wwPDB EM Validation Summary Report

May 19, 2024 – 09:11 PM JST

PDB ID	:	6L7P
EMDB ID	:	EMD-0850
Title	:	cryo-EM structure of cyanobacteria NDH-1LdelV complex
Authors	:	Zhang, C.; Shuai, J.; Wu, J.; Lei, M.
Deposited on	:	2019-11-02
Resolution	:	3.60 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

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

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

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

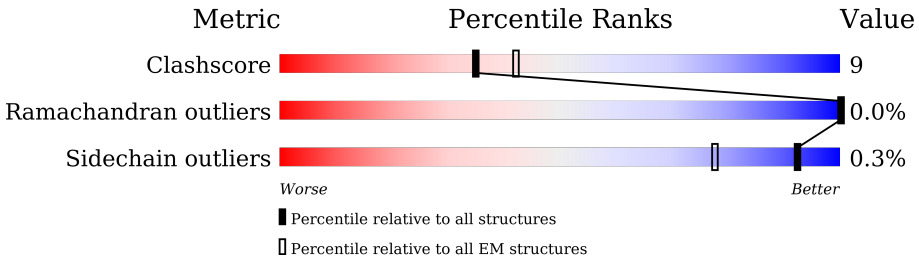
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	372	9% 87% 11% ·
2	B	515	· 83% 13% ·
3	C	132	16% 82% 10% 8%
4	D	529	· 83% 12% 5%
5	E	101	· 84% 16%
6	F	656	9% 87% 12% ·
7	G	200	8% 84% 12% ·
8	H	394	9% 84% 16%

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Mol	Chain	Length	Quality of chain
9	I	196	15% 87% 9%
10	J	168	7% 83% 10% 7%
11	K	237	8% 76% 8% 16%
12	L	76	11% 86% 11%
13	M	111	9% 93% 6%
14	N	150	8% 89% 9%
15	O	70	13% 90% 6%
16	P	44	9% 89% 5% 7%
17	Q	45	16% 82% 16%
18	S	110	15% 47% 50%

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
19	BCR	D	602	-	-	X	-
22	AJP	A	406	X	-	-	-
22	AJP	A	407	X	-	-	-
22	AJP	A	408	X	-	-	-
22	AJP	B	604	X	-	-	-
22	AJP	B	605	X	-	-	-
22	AJP	B	606	X	-	-	-
22	AJP	B	607	X	-	-	-
22	AJP	B	608	X	-	-	-
22	AJP	B	609	X	-	-	-
22	AJP	B	610	X	-	-	-
22	AJP	B	611	X	-	-	-
22	AJP	B	612	X	-	-	-
22	AJP	B	613	X	-	-	-
22	AJP	B	614	X	-	-	-
22	AJP	C	201	X	-	-	-
22	AJP	C	202	X	-	X	-
22	AJP	D	607	X	-	-	-
22	AJP	D	608	X	-	-	-
22	AJP	D	609	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	AJP	D	610	X	-	-	-
22	AJP	D	611	X	-	-	-
22	AJP	D	612	X	-	-	-
22	AJP	D	613	X	-	-	-
22	AJP	D	614	X	-	-	-
22	AJP	D	615	X	-	-	-
22	AJP	D	616	X	-	-	-
22	AJP	F	704	X	-	-	-
22	AJP	F	705	X	-	-	-
22	AJP	F	706	X	-	-	-
22	AJP	F	707	X	-	-	-
22	AJP	F	708	X	-	-	-
22	AJP	F	709	X	-	-	-
22	AJP	F	710	X	-	-	-
22	AJP	F	711	X	-	-	-
22	AJP	F	712	X	-	-	-
22	AJP	G	302	X	-	-	-
22	AJP	G	303	X	-	-	-
22	AJP	G	304	X	-	-	-
22	AJP	G	305	X	-	-	-
22	AJP	G	306	X	-	-	-
22	AJP	G	307	X	-	-	-
22	AJP	Q	101	X	-	-	-
22	AJP	Q	102	X	-	-	-
22	AJP	Q	103	X	-	-	-
25	SF4	I	202	-	-	X	-
25	SF4	K	301	-	-	X	-

2 Entry composition (i)

There are 25 unique types of molecules in this entry. The entry contains 32798 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	365	2820	1896	438	476	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	492	3723	2471	577	659	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	646	4997	3314	795	850	38	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	191	Total	C	N	O	S	0	0
			1454	969	228	253	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	189	Total	C	N	O	S	0	0
			1516	967	260	276	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	200	Total	C	N	O	S	0	0
			1550	996	269	272	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	67	Total	C	N	O	0	0
			533	346	90	97		

- 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		

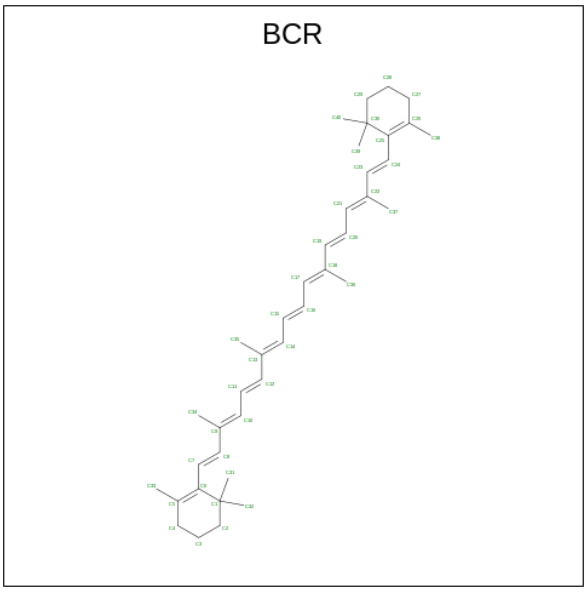
- Molecule 17 is a protein called NAD(P)H-quinone oxidoreductase subunit Q.

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 Tlr0636 protein.

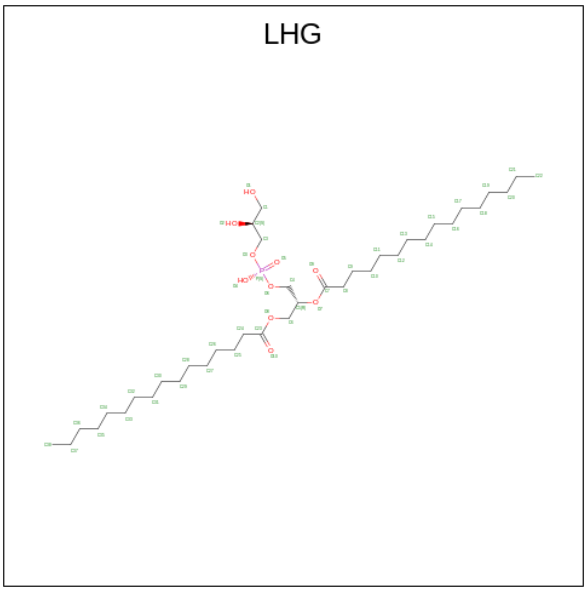
Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	55	Total	C	N	O	S	0	0
			432	280	69	82	1		

- Molecule 19 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



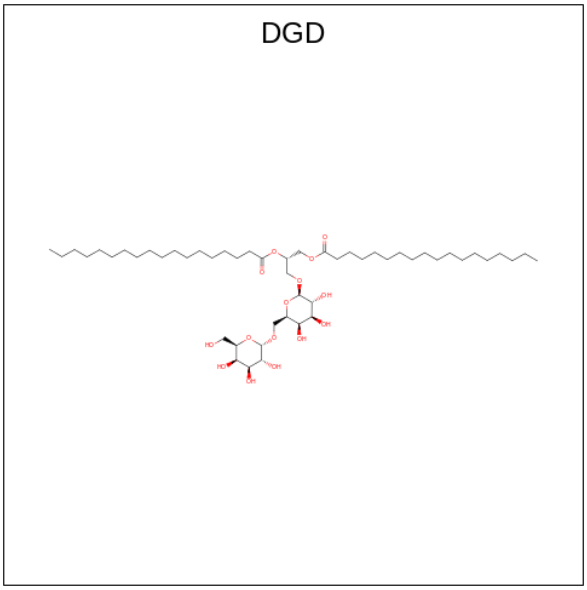
Mol	Chain	Residues	Atoms	AltConf
19	A	1	Total C 40 40	0
19	D	1	Total C 40 40	0
19	D	1	Total C 40 40	0

- Molecule 20 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



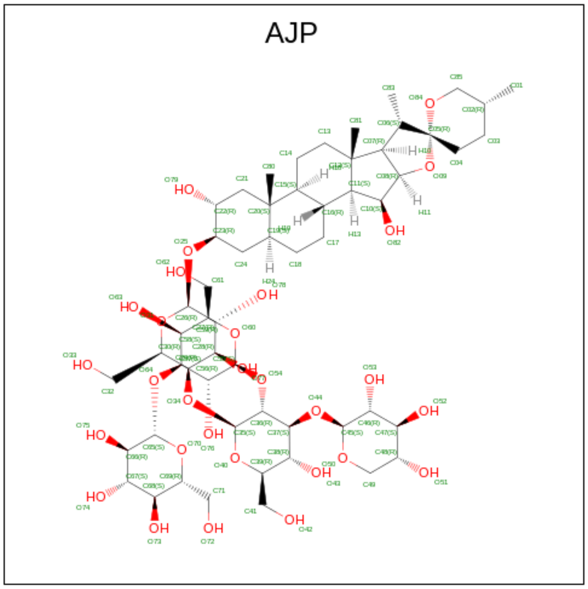
Mol	Chain	Residues	Atoms				AltConf
20	A	1	Total	C	O	P	0
			49	38	10	1	
20	A	1	Total	C	O	P	0
			49	38	10	1	
20	B	1	Total	C	O	P	0
			49	38	10	1	
20	B	1	Total	C	O	P	0
			49	38	10	1	
20	D	1	Total	C	O	P	0
			49	38	10	1	
20	D	1	Total	C	O	P	0
			49	38	10	1	
20	F	1	Total	C	O	P	0
			49	38	10	1	
20	F	1	Total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

- Molecule 21 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



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

- Molecule 22 is Digitonin (three-letter code: AJP) (formula: $C_{56}H_{92}O_{29}$).



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

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

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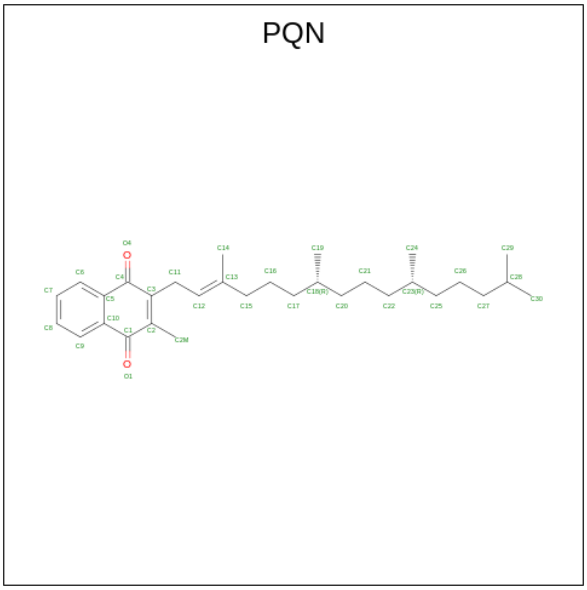
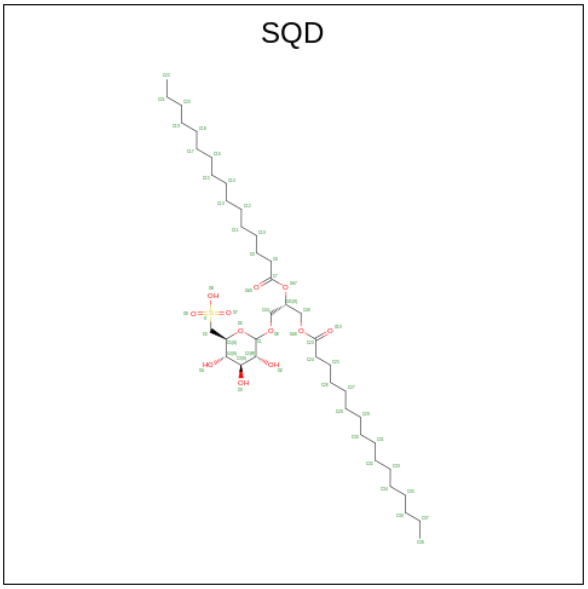
Mol	Chain	Residues	Atoms	AltConf
22	F	1	Total C O 32 27 5	0
22	G	1	Total C O 32 27 5	0
22	G	1	Total C O 32 27 5	0
22	G	1	Total C O 32 27 5	0
22	G	1	Total C O 32 27 5	0
22	G	1	Total C O 32 27 5	0
22	G	1	Total C O 32 27 5	0
22	Q	1	Total C O 32 27 5	0
22	Q	1	Total C O 32 27 5	0
22	Q	1	Total C O 32 27 5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

- Molecule 23 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).



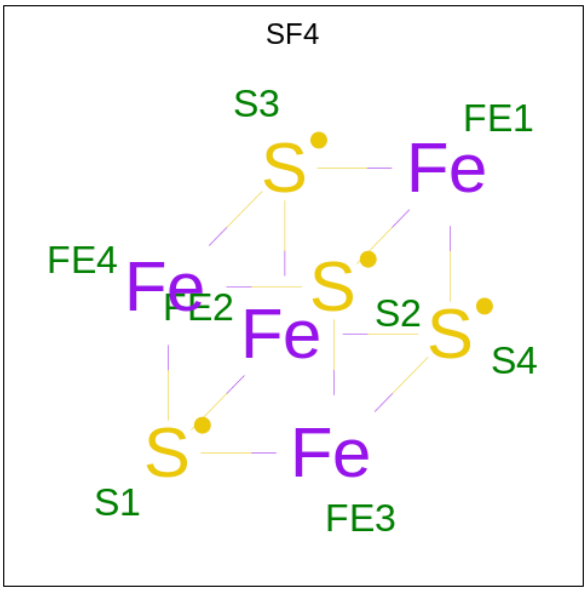
Mol	Chain	Residues	Atoms	AltConf
23	B	1	Total C O 33 31 2	0

- Molecule 24 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



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

- Molecule 25 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).

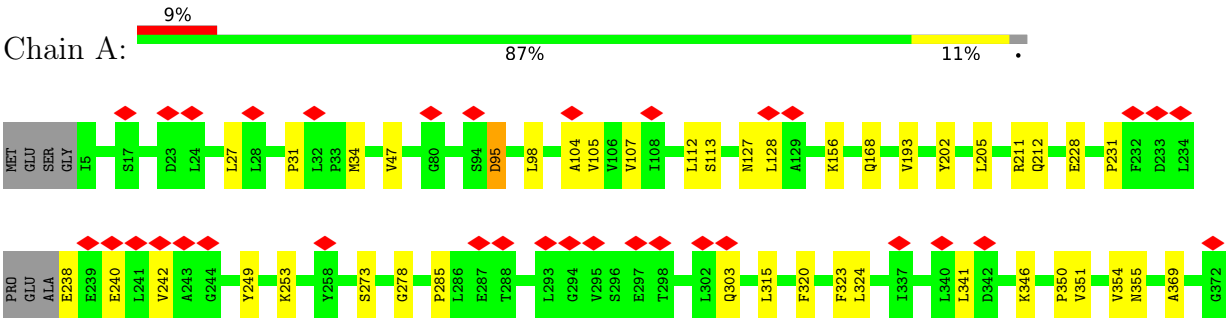


Mol	Chain	Residues	Atoms			AltConf
25	I	1	Total	Fe	S	0
			8	4	4	
25	I	1	Total	Fe	S	0
			8	4	4	
25	K	1	Total	Fe	S	0
			8	4	4	

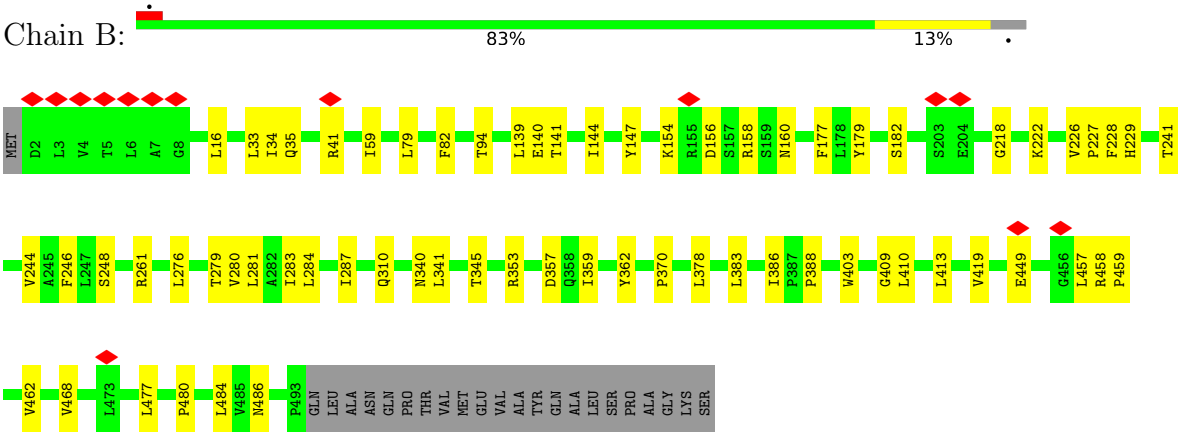
3 Residue-property plots (i)

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.

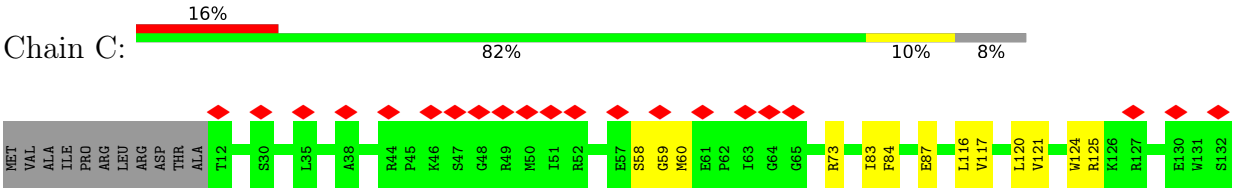
• Molecule 1: NAD(P)H-quinone oxidoreductase subunit 1



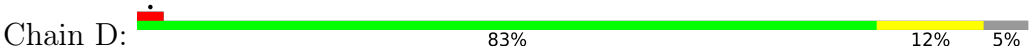
• Molecule 2: NAD(P)H-quinone oxidoreductase subunit 2

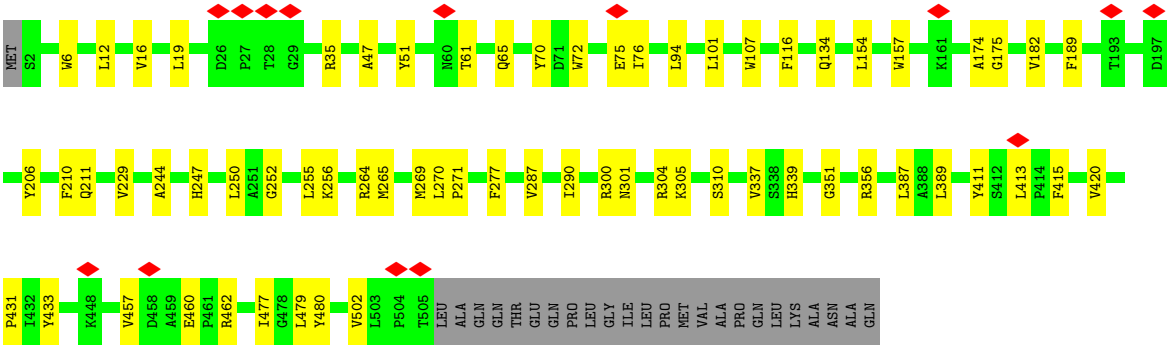


• Molecule 3: NAD(P)H-quinone oxidoreductase subunit 3

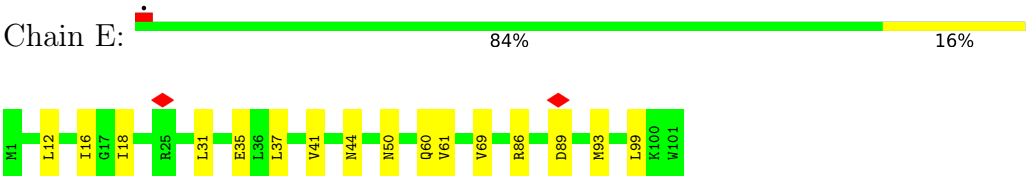


• Molecule 4: NAD(P)H-quinone oxidoreductase chain 4 1

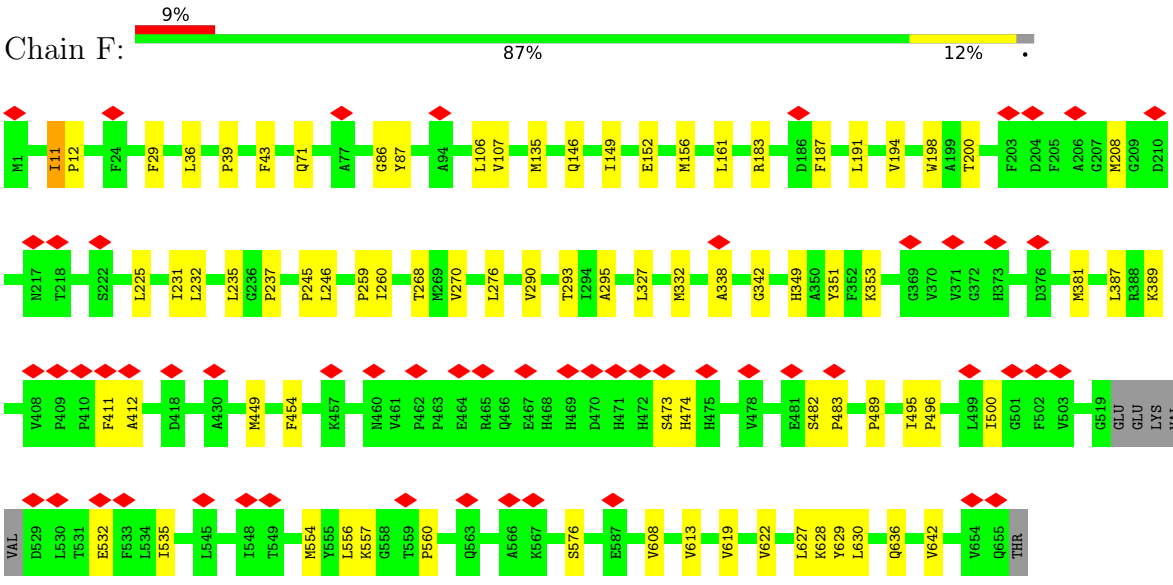




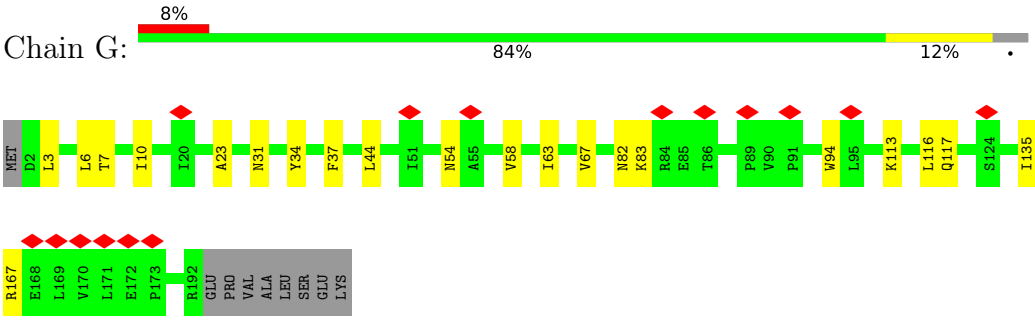
• Molecule 5: NAD(P)H-quinone oxidoreductase subunit 4L



• Molecule 6: NADH dehydrogenase subunit 5

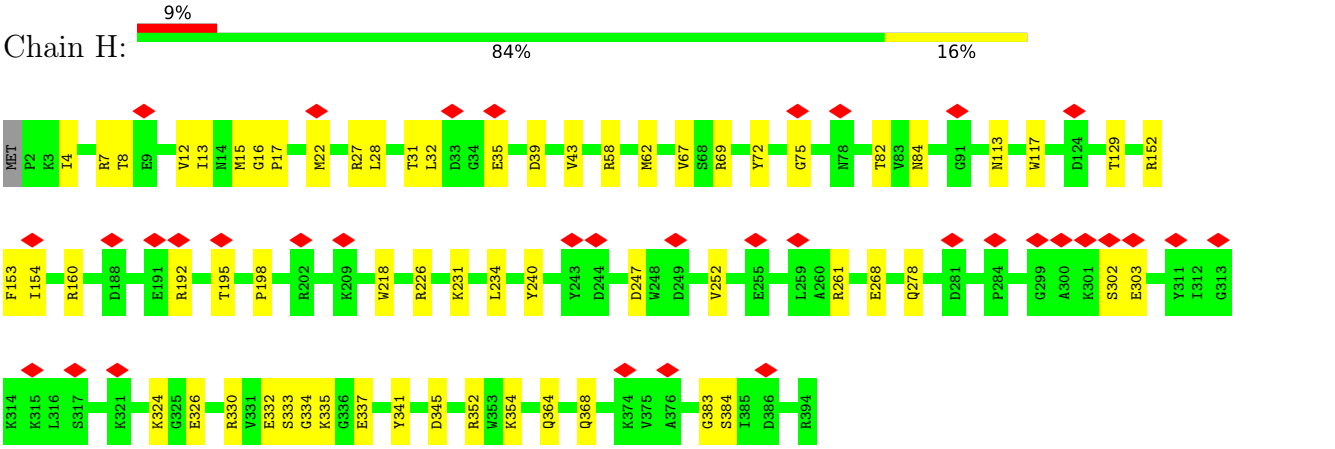


• Molecule 7: NADH-quinone oxidoreductase subunit J



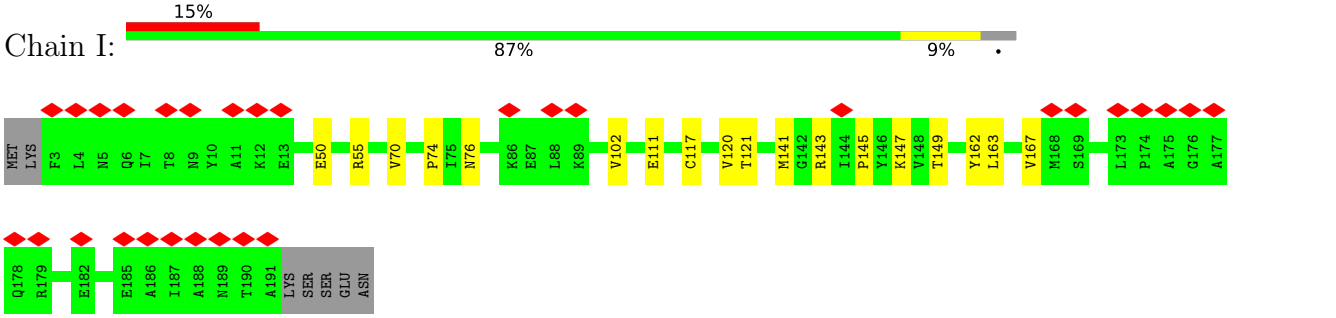
• Molecule 8: NAD(P)H-quinone oxidoreductase subunit H

Chain H:



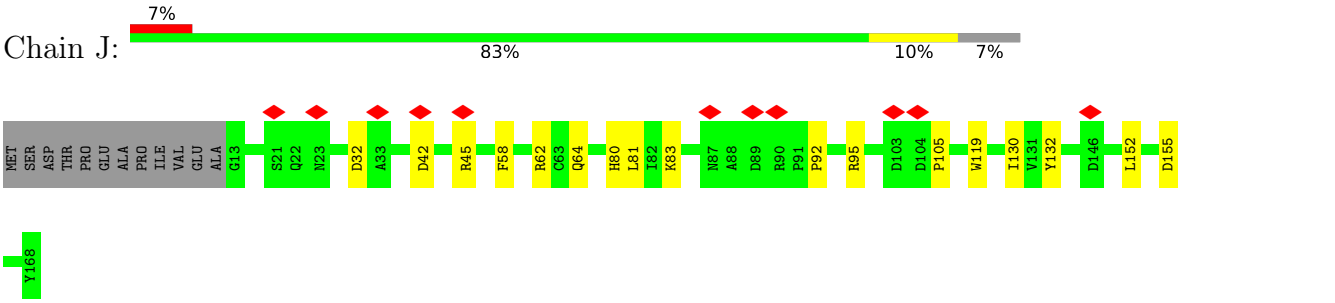
• Molecule 9: NAD(P)H-quinone oxidoreductase subunit I

Chain I:



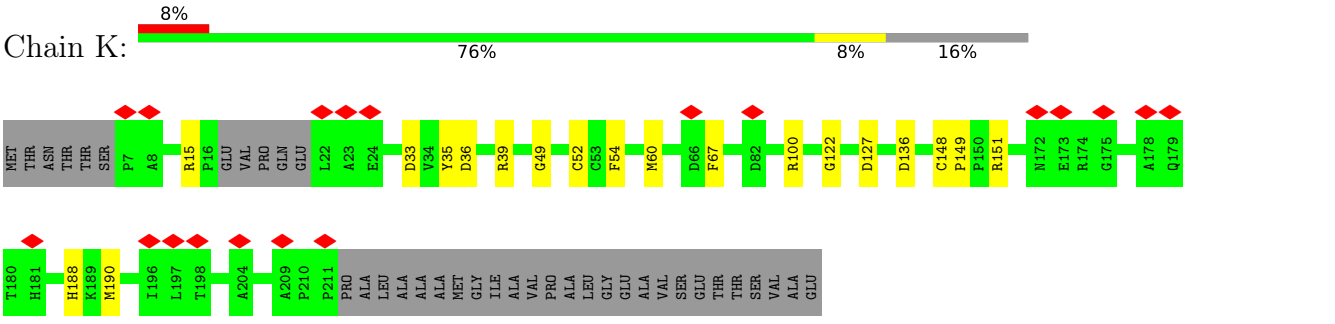
• Molecule 10: NAD(P)H-quinone oxidoreductase subunit J

Chain J:



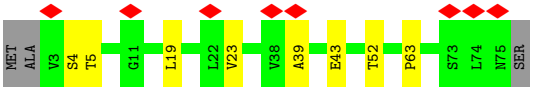
• Molecule 11: NAD(P)H-quinone oxidoreductase subunit K

Chain K:

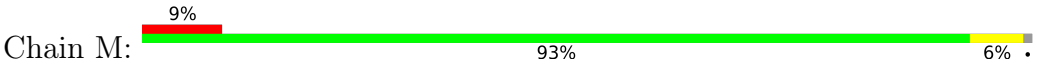


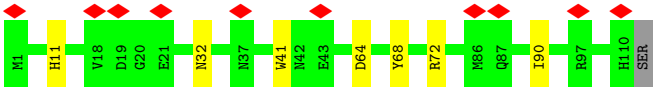
• Molecule 12: NAD(P)H-quinone oxidoreductase subunit L

Chain L:

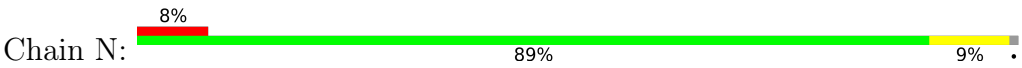


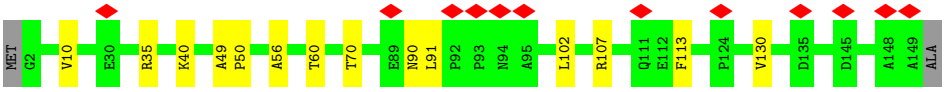
• Molecule 13: NAD(P)H-quinone oxidoreductase subunit M



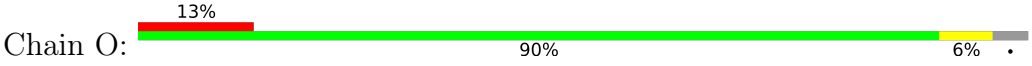


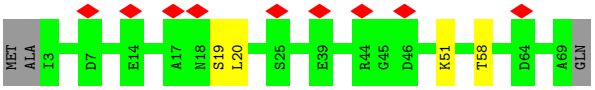
• Molecule 14: NAD(P)H-quinone oxidoreductase subunit N



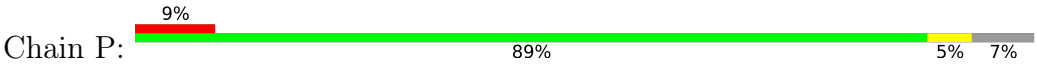


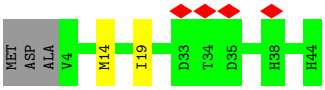
• Molecule 15: NAD(P)H-quinone oxidoreductase subunit O



