Full wwPDB EM Validation Report

May 12, 2025 – 08:21 PM EDT

PDB ID	:	8V63 / pdb_00008v63
EMDB ID	:	EMD-42988
Title	:	R207A mutant of human Slo1 in presence of EDTA - activated VSD
Authors	:	Pal, K.; Kallure, G.S.; Chowdhury, S.
Deposited on	:	2023-12-01
Resolution	:	2.72 Å(reported)

This is a Full wwPDB EM Validation 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:

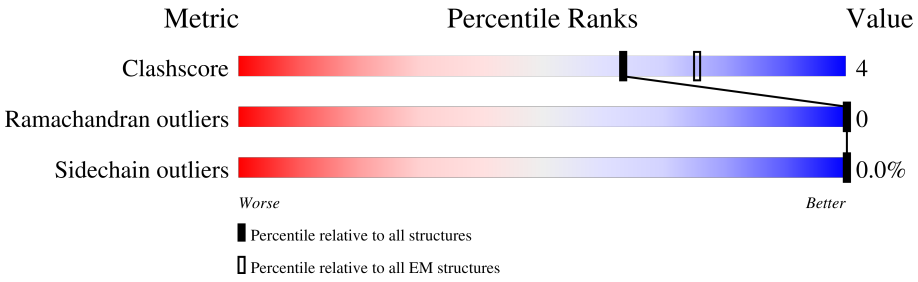
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.72 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	1065	76% 9% 15%
1	B	1065	76% 9% 15%
1	C	1065	76% 9% 15%
1	D	1065	77% 8% 15%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 31665 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 Calcium-activated potassium channel subunit alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	906	Total	C	N	O	S	0	0
			7212	4675	1179	1310	48		
1	B	906	Total	C	N	O	S	0	0
			7212	4675	1179	1310	48		
1	C	906	Total	C	N	O	S	0	0
			7212	4675	1179	1310	48		
1	D	906	Total	C	N	O	S	0	0
			7212	4675	1179	1310	48		

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	207	ALA	ARG	engineered mutation	UNP Q12791
A	1057	SER	-	expression tag	UNP Q12791
A	1058	ASN	-	expression tag	UNP Q12791
A	1059	SER	-	expression tag	UNP Q12791
A	1060	LEU	-	expression tag	UNP Q12791
A	1061	GLU	-	expression tag	UNP Q12791
A	1062	VAL	-	expression tag	UNP Q12791
A	1063	LEU	-	expression tag	UNP Q12791
A	1064	PHE	-	expression tag	UNP Q12791
A	1065	GLN	-	expression tag	UNP Q12791
B	207	ALA	ARG	engineered mutation	UNP Q12791
B	1057	SER	-	expression tag	UNP Q12791
B	1058	ASN	-	expression tag	UNP Q12791
B	1059	SER	-	expression tag	UNP Q12791
B	1060	LEU	-	expression tag	UNP Q12791
B	1061	GLU	-	expression tag	UNP Q12791
B	1062	VAL	-	expression tag	UNP Q12791
B	1063	LEU	-	expression tag	UNP Q12791
B	1064	PHE	-	expression tag	UNP Q12791
B	1065	GLN	-	expression tag	UNP Q12791
C	207	ALA	ARG	engineered mutation	UNP Q12791
C	1057	SER	-	expression tag	UNP Q12791

Continued on next page...

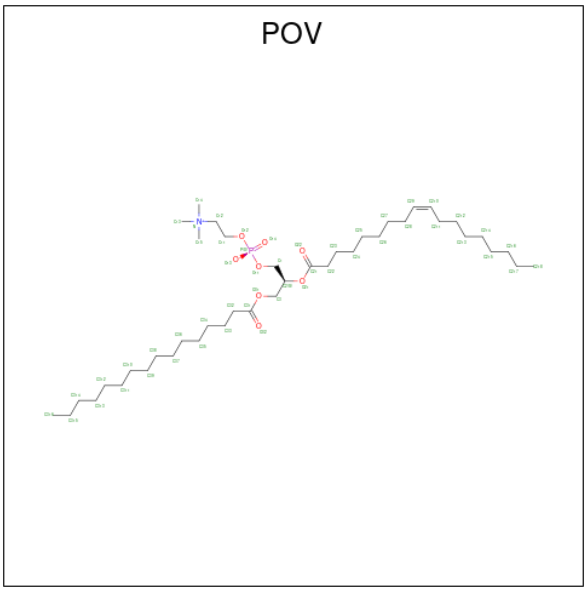
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	1058	ASN	-	expression tag	UNP Q12791
C	1059	SER	-	expression tag	UNP Q12791
C	1060	LEU	-	expression tag	UNP Q12791
C	1061	GLU	-	expression tag	UNP Q12791
C	1062	VAL	-	expression tag	UNP Q12791
C	1063	LEU	-	expression tag	UNP Q12791
C	1064	PHE	-	expression tag	UNP Q12791
C	1065	GLN	-	expression tag	UNP Q12791
D	207	ALA	ARG	engineered mutation	UNP Q12791
D	1057	SER	-	expression tag	UNP Q12791
D	1058	ASN	-	expression tag	UNP Q12791
D	1059	SER	-	expression tag	UNP Q12791
D	1060	LEU	-	expression tag	UNP Q12791
D	1061	GLU	-	expression tag	UNP Q12791
D	1062	VAL	-	expression tag	UNP Q12791
D	1063	LEU	-	expression tag	UNP Q12791
D	1064	PHE	-	expression tag	UNP Q12791
D	1065	GLN	-	expression tag	UNP Q12791

- Molecule 2 is POTASSIUM ION (CCD ID: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
2	A	6	Total K 6 6	0
2	B	1	Total K 1 1	0
2	C	1	Total K 1 1	0
2	D	1	Total K 1 1	0

- Molecule 3 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (CCD ID: POV) (formula: $C_{42}H_{82}NO_8P$) (labeled as "Ligand of Interest" by depositor).



