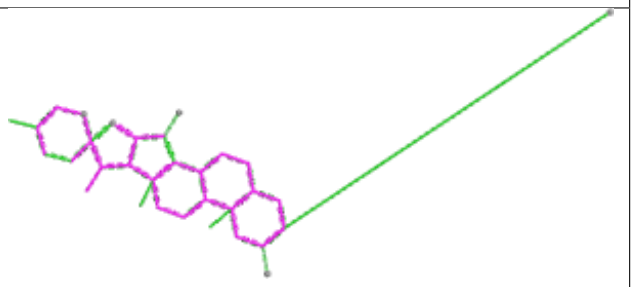


Rings

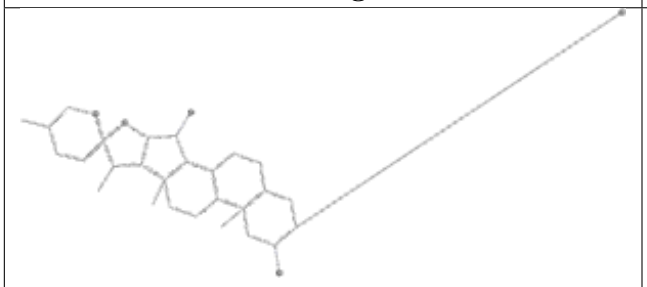
Ligand AJP F 710



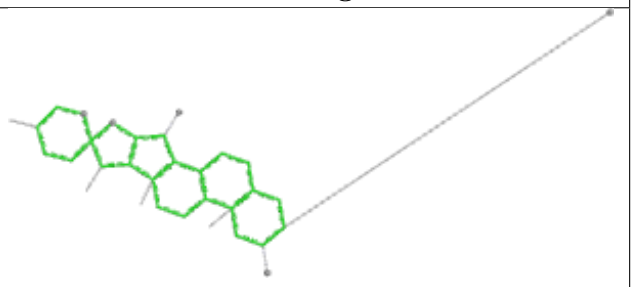
Bond lengths



Bond angles

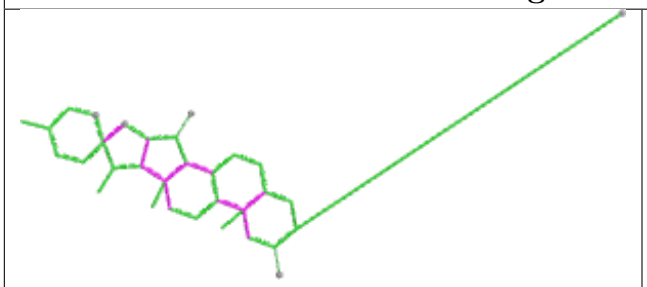


Torsions

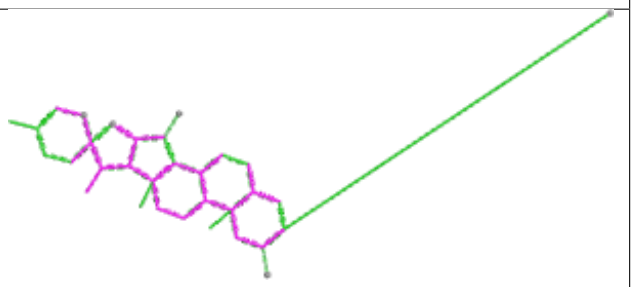


Rings

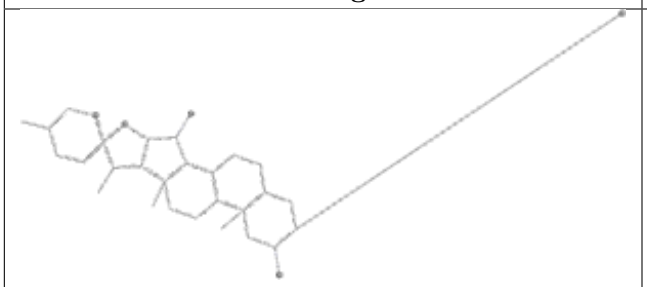
Ligand AJP B 611



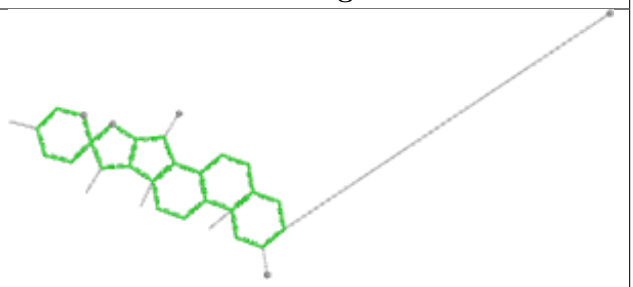
Bond lengths



Bond angles

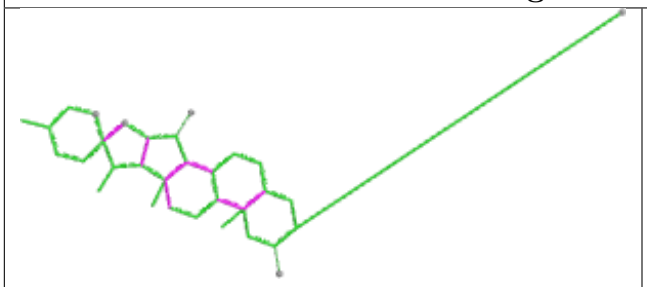


Torsions

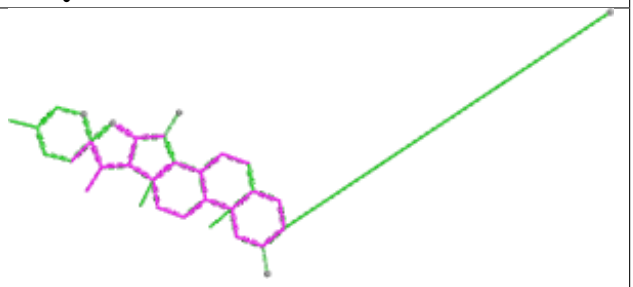


Rings

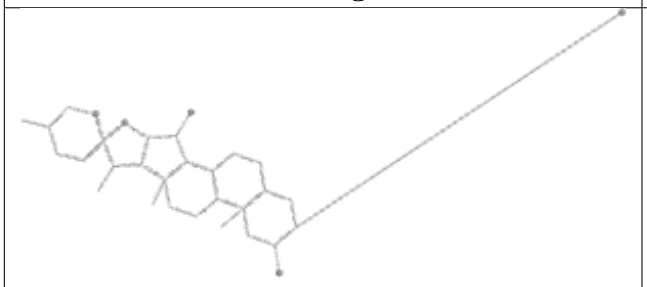
Ligand AJP Q 103



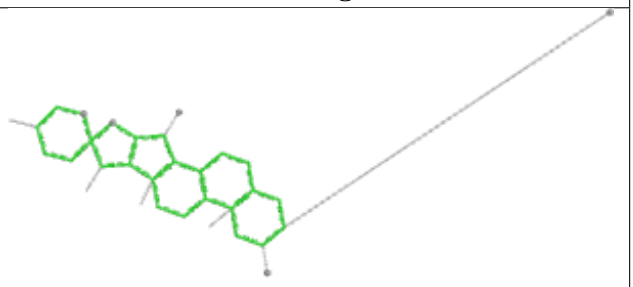
Bond lengths



Bond angles

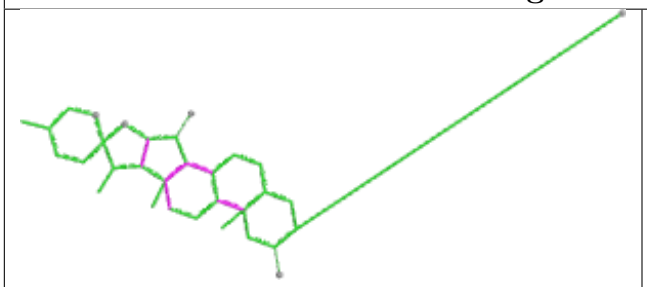


Torsions

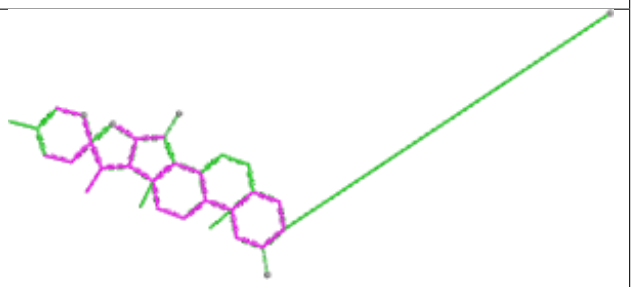


Rings

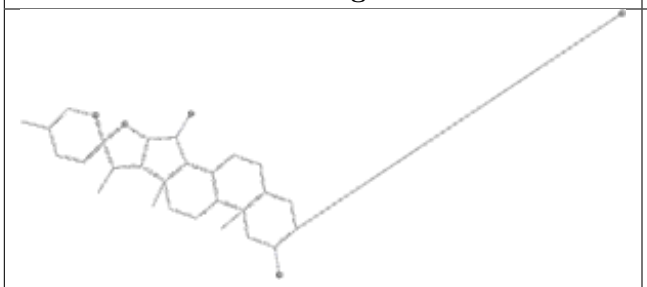
Ligand AJP D 613



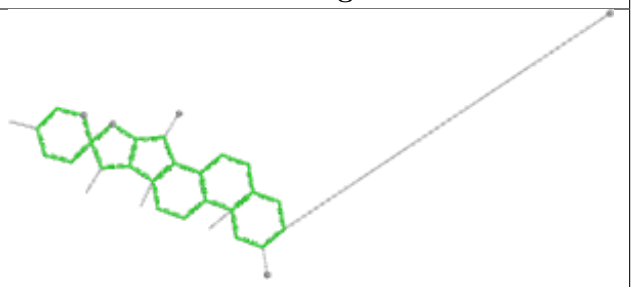
Bond lengths



Bond angles

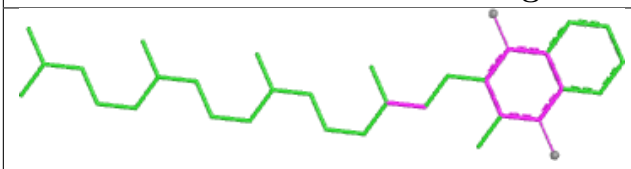


Torsions

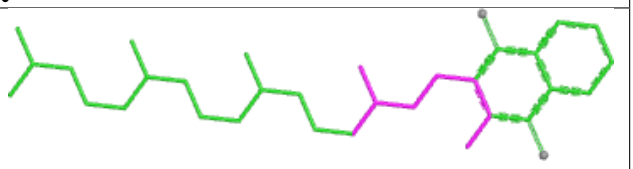


Rings

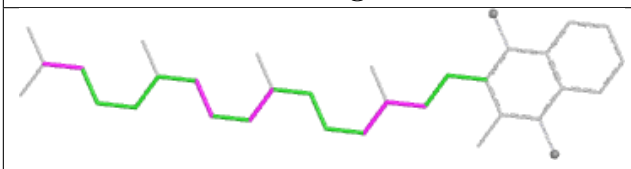
Ligand PQN B 601



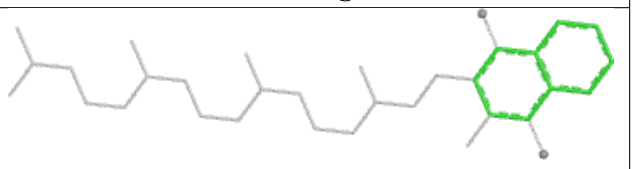
Bond lengths



Bond angles

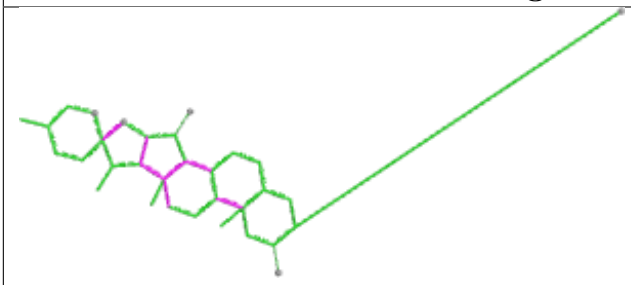


Torsions

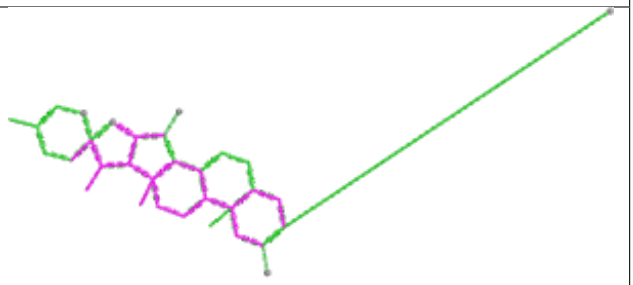


Rings