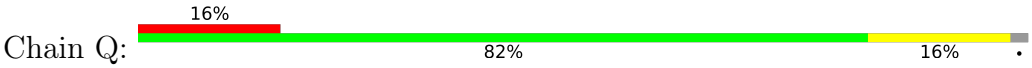


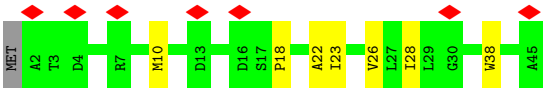
• Molecule 16: NAD(P)H-quinone oxidoreductase subunit P



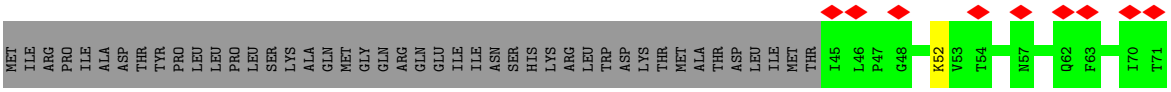


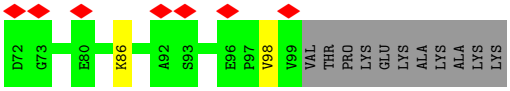
• Molecule 17: NAD(P)H-quinone oxidoreductase subunit Q





• Molecule 18: Tlr0636 protein




D72
G73
E80
K86
A92
S93
E96
P97
V98
V99
VAL
THR
PRO
LYS
GLU
LYS
ALA
LYS
ALA
LYS
LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	439946	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	0.529	Depositor
Minimum map value	-0.182	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.0403	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: BCR, PQN, AJP, DGD, LHG, SQD, 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	0.28	0/2891	0.54	2/3950 (0.1%)
2	B	0.28	0/3809	0.49	0/5197
3	C	0.30	0/1008	0.52	0/1375
4	D	0.28	0/4003	0.50	1/5464 (0.0%)
5	E	0.27	0/793	0.46	0/1077
6	F	0.28	0/5146	0.48	0/7010
7	G	0.27	0/1486	0.46	0/2038
8	H	0.26	0/3260	0.47	0/4417
9	I	0.26	0/1554	0.46	0/2108
10	J	0.24	0/1314	0.46	1/1789 (0.1%)
11	K	0.26	0/1589	0.48	0/2160
12	L	0.30	0/610	0.49	0/835
13	M	0.24	0/895	0.44	0/1214
14	N	0.25	0/1197	0.46	0/1628
15	O	0.24	0/545	0.45	0/741
16	P	0.34	0/330	0.56	0/448
17	Q	0.26	0/341	0.38	0/464
18	S	0.26	0/441	0.47	0/601
All	All	0.27	0/31212	0.48	4/42516 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
8	H	0	1
14	N	0	1
All	All	0	3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	128	LEU	CA-CB-CG	6.73	130.77	115.30
4	D	270	LEU	CA-CB-CG	5.83	128.72	115.30
1	A	112	LEU	CA-CB-CG	5.53	128.02	115.30
10	J	42	ASP	CB-CG-OD2	5.15	122.94	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	GLU	Peptide
8	H	129	THR	Peptide
14	N	91	LEU	Peptide

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	2820	0	2953	48	0
2	B	3723	0	3857	88	0
3	C	978	0	1008	43	0
4	D	3896	0	4040	75	0
5	E	783	0	837	15	0
6	F	4997	0	5026	69	0
7	G	1454	0	1540	43	0
8	H	3177	0	3157	42	0
9	I	1516	0	1484	14	0
10	J	1278	0	1233	11	0
11	K	1550	0	1588	16	0
12	L	590	0	603	5	0
13	M	879	0	860	4	0
14	N	1165	0	1176	8	0
15	O	533	0	544	2	0
16	P	321	0	317	3	0
17	Q	332	0	331	7	0
18	S	432	0	430	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	A	40	0	56	18	0
19	D	80	0	112	40	0
20	A	98	0	144	1	0
20	B	98	0	146	2	0
20	D	98	0	148	2	0
20	F	98	0	144	0	0
20	G	49	0	74	2	0
21	A	132	0	191	2	0
22	A	96	0	0	15	0
22	B	352	0	0	86	0
22	C	64	0	0	29	0
22	D	320	0	0	63	0
22	F	288	0	0	46	0
22	G	192	0	0	36	0
22	Q	96	0	0	11	0
23	B	33	0	46	1	0
24	D	108	0	156	10	0
24	F	54	0	78	2	0
24	L	54	0	78	1	0
25	I	16	0	0	2	0
25	K	8	0	0	3	0
All	All	32798	0	32357	565	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

The worst 5 of 565 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)
3:C:124:TRP:CZ3	22:C:202:AJP:C81	1.81	1.59
4:D:277:PHE:HE2	22:D:613:AJP:C81	1.08	1.57
2:B:287:ILE:CD1	22:B:614:AJP:C83	1.83	1.52
4:D:277:PHE:CE2	22:D:613:AJP:C81	1.93	1.51
1:A:323:PHE:CE2	19:A:401:BCR:H20C	1.45	1.50

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	361/372 (97%)	335 (93%)	26 (7%)	0	100	100
2	B	490/515 (95%)	470 (96%)	20 (4%)	0	100	100
3	C	119/132 (90%)	108 (91%)	11 (9%)	0	100	100
4	D	502/529 (95%)	475 (95%)	27 (5%)	0	100	100
5	E	99/101 (98%)	91 (92%)	8 (8%)	0	100	100
6	F	642/656 (98%)	605 (94%)	37 (6%)	0	100	100
7	G	189/200 (94%)	182 (96%)	7 (4%)	0	100	100
8	H	391/394 (99%)	356 (91%)	34 (9%)	1 (0%)	41	75
9	I	187/196 (95%)	175 (94%)	12 (6%)	0	100	100
10	J	154/168 (92%)	140 (91%)	14 (9%)	0	100	100
11	K	196/237 (83%)	182 (93%)	14 (7%)	0	100	100
12	L	71/76 (93%)	65 (92%)	6 (8%)	0	100	100
13	M	108/111 (97%)	98 (91%)	10 (9%)	0	100	100
14	N	146/150 (97%)	136 (93%)	10 (7%)	0	100	100
15	O	65/70 (93%)	55 (85%)	10 (15%)	0	100	100
16	P	39/44 (89%)	31 (80%)	8 (20%)	0	100	100
17	Q	42/45 (93%)	41 (98%)	1 (2%)	0	100	100
18	S	53/110 (48%)	53 (100%)	0	0	100	100
All	All	3854/4106 (94%)	3598 (93%)	255 (7%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	198	PRO

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	297/302 (98%)	296 (100%)	1 (0%)	92 97
2	B	395/413 (96%)	395 (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
6	F	518/527 (98%)	515 (99%)	3 (1%)	86 94
7	G	158/166 (95%)	158 (100%)	0	100 100
8	H	337/338 (100%)	336 (100%)	1 (0%)	92 97
9	I	165/172 (96%)	165 (100%)	0	100 100
10	J	138/148 (93%)	136 (99%)	2 (1%)	67 85
11	K	169/196 (86%)	169 (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%)	117 (98%)	2 (2%)	60 82
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	S	48/97 (50%)	48 (100%)	0	100 100
All	All	3209/3381 (95%)	3200 (100%)	9 (0%)	92 97

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	N	70	THR
14	N	107	ARG
6	F	628	LYS
8	H	8	THR
10	J	45	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
8	H	156	ASN
9	I	76	ASN
15	O	49	GLN
8	H	278	GLN
10	J	64	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

66 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	$\#\|Z\| > 2$
22	AJP	D	615	-	37,37,95	1.24	6 (16%)	58,62,149	2.24	16 (27%)
22	AJP	B	608	-	37,37,95	1.27	8 (21%)	58,62,149	2.20	17 (29%)
25	SF4	I	201	9	0,12,12	-	-	-		
20	LHG	F	702	-	48,48,48	0.57	0	51,54,54	1.25	6 (11%)
20	LHG	B	603	-	48,48,48	0.61	1 (2%)	51,54,54	1.24	6 (11%)
22	AJP	D	609	-	37,37,95	1.25	6 (16%)	58,62,149	2.19	18 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	LHG	G	301	-	48,48,48	0.61	1 (2%)	51,54,54	1.24	6 (11%)
22	AJP	B	604	-	37,37,95	1.50	7 (18%)	58,62,149	2.38	19 (32%)
22	AJP	B	609	-	37,37,95	1.44	9 (24%)	58,62,149	2.40	19 (32%)
22	AJP	A	406	-	37,37,95	1.34	6 (16%)	58,62,149	2.22	16 (27%)
22	AJP	D	608	-	37,37,95	1.51	7 (18%)	58,62,149	2.46	21 (36%)
22	AJP	F	707	-	37,37,95	1.31	6 (16%)	58,62,149	2.21	19 (32%)
22	AJP	F	709	-	37,37,95	1.30	7 (18%)	58,62,149	2.24	17 (29%)
22	AJP	Q	103	-	37,37,95	1.29	6 (16%)	58,62,149	2.25	18 (31%)
22	AJP	G	306	-	37,37,95	1.27	8 (21%)	58,62,149	2.20	17 (29%)
24	SQD	D	606	-	53,54,54	0.94	5 (9%)	62,65,65	1.53	11 (17%)
20	LHG	F	701	-	48,48,48	0.58	0	51,54,54	1.24	6 (11%)
22	AJP	B	606	-	37,37,95	1.16	7 (18%)	58,62,149	2.12	16 (27%)
22	AJP	D	607	-	37,37,95	1.55	7 (18%)	58,62,149	2.27	20 (34%)
22	AJP	D	614	-	37,37,95	1.43	7 (18%)	58,62,149	2.25	21 (36%)
22	AJP	B	610	-	37,37,95	1.29	7 (18%)	58,62,149	2.32	18 (31%)
22	AJP	Q	102	-	37,37,95	1.48	7 (18%)	58,62,149	2.37	18 (31%)
22	AJP	G	303	-	37,37,95	1.27	7 (18%)	58,62,149	2.22	18 (31%)
22	AJP	D	616	-	37,37,95	1.27	5 (13%)	58,62,149	2.23	17 (29%)
22	AJP	C	201	-	37,37,95	1.29	7 (18%)	58,62,149	2.19	16 (27%)
22	AJP	F	708	-	37,37,95	1.33	4 (10%)	58,62,149	2.33	21 (36%)
22	AJP	D	610	-	37,37,95	1.37	6 (16%)	58,62,149	2.22	18 (31%)
22	AJP	Q	101	-	37,37,95	1.23	6 (16%)	58,62,149	2.15	16 (27%)
23	PQN	B	601	-	34,34,34	2.85	9 (26%)	42,45,45	1.98	5 (11%)
25	SF4	I	202	9	0,12,12	-	-	-		
22	AJP	F	710	-	37,37,95	1.18	6 (16%)	58,62,149	2.11	16 (27%)
22	AJP	D	612	-	37,37,95	1.30	6 (16%)	58,62,149	2.29	19 (32%)
24	SQD	L	101	-	53,54,54	0.95	5 (9%)	62,65,65	1.56	10 (16%)
24	SQD	D	605	-	53,54,54	0.95	5 (9%)	62,65,65	1.52	11 (17%)
22	AJP	C	202	-	37,37,95	1.37	8 (21%)	58,62,149	2.21	17 (29%)
25	SF4	K	301	11	0,12,12	-	-	-		
22	AJP	G	305	-	37,37,95	1.34	8 (21%)	58,62,149	2.21	19 (32%)
22	AJP	B	607	-	37,37,95	1.27	7 (18%)	58,62,149	2.26	17 (29%)
22	AJP	G	307	-	37,37,95	1.39	7 (18%)	58,62,149	2.23	20 (34%)
22	AJP	A	407	-	37,37,95	1.27	3 (8%)	58,62,149	2.26	19 (32%)
22	AJP	F	711	-	37,37,95	1.35	7 (18%)	58,62,149	2.24	18 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	AJP	B	614	-	37,37,95	1.33	7 (18%)	58,62,149	2.23	18 (31%)
22	AJP	D	613	-	37,37,95	1.36	7 (18%)	58,62,149	2.34	13 (22%)
22	AJP	F	712	-	37,37,95	1.37	8 (21%)	58,62,149	2.25	18 (31%)
22	AJP	G	302	-	37,37,95	1.52	7 (18%)	58,62,149	2.31	20 (34%)
20	LHG	B	602	-	48,48,48	0.61	0	51,54,54	1.25	6 (11%)
22	AJP	D	611	-	37,37,95	1.26	5 (13%)	58,62,149	2.30	17 (29%)
21	DGD	A	404	-	67,67,67	0.89	2 (2%)	81,81,81	1.39	11 (13%)
19	BCR	A	401	-	41,41,41	1.74	8 (19%)	56,56,56	1.60	10 (17%)
22	AJP	B	612	-	37,37,95	1.18	6 (16%)	58,62,149	2.12	16 (27%)
22	AJP	F	705	-	37,37,95	1.39	8 (21%)	58,62,149	2.19	18 (31%)
19	BCR	D	601	-	41,41,41	1.69	8 (19%)	56,56,56	1.65	12 (21%)
24	SQD	F	703	-	53,54,54	0.95	5 (9%)	62,65,65	1.56	12 (19%)
22	AJP	F	706	-	37,37,95	1.33	7 (18%)	58,62,149	2.23	19 (32%)
21	DGD	A	405	-	67,67,67	0.91	3 (4%)	81,81,81	1.42	12 (14%)
20	LHG	A	402	-	48,48,48	0.58	0	51,54,54	1.24	6 (11%)
22	AJP	B	605	-	37,37,95	1.28	5 (13%)	58,62,149	2.16	17 (29%)
19	BCR	D	602	-	41,41,41	1.72	8 (19%)	56,56,56	1.67	11 (19%)
20	LHG	D	603	-	48,48,48	0.62	1 (2%)	51,54,54	1.26	6 (11%)
22	AJP	B	611	-	37,37,95	1.32	7 (18%)	58,62,149	2.17	19 (32%)
20	LHG	A	403	-	48,48,48	0.62	1 (2%)	51,54,54	1.25	5 (9%)
22	AJP	F	704	-	37,37,95	1.30	6 (16%)	58,62,149	2.16	19 (32%)
22	AJP	G	304	-	37,37,95	1.29	8 (21%)	58,62,149	2.42	17 (29%)
22	AJP	A	408	-	37,37,95	1.25	6 (16%)	58,62,149	2.25	17 (29%)
20	LHG	D	604	-	48,48,48	0.61	1 (2%)	51,54,54	1.26	6 (11%)
22	AJP	B	613	-	37,37,95	1.16	5 (13%)	58,62,149	2.14	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
22	AJP	D	615	-	12/12/14/38	-	0/6/6/11
22	AJP	B	608	-	12/12/14/38	-	0/6/6/11
25	SF4	I	201	9	-	-	0/6/5/5
20	LHG	F	702	-	-	21/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	LHG	B	603	-	-	20/53/53/53	-
22	AJP	D	609	-	12/12/14/38	-	0/6/6/11
22	AJP	B	604	-	12/12/14/38	-	0/6/6/11
22	AJP	B	609	-	12/12/14/38	-	0/6/6/11
22	AJP	D	608	-	12/12/14/38	-	0/6/6/11
22	AJP	A	406	-	12/12/14/38	-	0/6/6/11
22	AJP	F	707	-	12/12/14/38	-	0/6/6/11
22	AJP	F	709	-	12/12/14/38	-	0/6/6/11
22	AJP	Q	103	-	12/12/14/38	-	0/6/6/11
20	LHG	G	301	-	-	22/53/53/53	-
22	AJP	G	306	-	12/12/14/38	-	0/6/6/11
24	SQD	D	606	-	-	16/49/69/69	0/1/1/1
20	LHG	F	701	-	-	26/53/53/53	-
22	AJP	B	606	-	12/12/14/38	-	0/6/6/11
22	AJP	D	607	-	12/12/14/38	-	0/6/6/11
22	AJP	D	614	-	12/12/14/38	-	0/6/6/11
22	AJP	B	610	-	12/12/14/38	-	0/6/6/11
22	AJP	Q	102	-	12/12/14/38	-	0/6/6/11
22	AJP	G	303	-	12/12/14/38	-	0/6/6/11
22	AJP	D	616	-	12/12/14/38	-	0/6/6/11
22	AJP	C	201	-	12/12/14/38	-	0/6/6/11
22	AJP	F	708	-	12/12/14/38	-	0/6/6/11
22	AJP	D	610	-	12/12/14/38	-	0/6/6/11
22	AJP	Q	101	-	12/12/14/38	-	0/6/6/11
23	PQN	B	601	-	-	9/23/43/43	0/2/2/2
25	SF4	I	202	9	-	-	0/6/5/5
22	AJP	F	710	-	12/12/14/38	-	0/6/6/11
22	AJP	D	612	-	12/12/14/38	-	0/6/6/11
24	SQD	L	101	-	-	18/49/69/69	0/1/1/1
24	SQD	D	605	-	-	18/49/69/69	0/1/1/1
22	AJP	C	202	-	12/12/14/38	-	0/6/6/11
25	SF4	K	301	11	-	-	0/6/5/5
22	AJP	G	305	-	12/12/14/38	-	0/6/6/11
22	AJP	B	607	-	12/12/14/38	-	0/6/6/11

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	AJP	G	307	-	12/12/14/38	-	0/6/6/11
22	AJP	A	407	-	12/12/14/38	-	0/6/6/11
22	AJP	F	711	-	12/12/14/38	-	0/6/6/11
22	AJP	B	614	-	12/12/14/38	-	0/6/6/11
22	AJP	D	613	-	12/12/14/38	-	0/6/6/11
22	AJP	F	712	-	12/12/14/38	-	0/6/6/11
22	AJP	G	302	-	12/12/14/38	-	0/6/6/11
22	AJP	D	611	-	12/12/14/38	-	0/6/6/11
20	LHG	B	602	-	-	26/53/53/53	-
19	BCR	A	401	-	-	23/29/63/63	0/2/2/2
21	DGD	A	404	-	-	18/55/95/95	0/2/2/2
22	AJP	B	612	-	12/12/14/38	-	0/6/6/11
22	AJP	F	705	-	12/12/14/38	-	0/6/6/11
19	BCR	D	601	-	-	26/29/63/63	0/2/2/2
24	SQD	F	703	-	-	21/49/69/69	0/1/1/1
22	AJP	F	706	-	12/12/14/38	-	0/6/6/11
21	DGD	A	405	-	-	20/55/95/95	0/2/2/2
20	LHG	A	402	-	-	21/53/53/53	-
22	AJP	B	605	-	12/12/14/38	-	0/6/6/11
19	BCR	D	602	-	-	19/29/63/63	0/2/2/2
20	LHG	D	603	-	-	25/53/53/53	-
22	AJP	B	611	-	12/12/14/38	-	0/6/6/11
22	AJP	F	704	-	12/12/14/38	-	0/6/6/11
22	AJP	G	304	-	12/12/14/38	-	0/6/6/11
20	LHG	A	403	-	-	17/53/53/53	-
22	AJP	A	408	-	12/12/14/38	-	0/6/6/11
20	LHG	D	604	-	-	23/53/53/53	-
22	AJP	B	613	-	12/12/14/38	-	0/6/6/11

The worst 5 of 353 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	601	PQN	C12-C13	8.31	1.52	1.33
23	B	601	PQN	O4-C4	8.17	1.40	1.23
23	B	601	PQN	O1-C1	8.12	1.40	1.23
19	A	401	BCR	C10-C9	4.19	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	D	602	BCR	C21-C22	4.17	1.41	1.35

The worst 5 of 943 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	D	613	AJP	C12-C07-C08	-9.65	94.45	104.88
22	B	610	AJP	C12-C07-C08	-9.22	94.92	104.88
22	F	709	AJP	C12-C07-C08	-9.16	94.98	104.88
22	D	611	AJP	C12-C07-C08	-9.15	94.99	104.88
22	G	304	AJP	C12-C07-C08	-9.04	95.12	104.88

5 of 528 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	A	406	AJP	C12
22	A	406	AJP	C02
22	A	406	AJP	C22
22	A	406	AJP	C07
22	A	406	AJP	C20

5 of 389 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	A	401	BCR	C1-C6-C7-C8
19	A	401	BCR	C5-C6-C7-C8
19	A	401	BCR	C10-C11-C12-C13
19	A	401	BCR	C11-C12-C13-C14
19	A	401	BCR	C11-C12-C13-C35

There are no ring outliers.

61 monomers are involved in 358 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	D	615	AJP	7	0
22	B	608	AJP	3	0
20	B	603	LHG	1	0
22	D	609	AJP	6	0
20	G	301	LHG	2	0
22	B	604	AJP	17	0
22	B	609	AJP	13	0
22	A	406	AJP	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	D	608	AJP	5	0
22	F	707	AJP	1	0
22	F	709	AJP	7	0
22	Q	103	AJP	1	0
22	G	306	AJP	10	0
24	D	606	SQD	2	0
22	B	606	AJP	4	0
22	D	607	AJP	10	0
22	D	614	AJP	9	0
22	B	610	AJP	6	0
22	Q	102	AJP	8	0
22	G	303	AJP	6	0
22	D	616	AJP	5	0
22	C	201	AJP	8	0
22	F	708	AJP	4	0
22	D	610	AJP	6	0
22	Q	101	AJP	2	0
23	B	601	PQN	1	0
25	I	202	SF4	2	0
22	F	710	AJP	6	0
22	D	612	AJP	4	0
24	L	101	SQD	1	0
24	D	605	SQD	8	0
22	C	202	AJP	21	0
25	K	301	SF4	3	0
22	G	305	AJP	5	0
22	B	607	AJP	4	0
22	G	307	AJP	5	0
22	A	407	AJP	7	0
22	F	711	AJP	2	0
22	B	614	AJP	20	0
22	D	613	AJP	7	0
22	F	712	AJP	7	0
22	G	302	AJP	4	0
20	B	602	LHG	1	0
22	D	611	AJP	9	0
19	A	401	BCR	18	0
22	B	612	AJP	8	0
22	F	705	AJP	8	0
19	D	601	BCR	13	0
24	F	703	SQD	2	0
22	F	706	AJP	11	0

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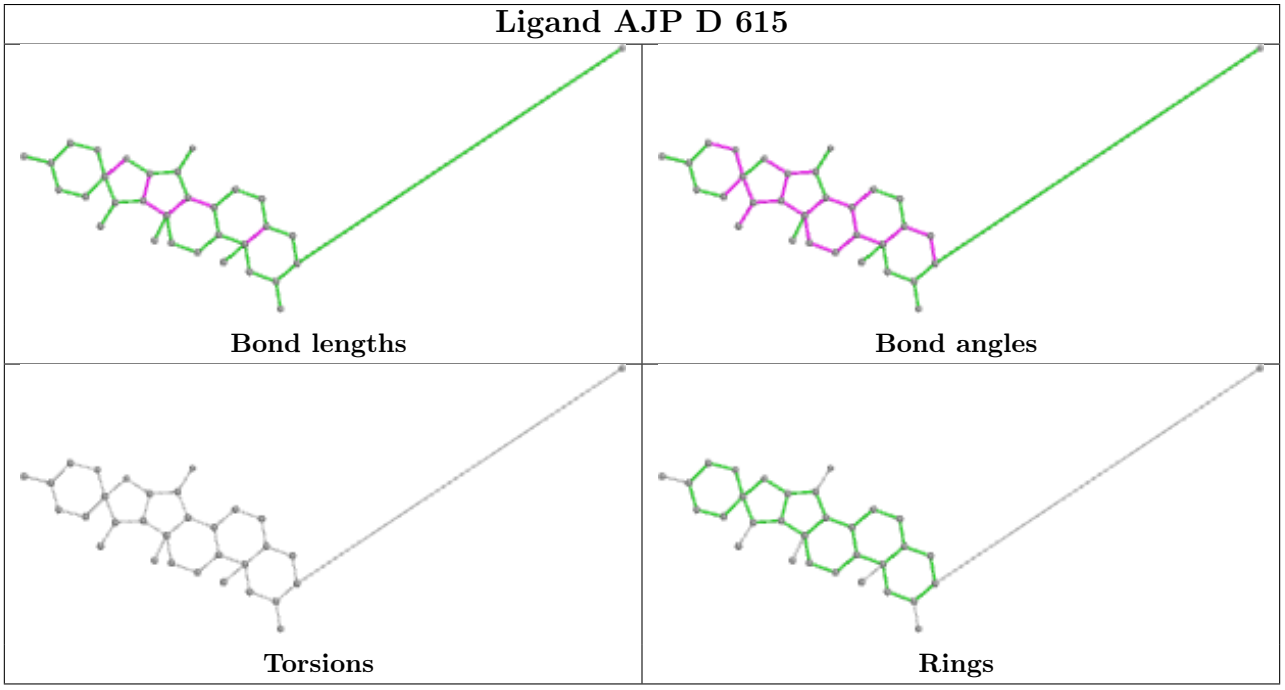
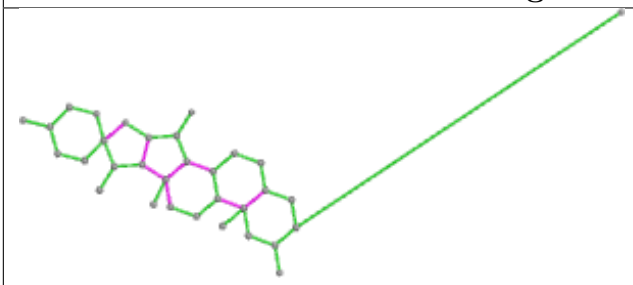
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	A	405	DGD	2	0
22	B	605	AJP	6	0
19	D	602	BCR	27	0
20	D	603	LHG	1	0
22	B	611	AJP	1	0
20	A	403	LHG	1	0
22	F	704	AJP	1	0
22	G	304	AJP	7	0
22	A	408	AJP	7	0
20	D	604	LHG	1	0
22	B	613	AJP	8	0

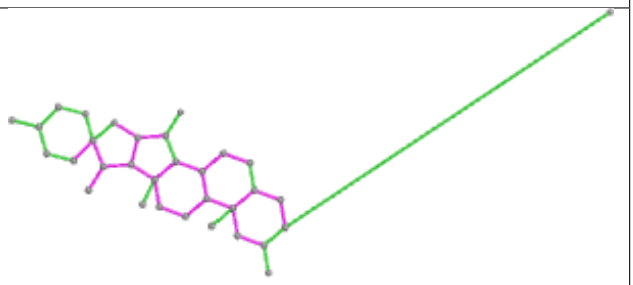
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



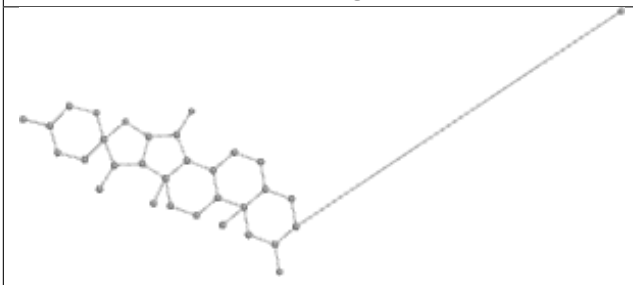
Ligand AJP B 608



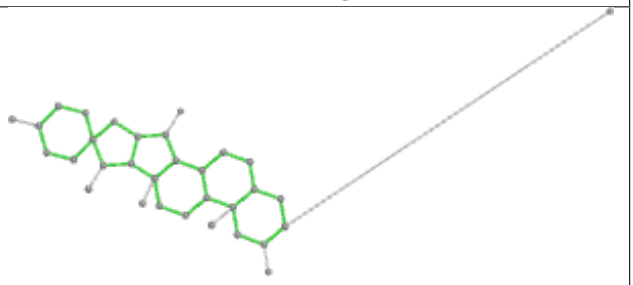
Bond lengths



Bond angles

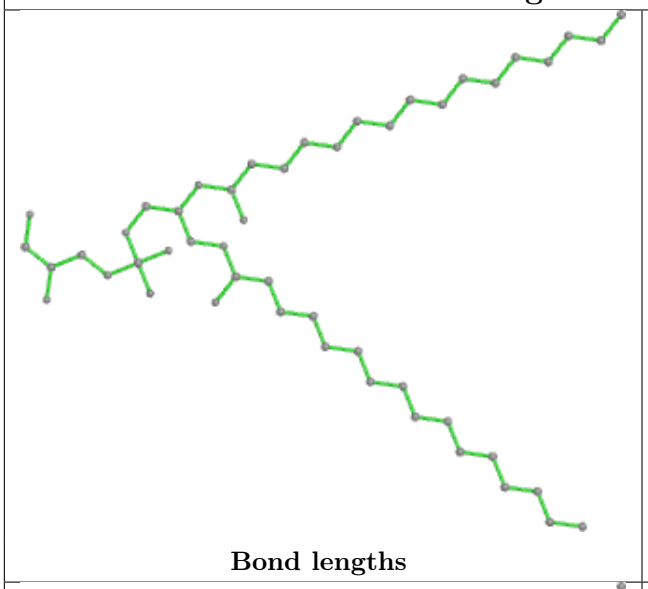


Torsions

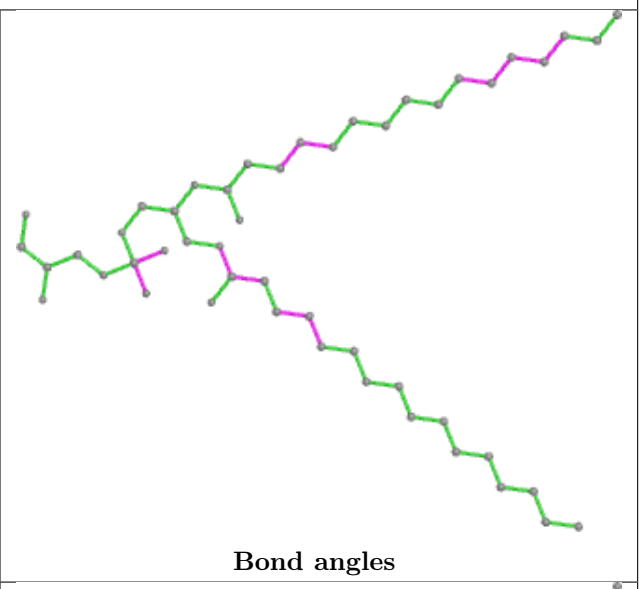


Rings

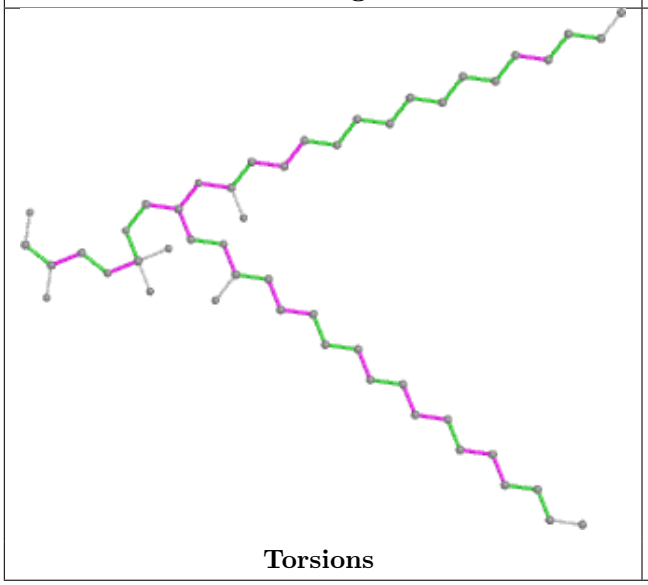
Ligand LHG F 702



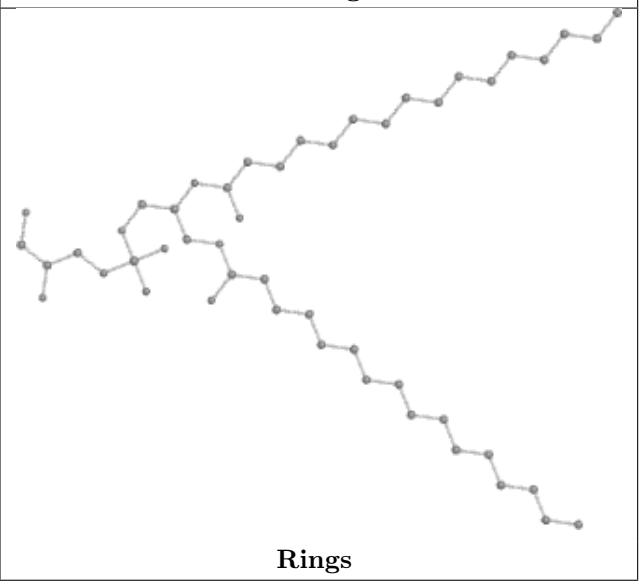
Bond lengths



Bond angles

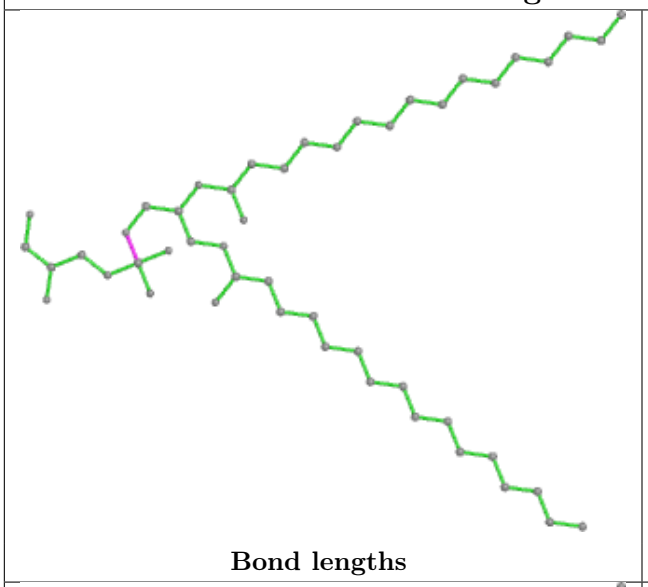


Torsions

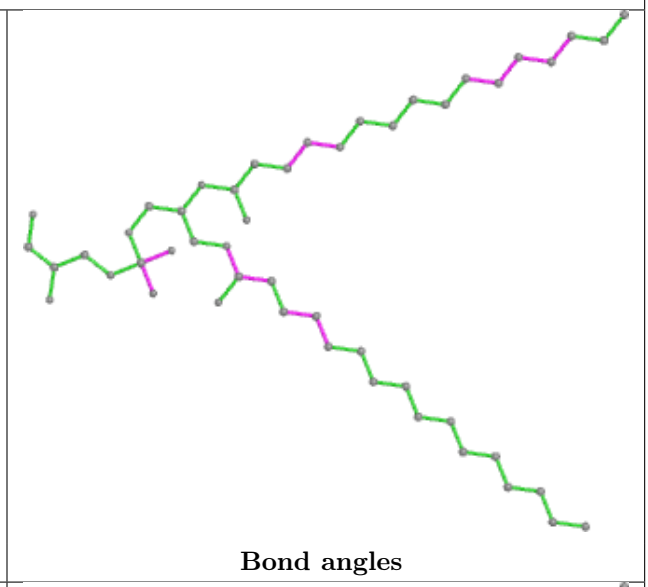


Rings

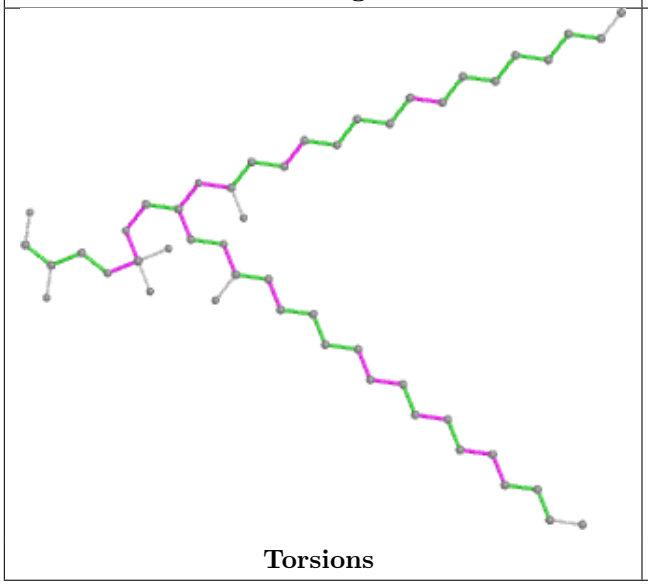
Ligand LHG B 603



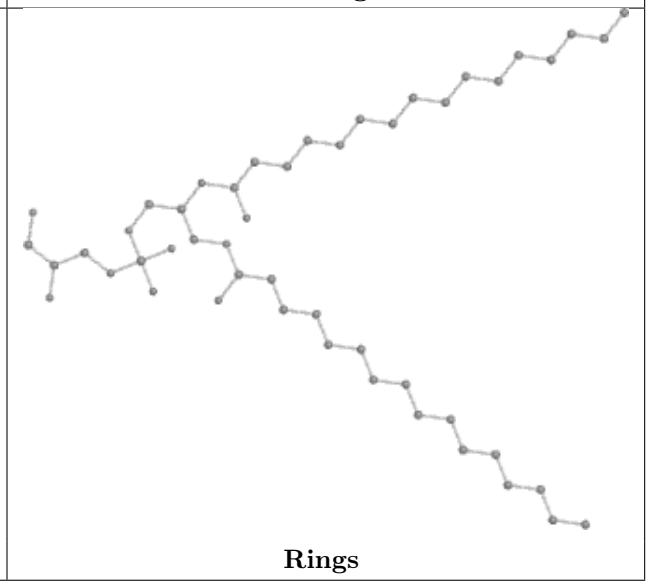
Bond lengths



Bond angles

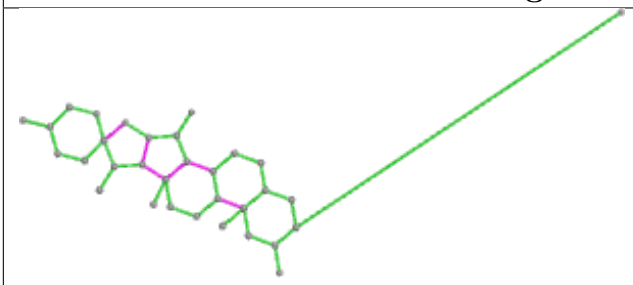


Torsions

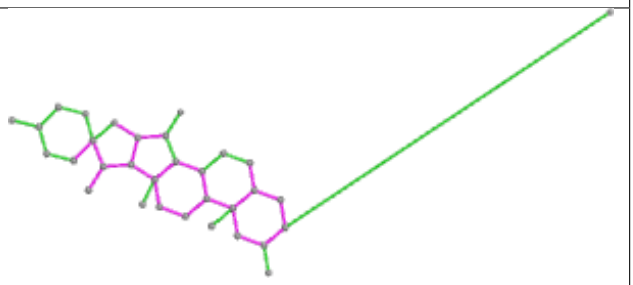


Rings

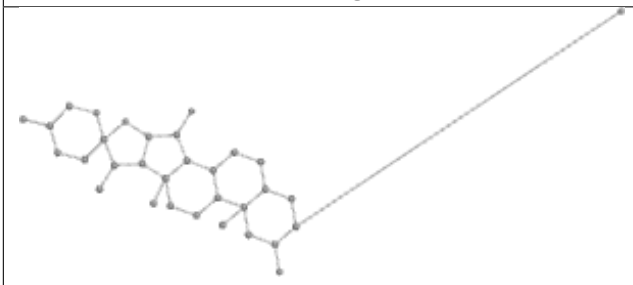
Ligand AJP D 609



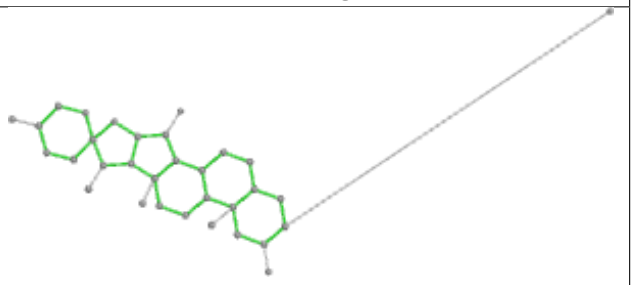
Bond lengths



Bond angles

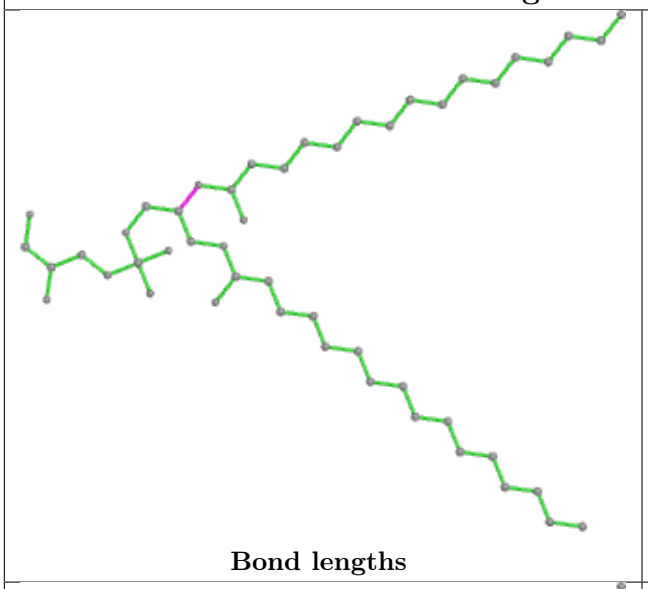


Torsions

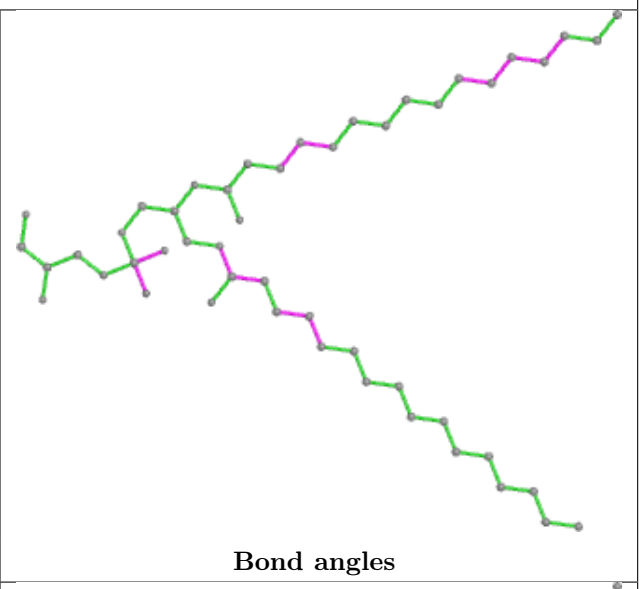


Rings

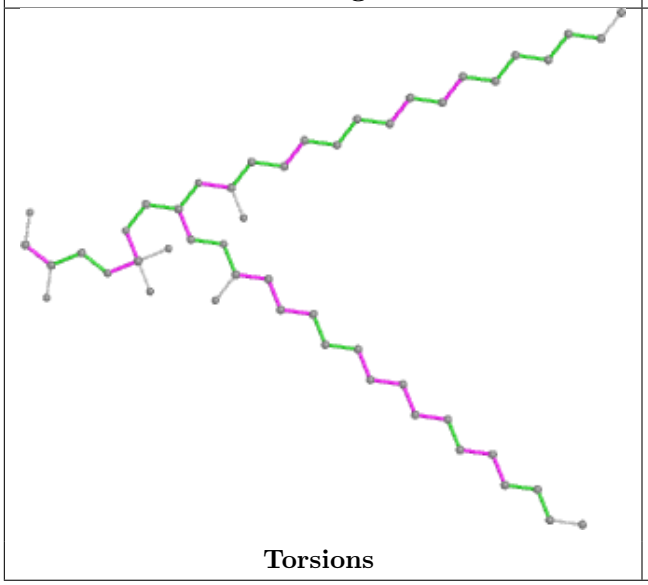
Ligand LHG G 301



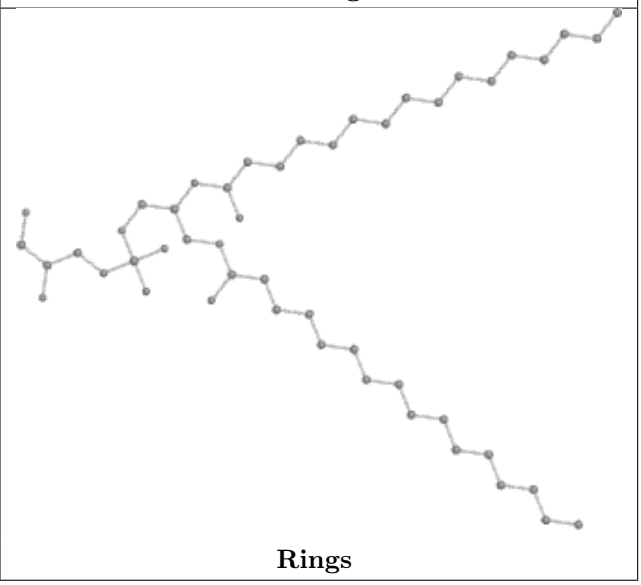
Bond lengths



Bond angles

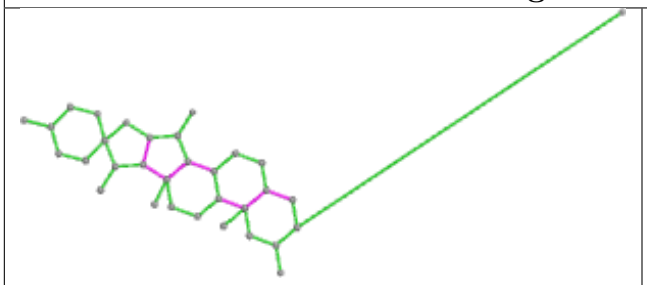


Torsions

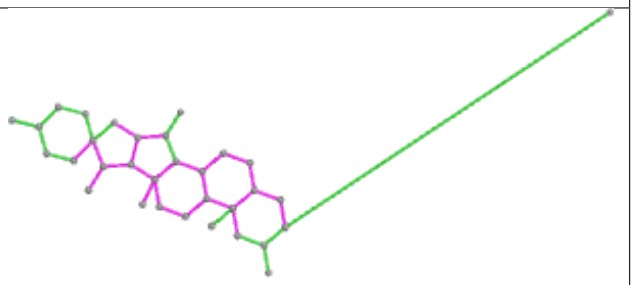


Rings

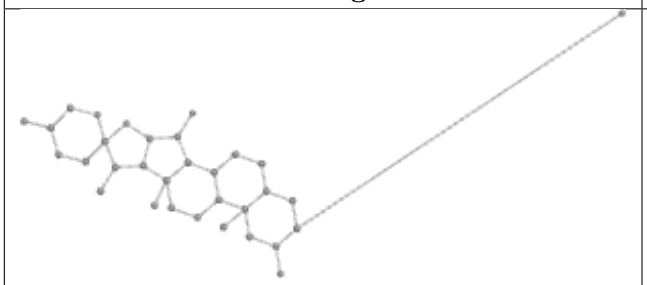
Ligand AJP B 604



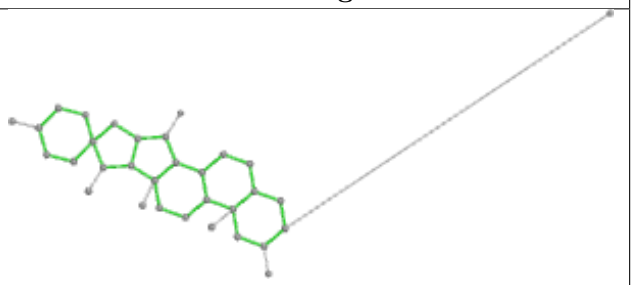
Bond lengths



Bond angles

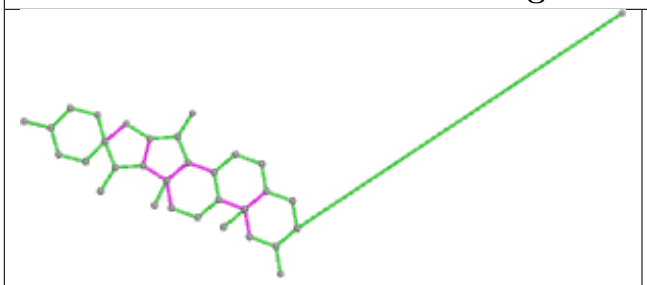


Torsions

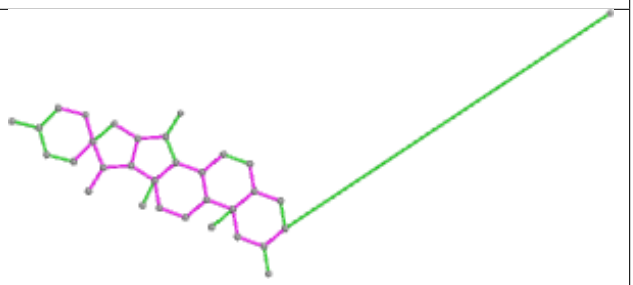


Rings

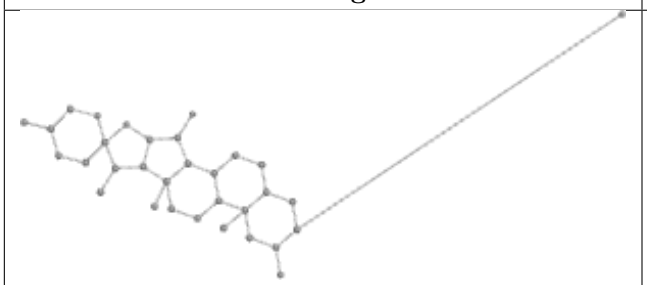
Ligand AJP B 609



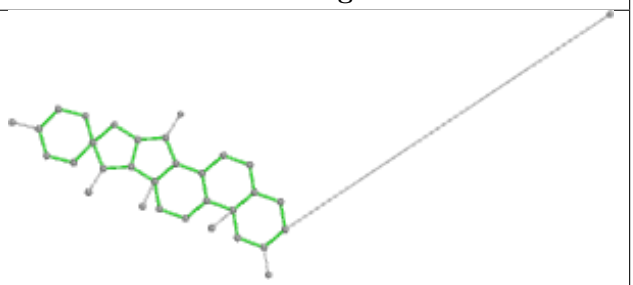
Bond lengths



Bond angles

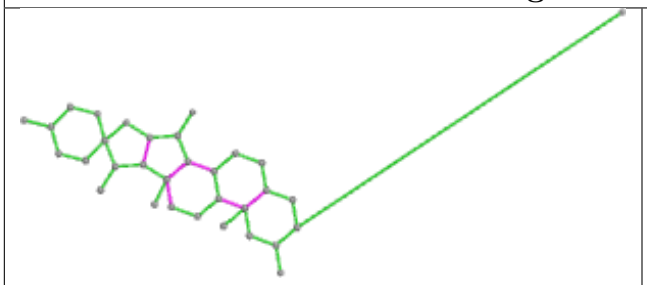


Torsions

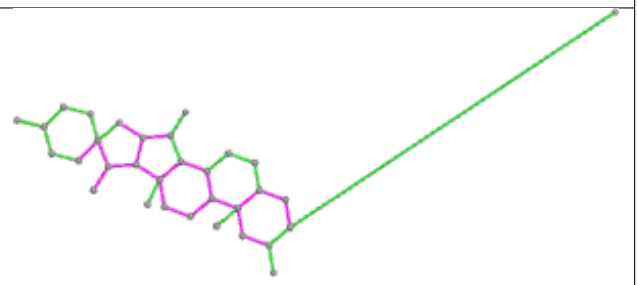


Rings

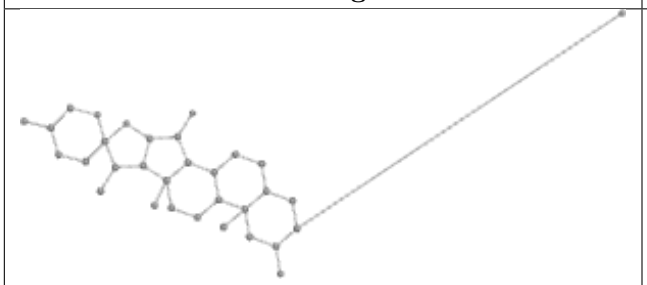
Ligand AJP A 406



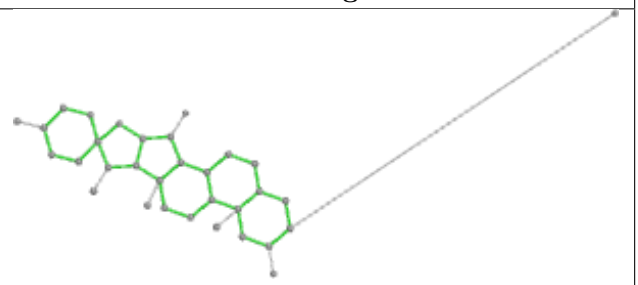
Bond lengths



Bond angles

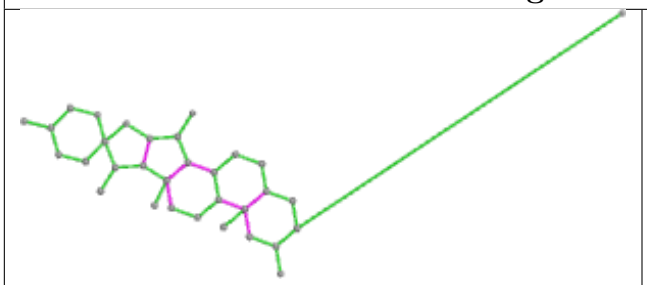


Torsions

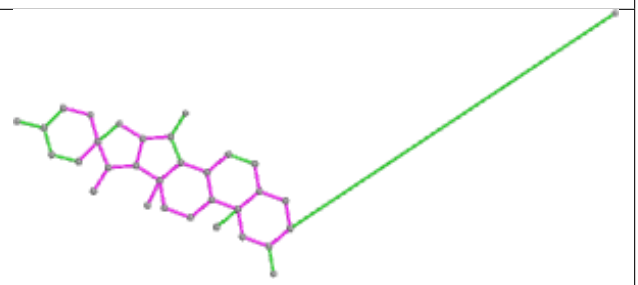


Rings

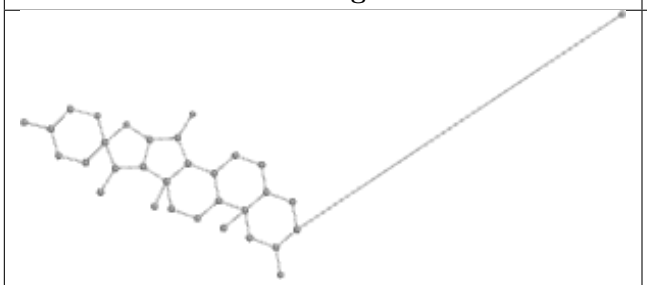
Ligand AJP D 608



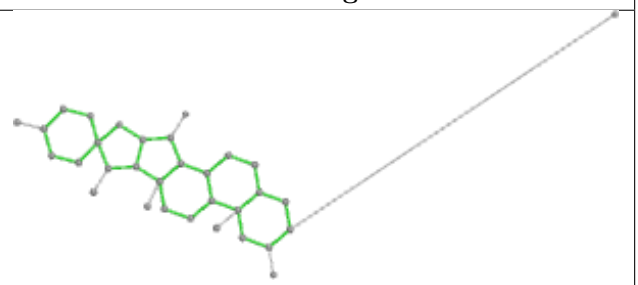
Bond lengths



Bond angles

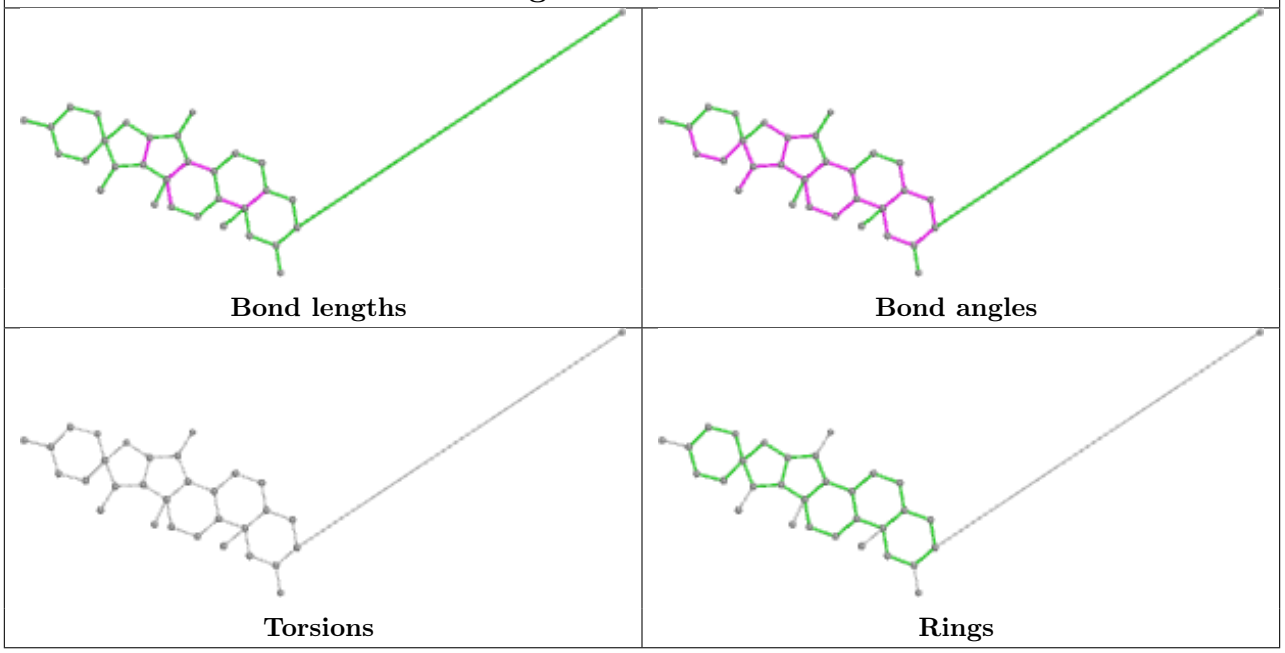


Torsions

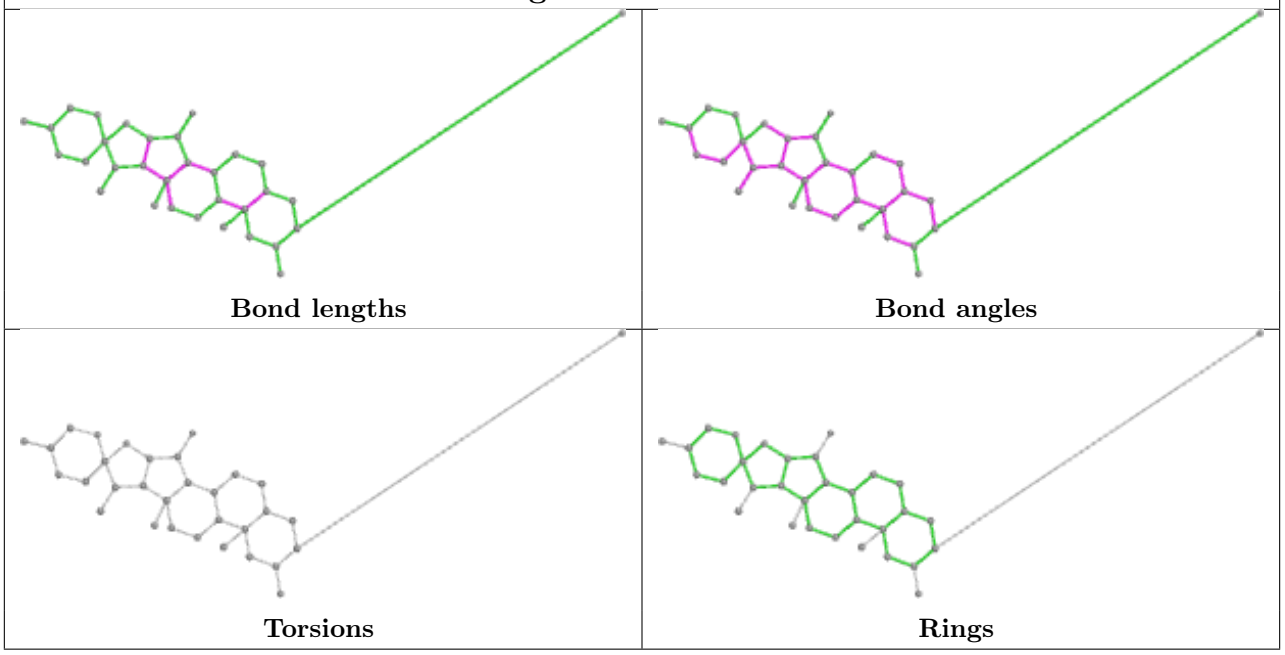


Rings

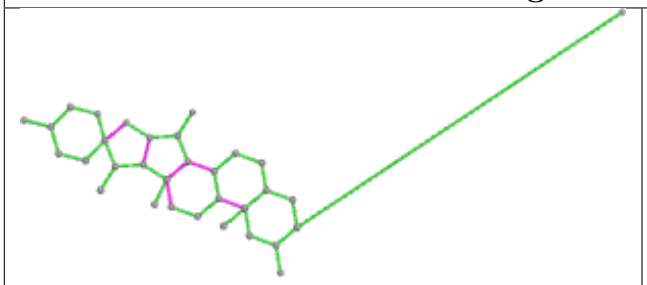
Ligand AJP F 707



Ligand AJP F 709



Ligand AJP Q 103



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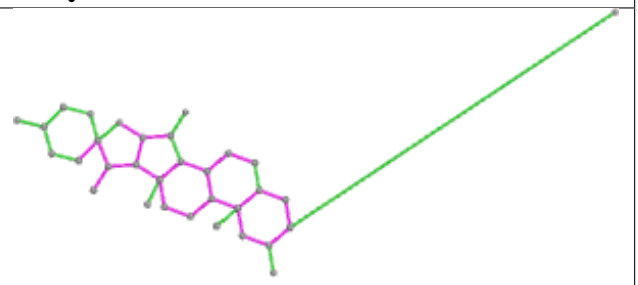
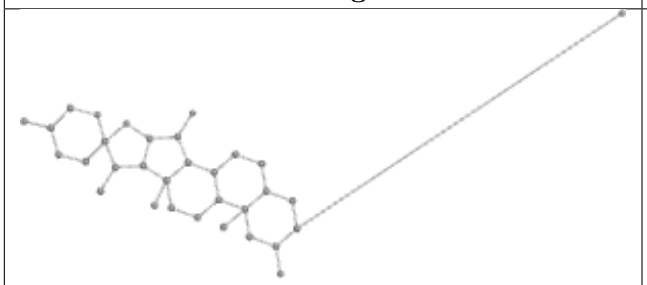


Bond angles



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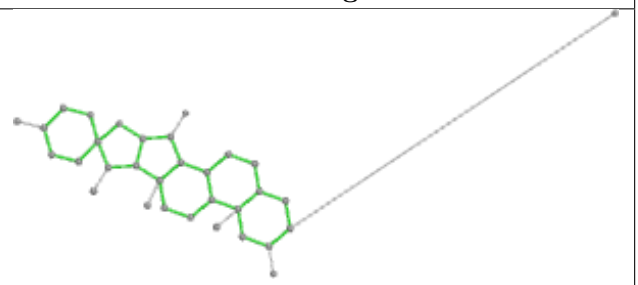
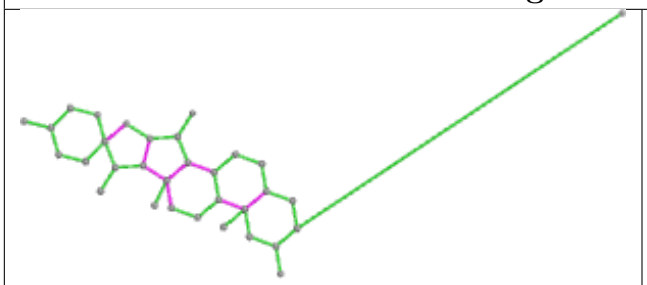


Rings

Ligand AJP G 306



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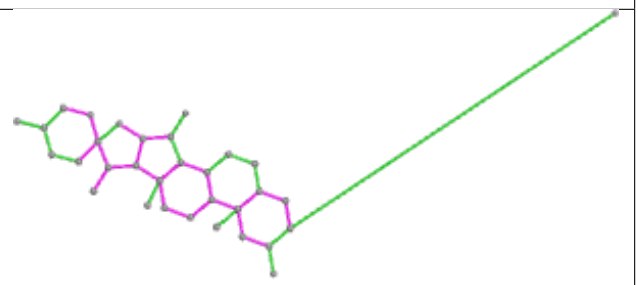
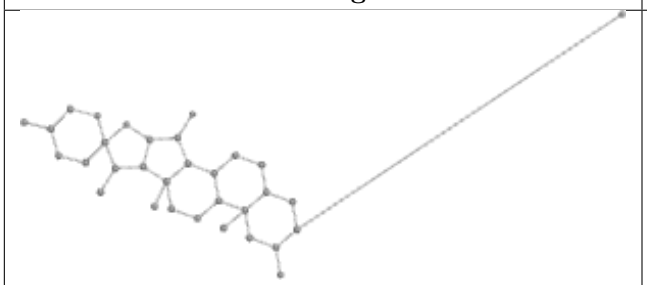
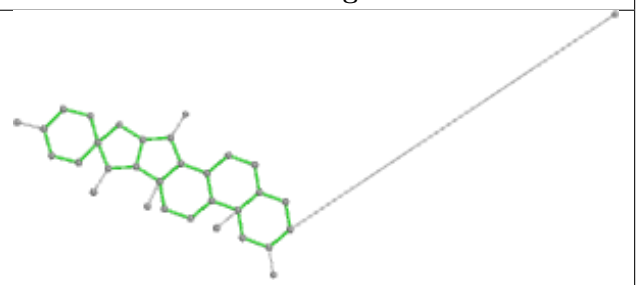