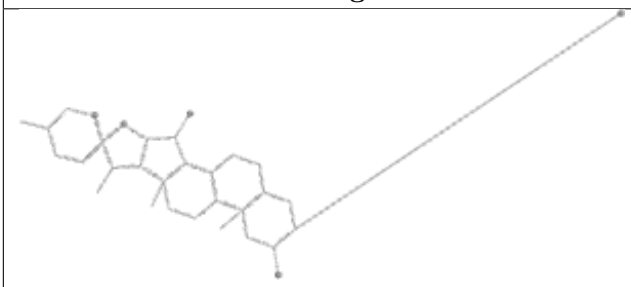
Ligand AJP B 608



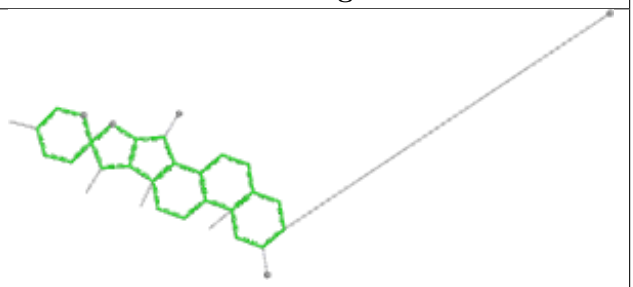
Bond lengths



Bond angles

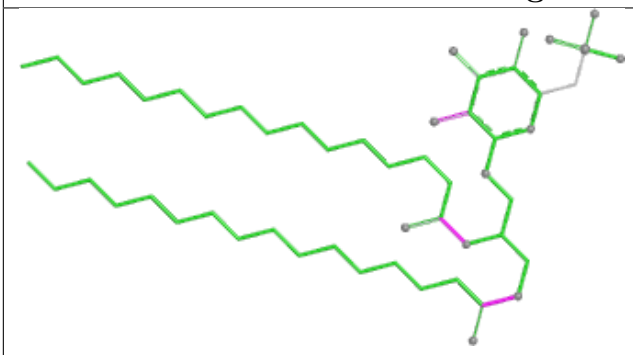


Torsions

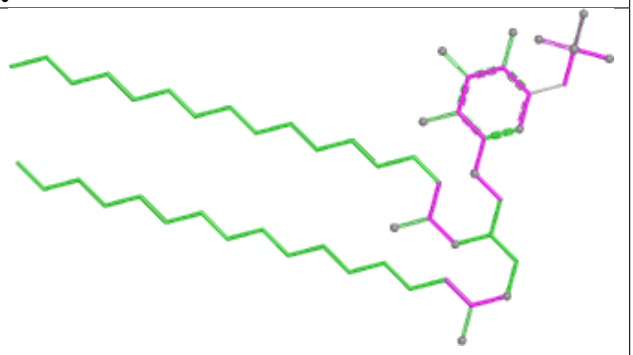


Rings

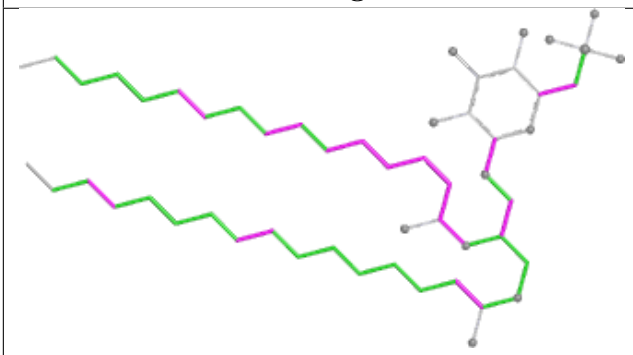
Ligand SQD L 101



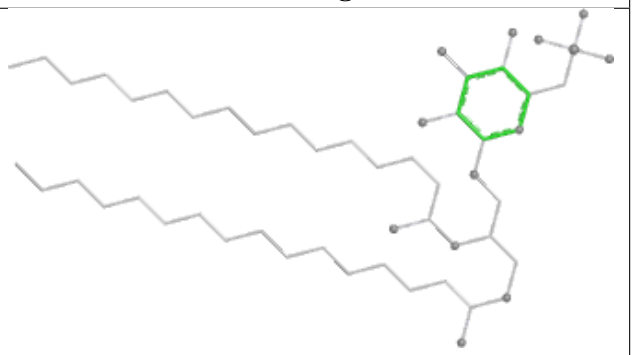
Bond lengths



Bond angles

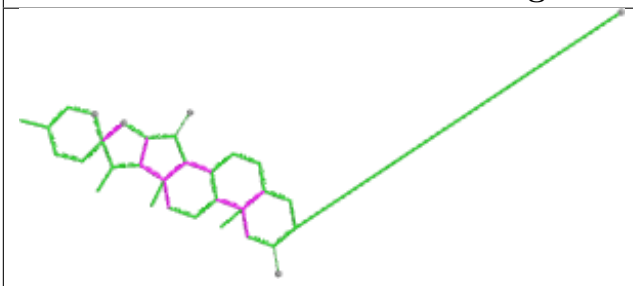


Torsions

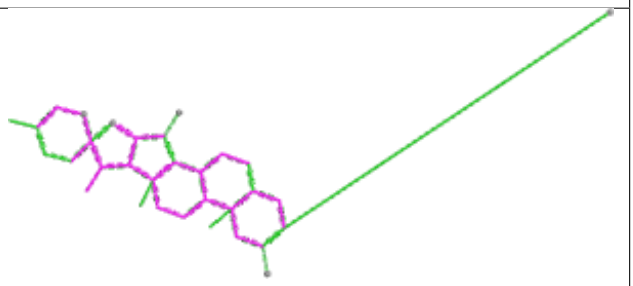


Rings

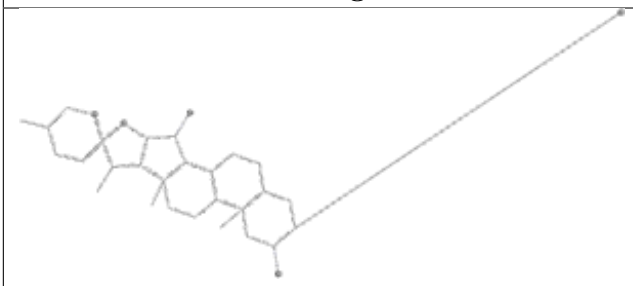
Ligand AJP F 714



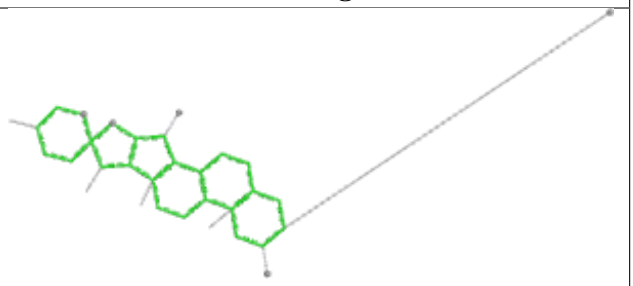
Bond lengths



Bond angles

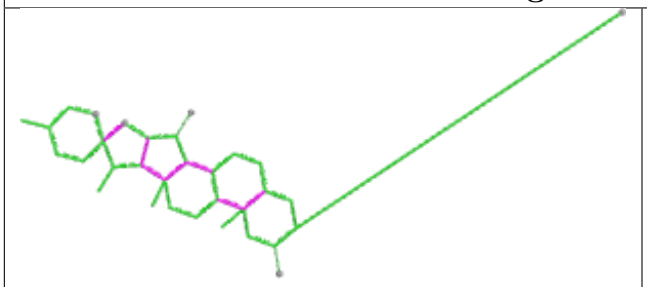


Torsions

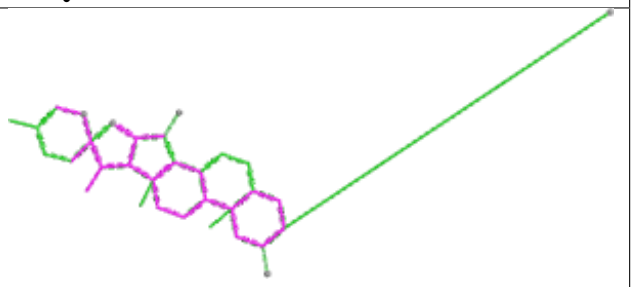


Rings

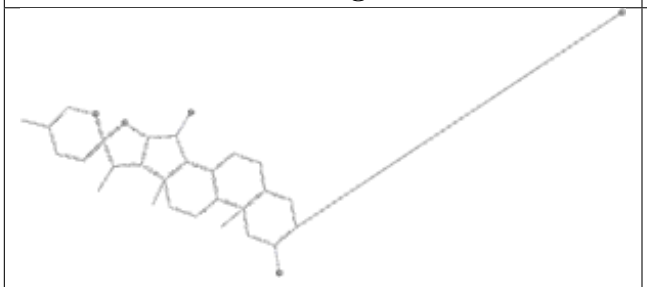
Ligand AJP Q 107



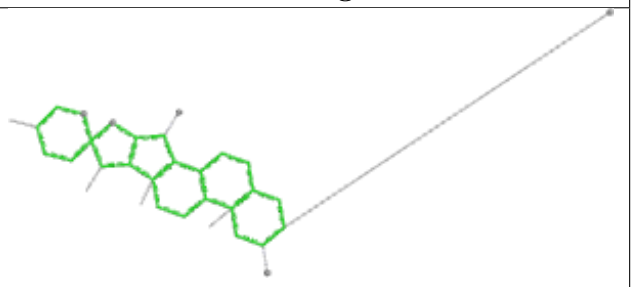
Bond lengths



Bond angles

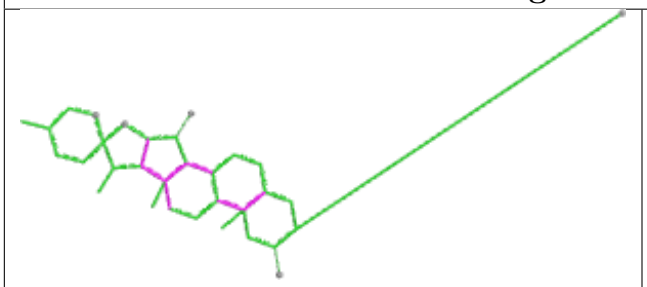


Torsions

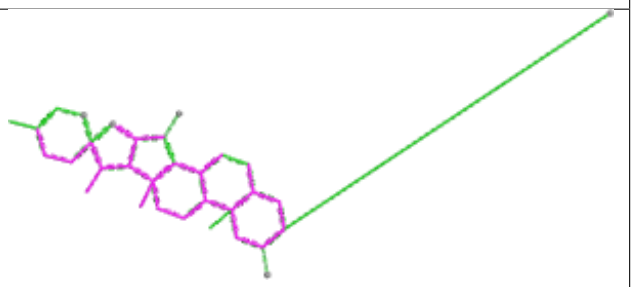


Rings

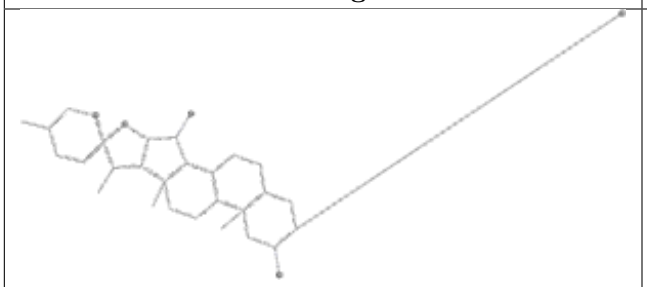
Ligand AJP F 709



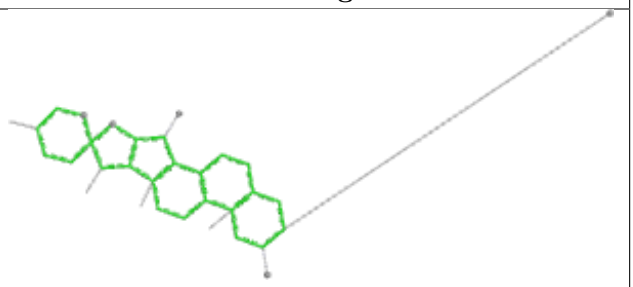
Bond lengths



Bond angles

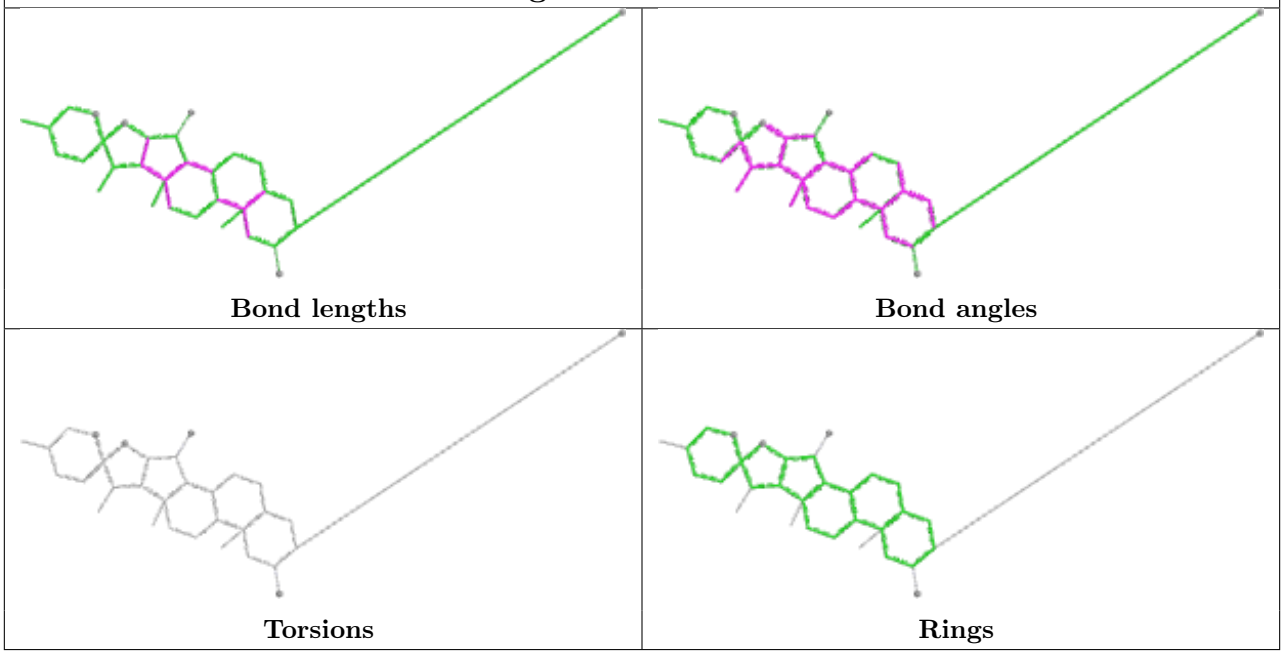


Torsions

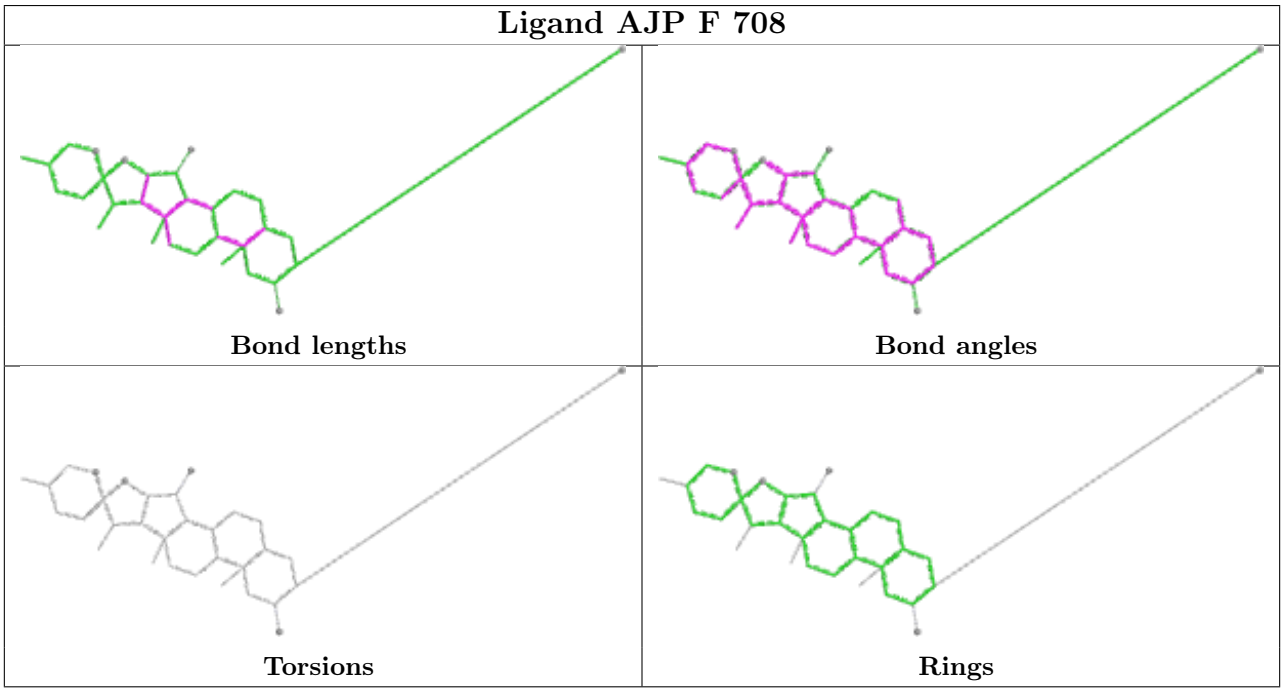


Rings

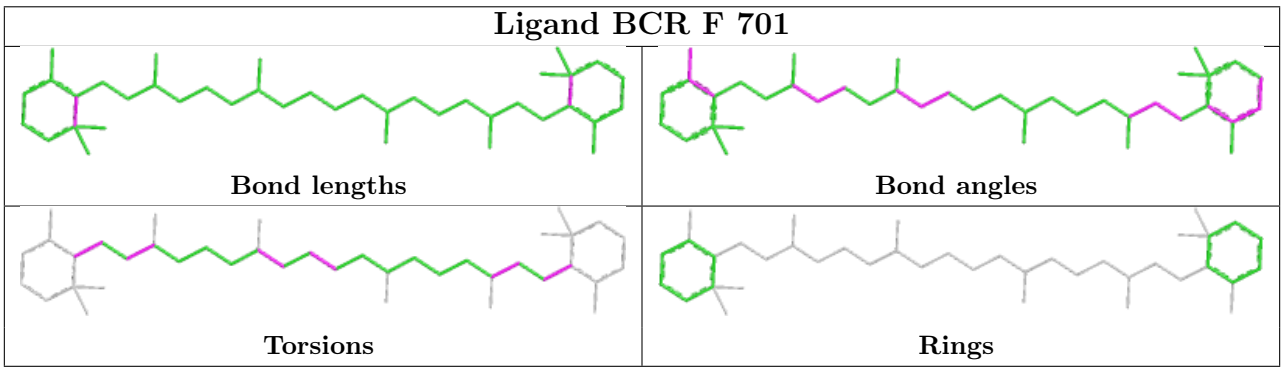
Ligand AJP F 707