Bond angles

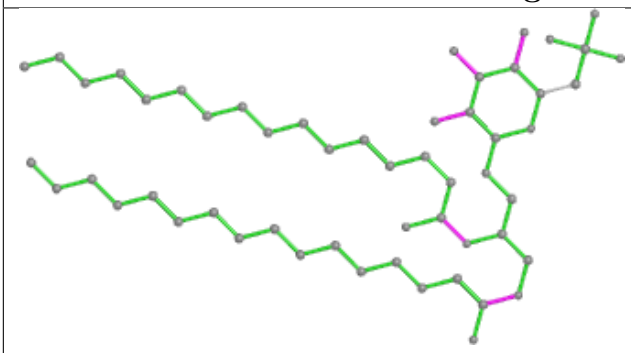


Torsions



Rings

Ligand SQD D 606



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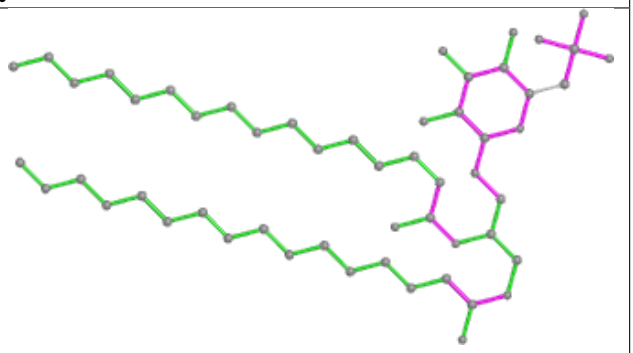
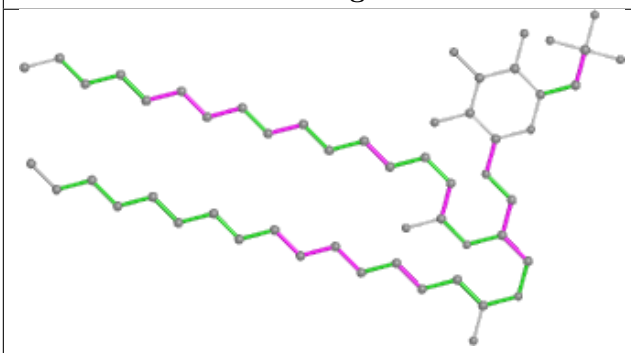


Bond angles



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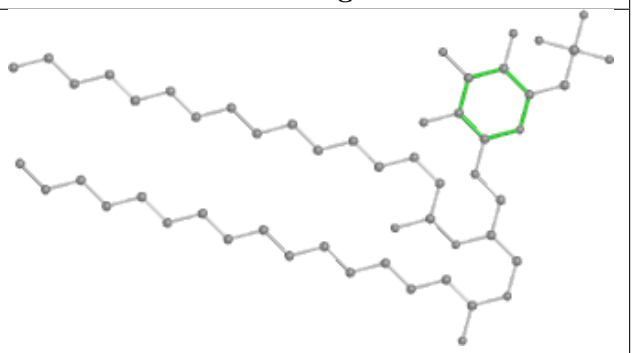
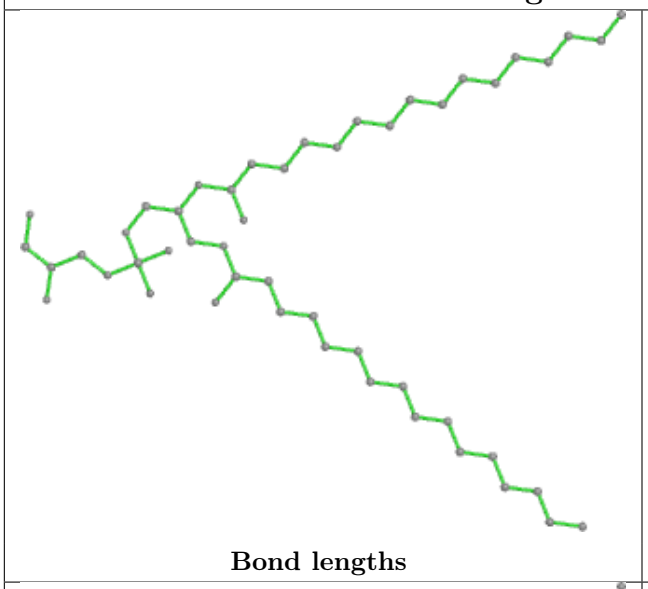


Rings

Ligand LHG F 701



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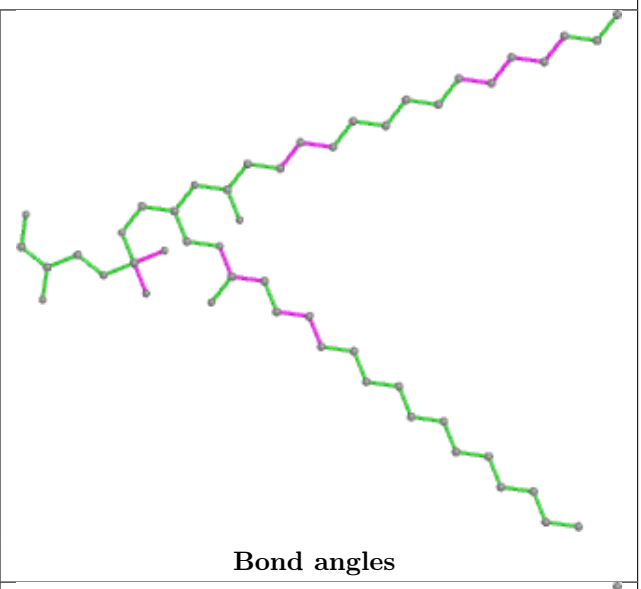
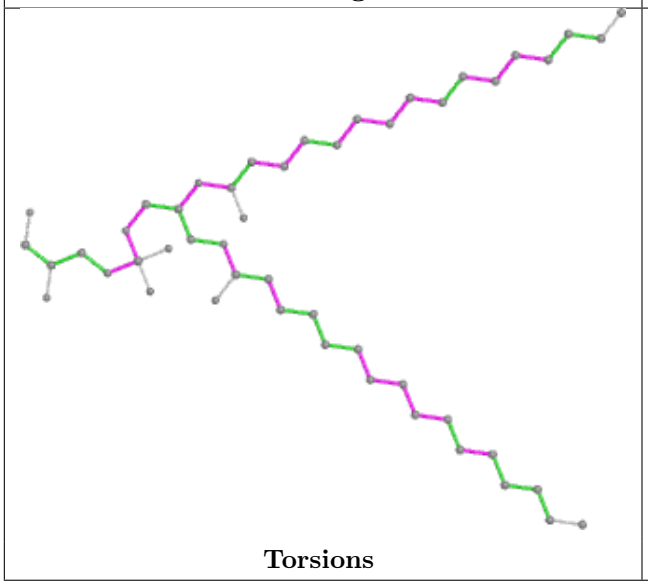
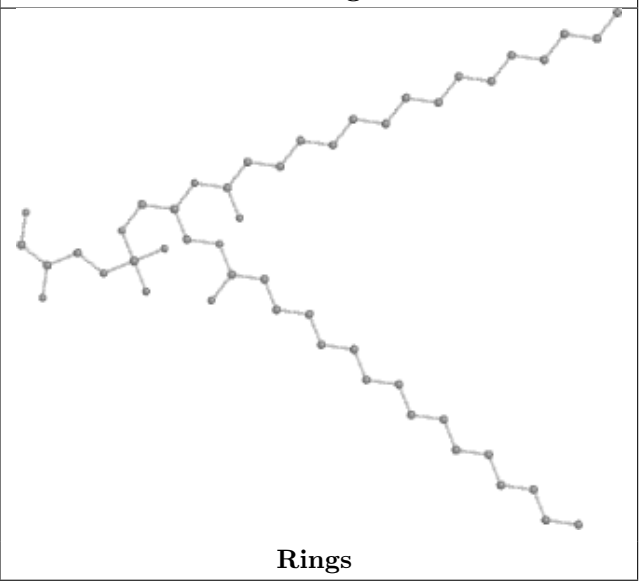


Bond angles

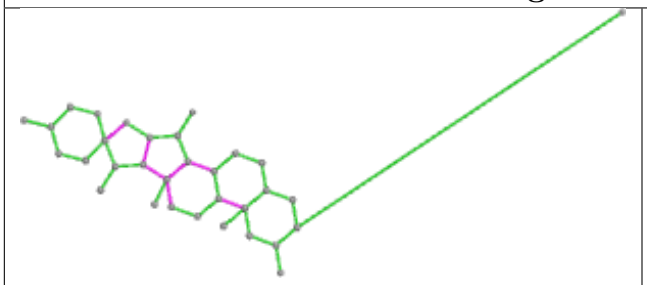


Torsions



Rings

Ligand AJP B 606



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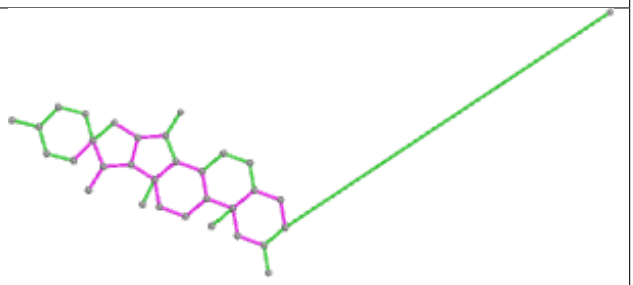
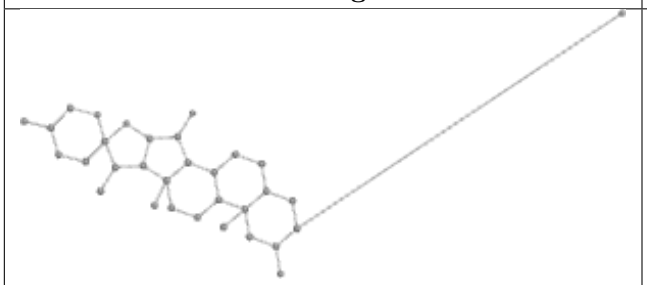
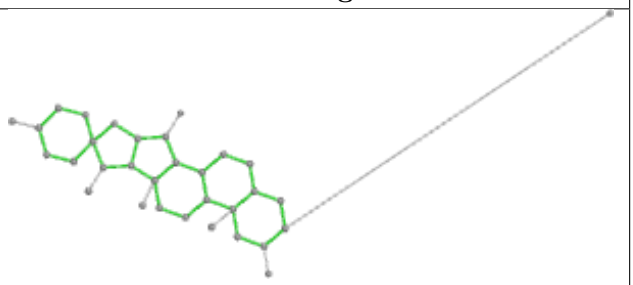


Bond angles

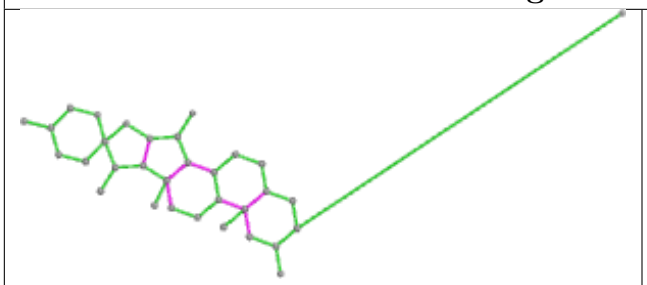


Torsions



Rings

Ligand AJP D 607



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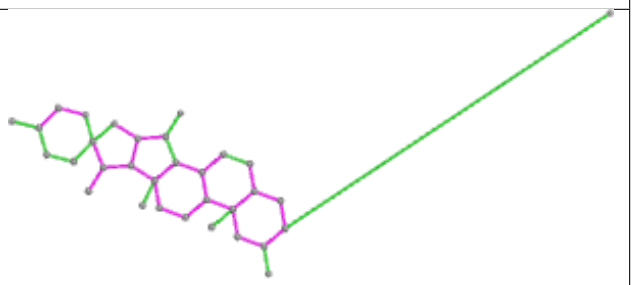
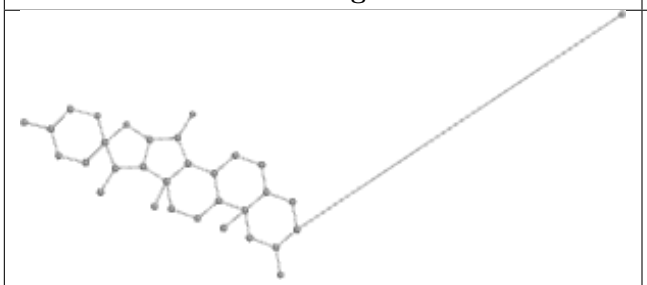
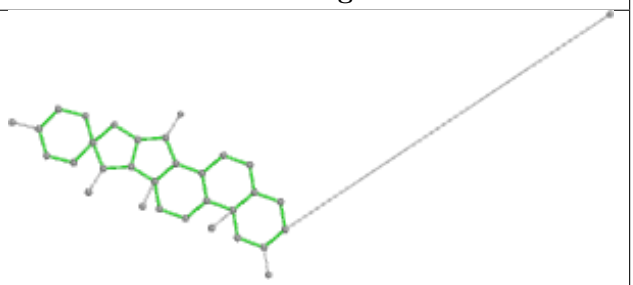


Bond angles

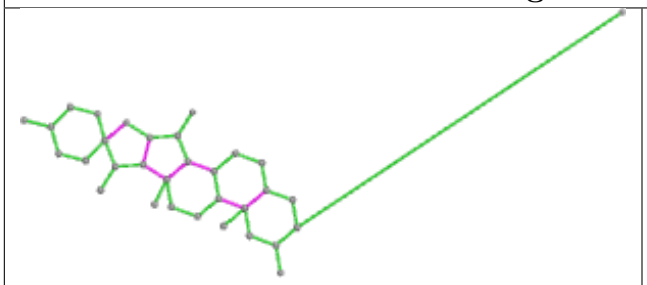


Torsions



Rings

Ligand AJP D 614



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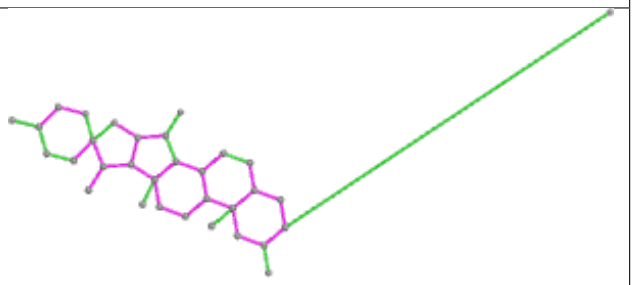
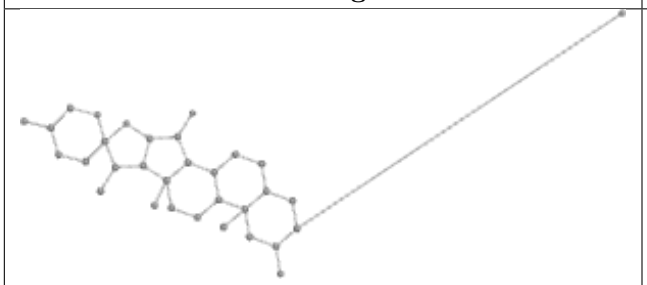


Bond angles



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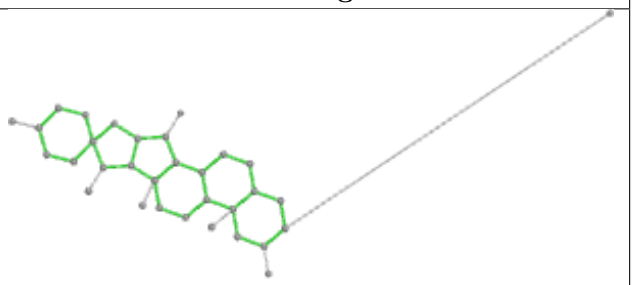
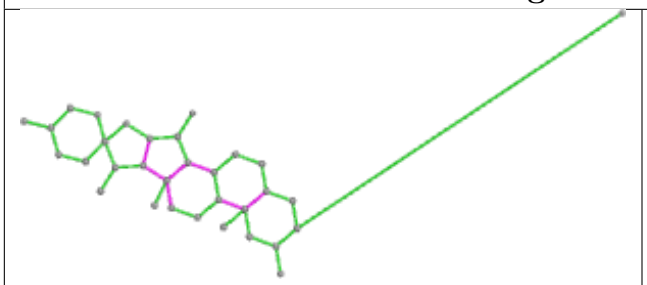


Rings

Ligand AJP B 610



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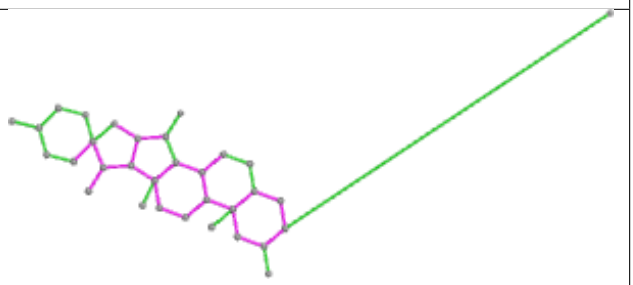
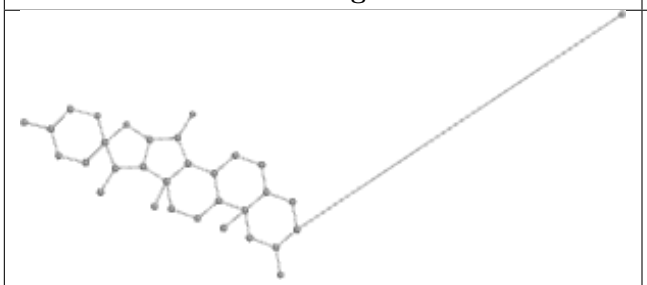
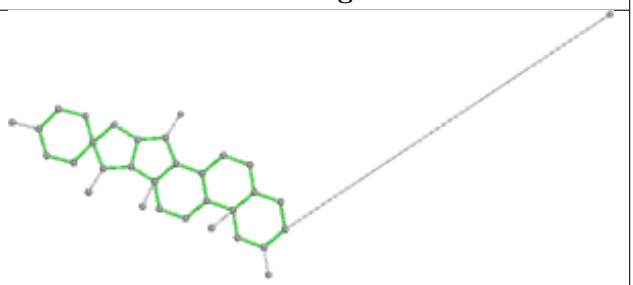


Bond angles

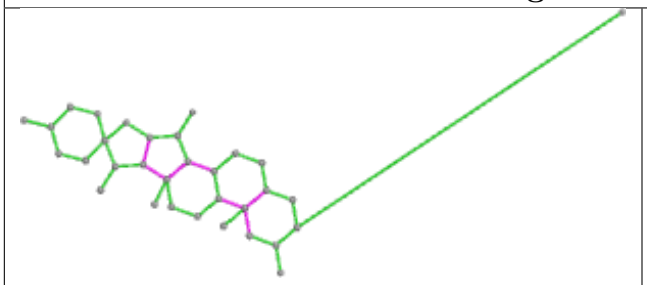


Torsions

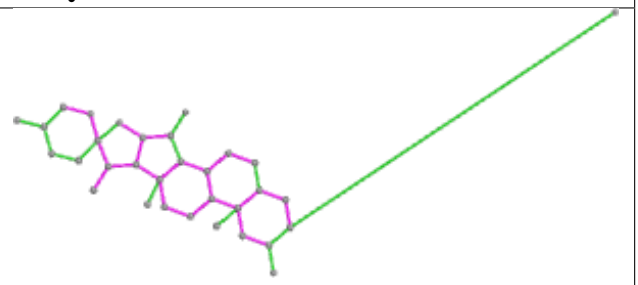


Rings

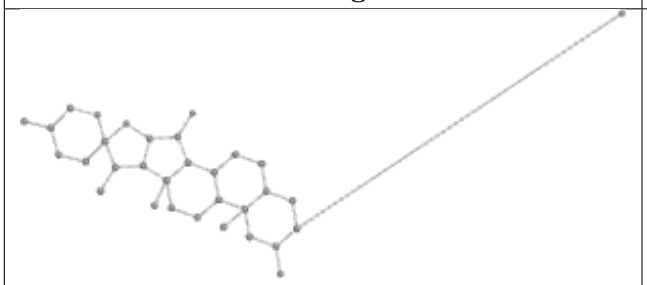
Ligand AJP Q 102



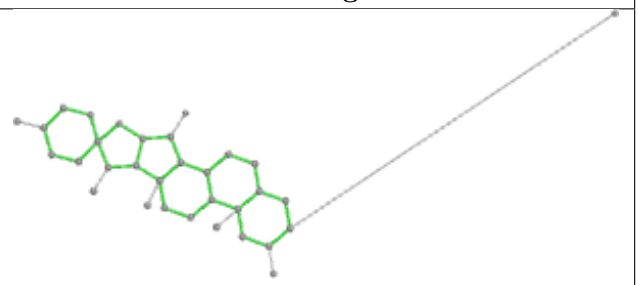
Bond lengths



Bond angles

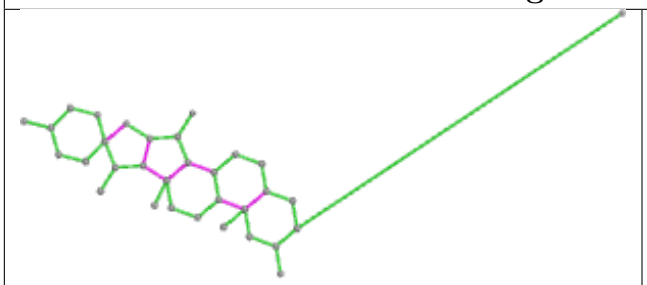


Torsions



Rings

Ligand AJP G 303



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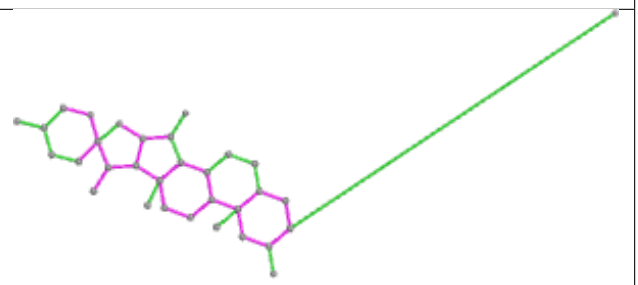
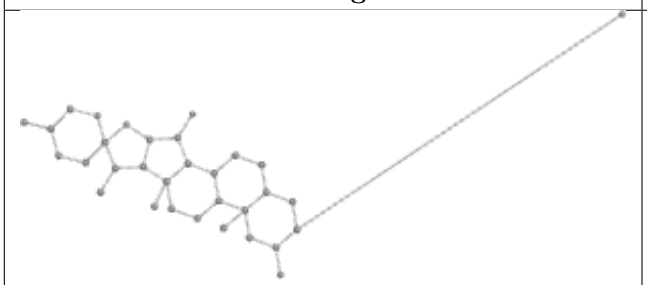
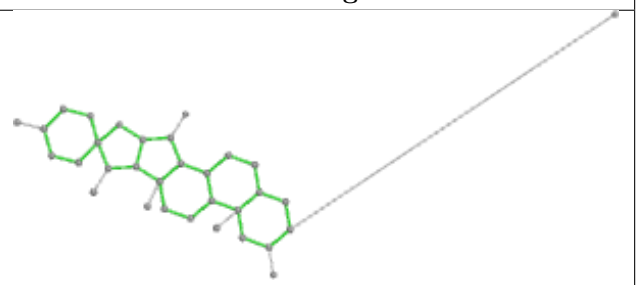


Bond angles

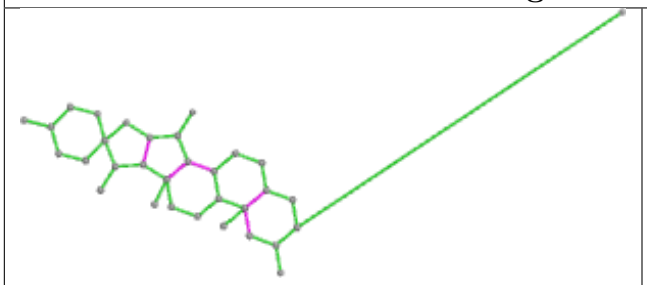


Torsions

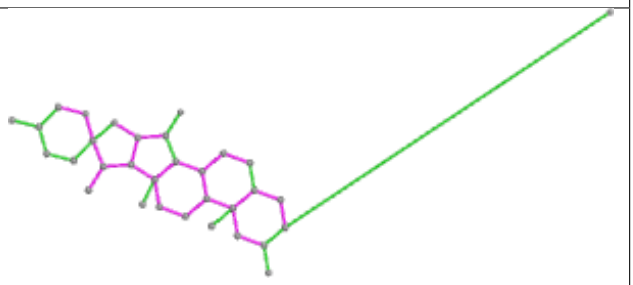


Rings

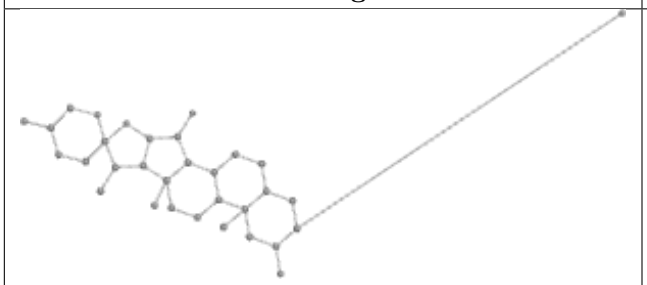
Ligand AJP D 616



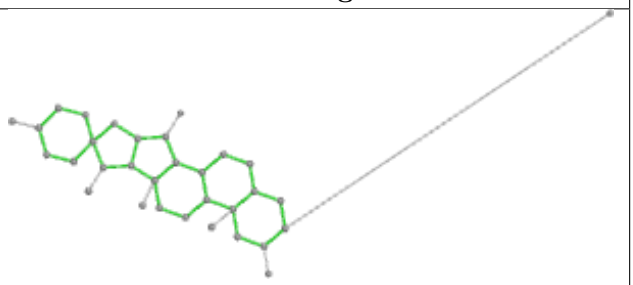
Bond lengths



Bond angles

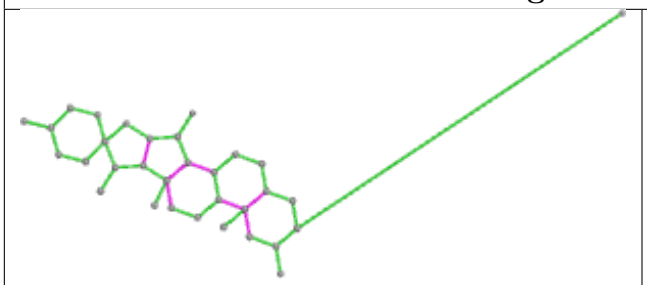


Torsions

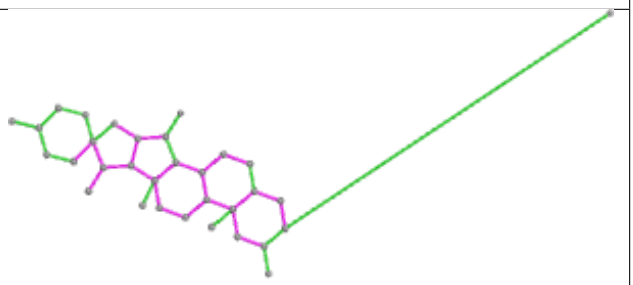


Rings

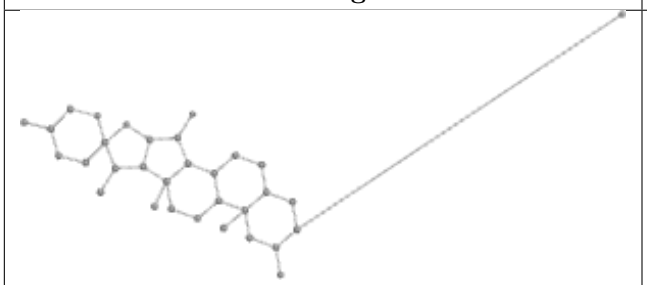
Ligand AJP C 201



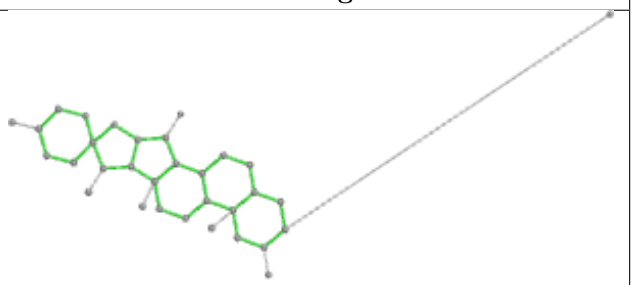
Bond lengths



Bond angles

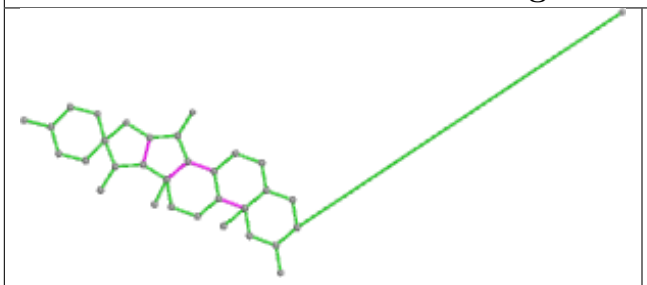


Torsions

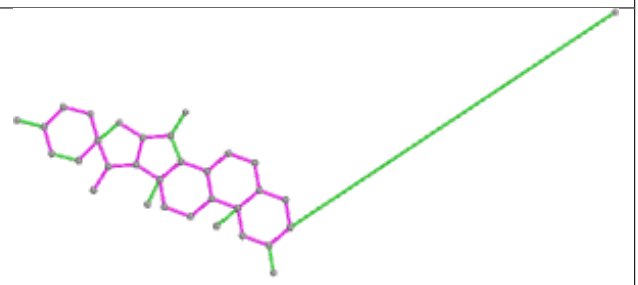


Rings

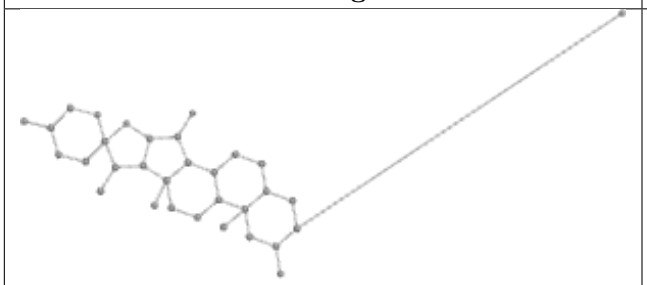
Ligand AJP F 708



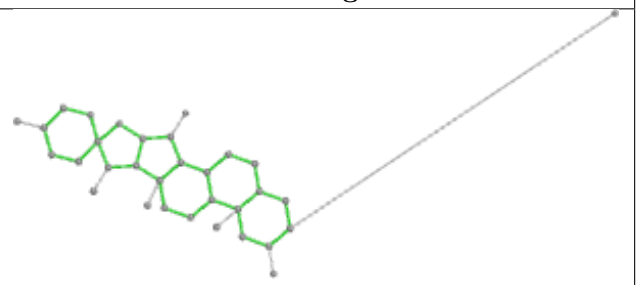
Bond lengths



Bond angles

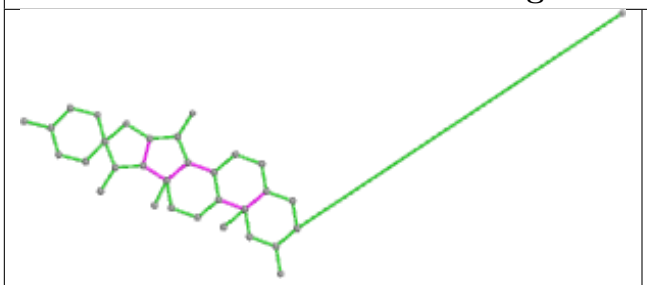


Torsions

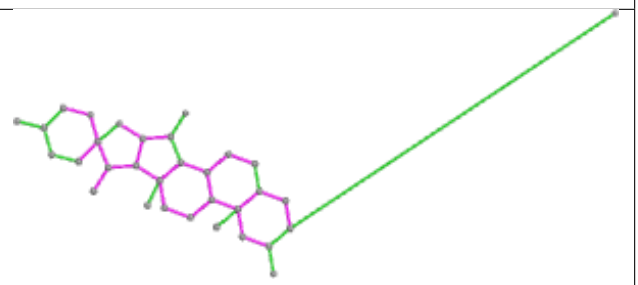


Rings

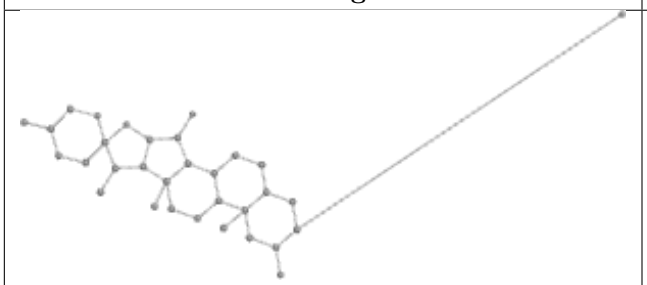
Ligand AJP D 610



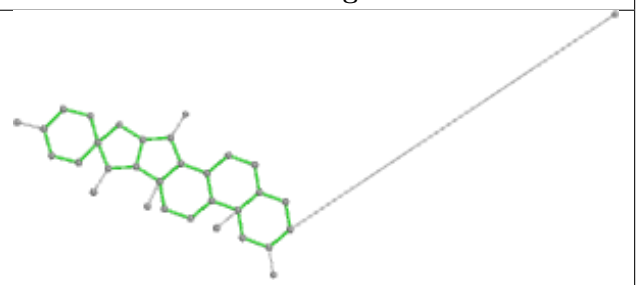
Bond lengths



Bond angles

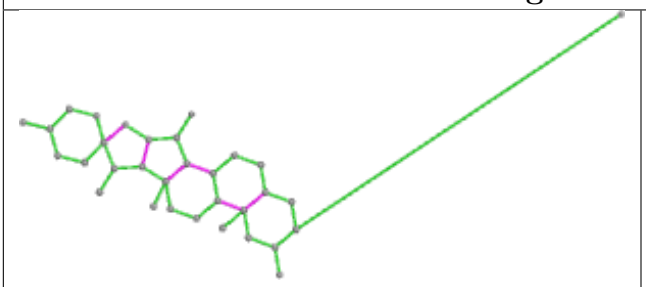


Torsions



Rings

Ligand AJP Q 101



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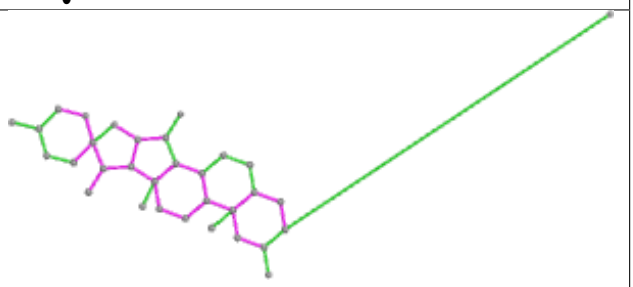
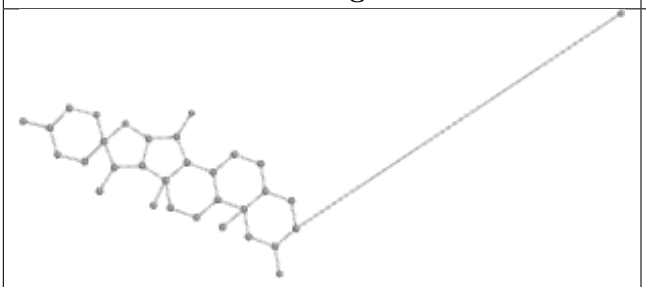
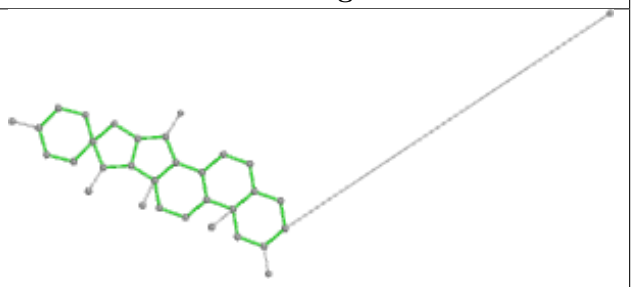


Bond angles

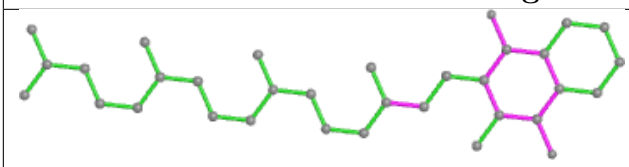


Torsions

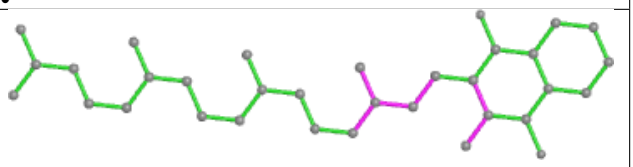


Rings

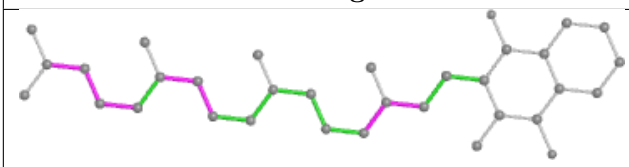
Ligand PQN B 601



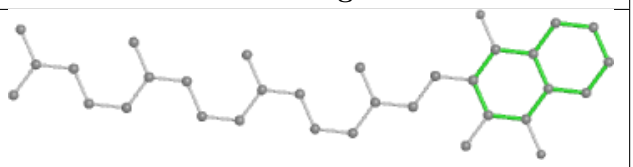
Bond lengths



Bond angles

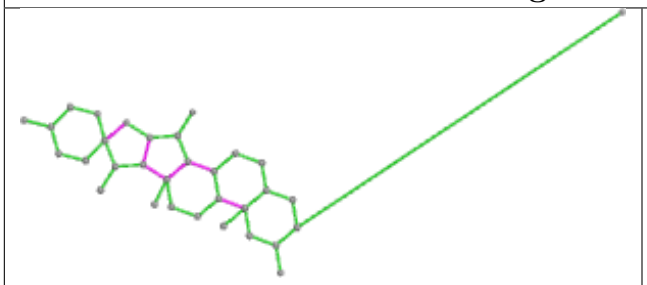


Torsions

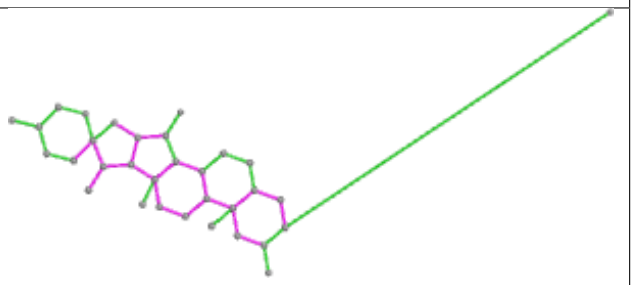


Rings

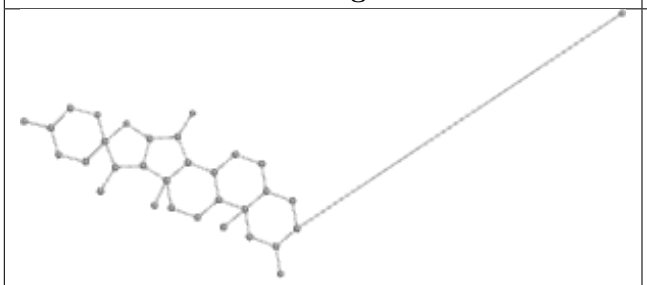
Ligand AJP F 710



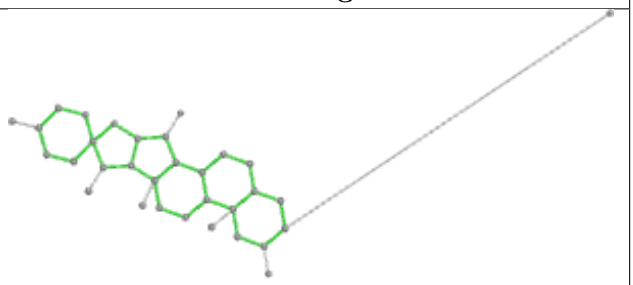
Bond lengths



Bond angles

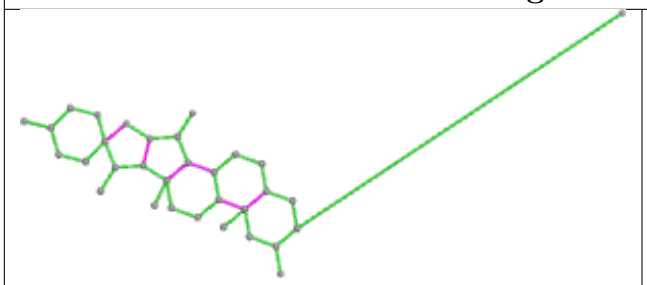


Torsions



Rings

Ligand AJP D 612



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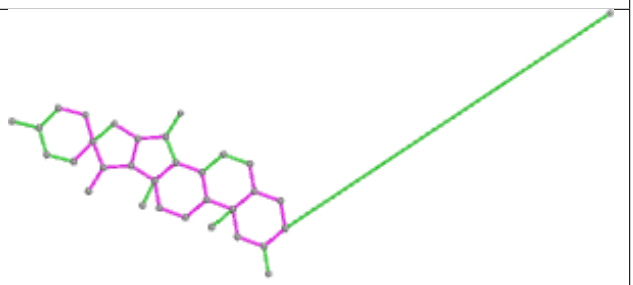
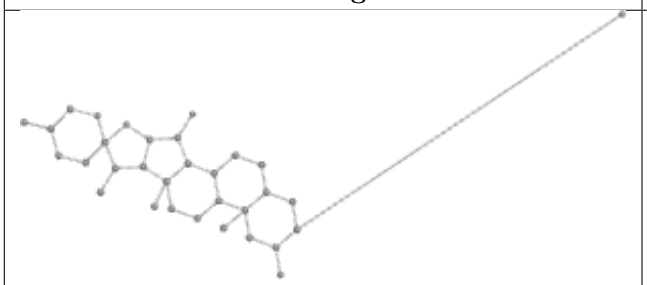
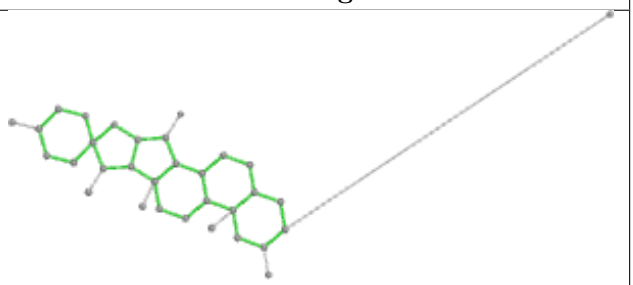