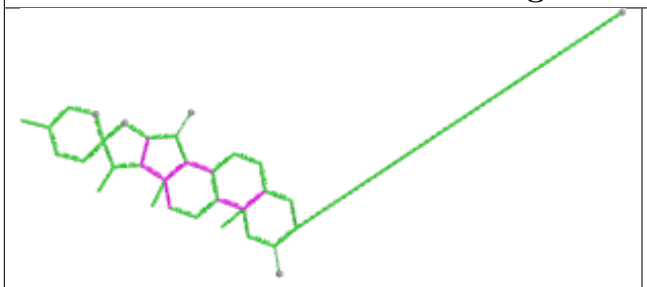
Ligand AJP F 708



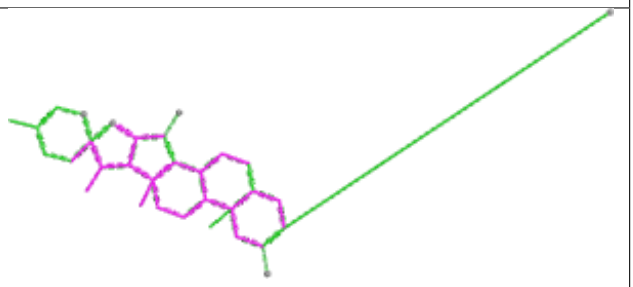
Ligand BCR F 701



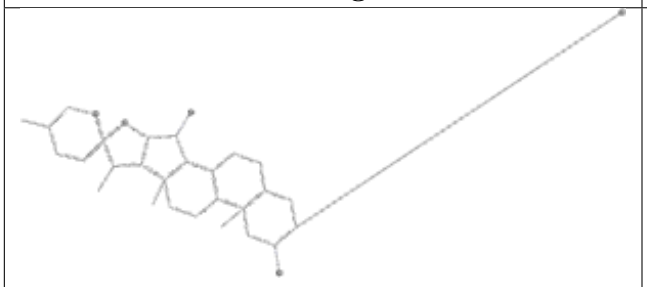
Ligand AJP A 405



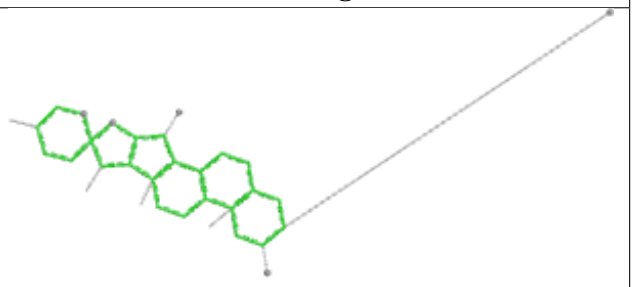
Bond lengths



Bond angles

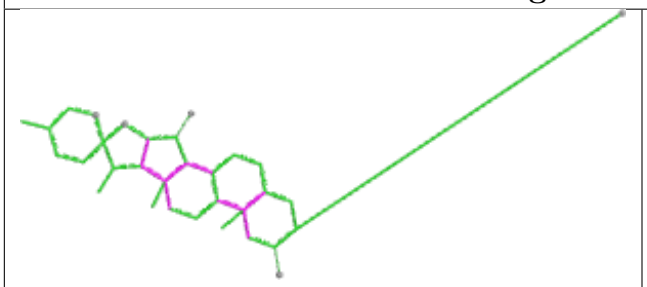


Torsions

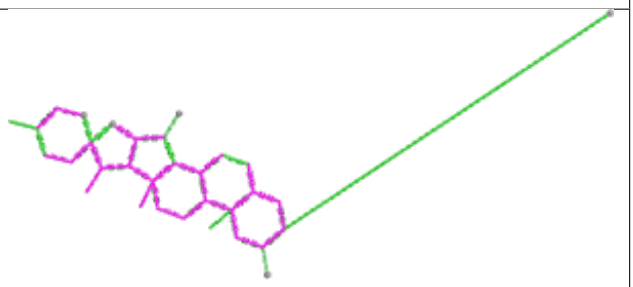


Rings

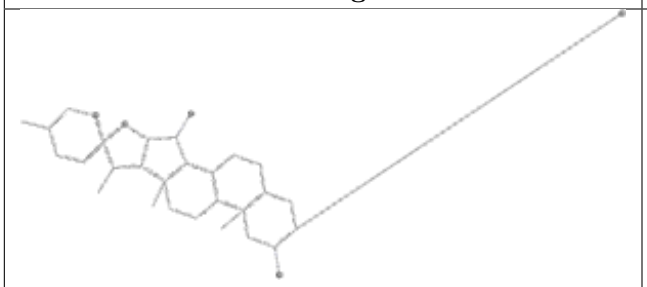
Ligand AJP F 716



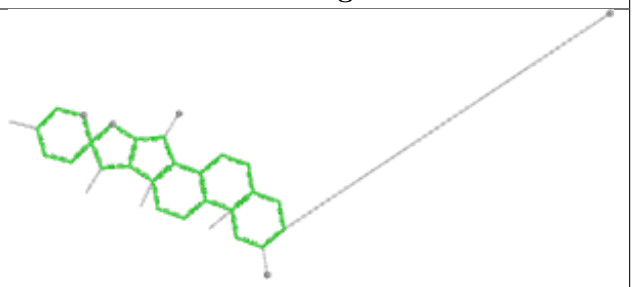
Bond lengths



Bond angles

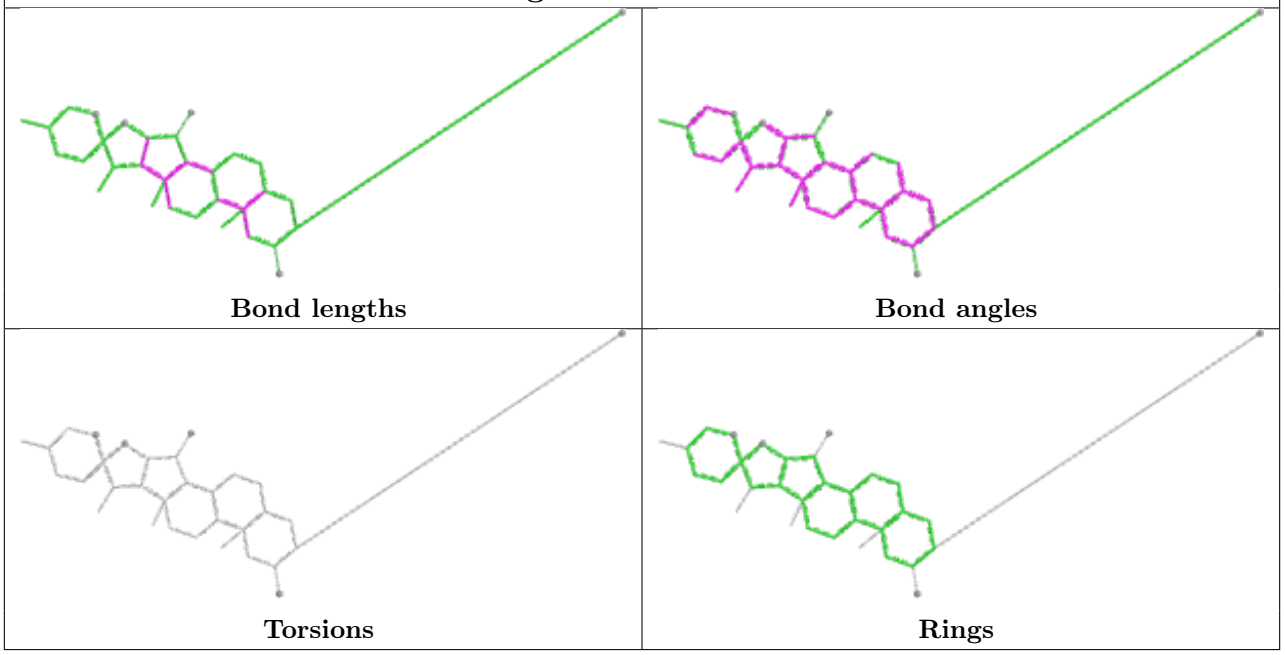


Torsions

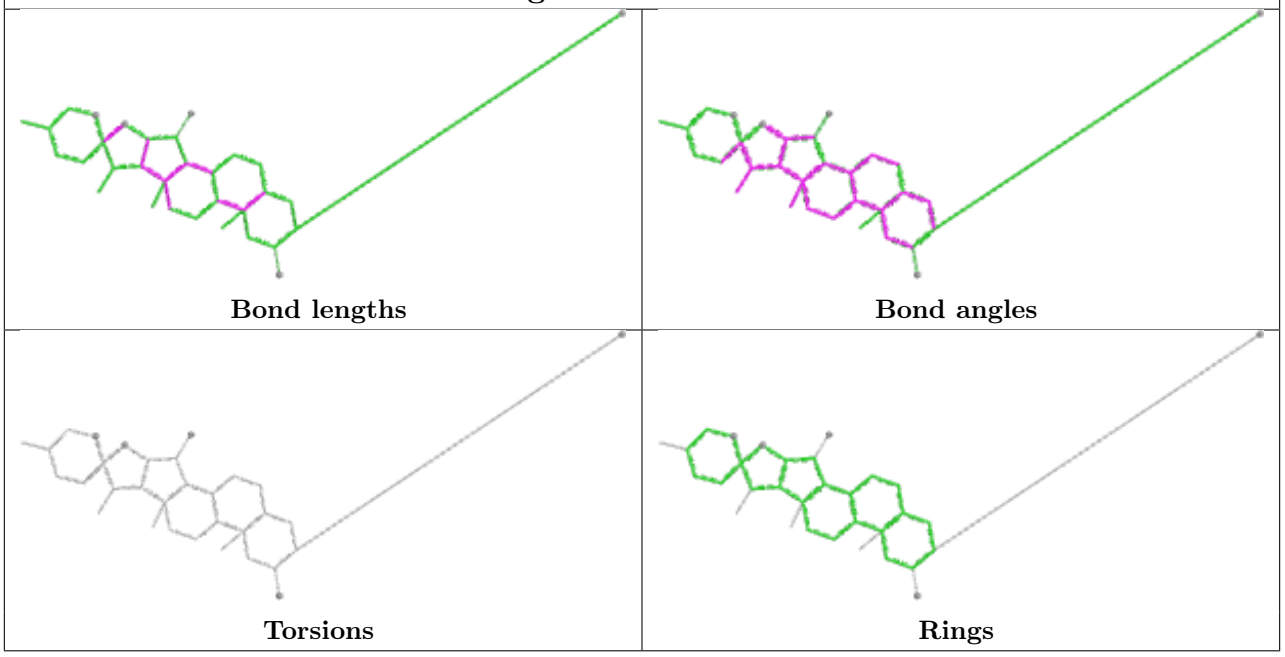


Rings

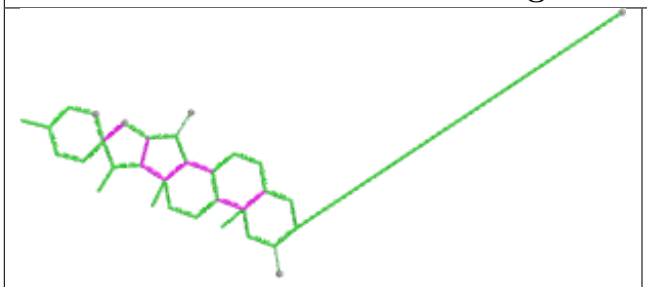
Ligand AJP D 603



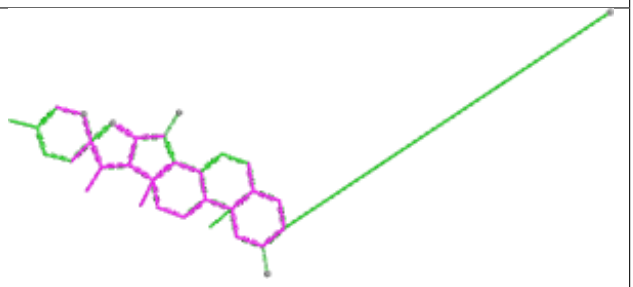
Ligand AJP B 610



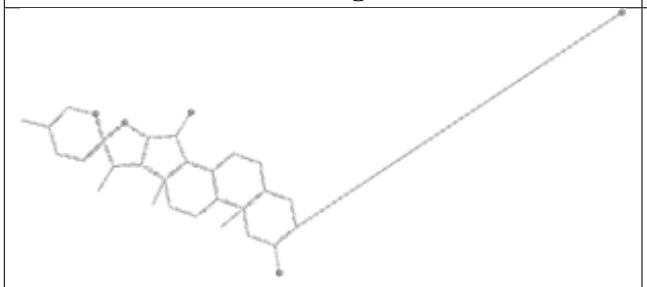
Ligand AJP B 613



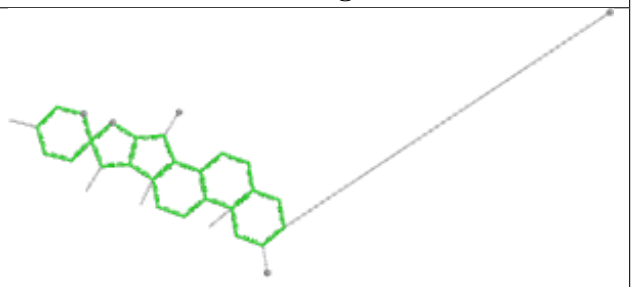
Bond lengths



Bond angles

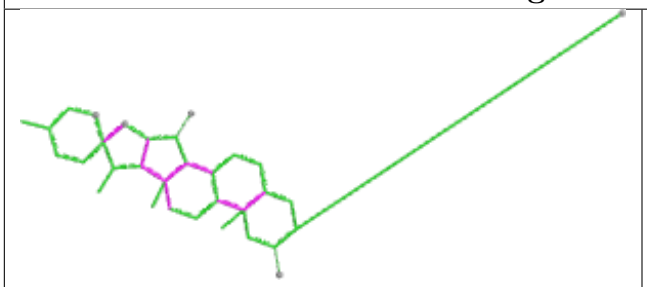


Torsions

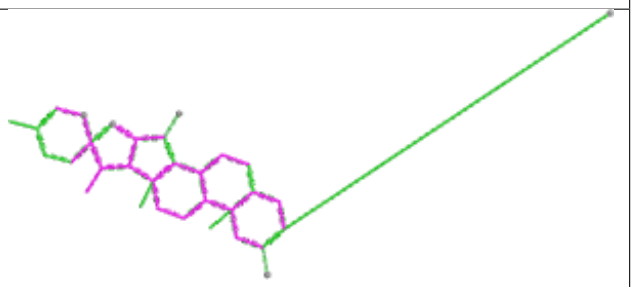


Rings

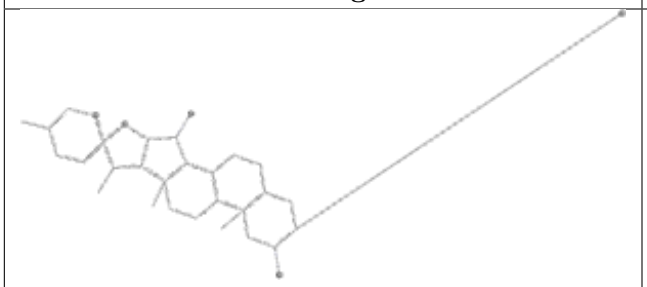
Ligand AJP B 607



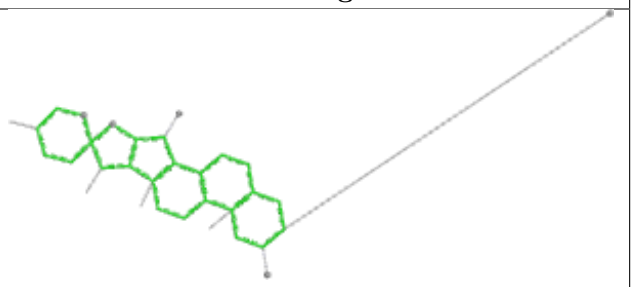
Bond lengths



Bond angles

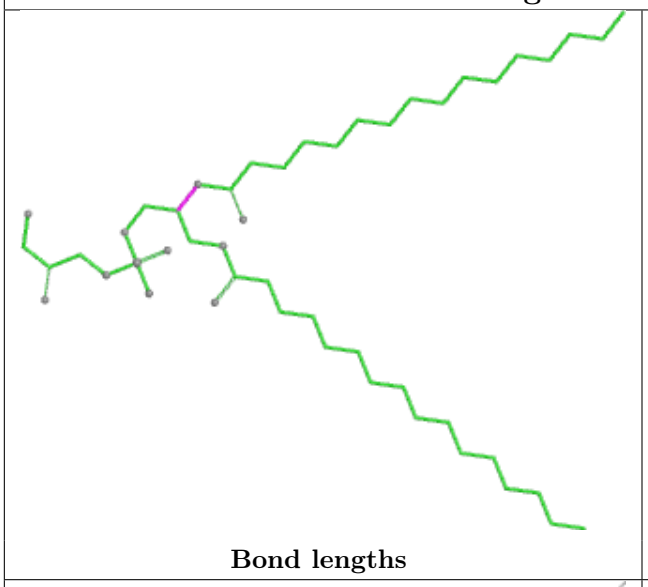


Torsions

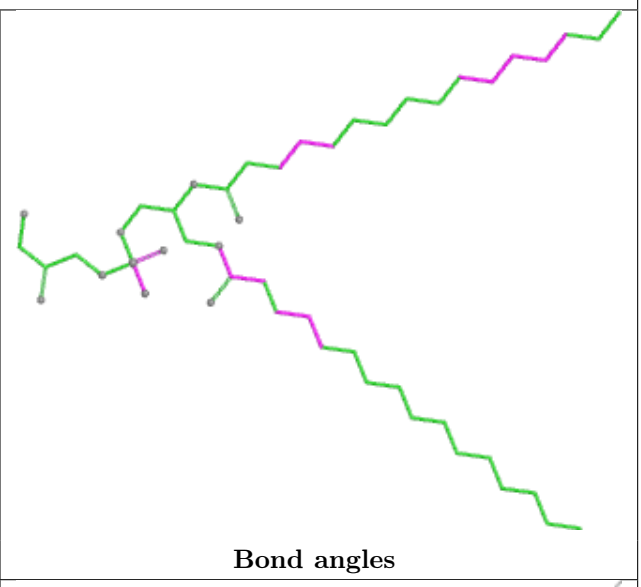


Rings

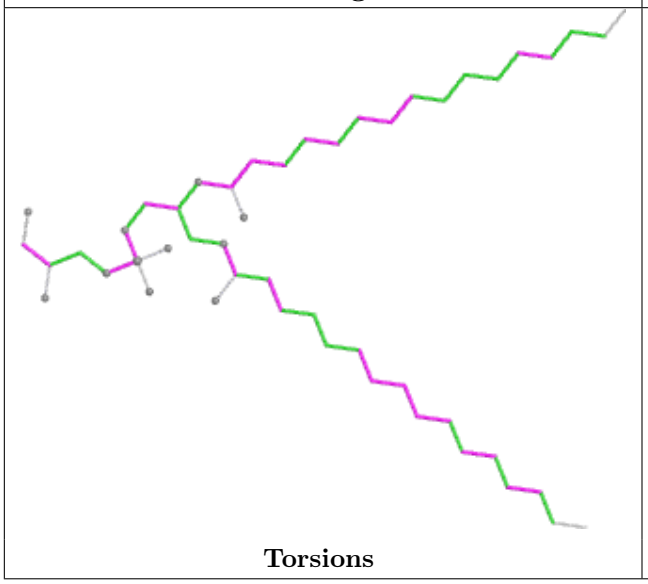
Ligand LHG B 604