Bond angles

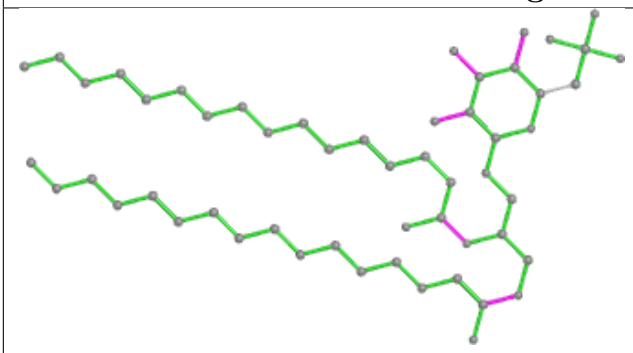


Torsions

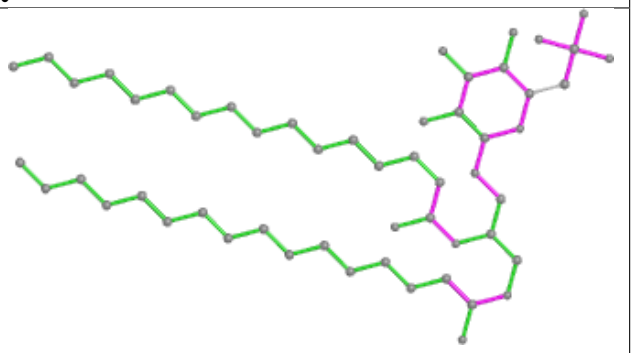


Rings

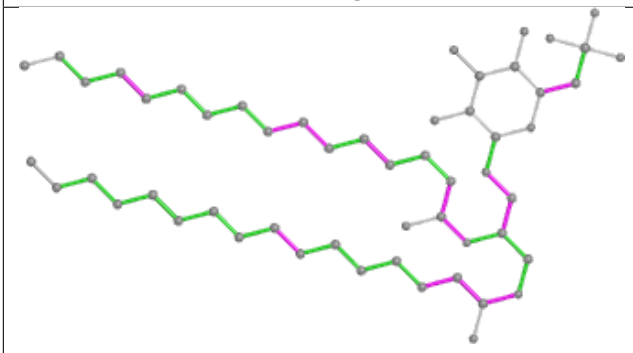
Ligand SQD L 101



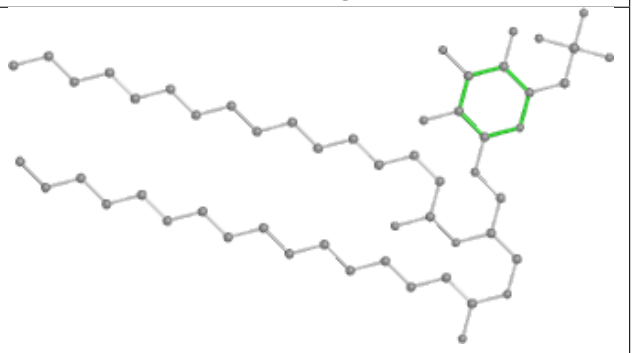
Bond lengths



Bond angles

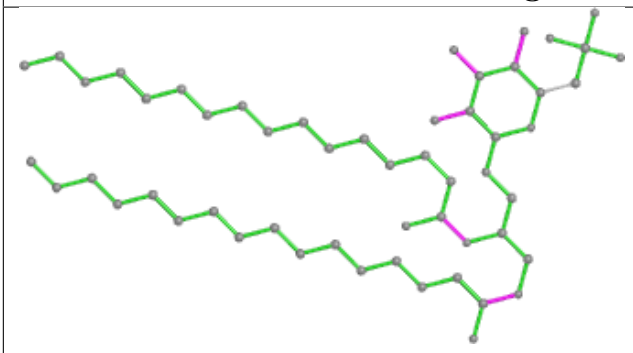


Torsions

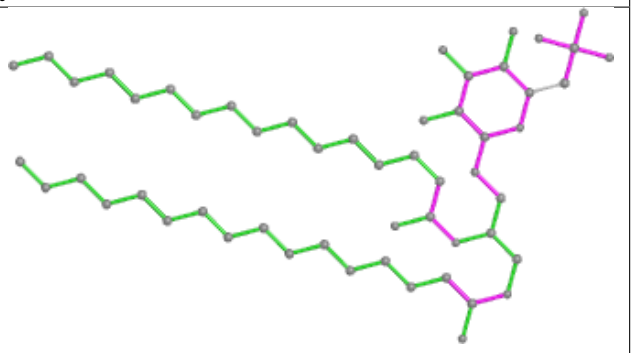


Rings

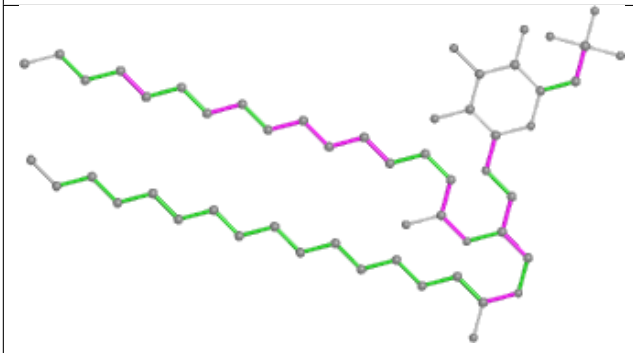
Ligand SQD D 605



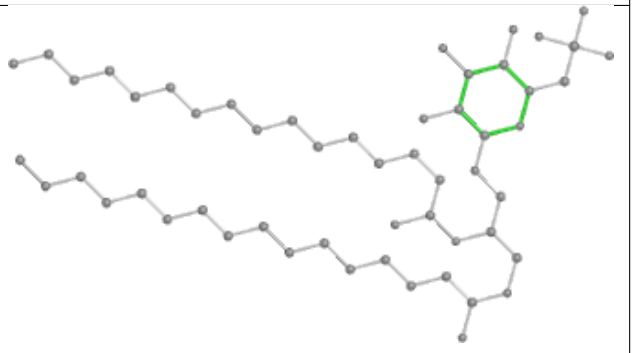
Bond lengths



Bond angles

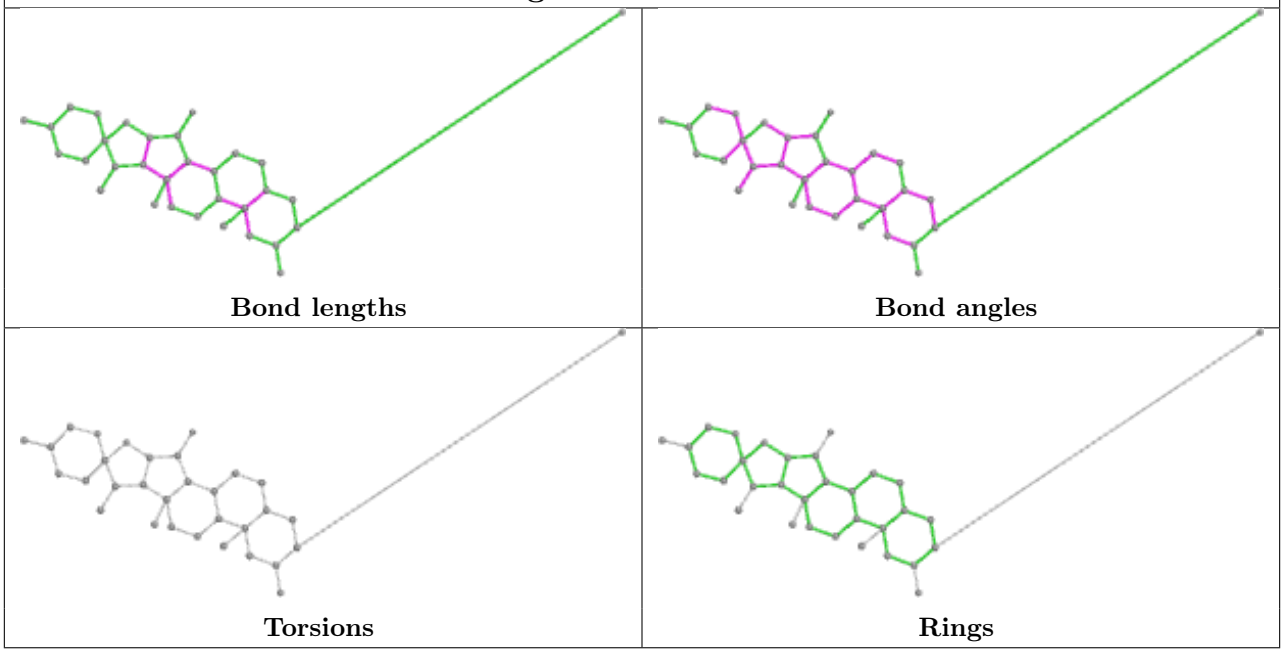


Torsions

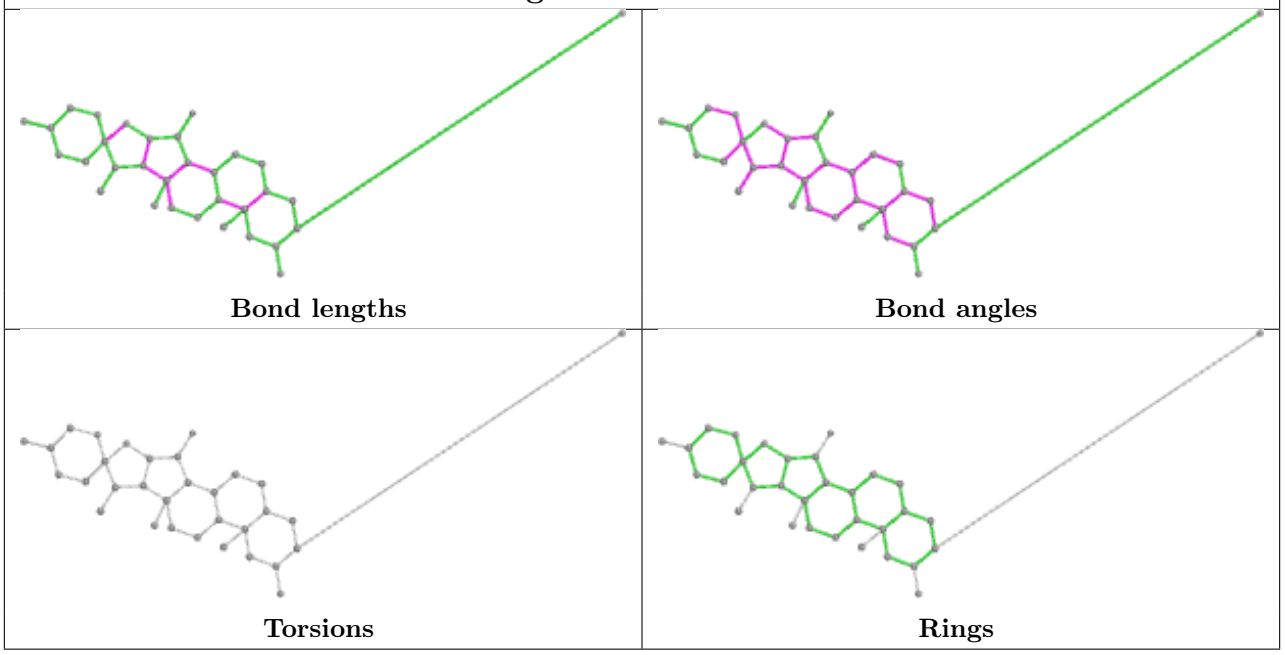


Rings

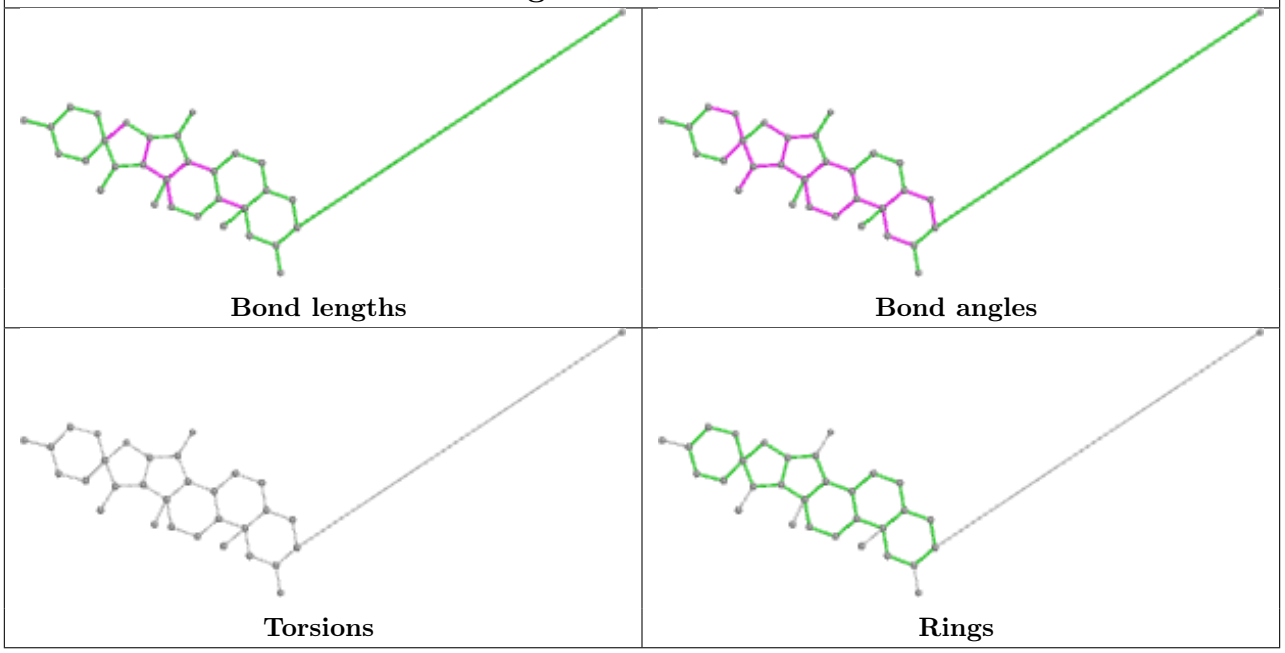
Ligand AJP C 202



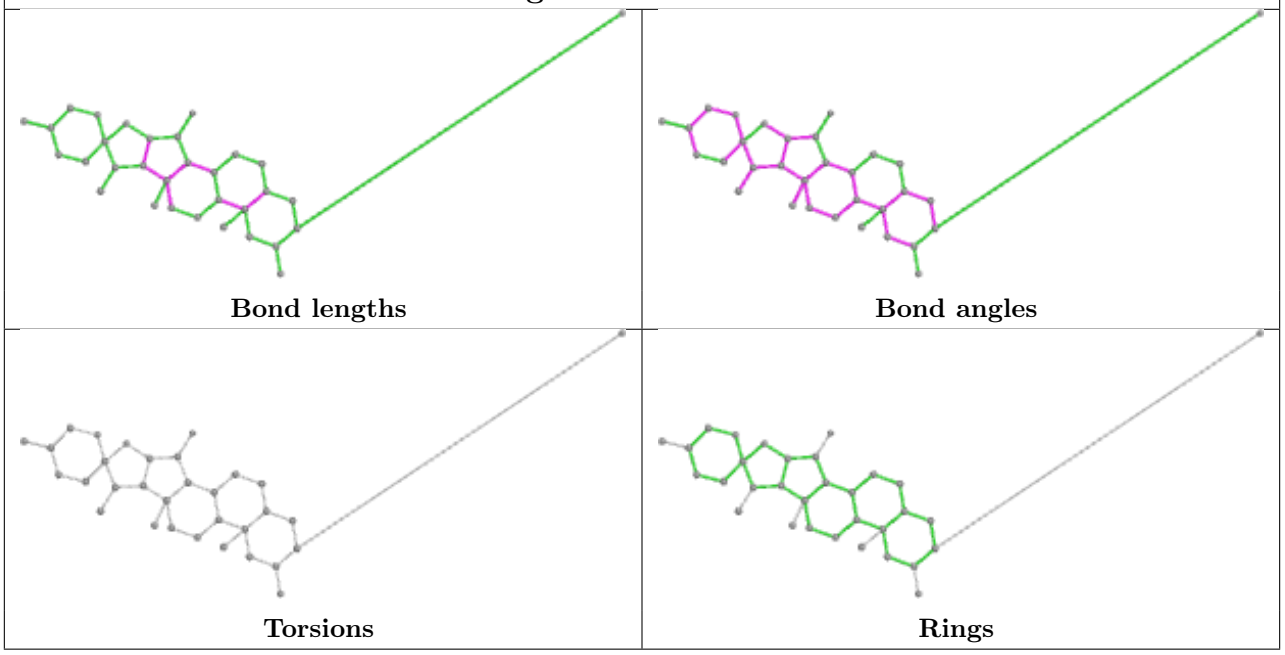
Ligand AJP G 305



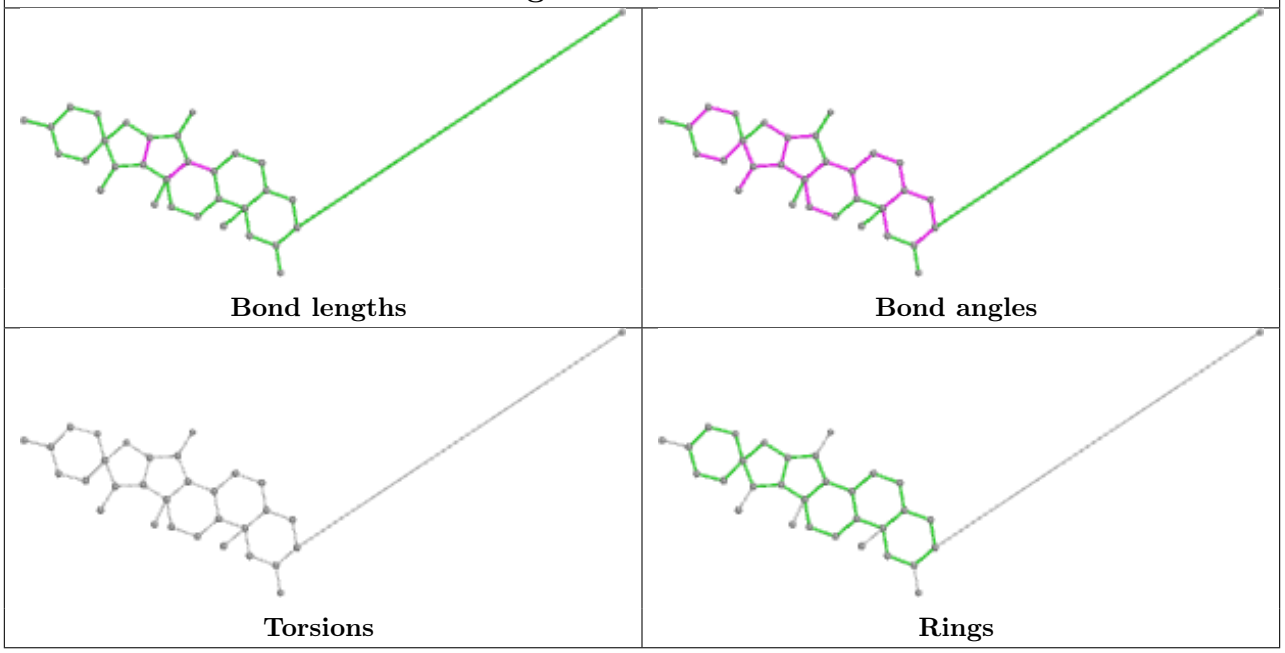
Ligand AJP B 607



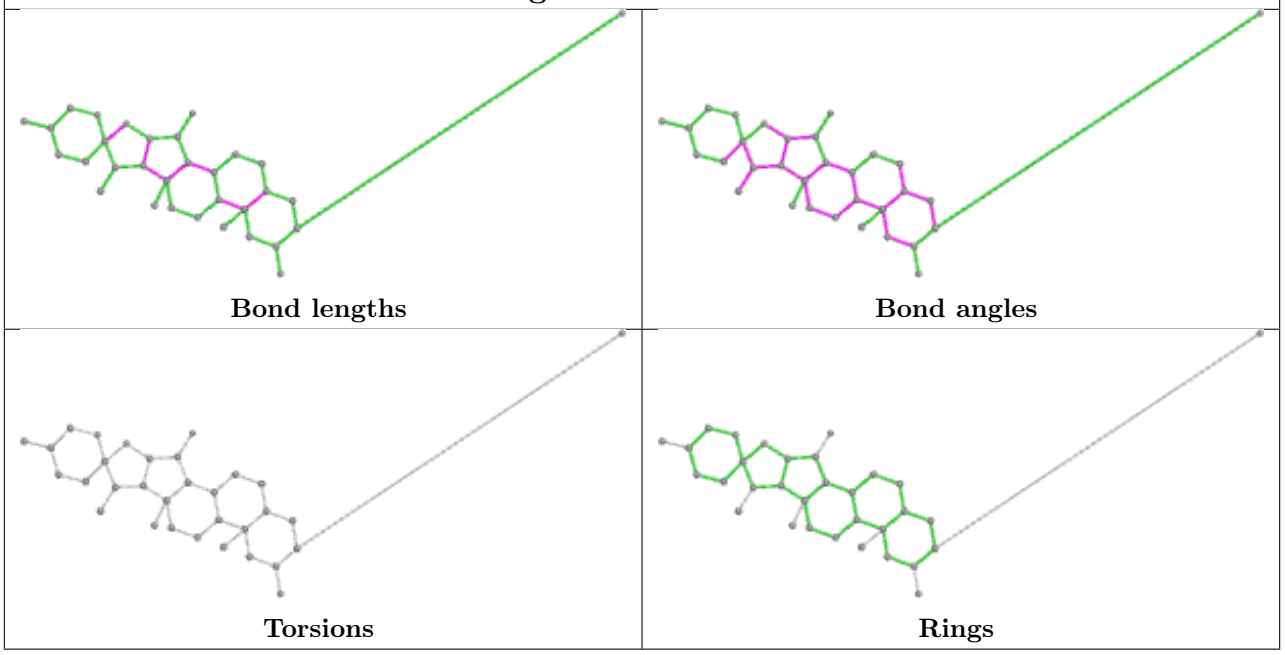
Ligand AJP G 307



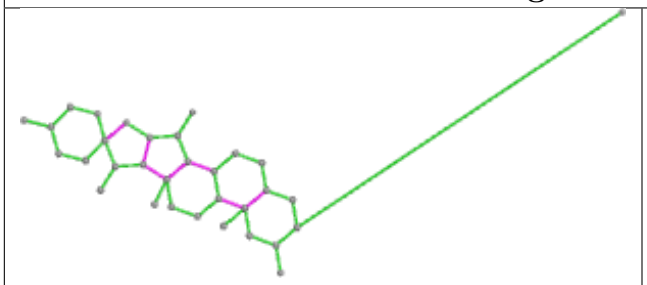
Ligand AJP A 407



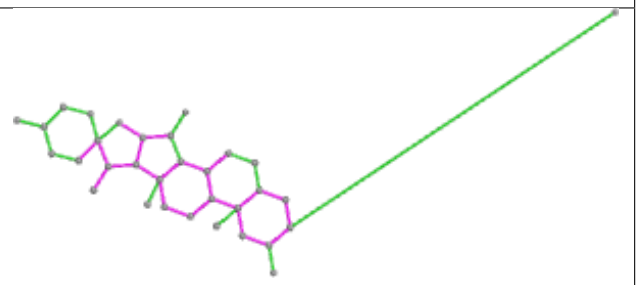
Ligand AJP F 711



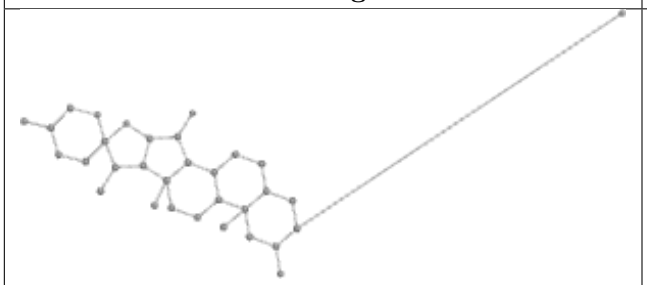
Ligand AJP B 614



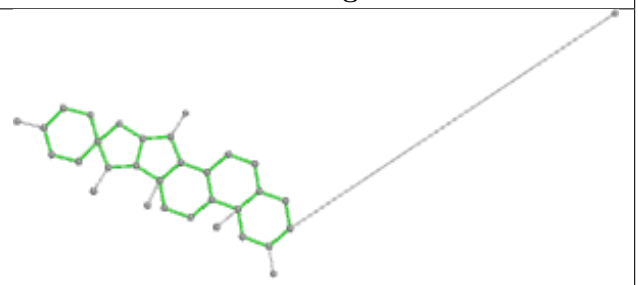
Bond lengths



Bond angles

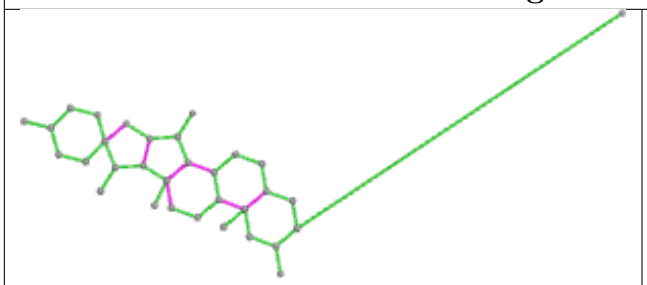


Torsions

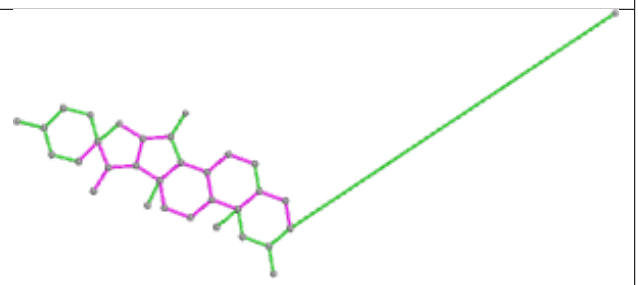


Rings

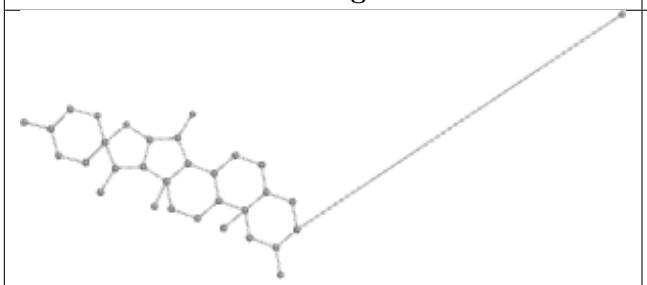
Ligand AJP D 613



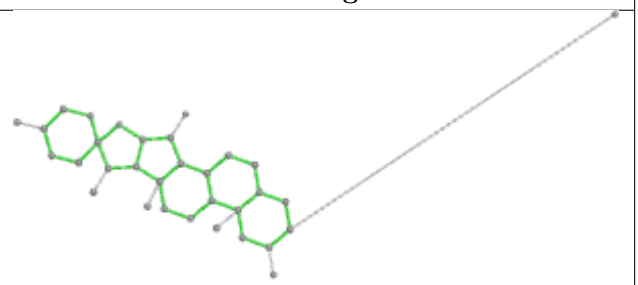
Bond lengths



Bond angles

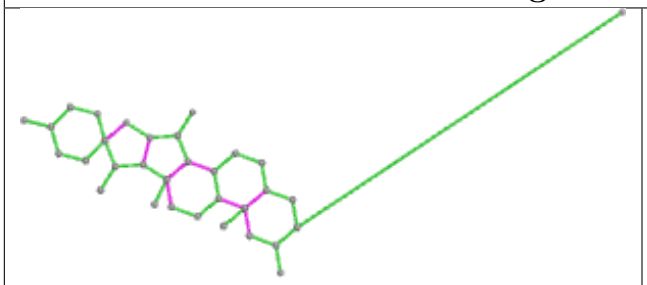


Torsions

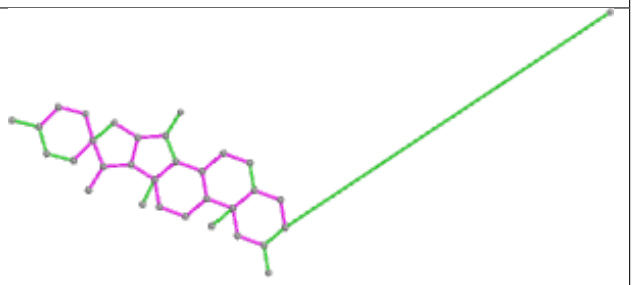


Rings

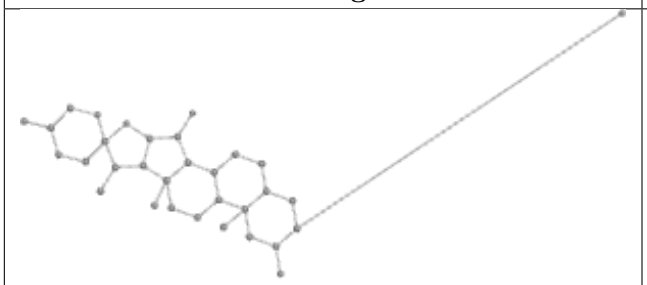
Ligand AJP F 712



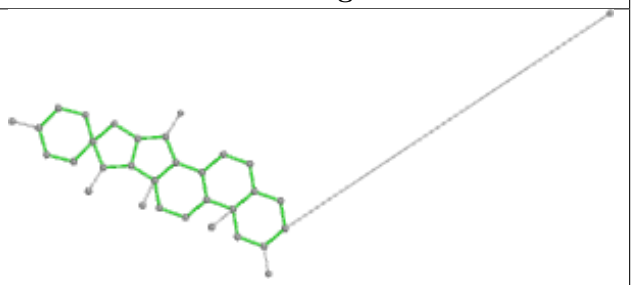
Bond lengths



Bond angles

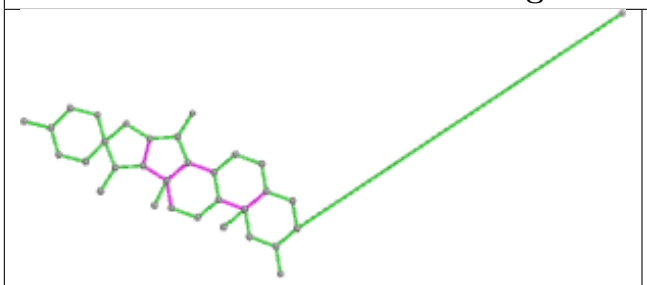


Torsions

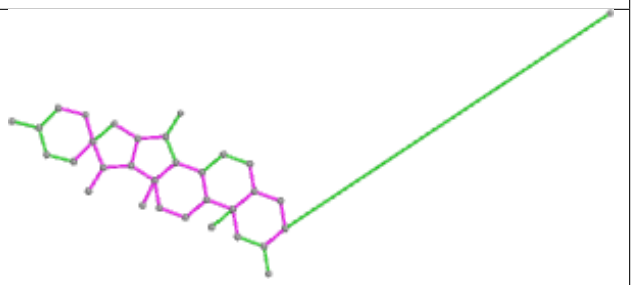


Rings

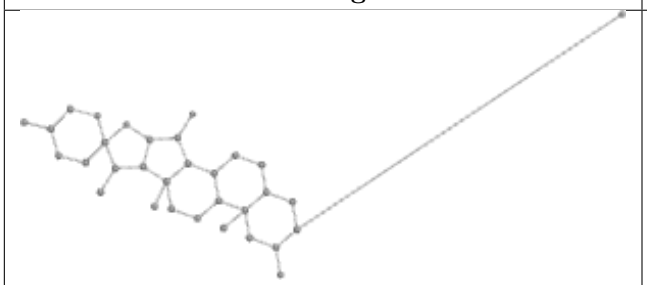
Ligand AJP G 302



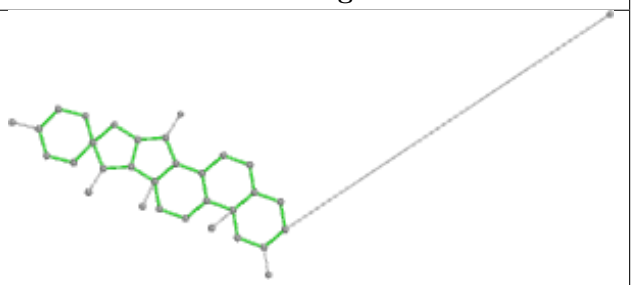
Bond lengths



Bond angles

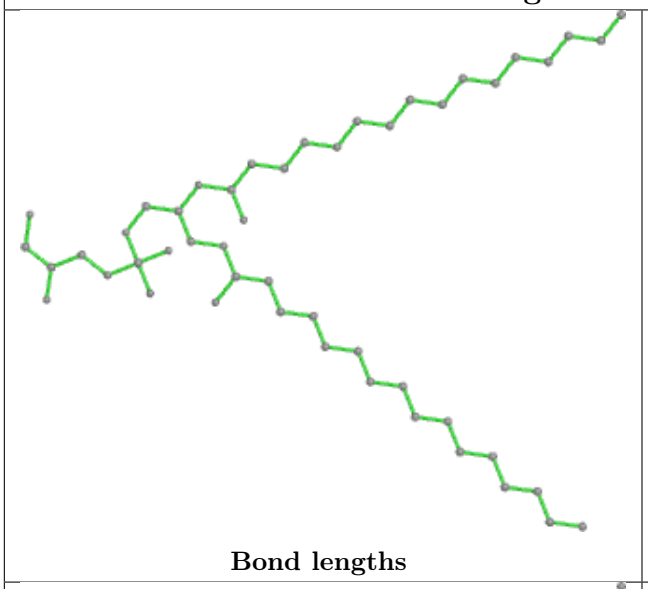


Torsions

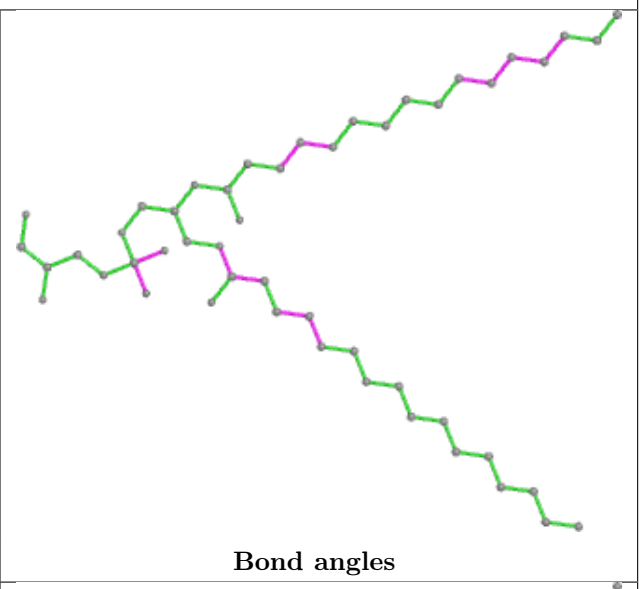


Rings

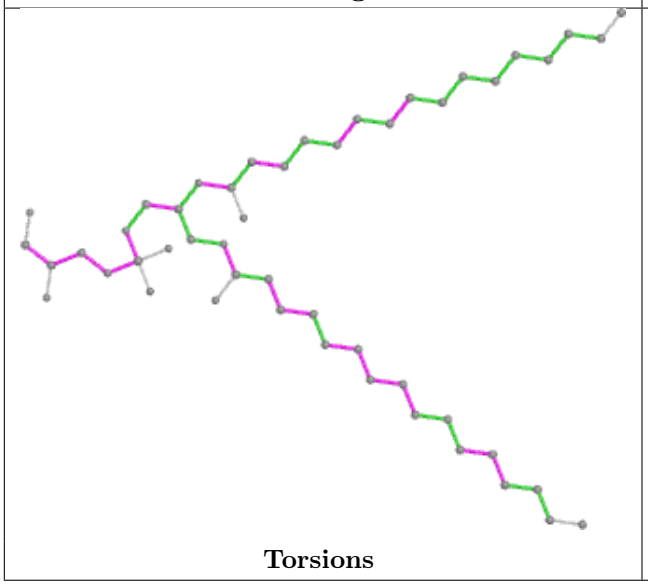
Ligand LHG B 602



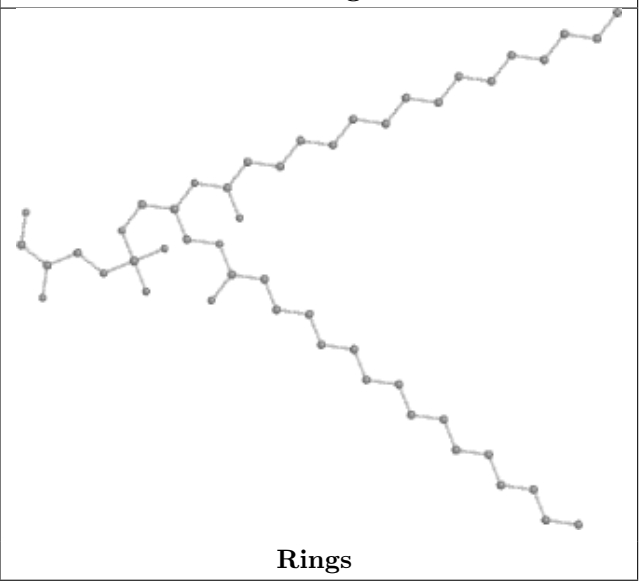
Bond lengths



Bond angles

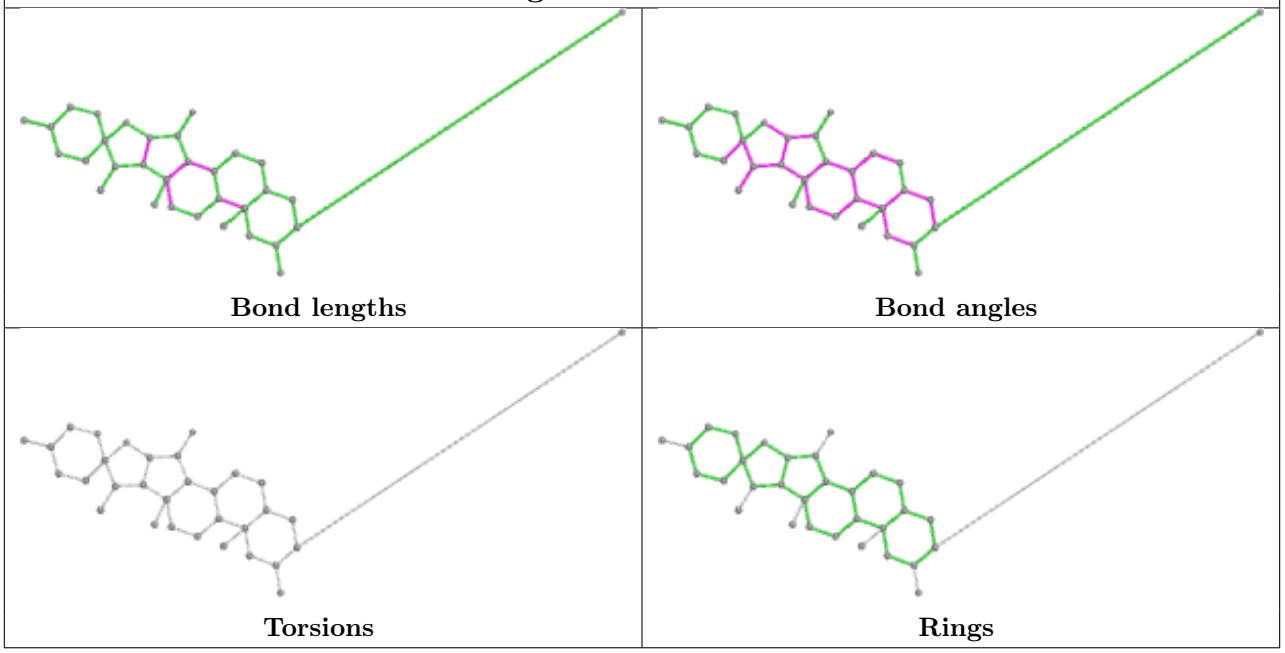


Torsions

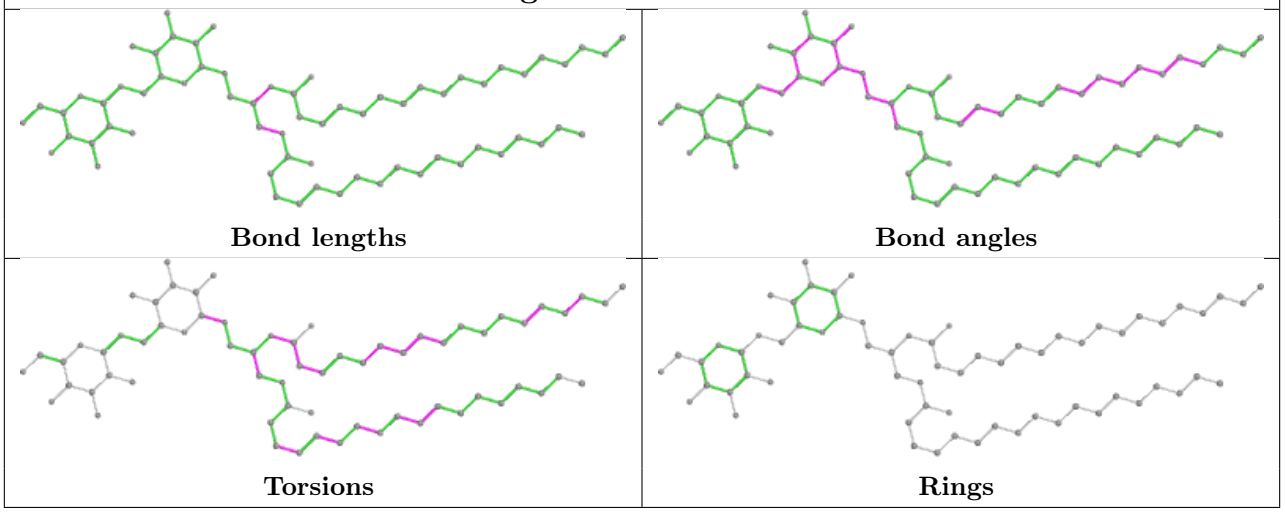


Rings

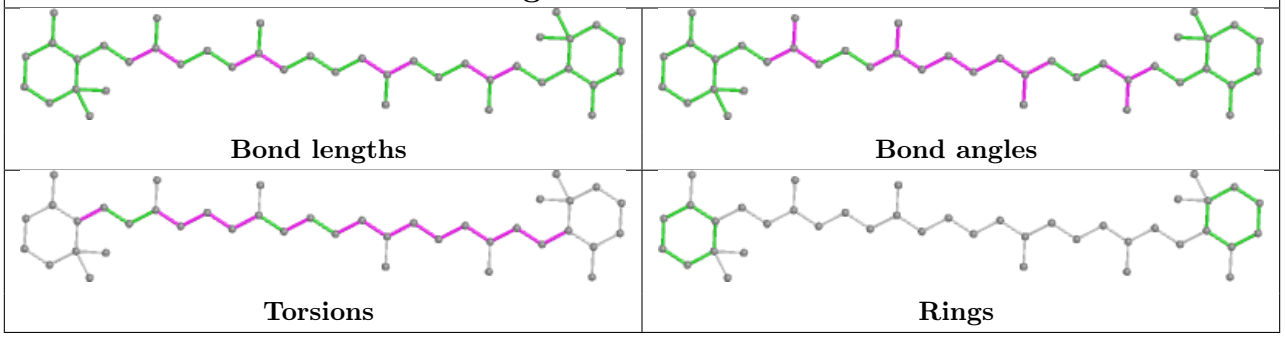
Ligand AJP D 611



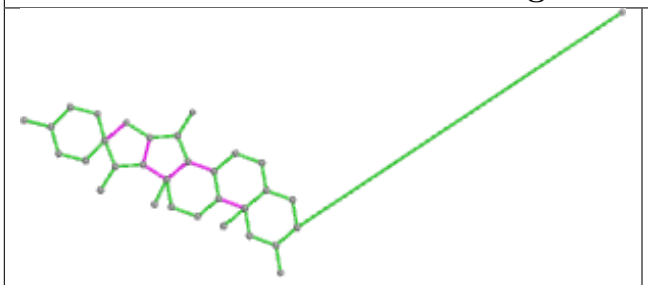
Ligand DGD A 404



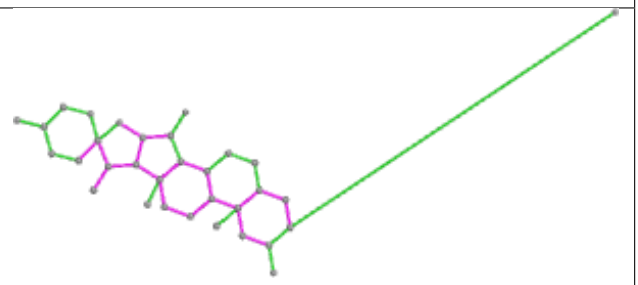
Ligand BCR A 401



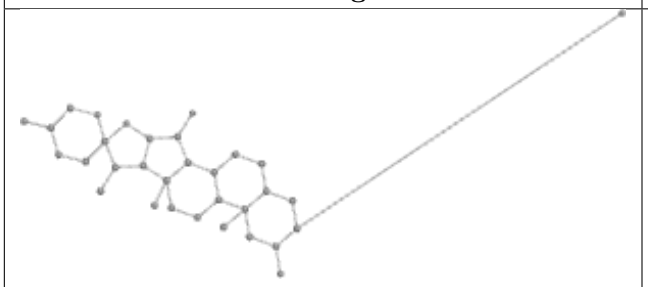
Ligand AJP B 612



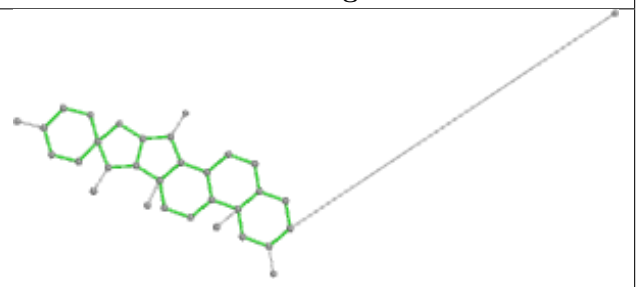
Bond lengths



Bond angles

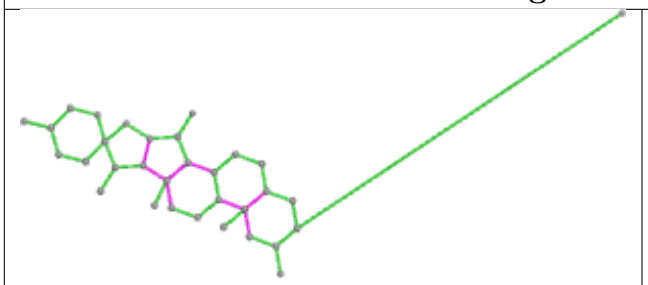


Torsions

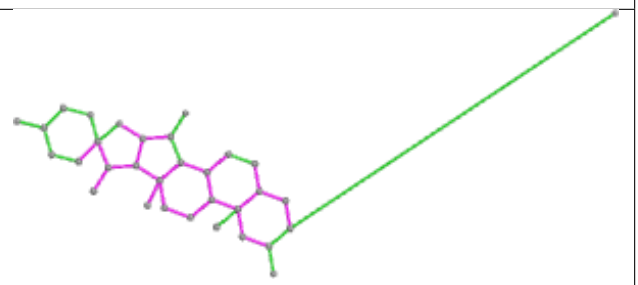


Rings

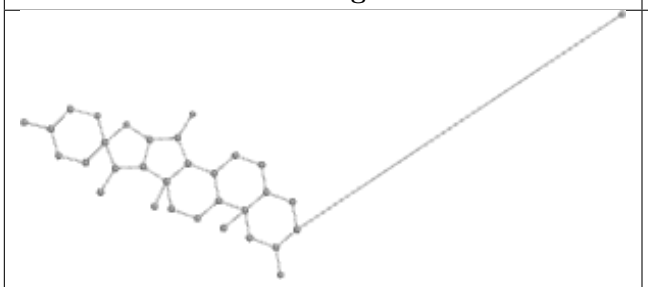
Ligand AJP F 705



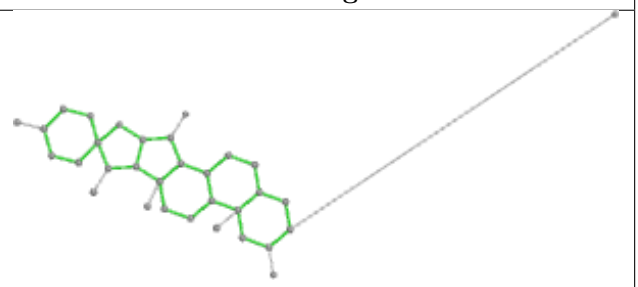
Bond lengths



Bond angles

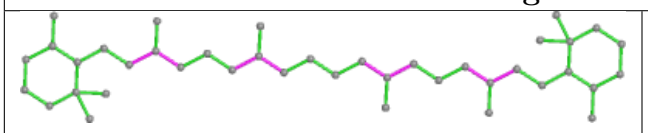


Torsions

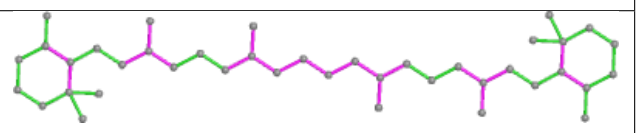


Rings

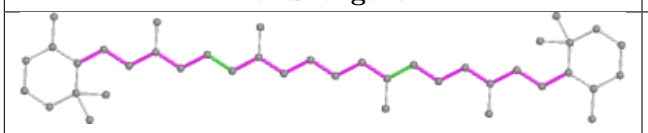
Ligand BCR D 601



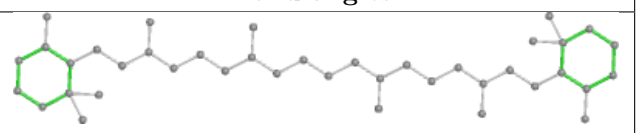
Bond lengths



Bond angles

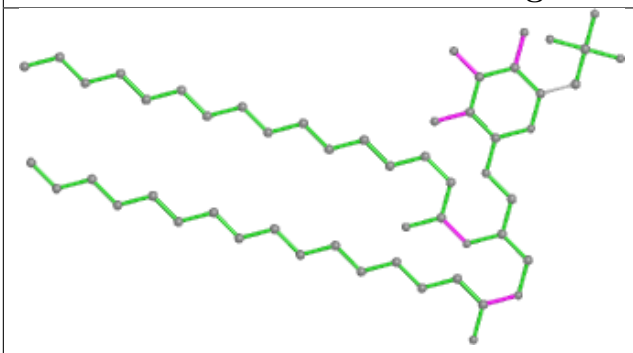


Torsions

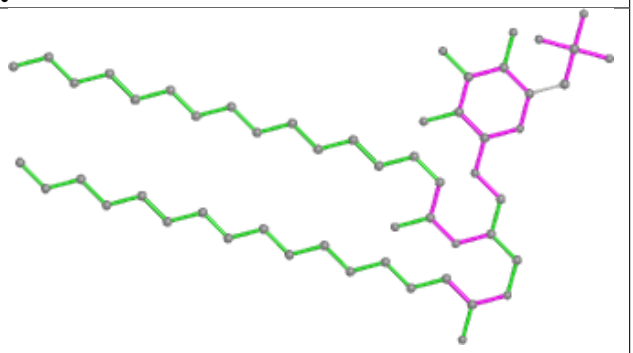


Rings

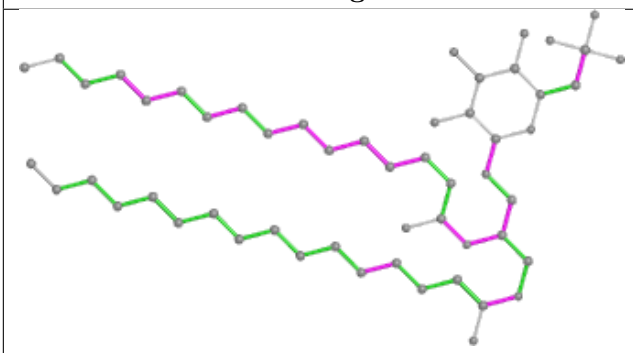
Ligand SQD F 703



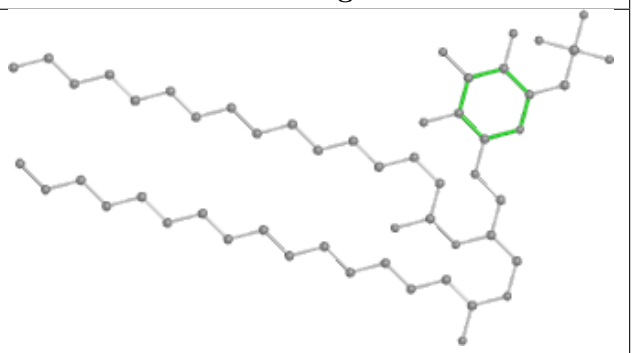
Bond lengths



Bond angles

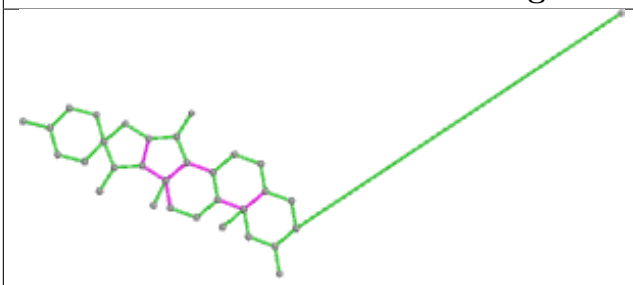


Torsions

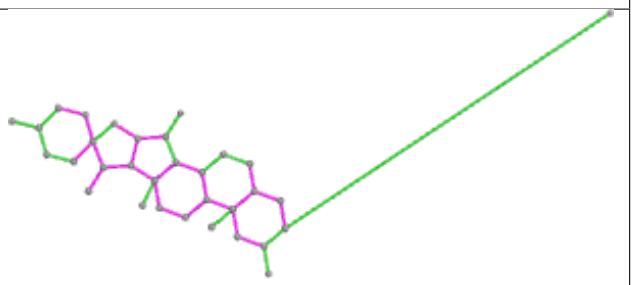


Rings

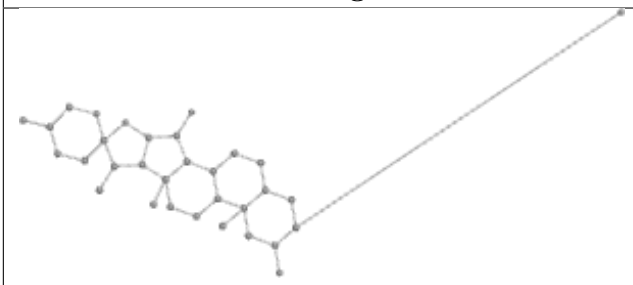
Ligand AJP F 706



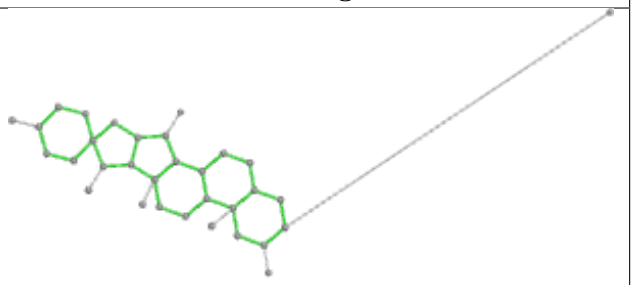
Bond lengths



Bond angles

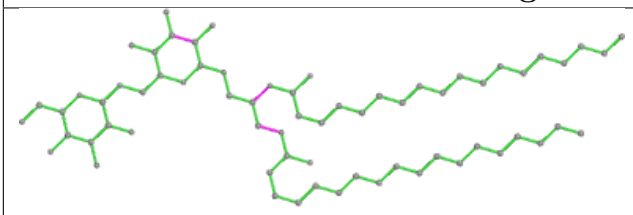


Torsions

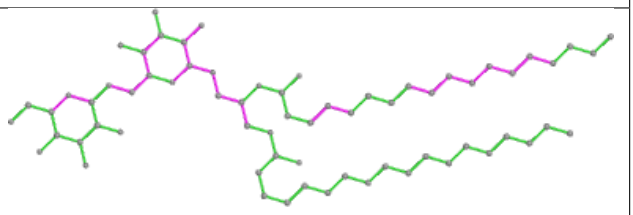


Rings

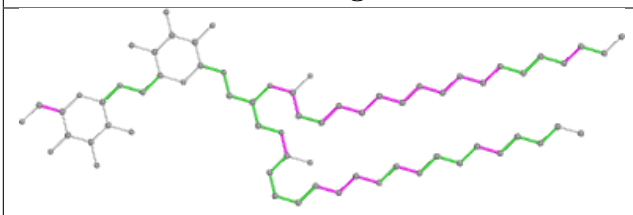
Ligand DGD A 405



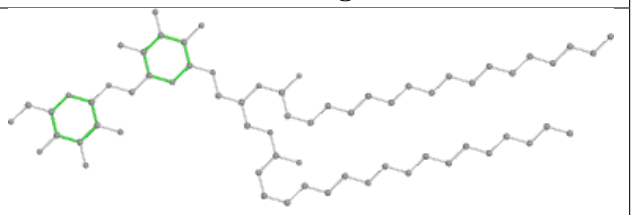
Bond lengths



Bond angles

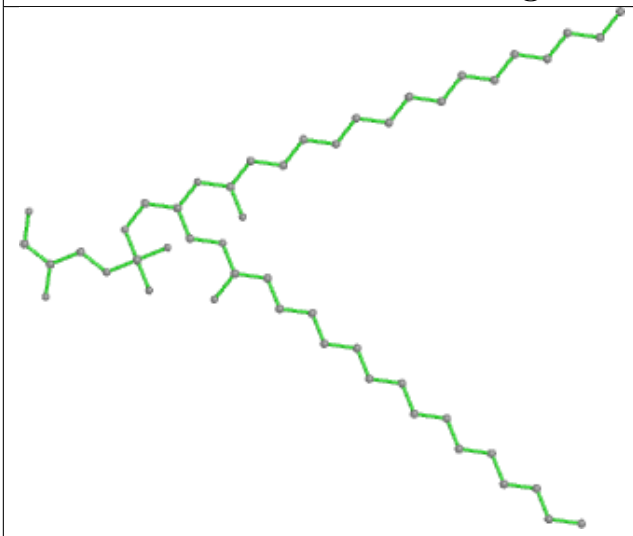


Torsions

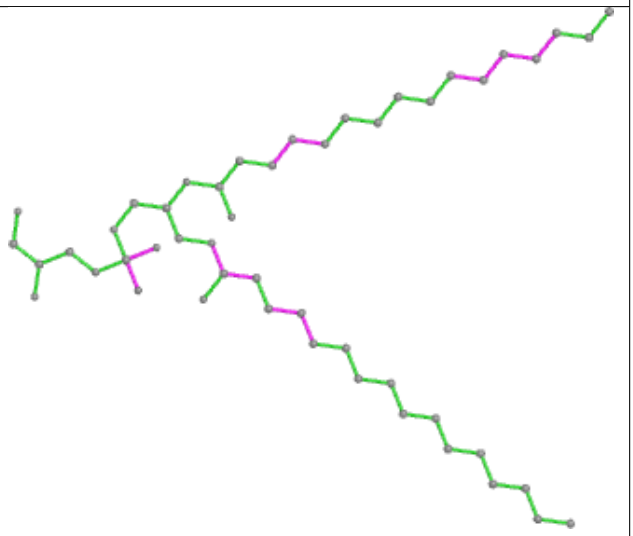


Rings

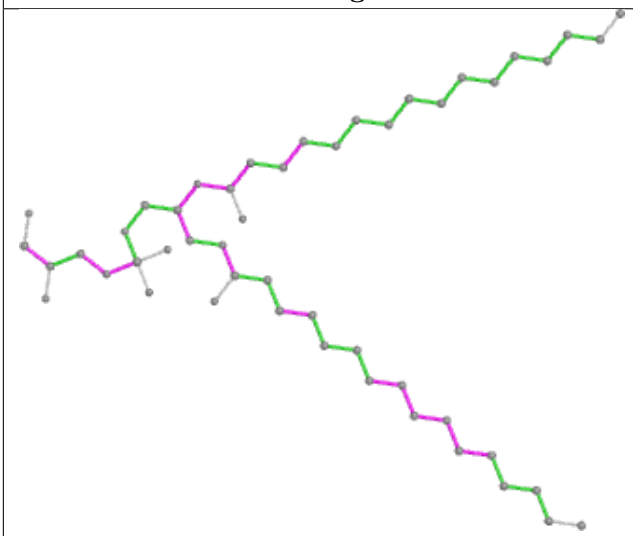
Ligand LHG A 402



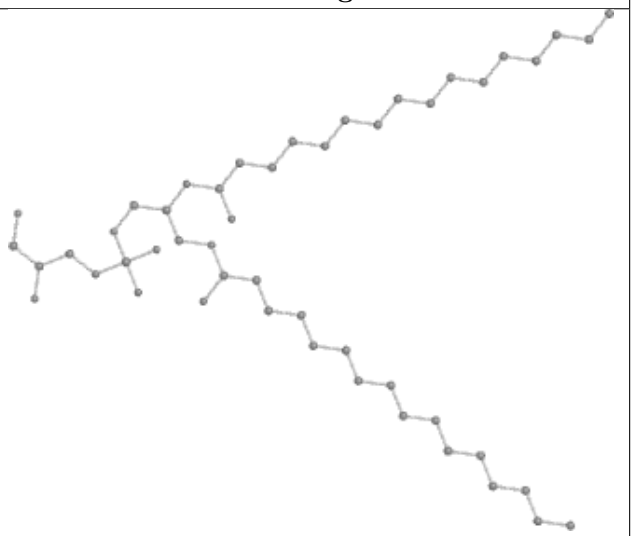
Bond lengths



Bond angles

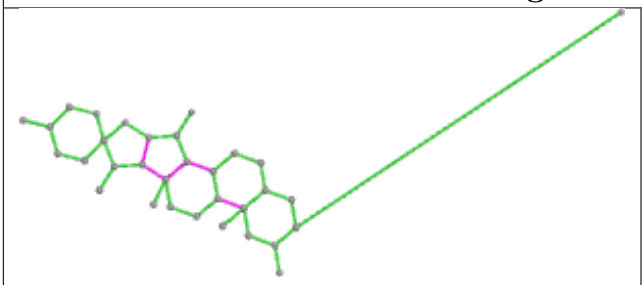


Torsions

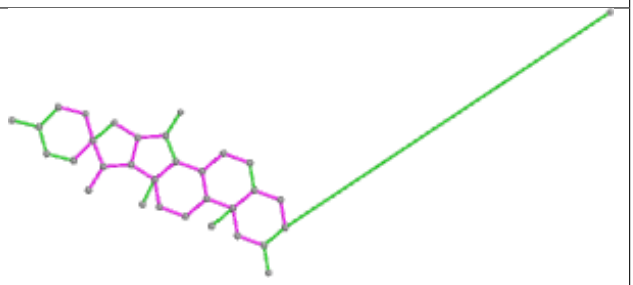


Rings

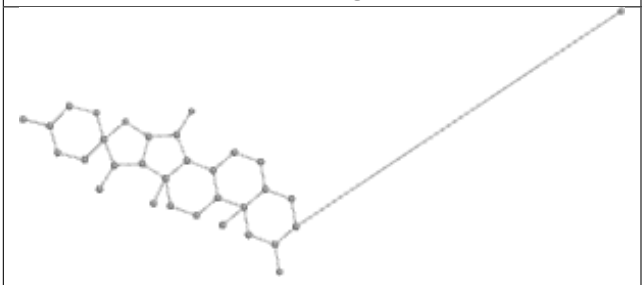
Ligand AJP B 605



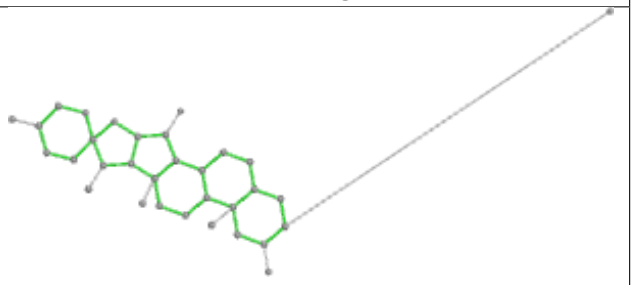
Bond lengths



Bond angles

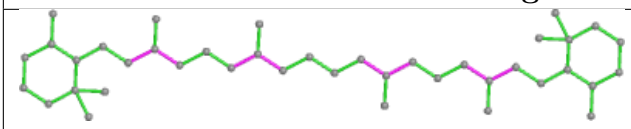


Torsions



Rings

Ligand BCR D 602



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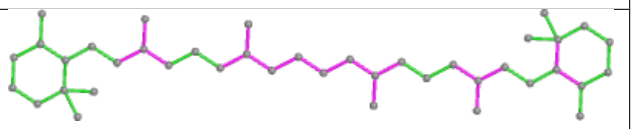
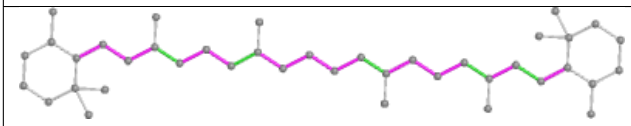
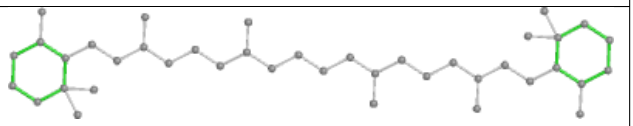