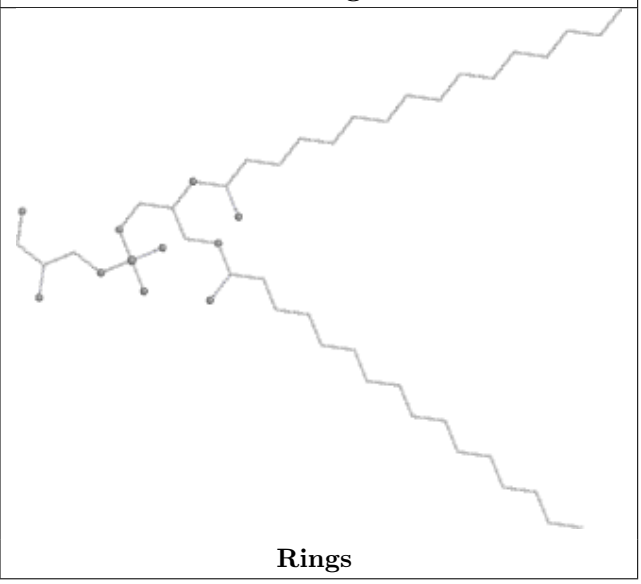
Bond lengths



Bond angles

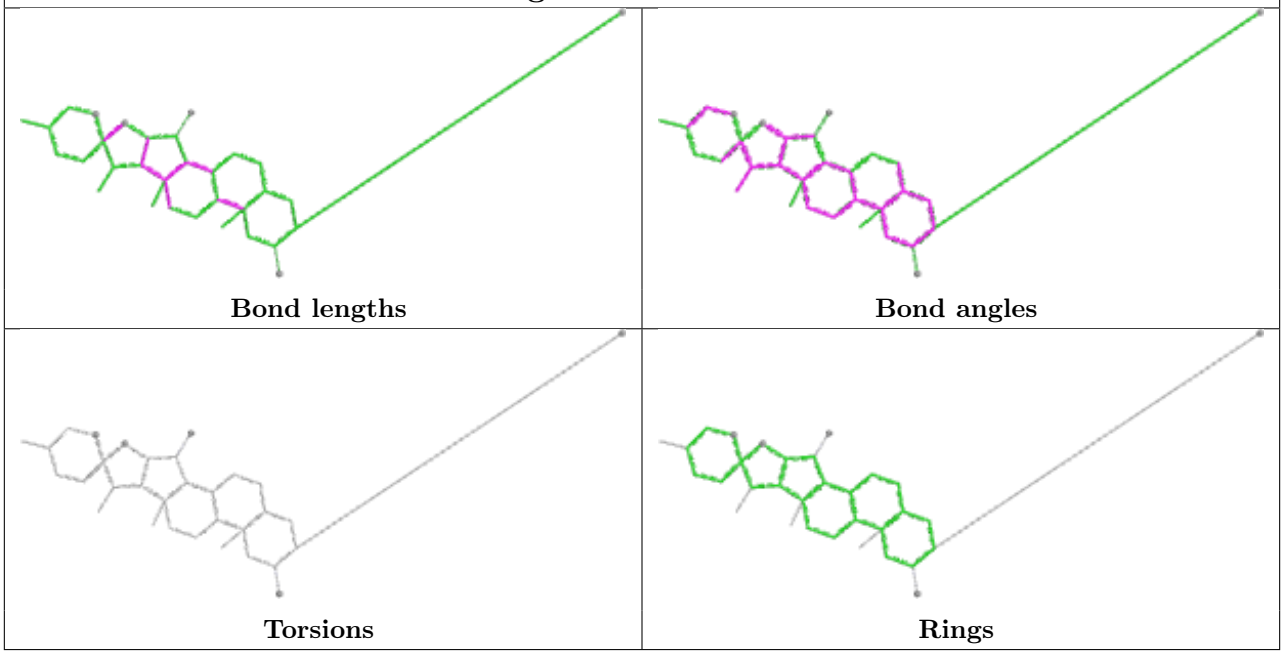


Torsions

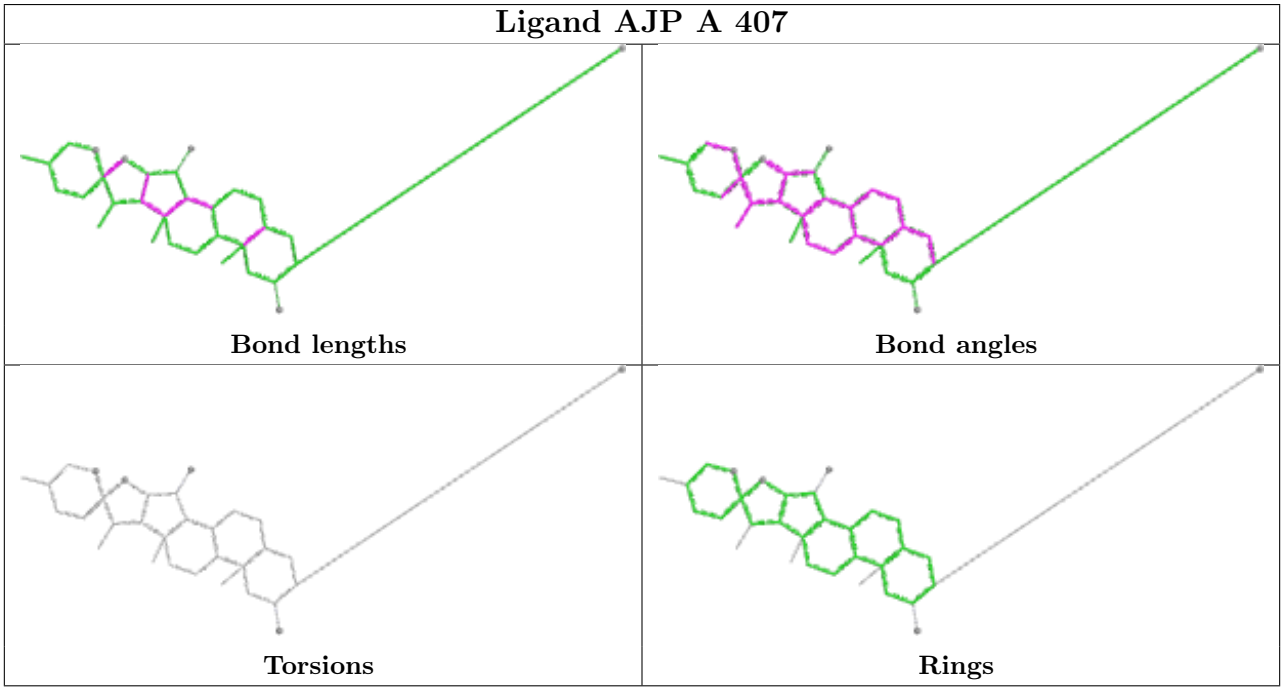


Rings

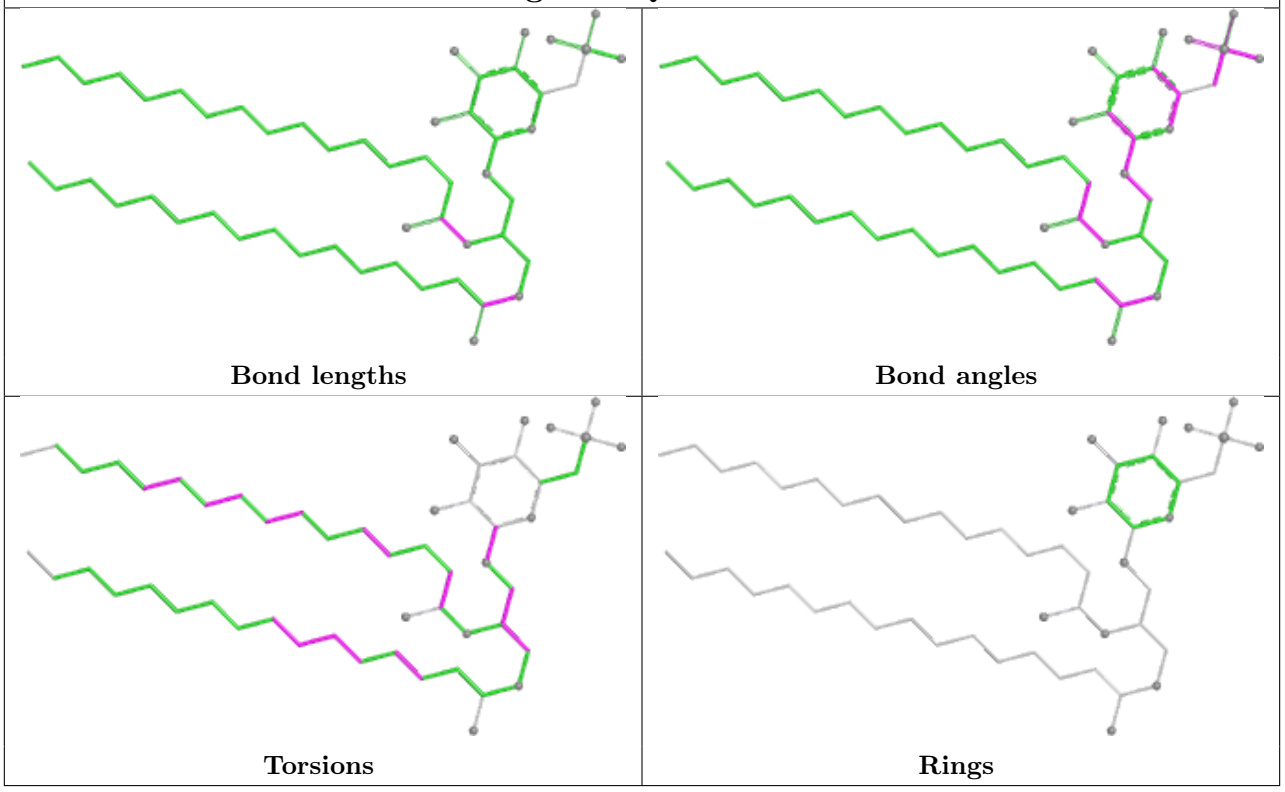
Ligand AJP B 617



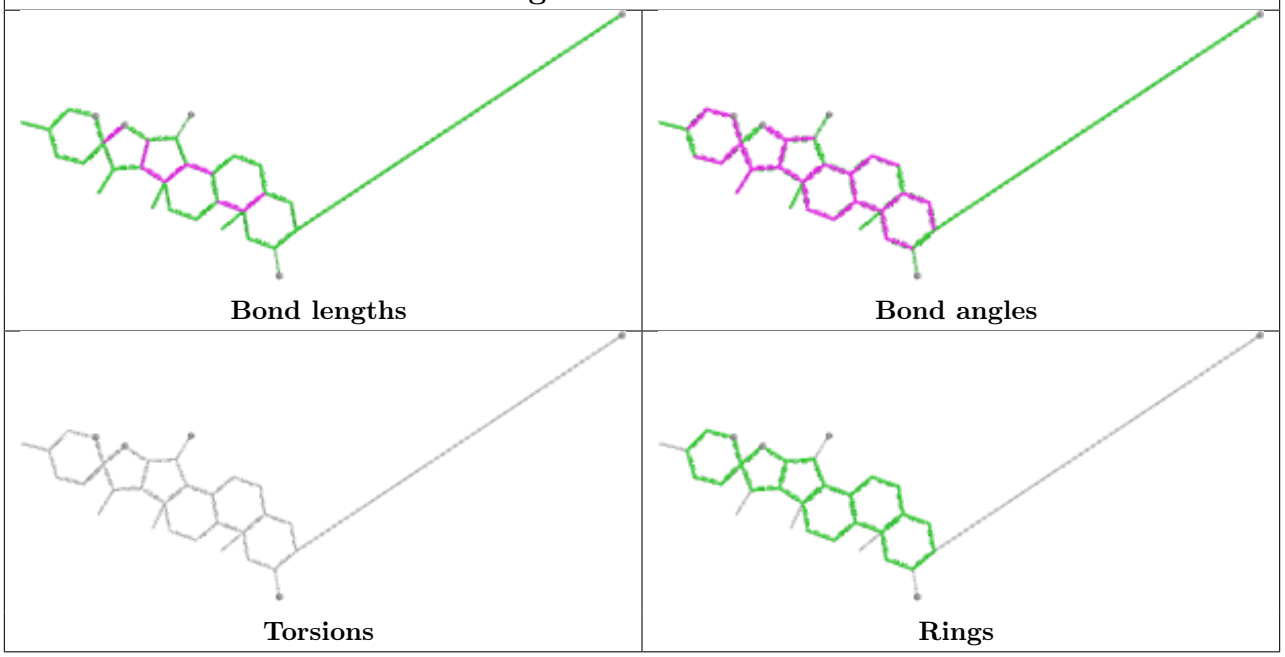
Ligand AJP A 407



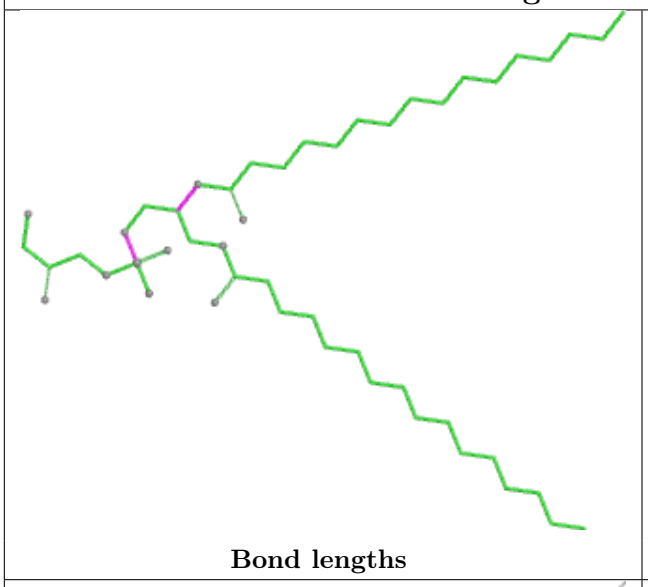
Ligand SQD B 605



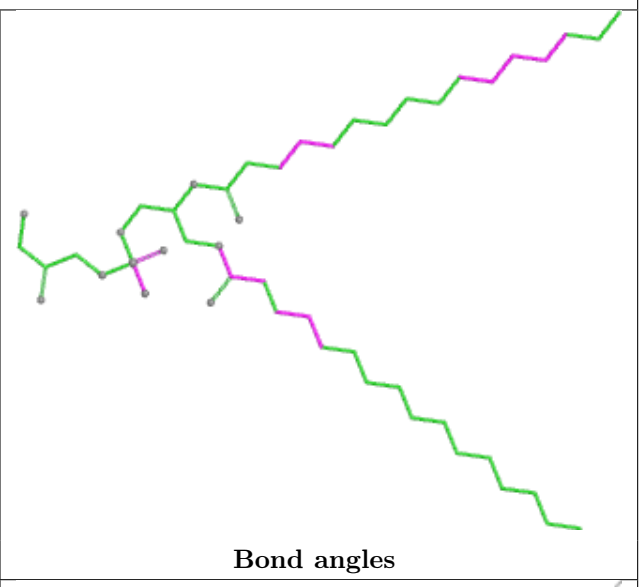
Ligand AJP E 201



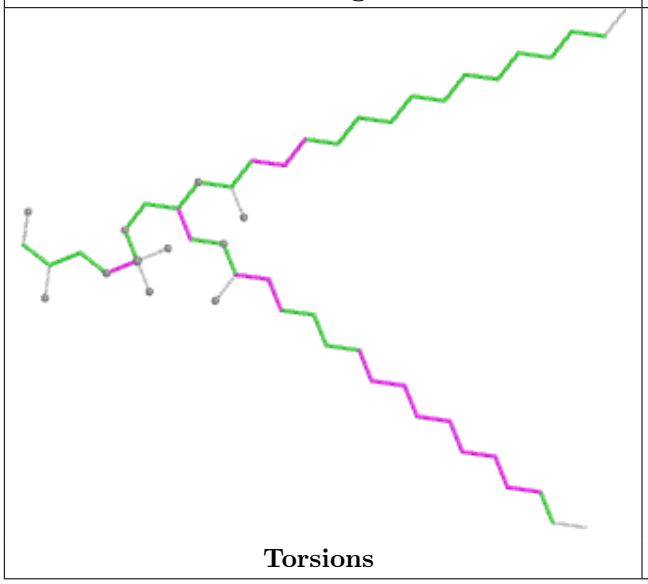
Ligand LHG D 601



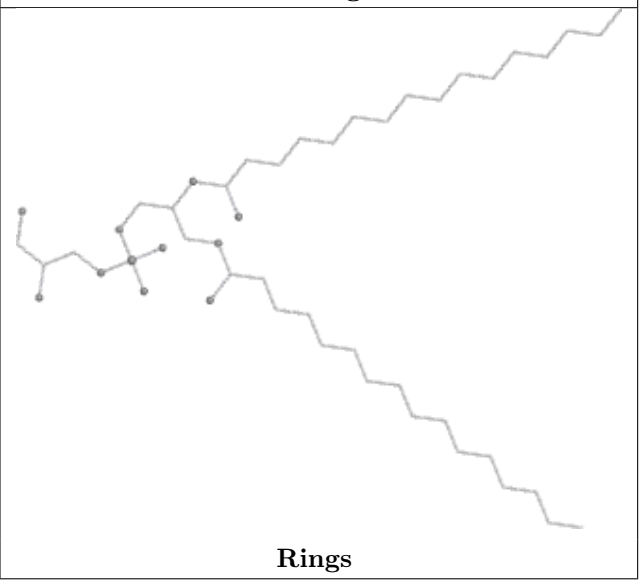
Bond lengths



Bond angles

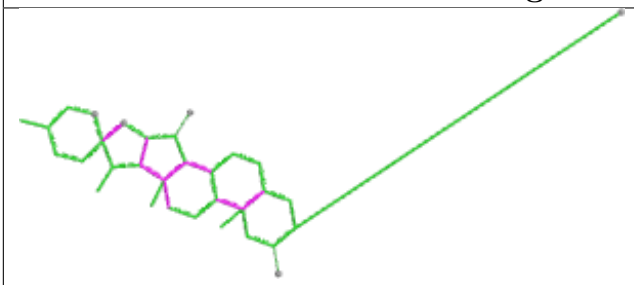


Torsions

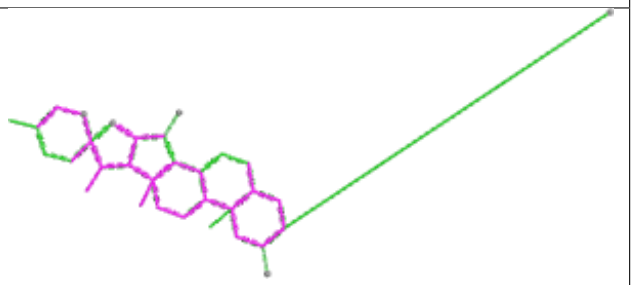


Rings

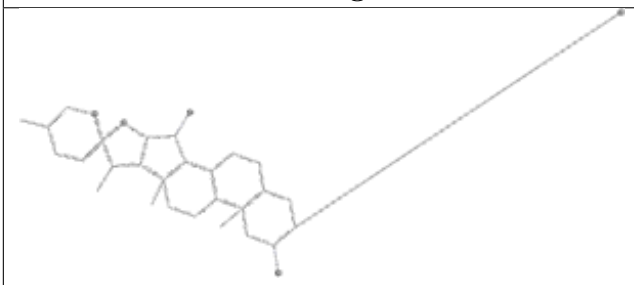
Ligand AJP A 408



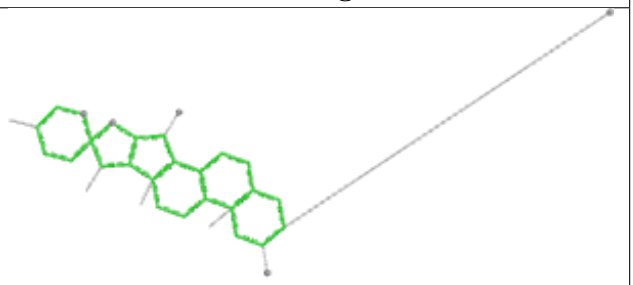
Bond lengths



Bond angles

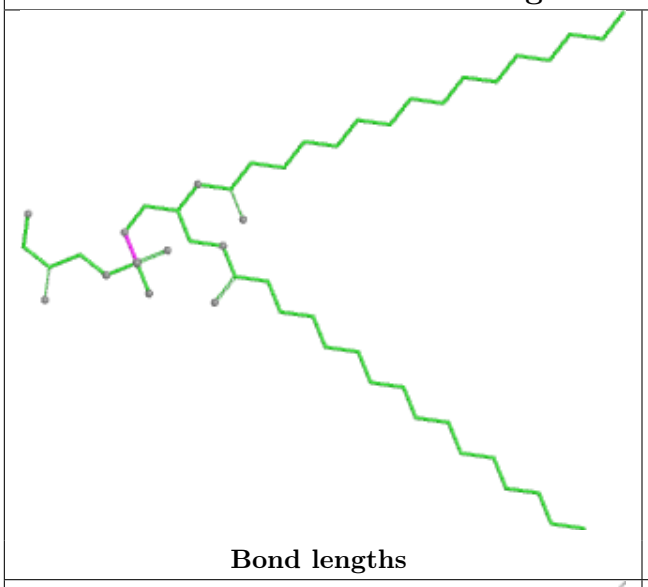


Torsions

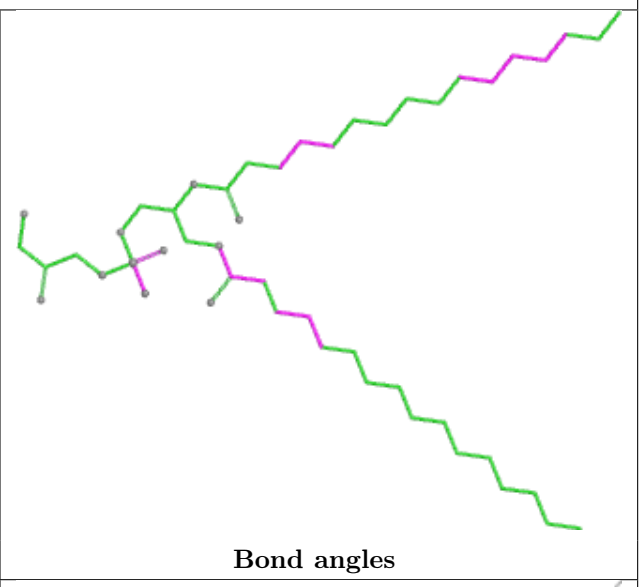


Rings

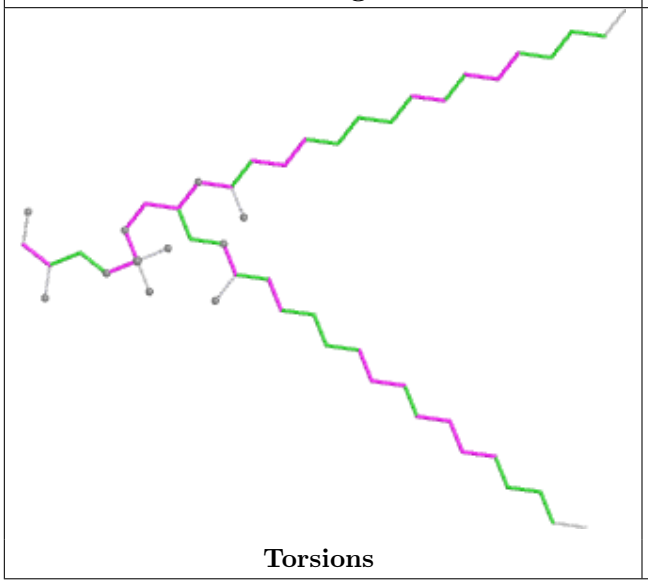
Ligand LHG F 702



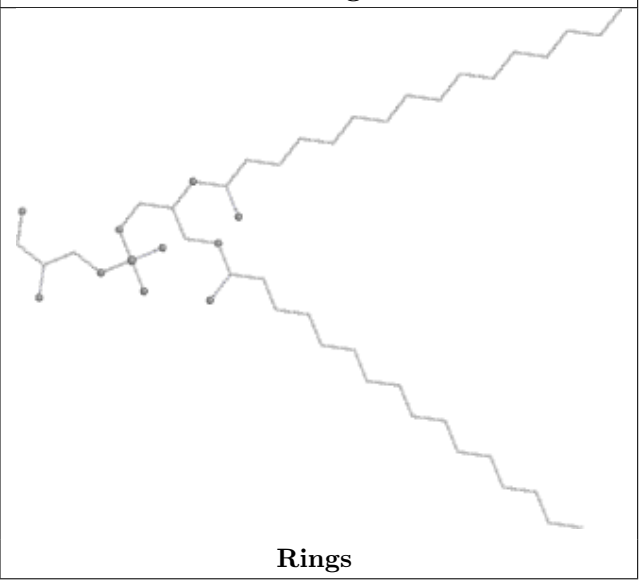
Bond lengths



Bond angles

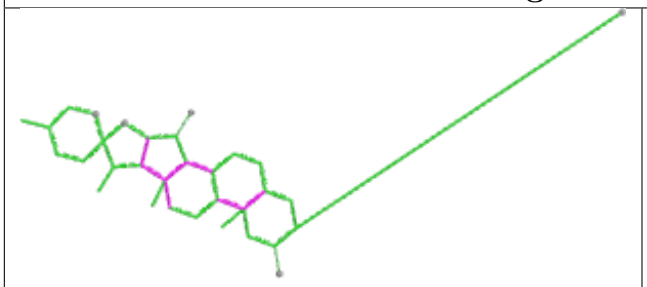


Torsions

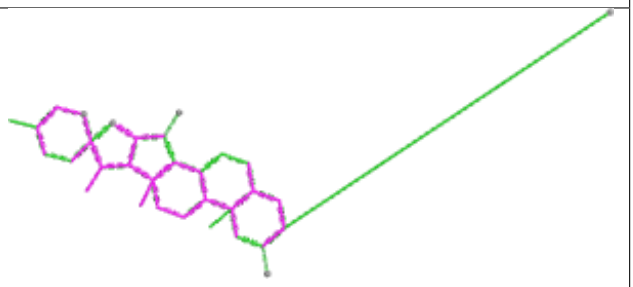


Rings

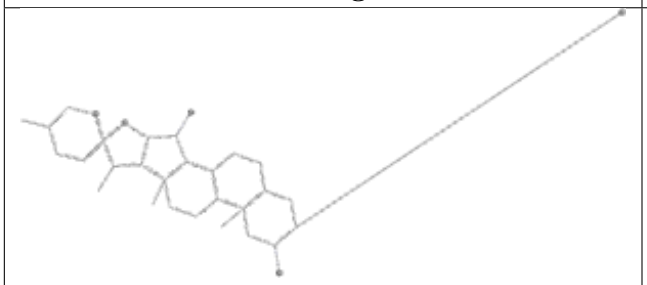
Ligand AJP G 301



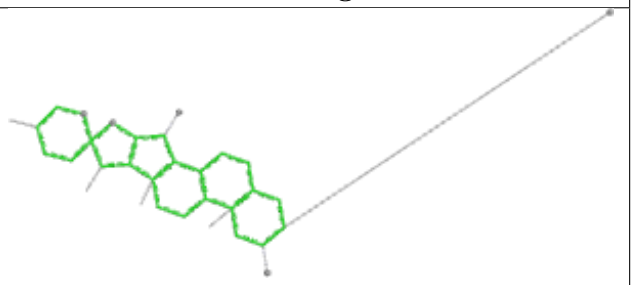
Bond lengths



Bond angles

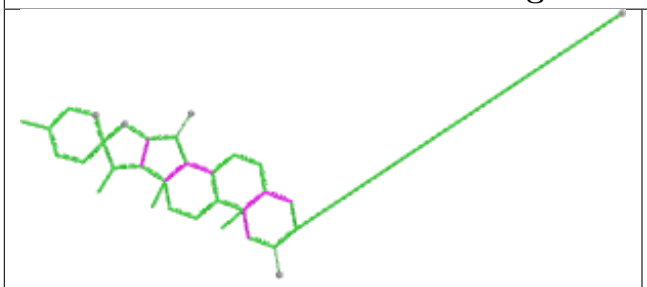


Torsions

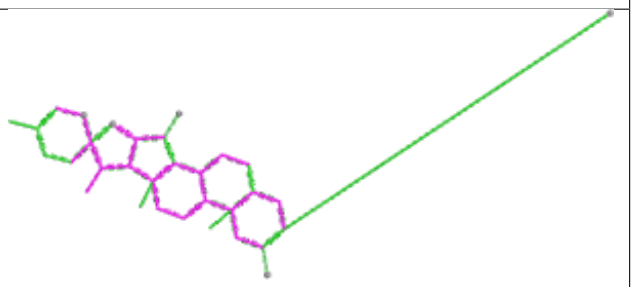


Rings

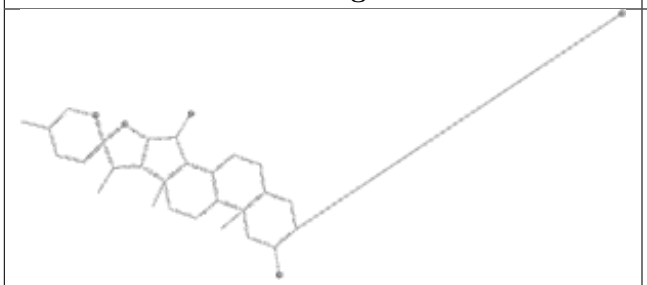
Ligand AJP D 612



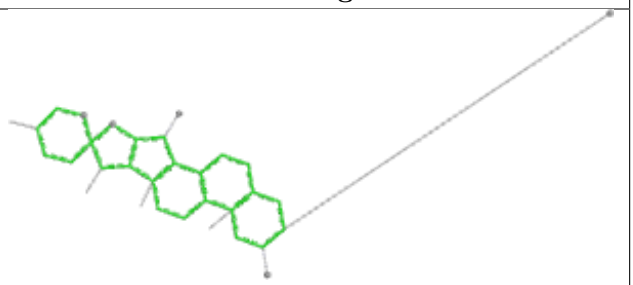
Bond lengths



Bond angles

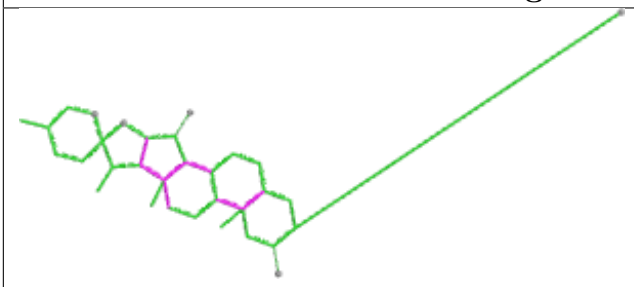


Torsions

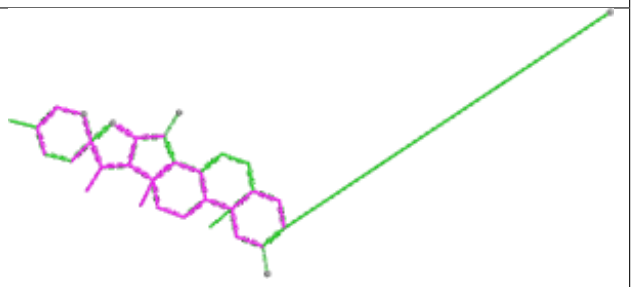


Rings

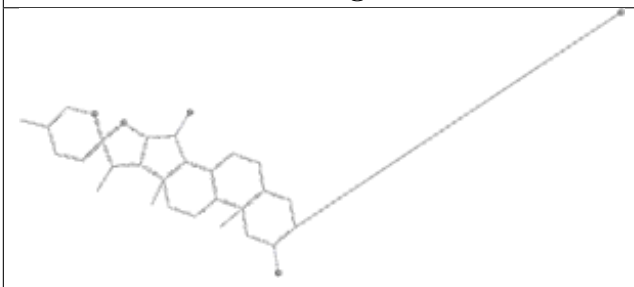
Ligand AJP G 306



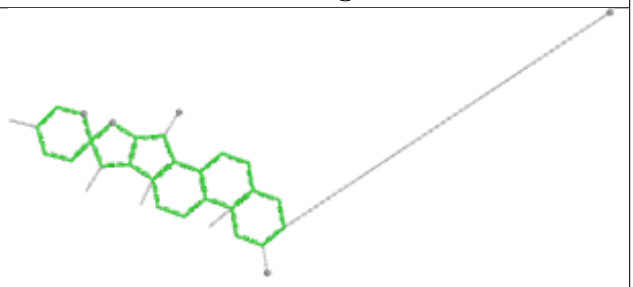
Bond lengths



Bond angles

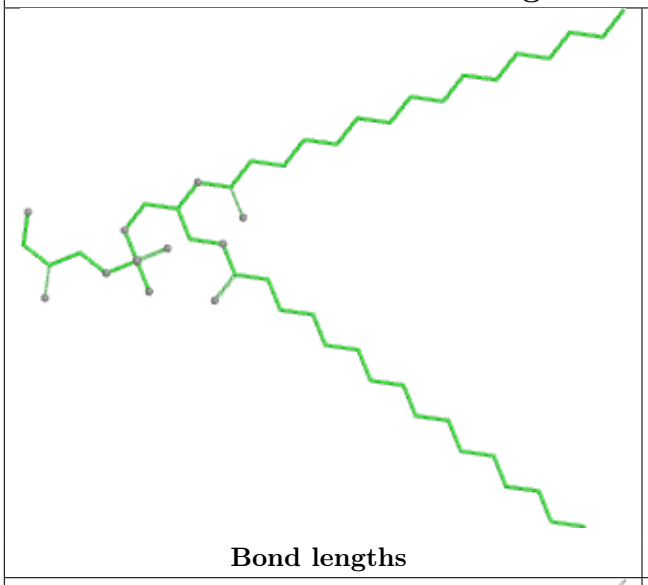


Torsions

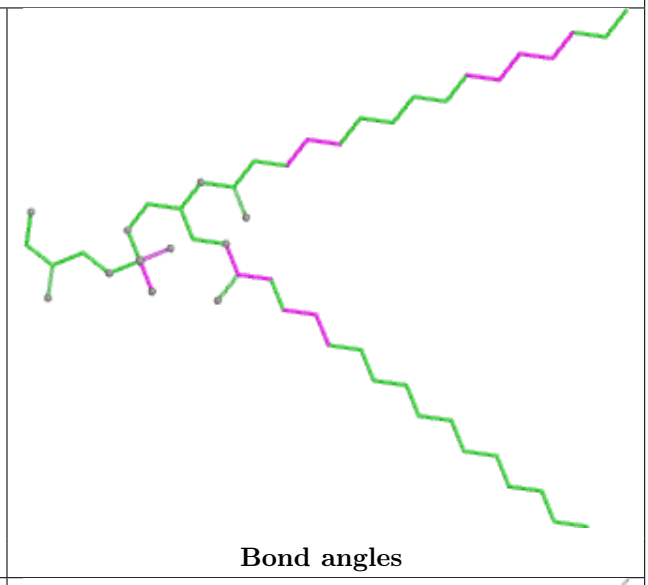


Rings

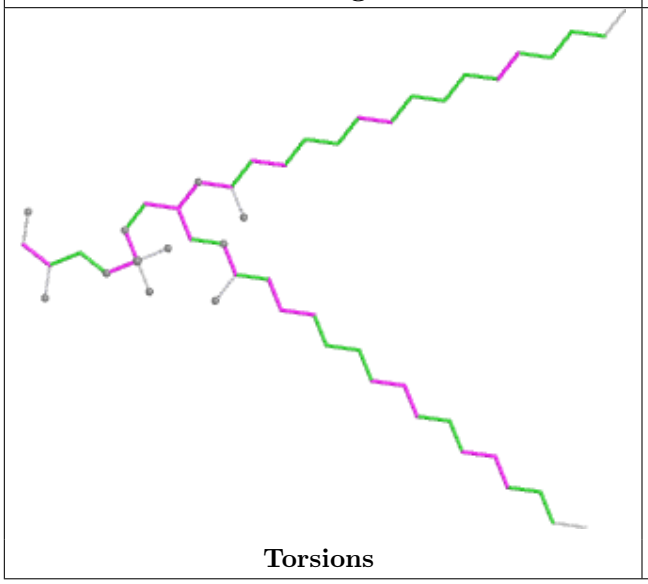
Ligand LHG H 401



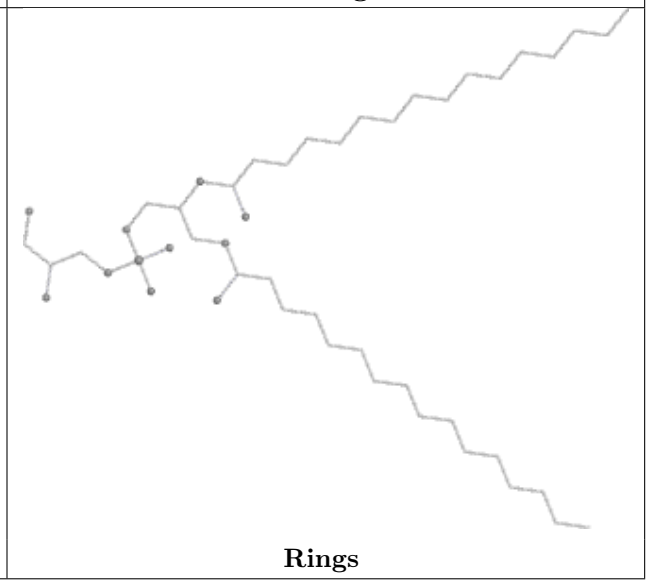
Bond lengths



Bond angles

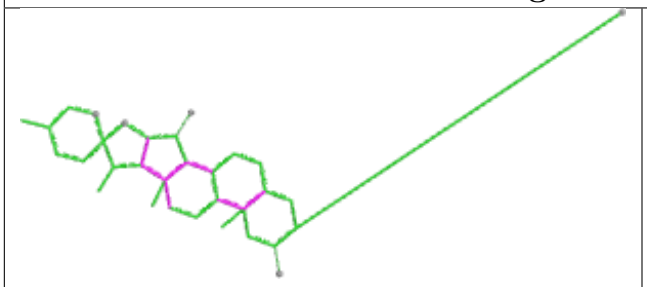


Torsions

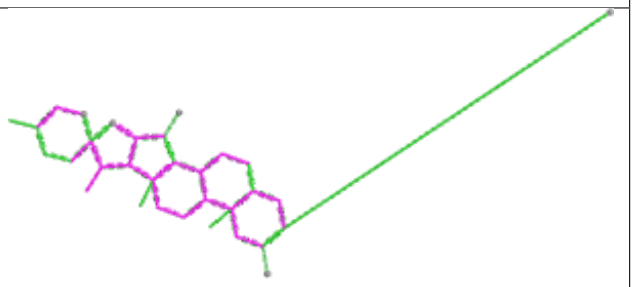


Rings

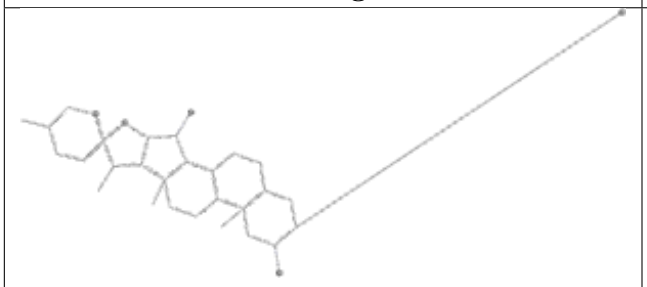
Ligand AJP F 715



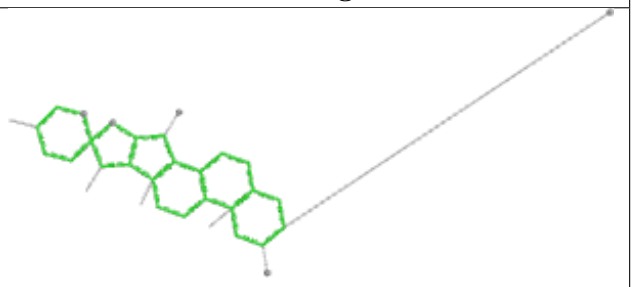
Bond lengths



Bond angles

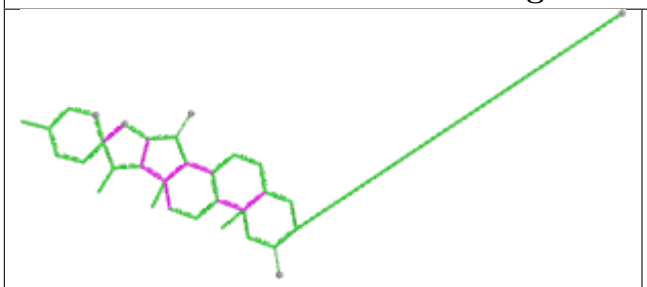


Torsions

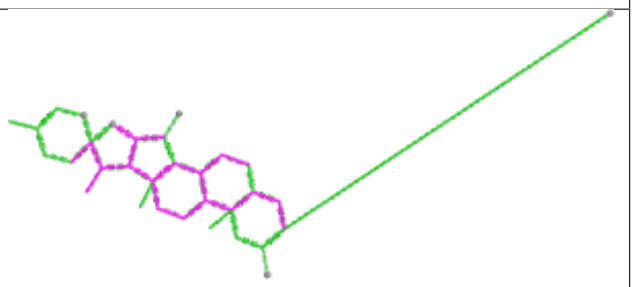


Rings

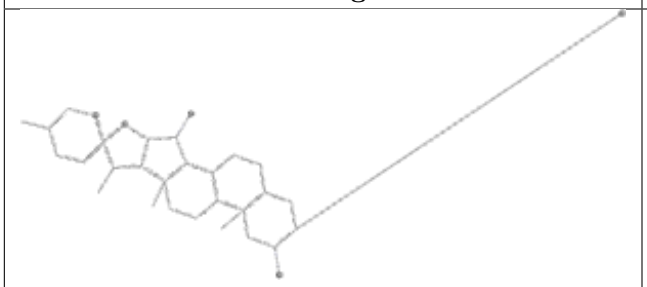
Ligand AJP D 609



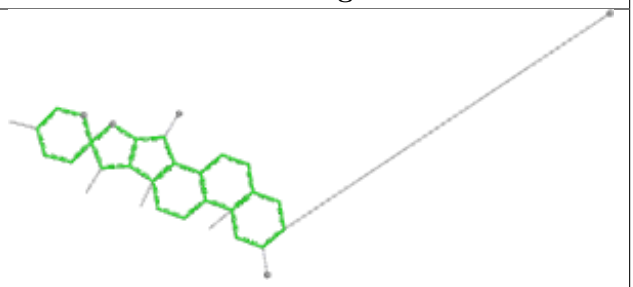
Bond lengths



Bond angles

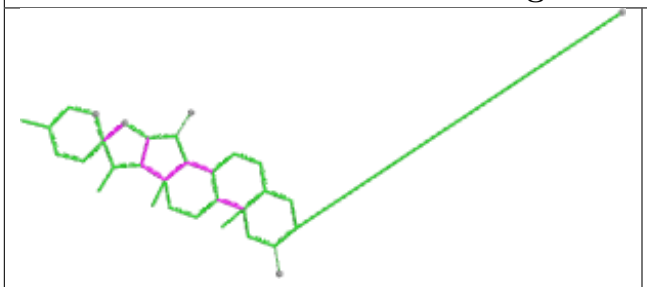