Bond angles

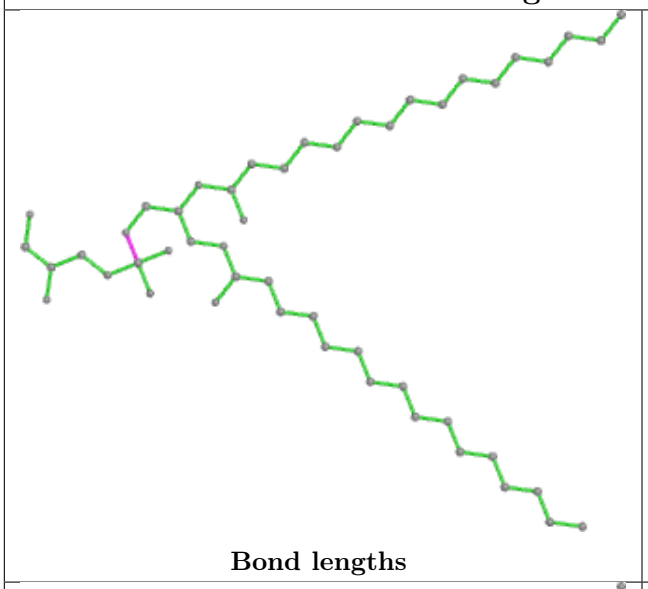


Torsions

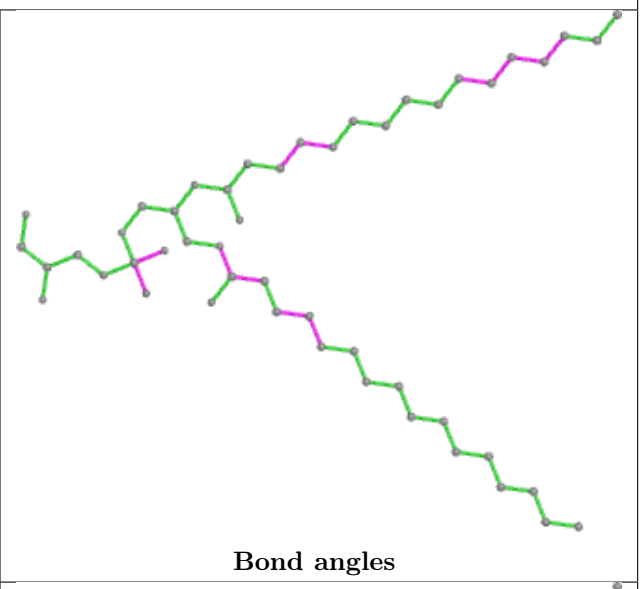


Rings

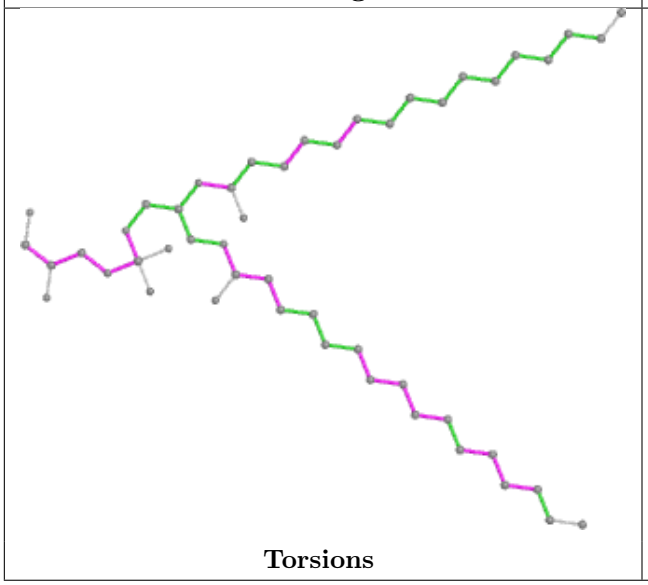
Ligand LHG D 603



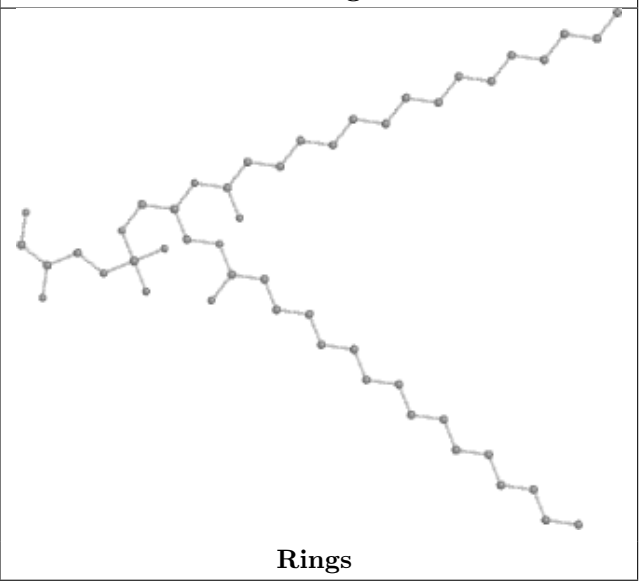
Bond lengths



Bond angles

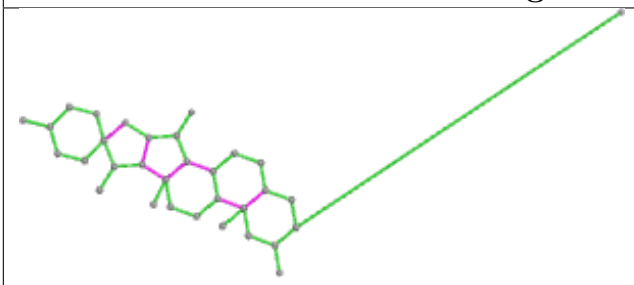


Torsions

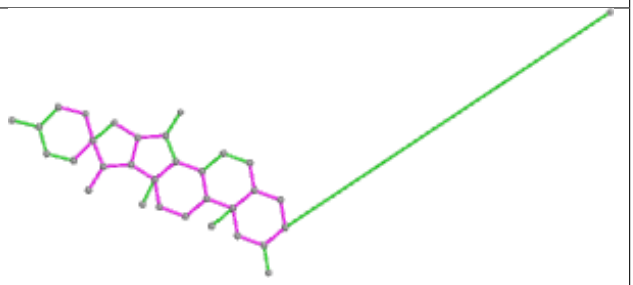


Rings

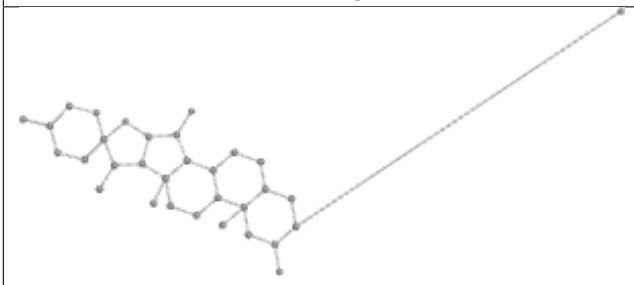
Ligand AJP B 611



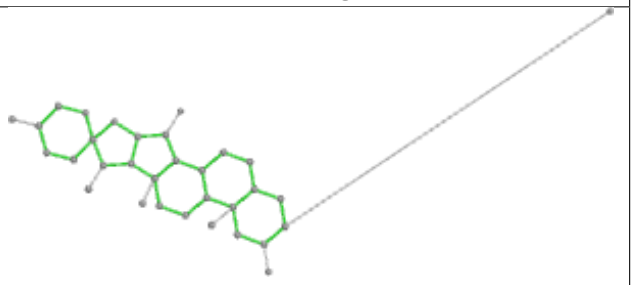
Bond lengths



Bond angles

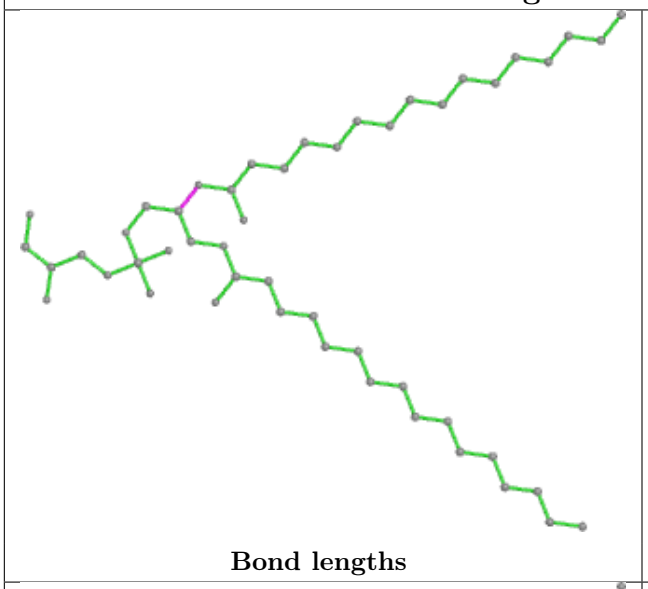


Torsions

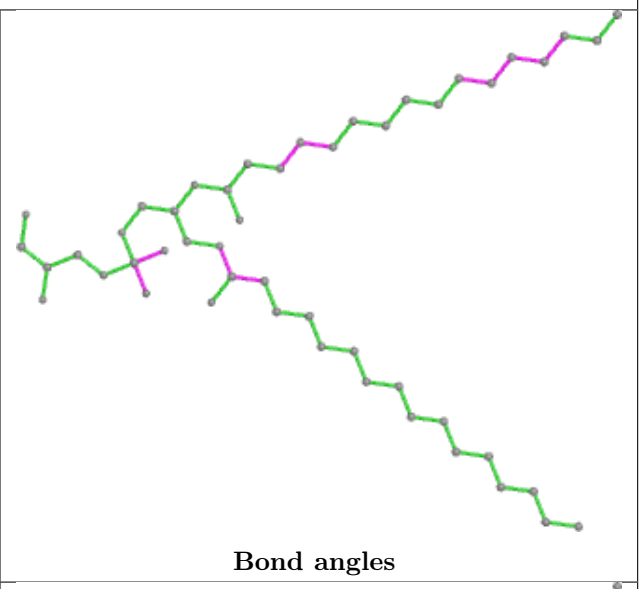


Rings

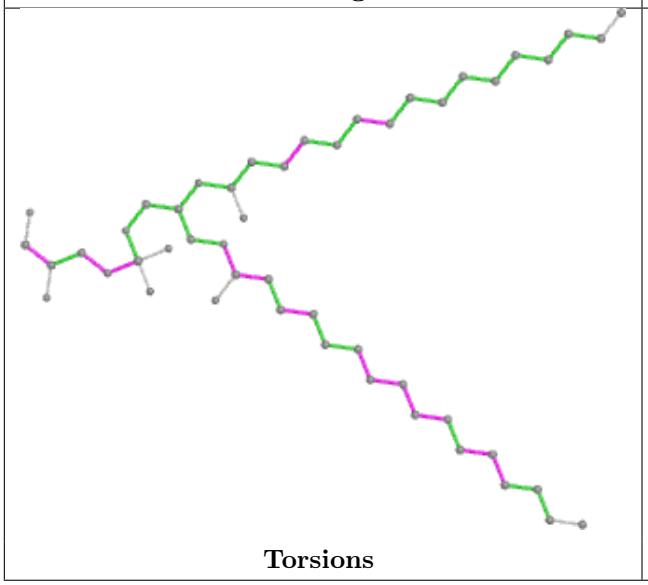
Ligand LHG A 403



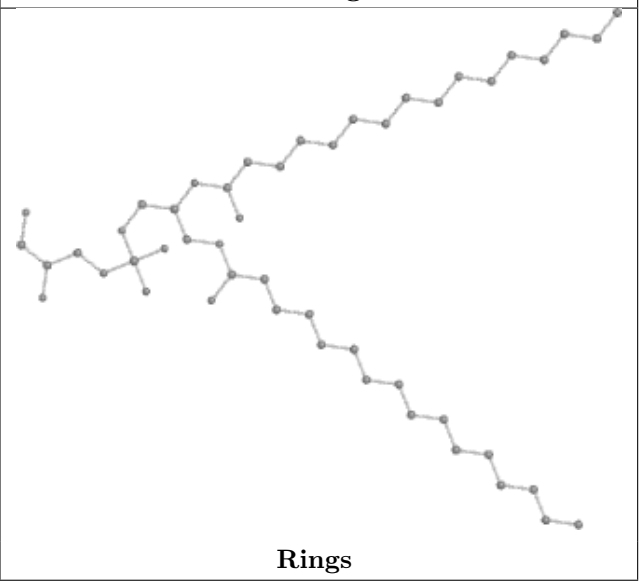
Bond lengths



Bond angles

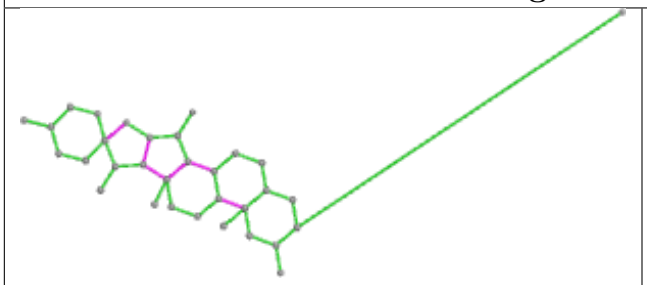


Torsions

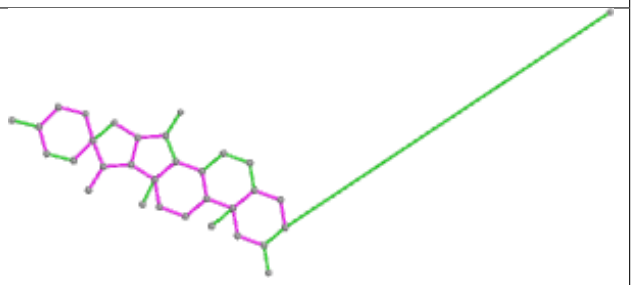


Rings

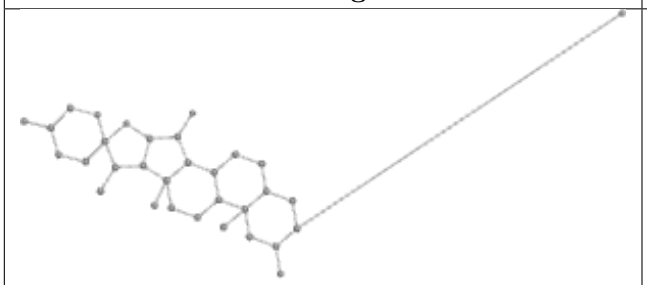
Ligand AJP F 704



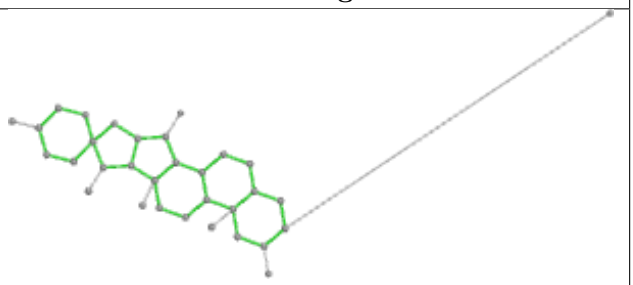
Bond lengths



Bond angles

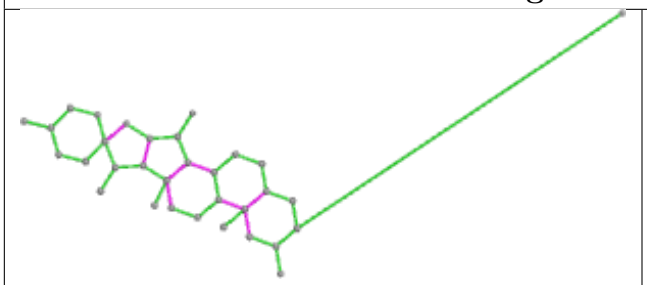


Torsions

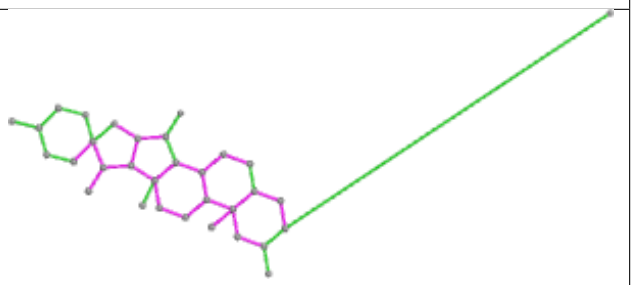


Rings

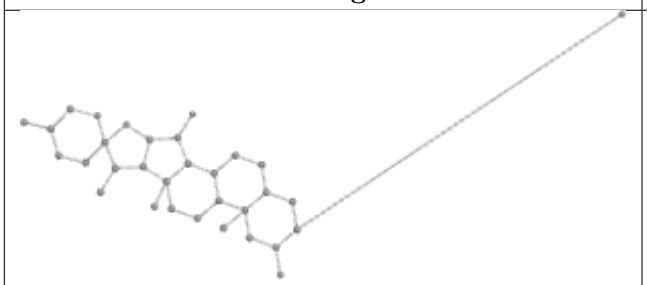
Ligand AJP G 304



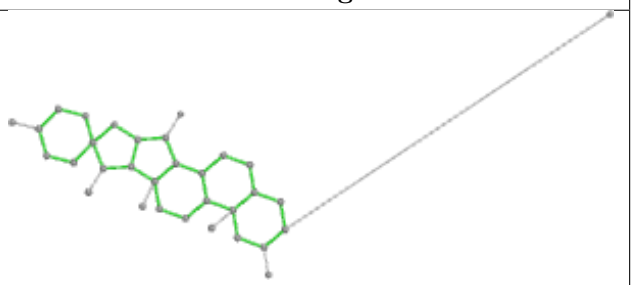
Bond lengths



Bond angles

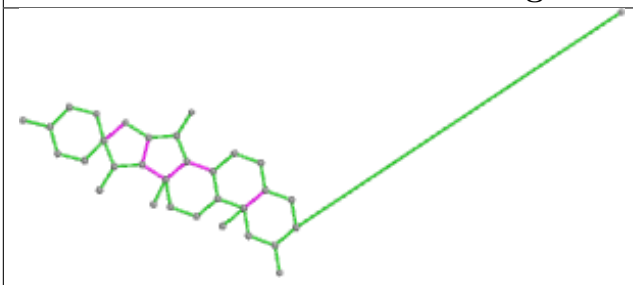


Torsions

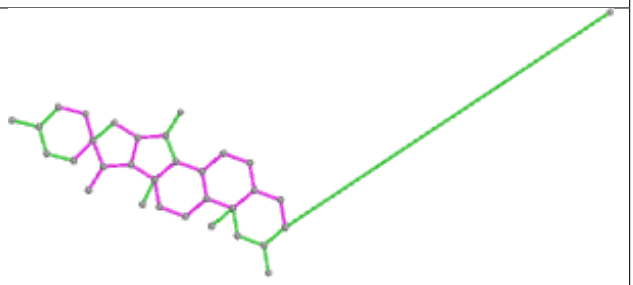


Rings

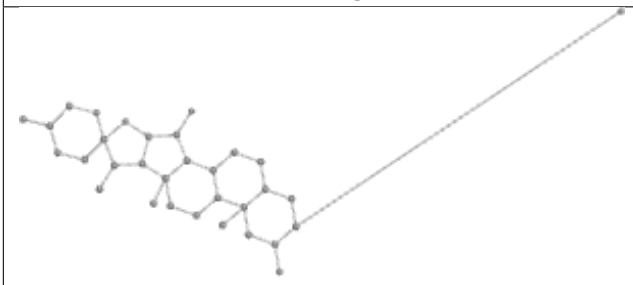
Ligand AJP A 408



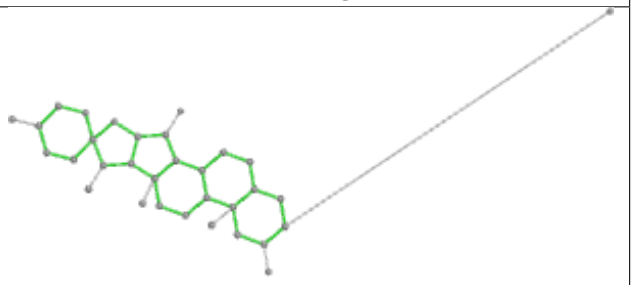
Bond lengths



Bond angles

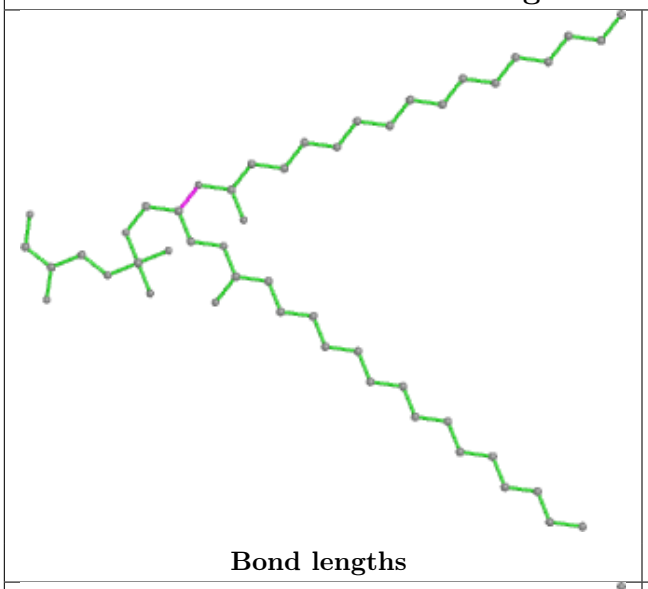


Torsions

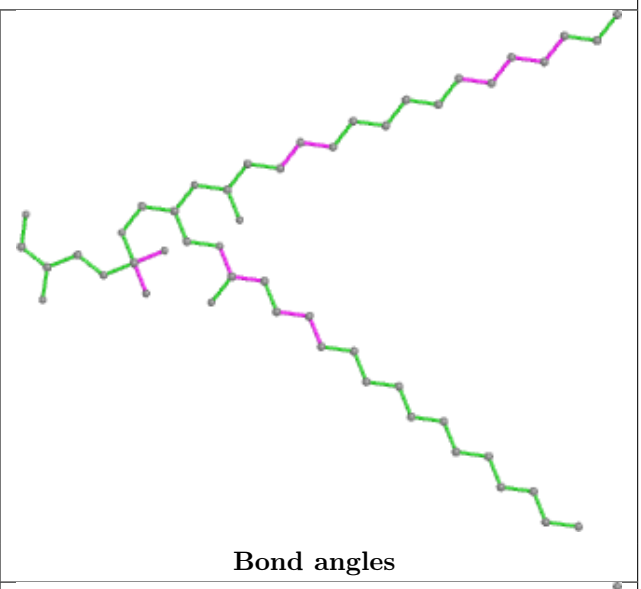


Rings

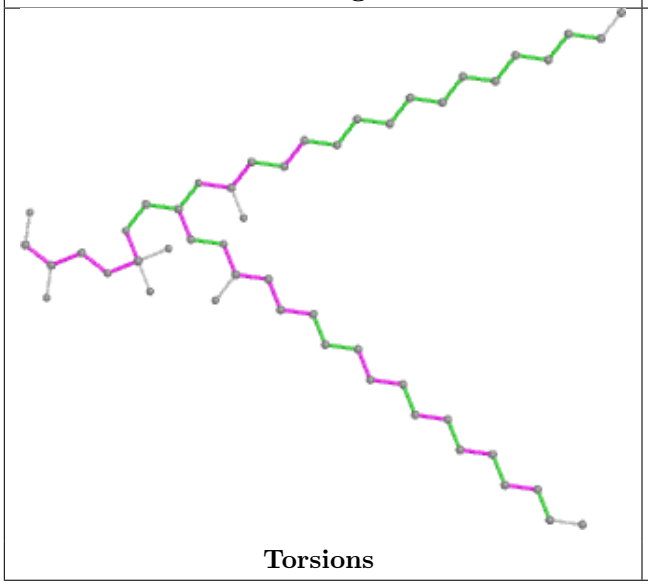
Ligand LHG D 604



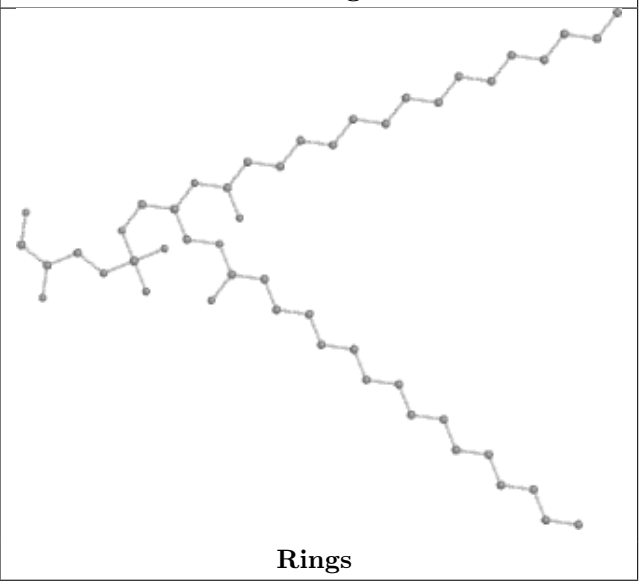
Bond lengths



Bond angles

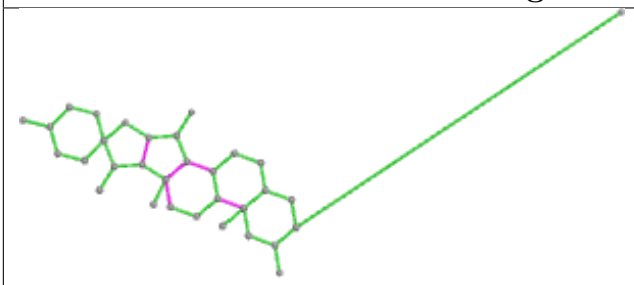


Torsions

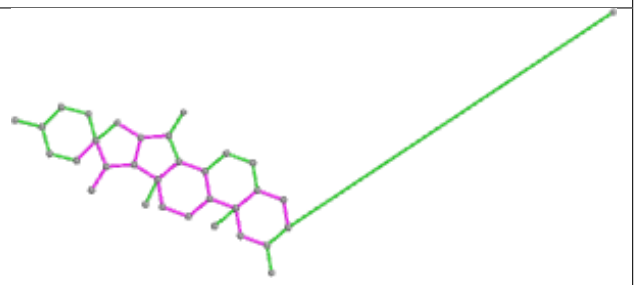


Rings

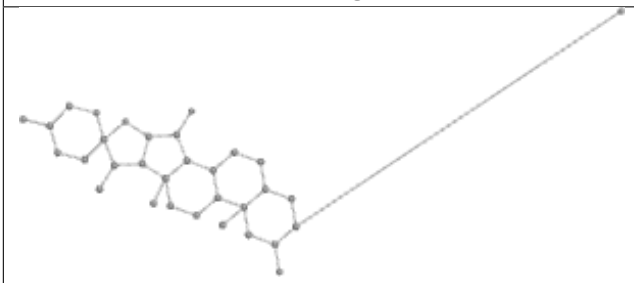
Ligand AJP B 613



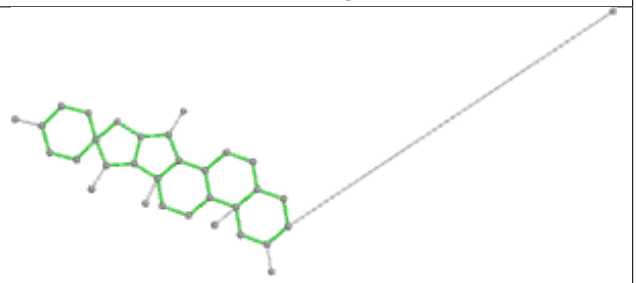
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Map visualisation

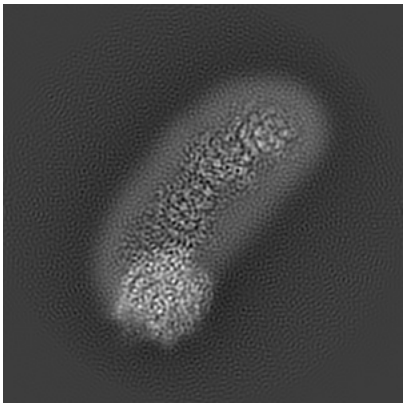
This section contains visualisations of the EMDB entry EMD-0850. These allow visual inspection of the internal detail of the map and identification of artifacts.

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.

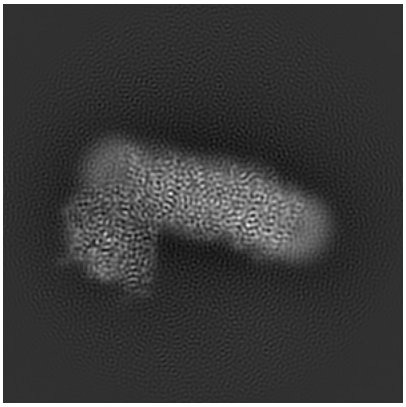
6.1 Orthogonal projections

6.1.1 Primary map

X



Y

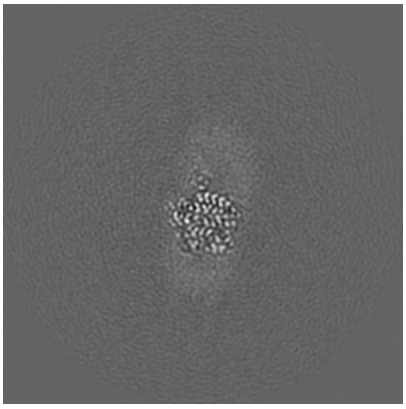


Z

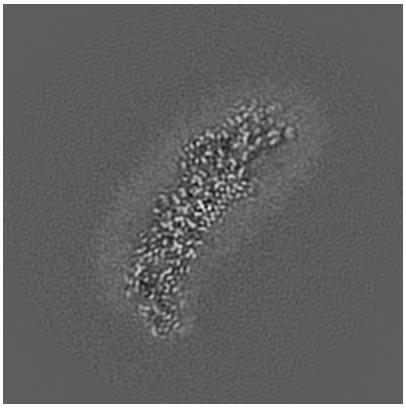
The images above show the map projected in three orthogonal directions.

6.2 Central slices

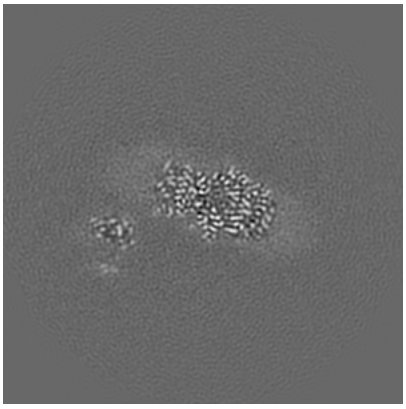
6.2.1 Primary map



X Index: 150



Y Index: 150

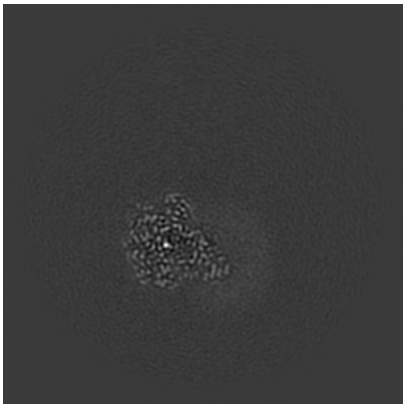


Z Index: 150

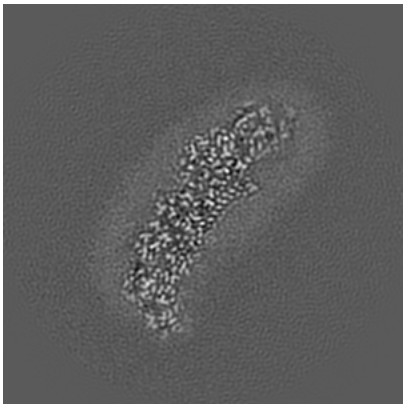
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

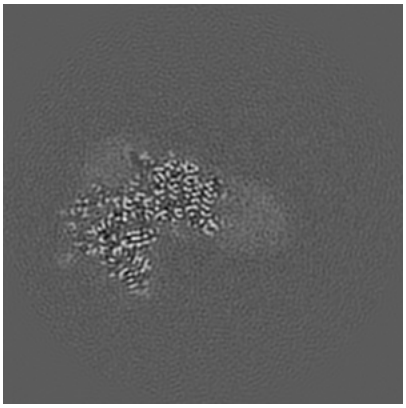
6.3.1 Primary map



X Index: 80



Y Index: 152

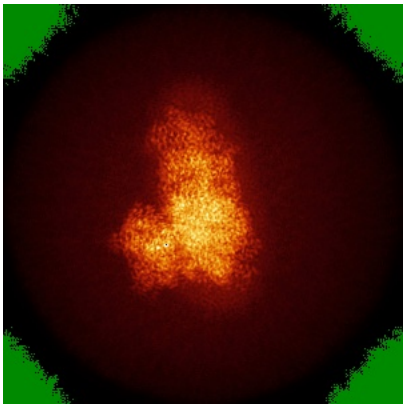


Z Index: 127

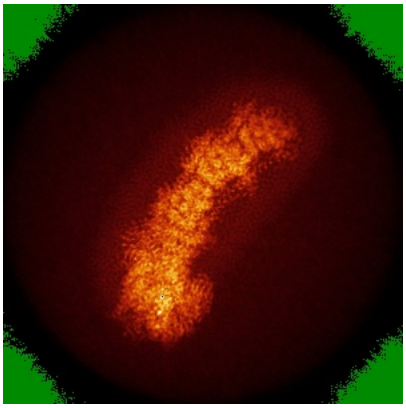
The images above show the largest variance slices of the map in three orthogonal directions.

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

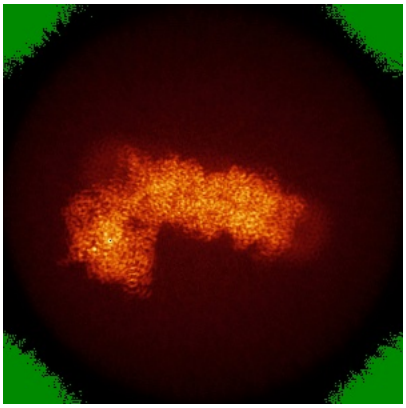
6.4.1 Primary map



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 0.0403. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

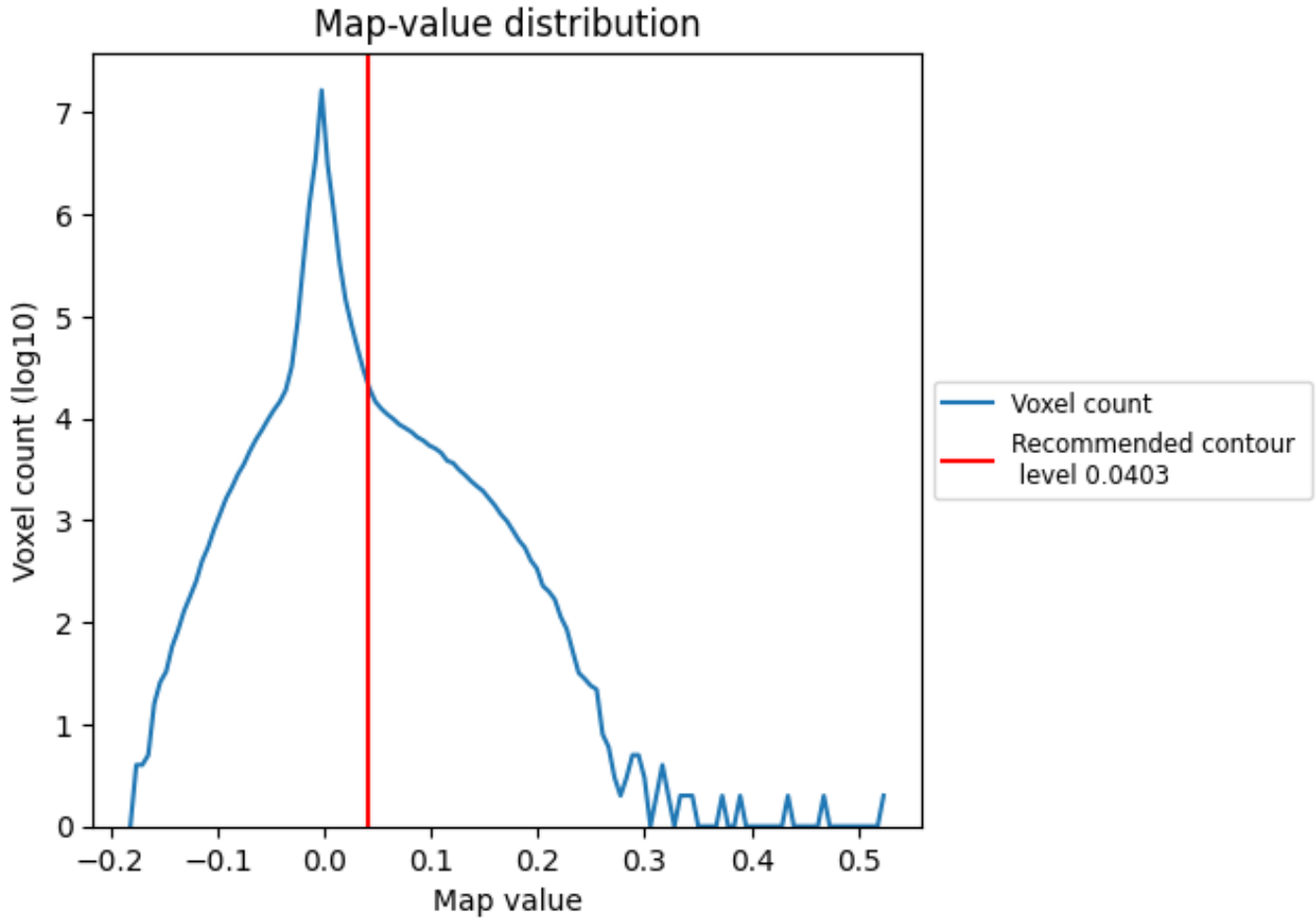
6.6 Mask visualisation (i)

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

7 Map analysis

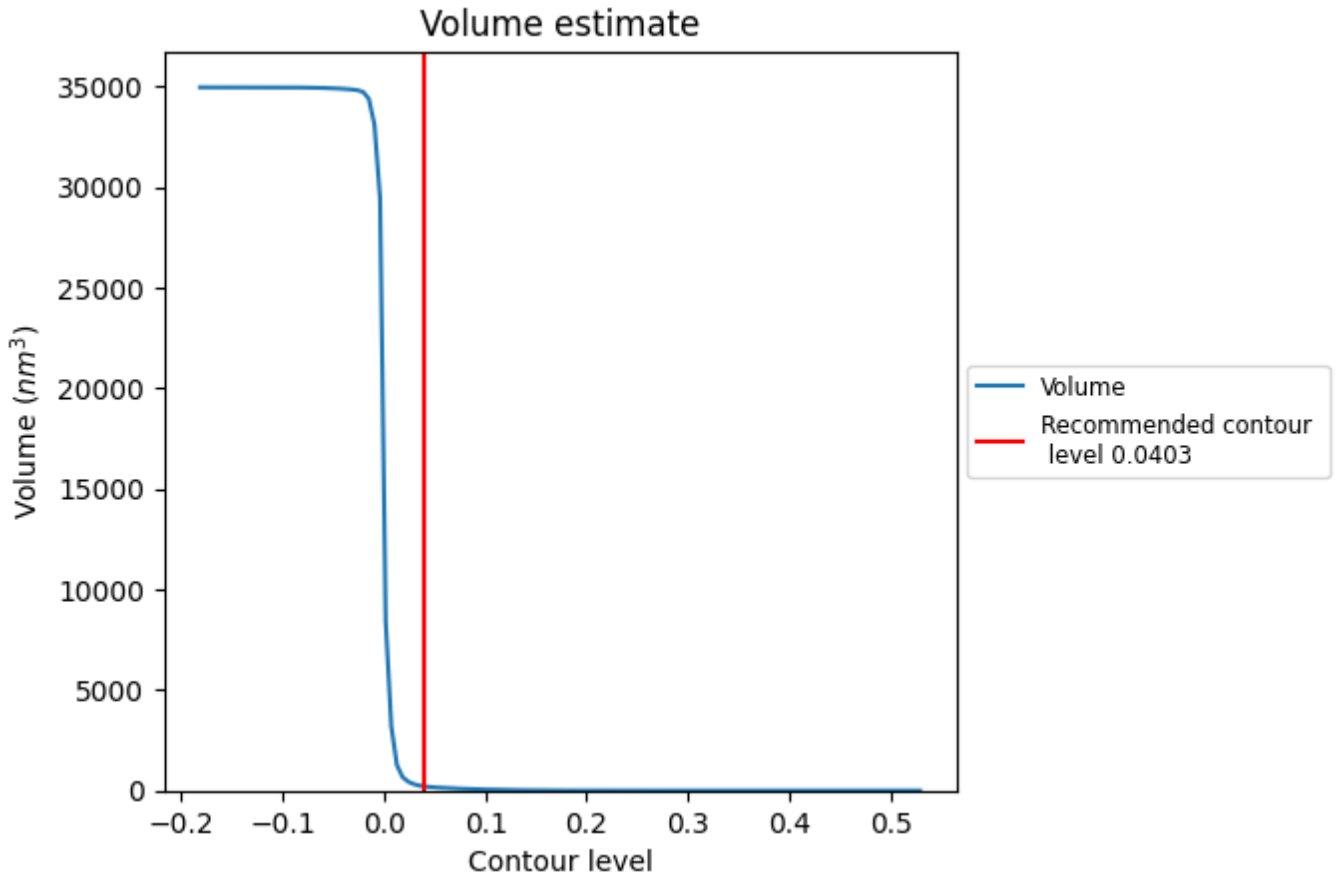
This section contains the results of statistical analysis of the map.

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.

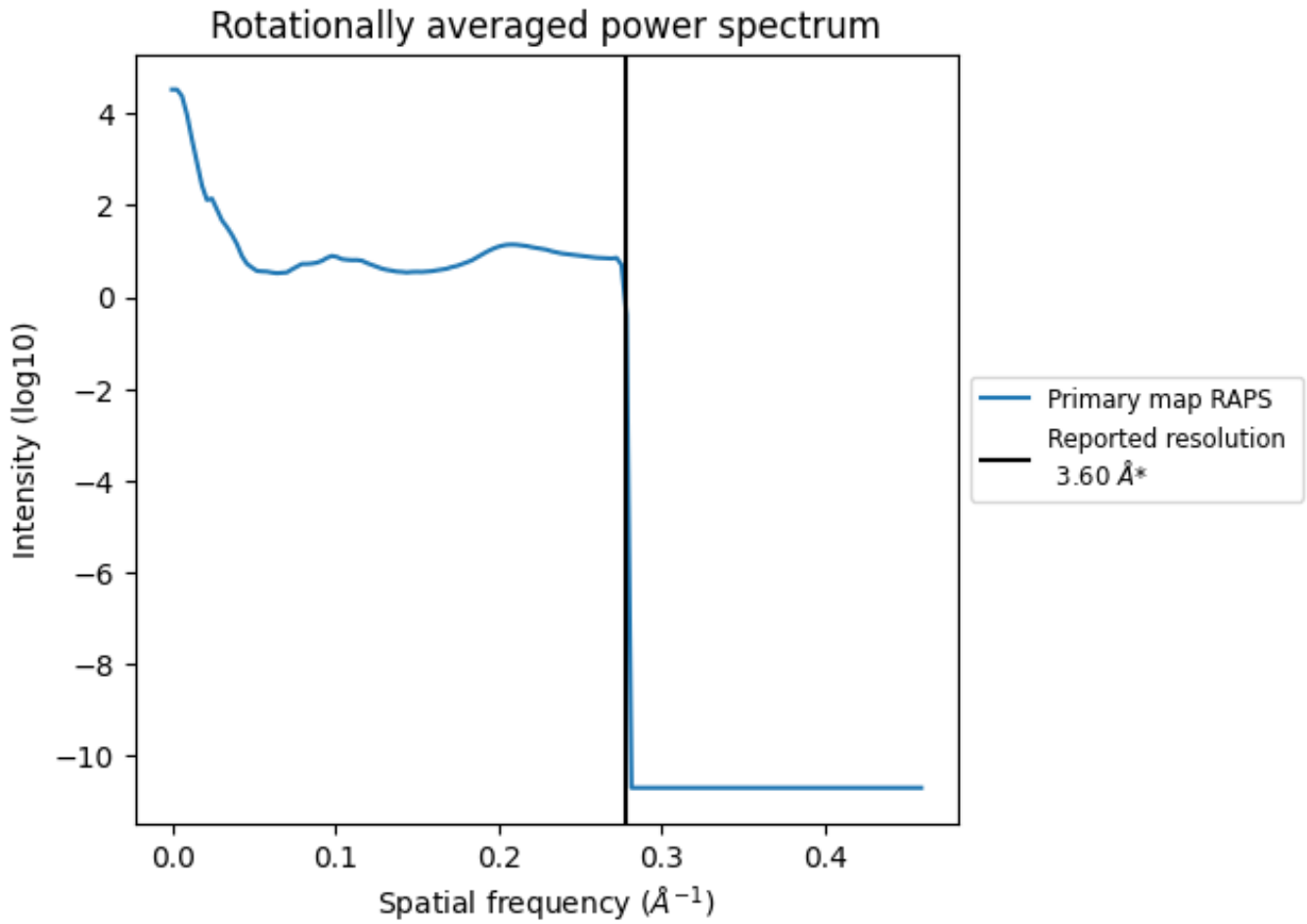
7.2 Volume estimate (i)



The volume at the recommended contour level is 204 nm^3; this corresponds to an approximate mass of 185 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 0.278 Å^{-1}

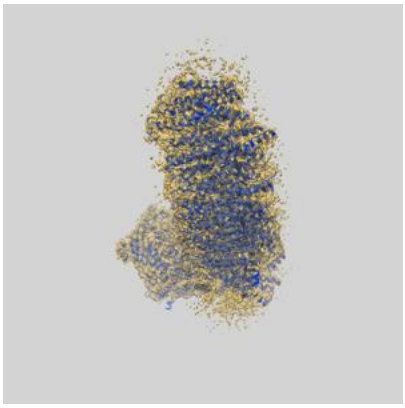
8 Fourier-Shell correlation (i)

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

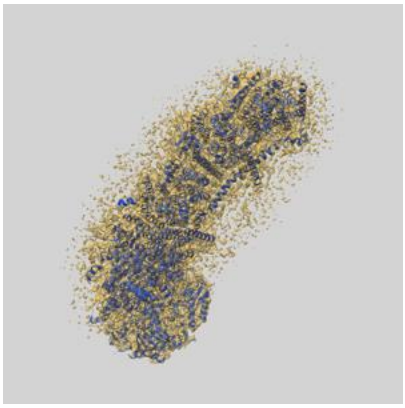
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-0850 and PDB model 6L7P. Per-residue inclusion information can be found in section 3 on page 15.

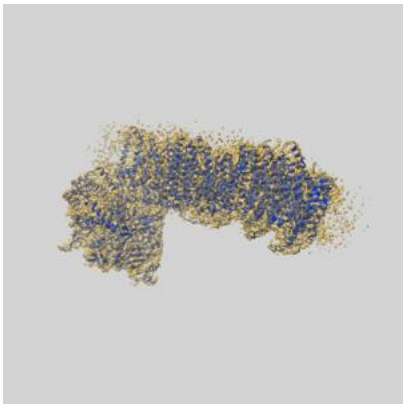
9.1 Map-model overlay



X



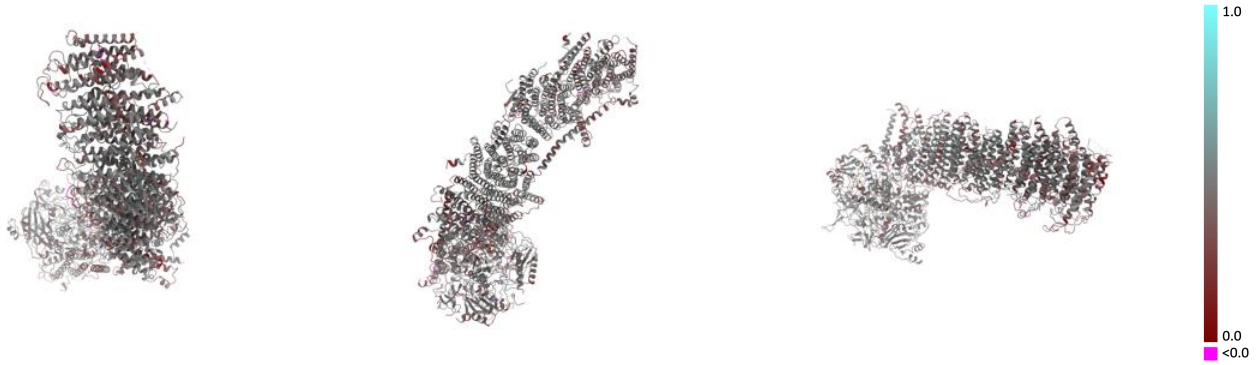
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0403 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.

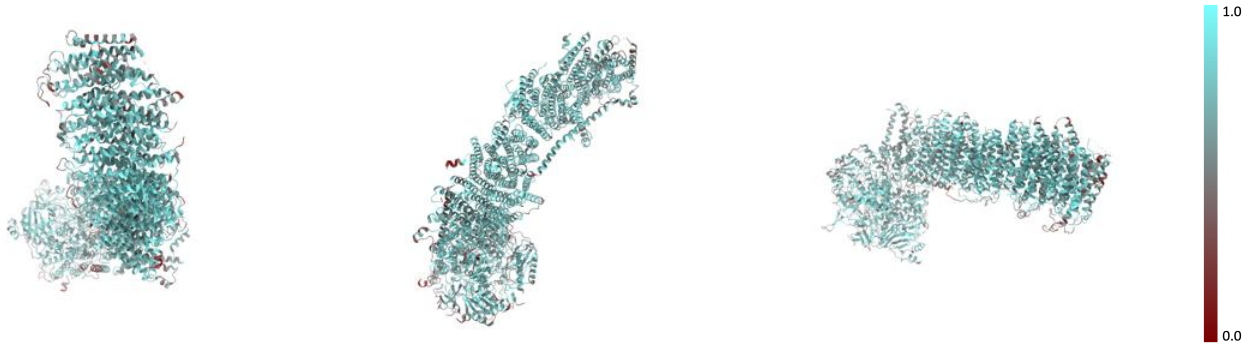
9.2 Q-score mapped to coordinate model (i)



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.

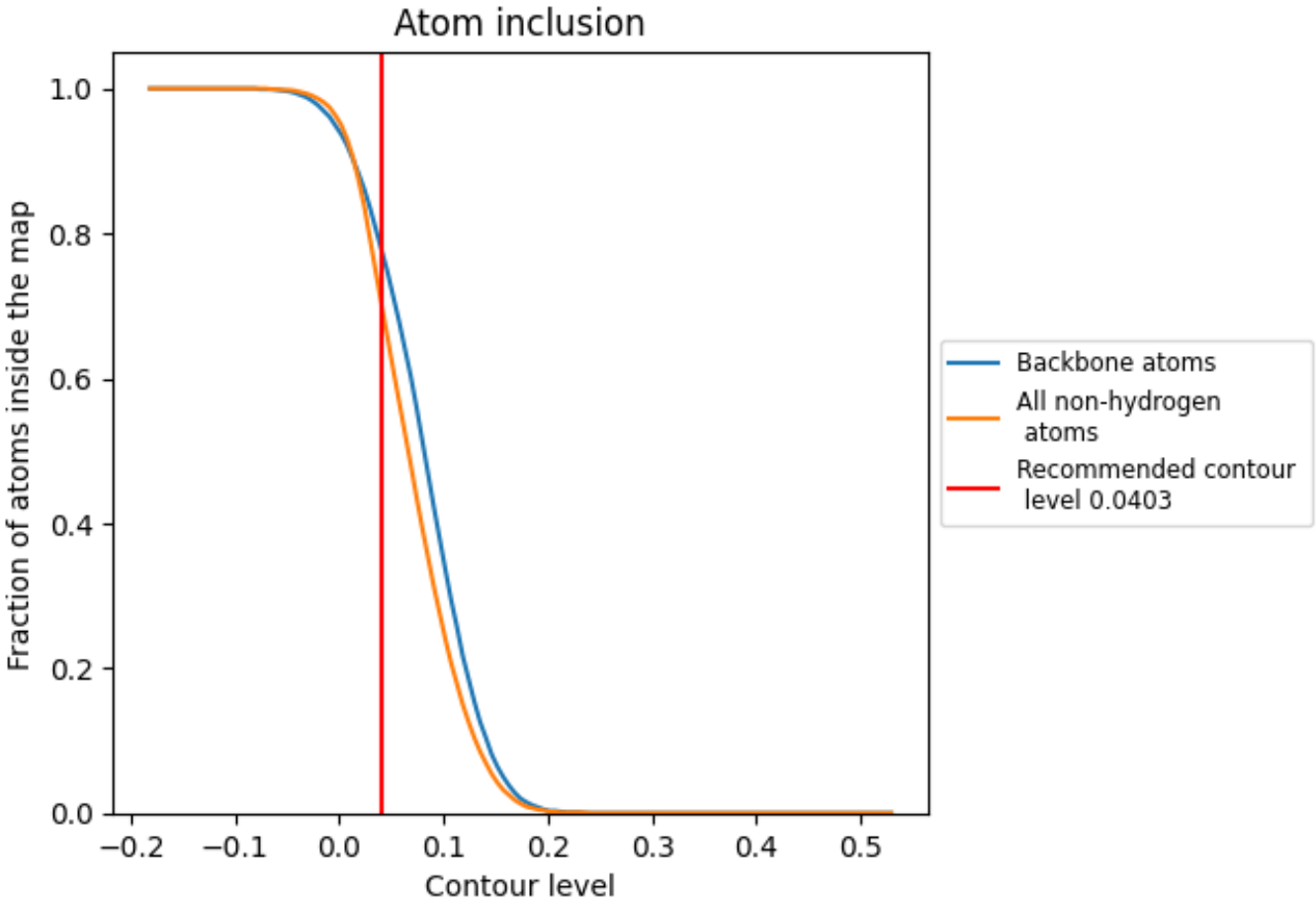
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0403).

9.4 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 70% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0403) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7030	0.4260
A	0.6860	0.4140
B	0.7410	0.4430
C	0.6350	0.4060
D	0.7570	0.4430
E	0.7660	0.4240
F	0.6770	0.4120
G	0.7020	0.4330
H	0.6910	0.4080
I	0.6620	0.4210
J	0.7260	0.4430
K	0.7200	0.4380
L	0.6710	0.4060
M	0.7030	0.4370
N	0.6900	0.4290
O	0.6540	0.4310
P	0.7190	0.4130
Q	0.6380	0.4110
S	0.5390	0.4240