Torsions

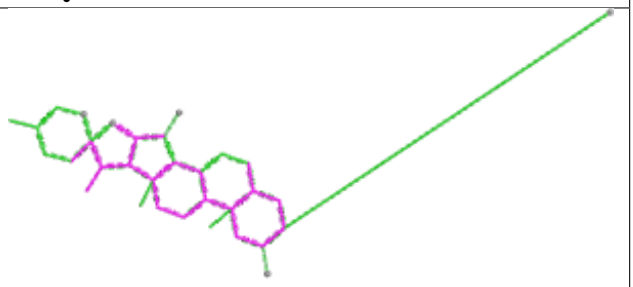


Rings

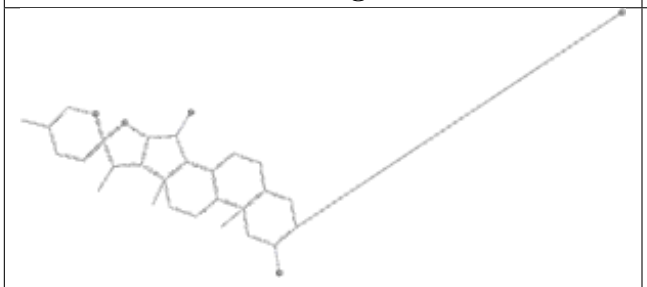
Ligand AJP Q 105



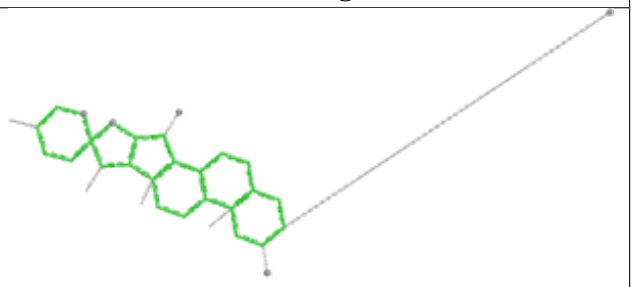
Bond lengths



Bond angles

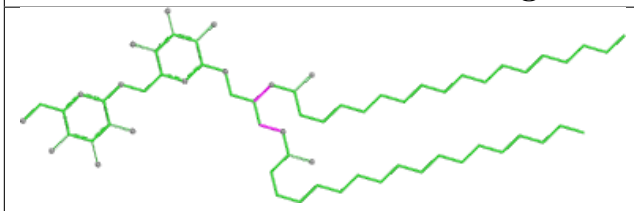


Torsions

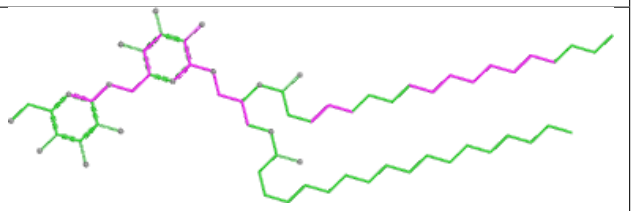


Rings

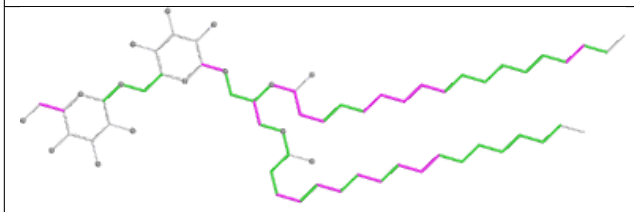
Ligand DGD A 403



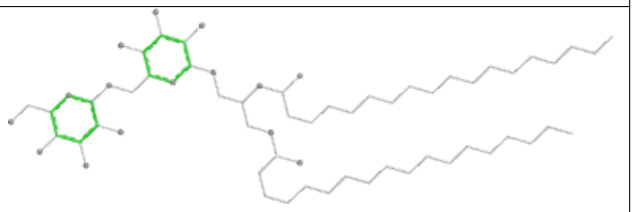
Bond lengths



Bond angles

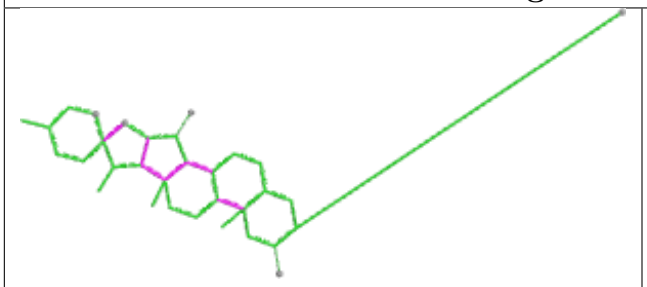


Torsions

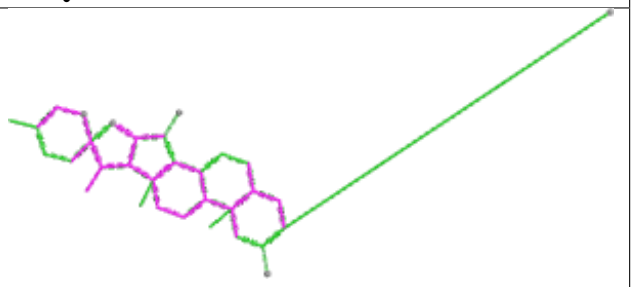


Rings

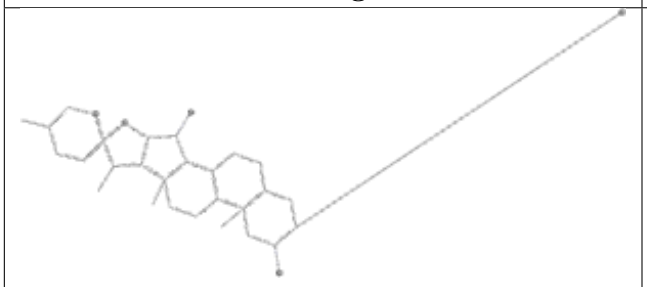
Ligand AJP Q 106



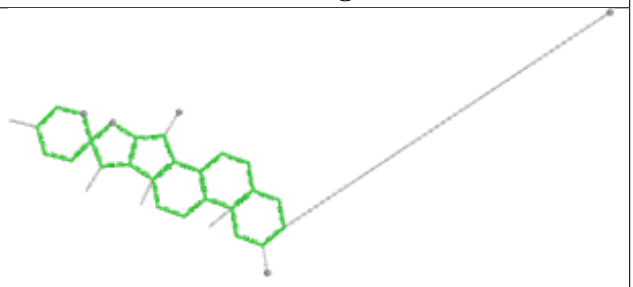
Bond lengths



Bond angles

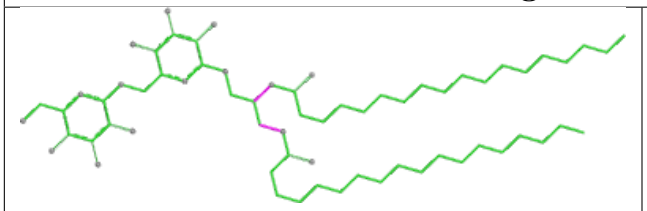


Torsions

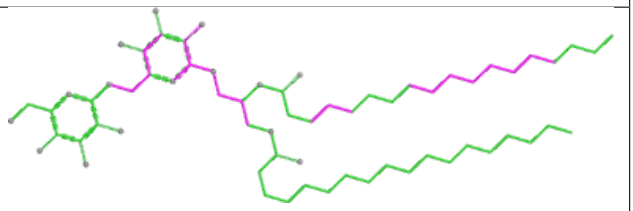


Rings

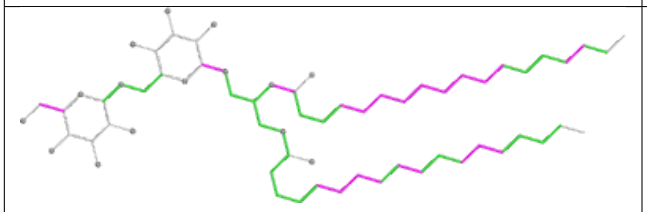
Ligand DGD A 404



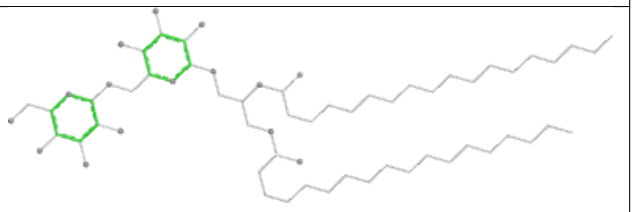
Bond lengths



Bond angles

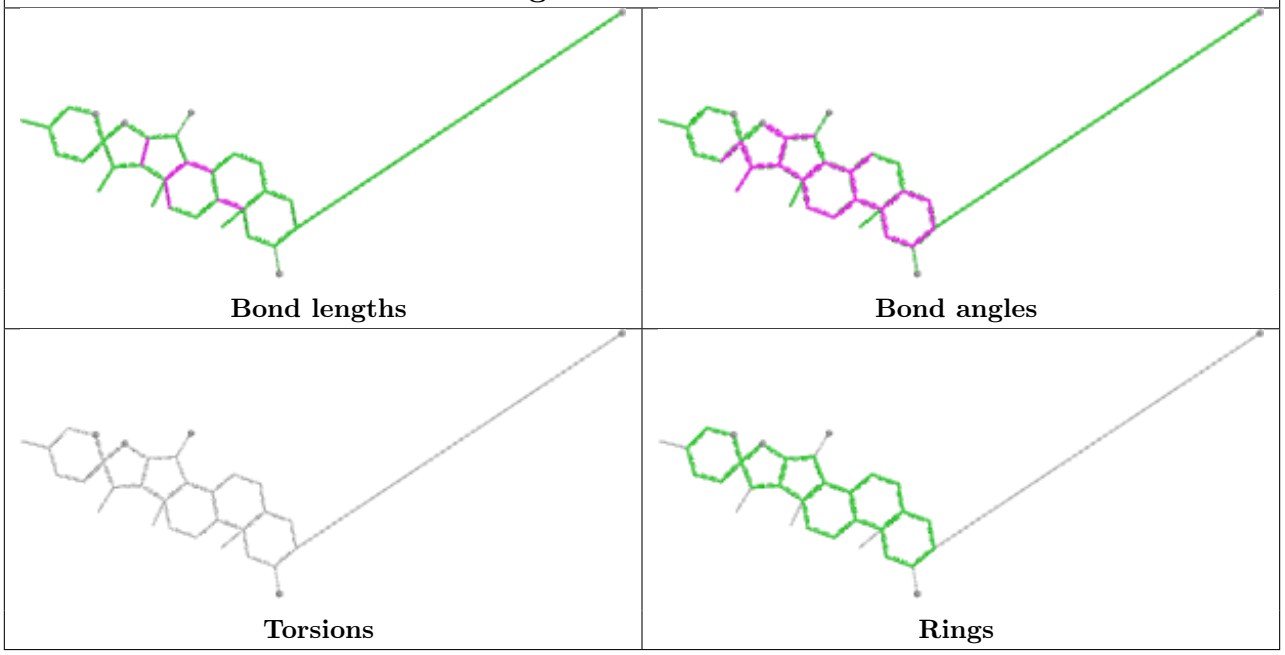


Torsions

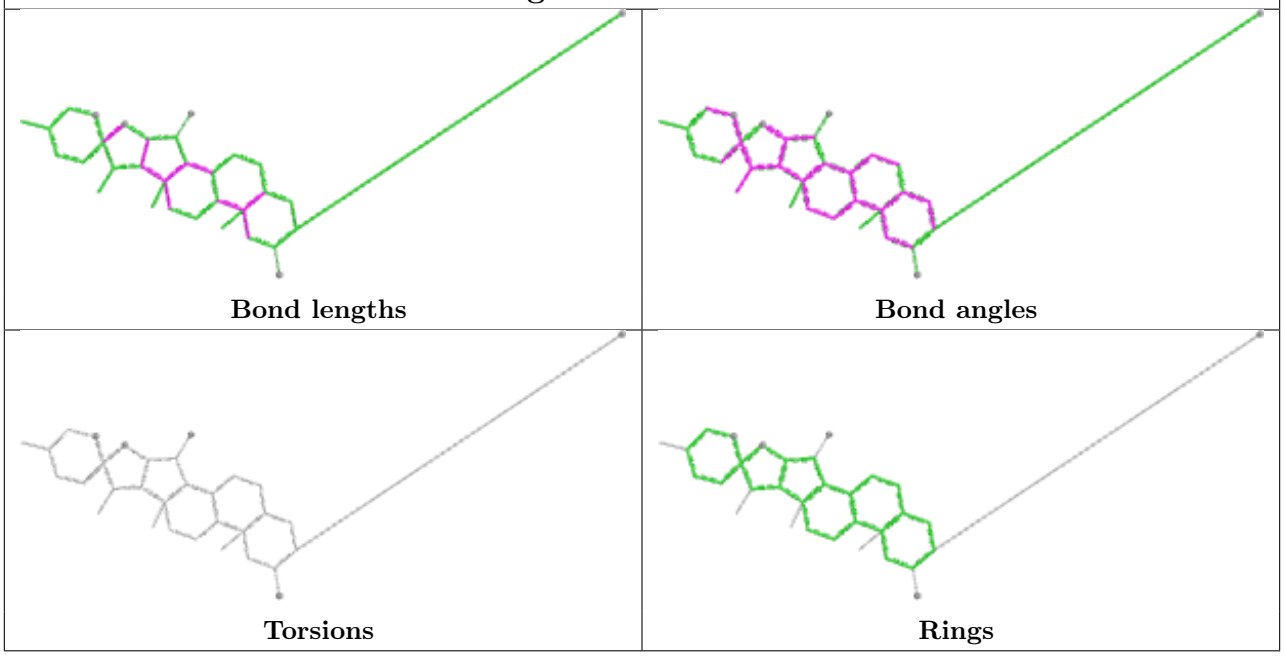


Rings

Ligand AJP F 718



Ligand AJP C 202



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.

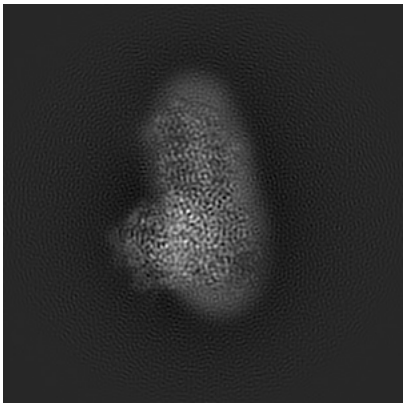
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-0849. These allow visual inspection of the internal detail of the map and identification of artifacts.

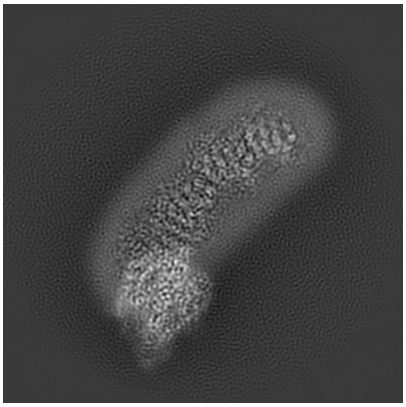
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

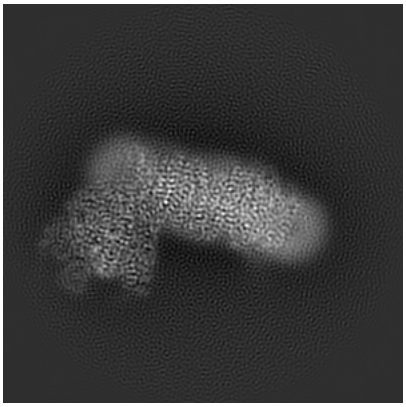
6.1.1 Primary map



X



Y

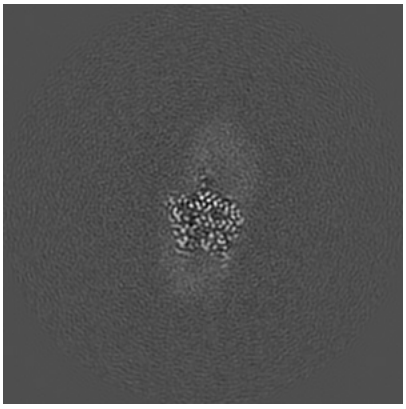


Z

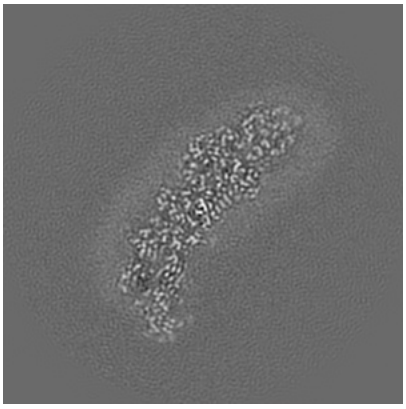
The images above show the map projected in three orthogonal directions.

6.2 Central slices

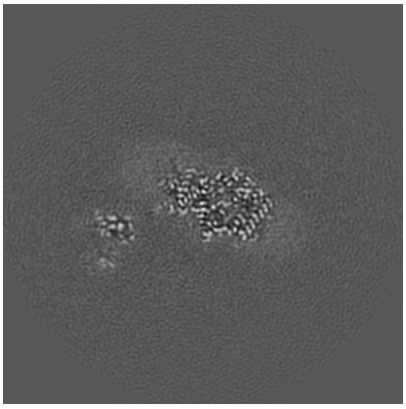
6.2.1 Primary map



X Index: 150



Y Index: 150

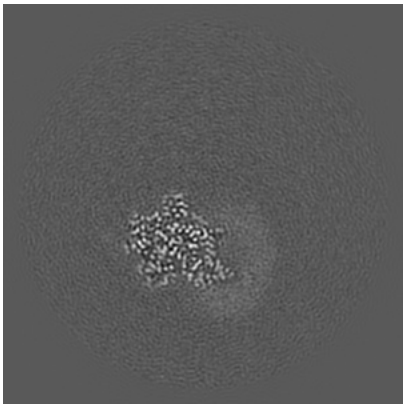


Z Index: 150

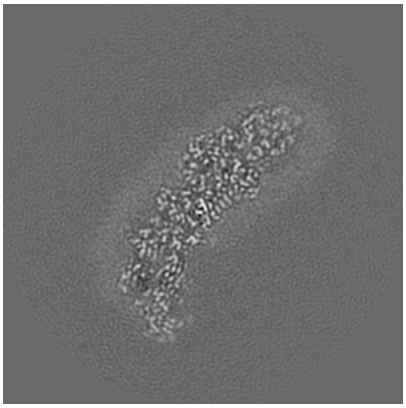
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

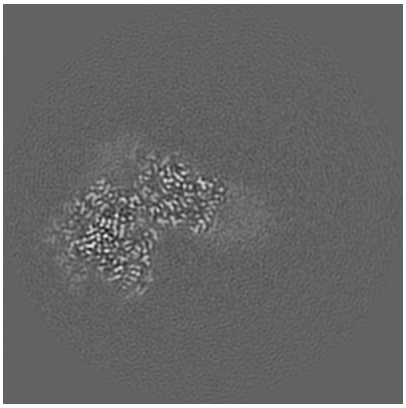
6.3.1 Primary map



X Index: 88



Y Index: 150

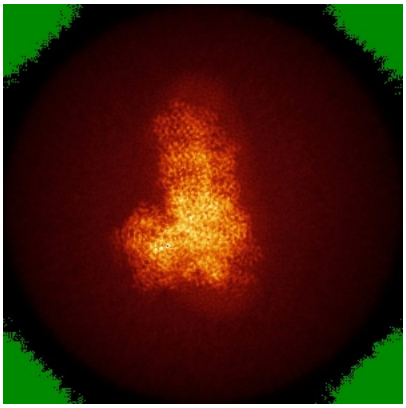


Z Index: 121

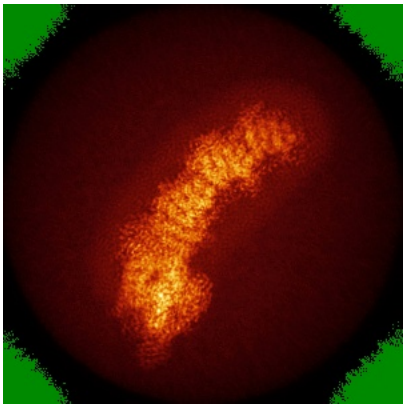
The images above show the largest variance slices of the map in three orthogonal directions.

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

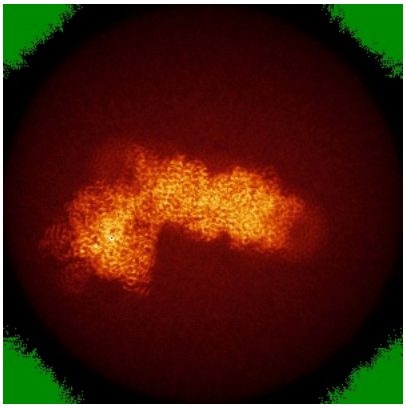
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.038. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

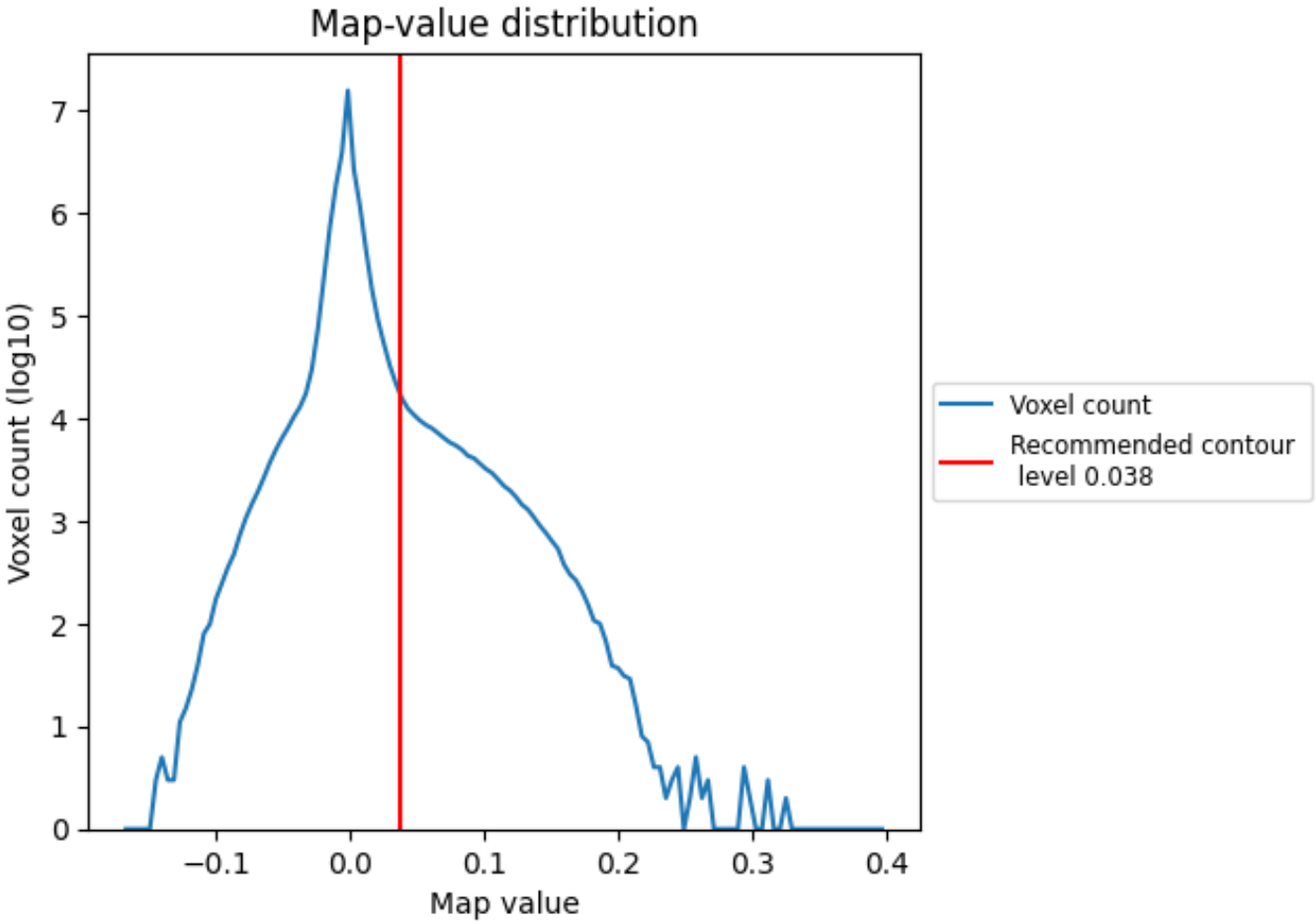
6.6 Mask visualisation (i)

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

7 Map analysis

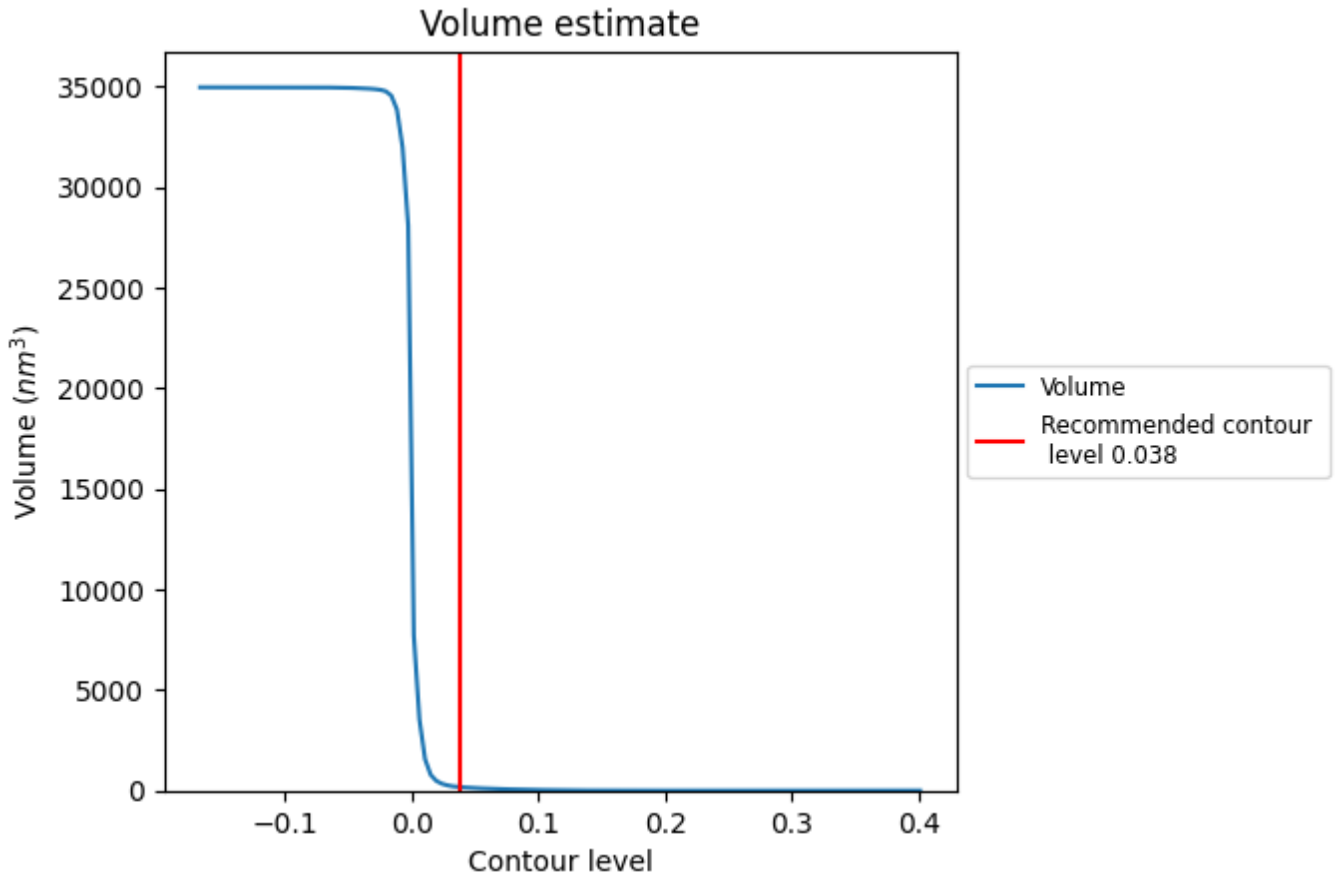
This section contains the results of statistical analysis of the map.

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.

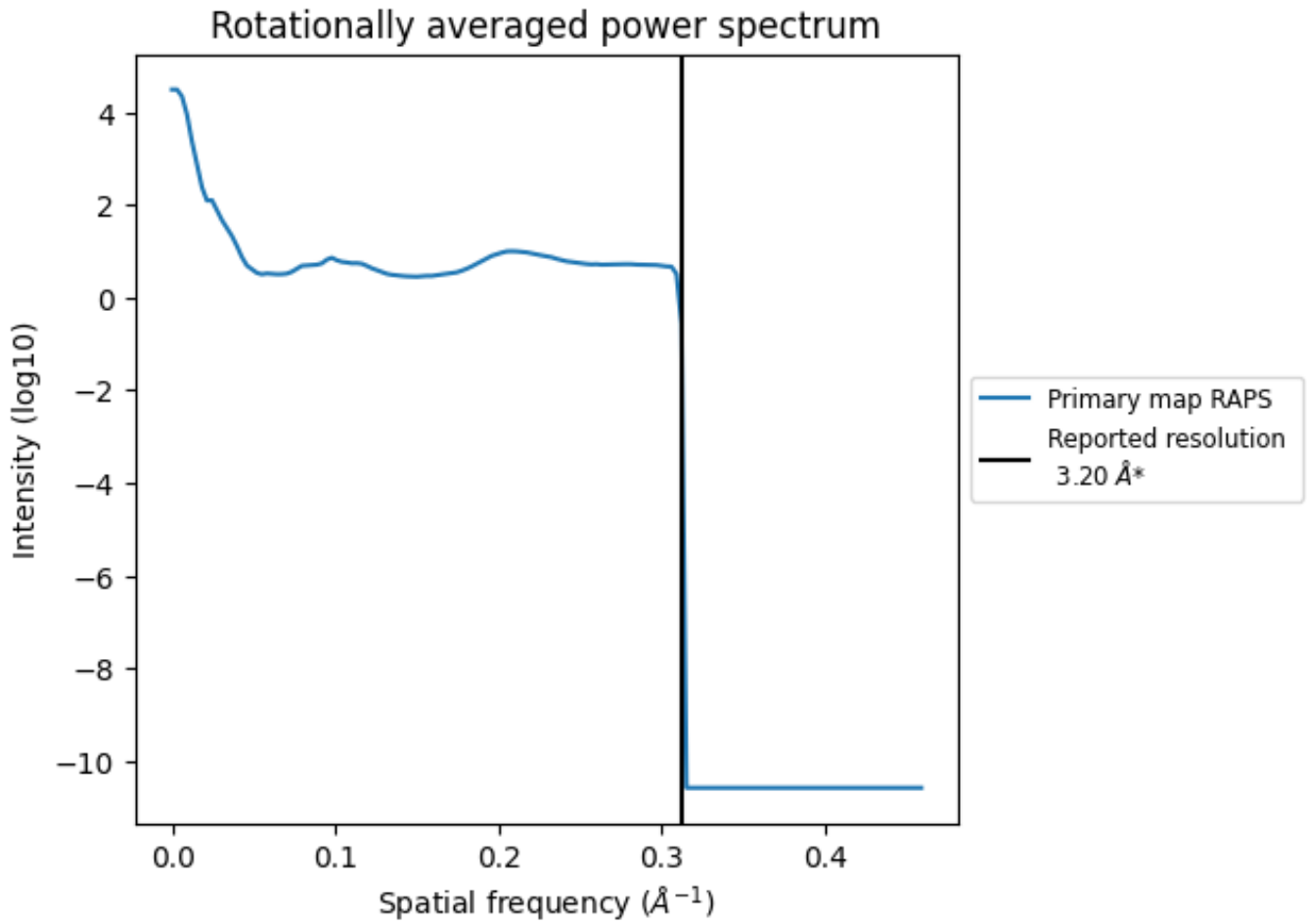
7.2 Volume estimate



The volume at the recommended contour level is 172 nm^3; this corresponds to an approximate mass of 155 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 0.312 Å^{-1}

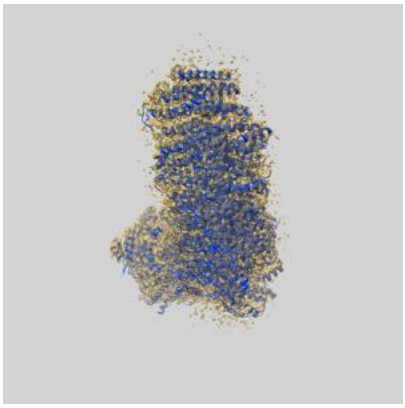
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

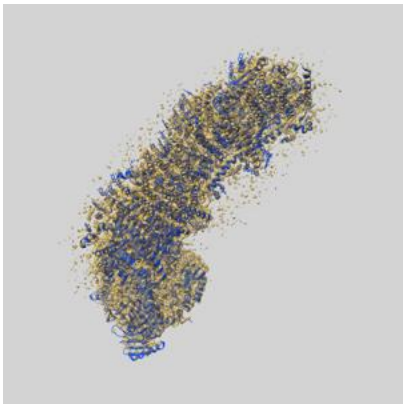
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-0849 and PDB model 6L7O. Per-residue inclusion information can be found in section 3 on page 17.

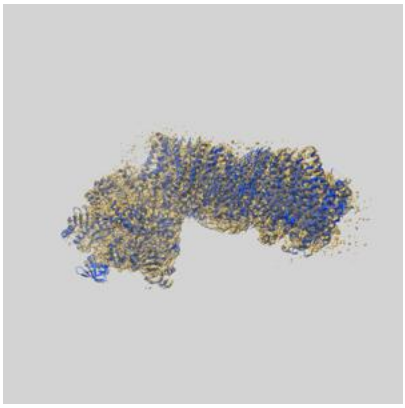
9.1 Map-model overlay



X



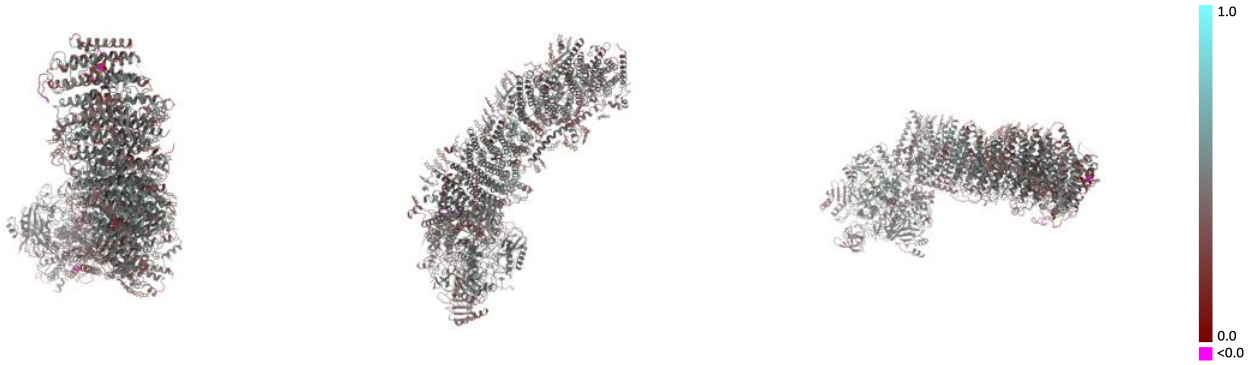
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.038 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.

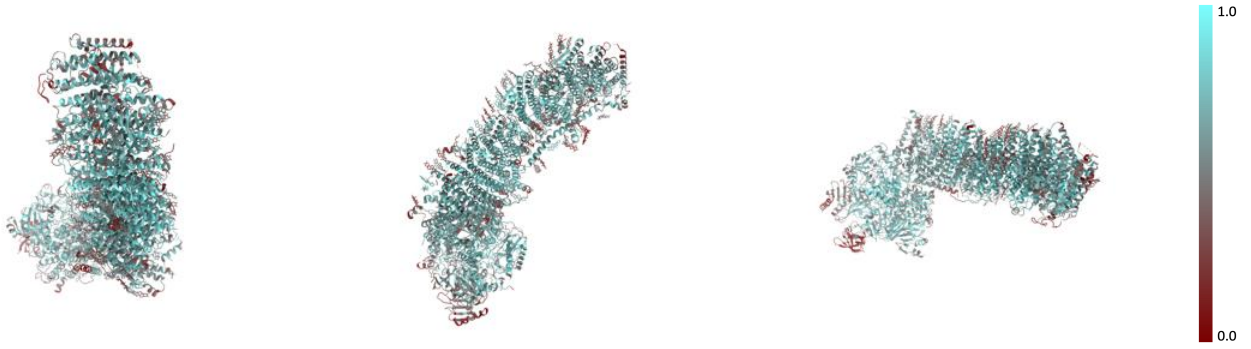
9.2 Q-score mapped to coordinate model



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.

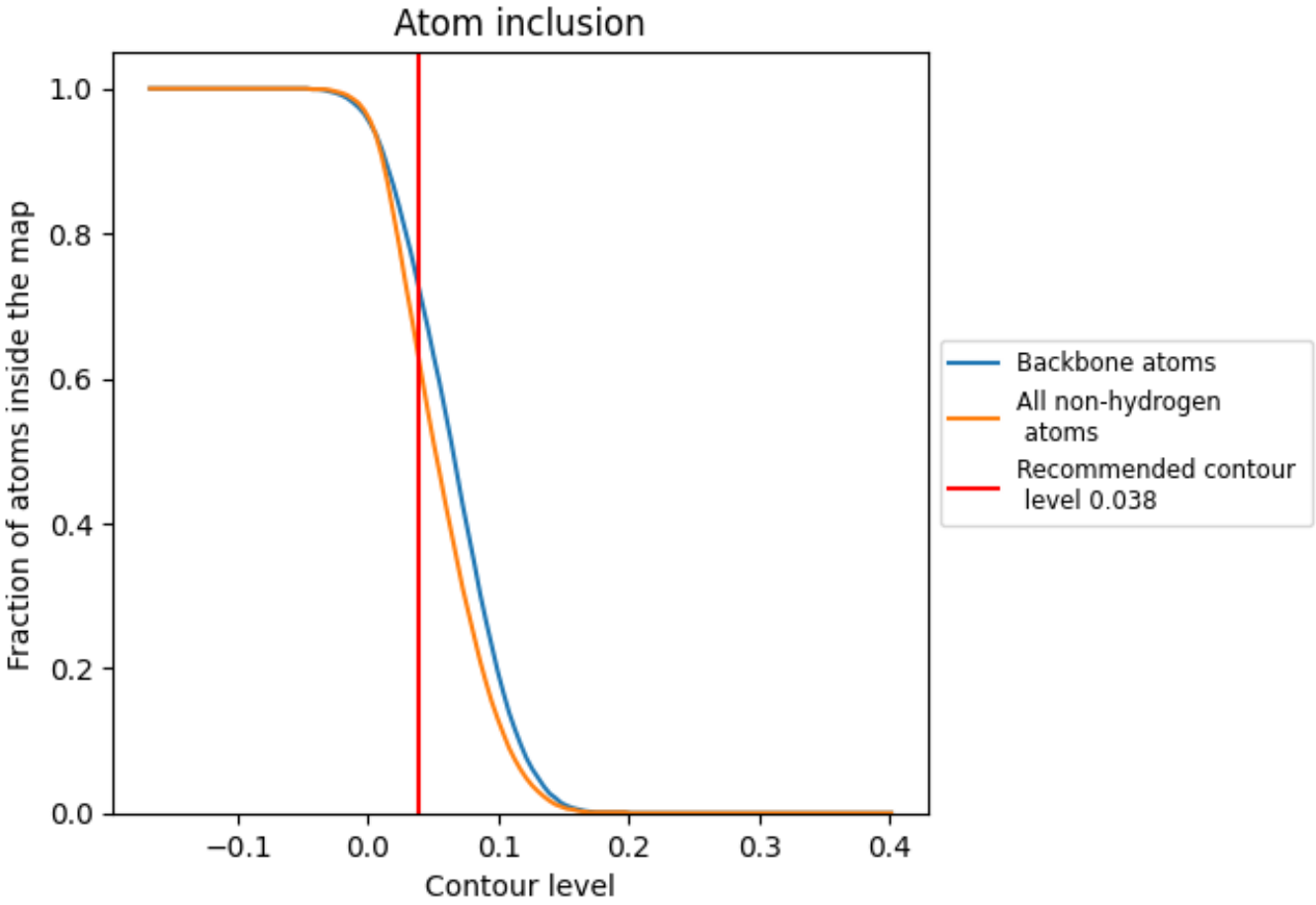
9.3 Atom inclusion mapped to coordinate model



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 (0.038).

9.4 Atom inclusion (i)



At the recommended contour level, 73% of all backbone atoms, 64% 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 (0.038) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6360	0.4330
A	0.6510	0.4290
B	0.6920	0.4540
C	0.6580	0.4240
D	0.7160	0.4480
E	0.7290	0.4560
F	0.6000	0.4130
G	0.6320	0.4350
H	0.6380	0.4150
I	0.6330	0.4280
J	0.6950	0.4530
K	0.7290	0.4760
L	0.6120	0.4340
M	0.6940	0.4610
N	0.6480	0.4380
O	0.6220	0.4420
P	0.6410	0.4420
Q	0.4630	0.3720
R	0.1930	0.3750
S	0.4230	0.4150
V	0.3120	0.3830