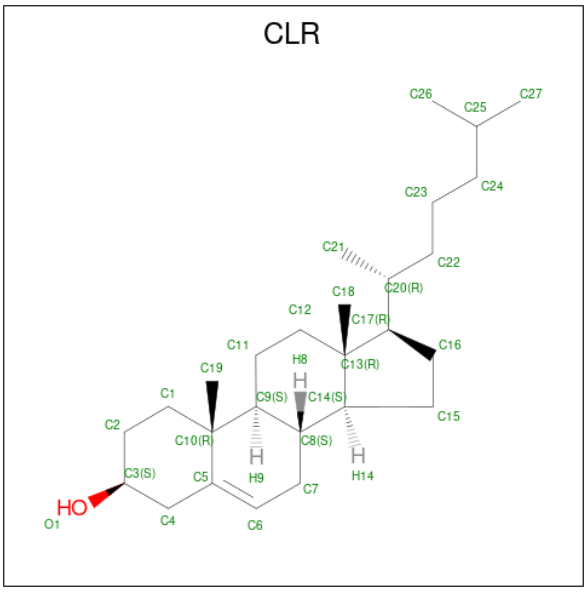
Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total C O P 37 28 8 1	0
3	A	1	Total C O P 26 19 6 1	0
3	A	1	Total C O P 39 30 8 1	0
3	A	1	Total C O 10 9 1	0
3	A	1	Total C O P 32 23 8 1	0
3	A	1	Total C O 15 13 2	0
3	A	1	Total C O P 28 19 8 1	0
3	B	1	Total C O P 37 28 8 1	0
3	B	1	Total C O P 26 19 6 1	0
3	B	1	Total C O P 39 30 8 1	0
3	B	1	Total C O 10 9 1	0
3	B	1	Total C O P 32 23 8 1	0
3	B	1	Total C O 15 13 2	0
3	B	1	Total C O P 28 19 8 1	0

Continued on next page...

Continued from previous page...

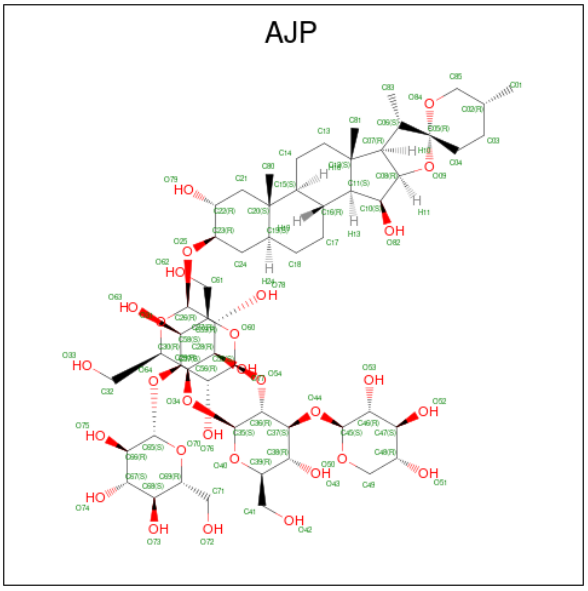
Mol	Chain	Residues	Atoms	AltConf
3	C	1	Total C O P 37 28 8 1	0
3	C	1	Total C O P 37 28 8 1	0
3	C	1	Total C O P 26 19 6 1	0
3	C	1	Total C O P 39 30 8 1	0
3	C	1	Total C O 10 9 1	0
3	C	1	Total C O P 32 23 8 1	0
3	C	1	Total C O 15 13 2	0
3	C	1	Total C O P 28 19 8 1	0
3	D	1	Total C O P 39 30 8 1	0
3	D	1	Total C O 10 9 1	0
3	D	1	Total C O P 26 19 6 1	0
3	D	1	Total C O P 32 23 8 1	0
3	D	1	Total C O 15 13 2	0
3	D	1	Total C O P 28 19 8 1	0

- Molecule 4 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total C O 28 27 1	0
4	B	1	Total C O 28 27 1	0
4	C	1	Total C O 28 27 1	0
4	D	1	Total C O 28 27 1	0

- Molecule 5 is Digitonin (CCD ID: AJP) (formula: $C_{56}H_{92}O_{29}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
5	A	1	Total C O 54 39 15	0
5	A	1	Total C O 54 39 15	0
5	A	1	Total C O 43 33 10	0
5	A	1	Total C O 43 33 10	0
5	A	1	Total C O 43 33 10	0
5	A	1	Total C O 65 45 20	0
5	A	1	Total C O 43 33 10	0
5	A	1	Total C O 43 33 10	0
5	A	1	Total C O 43 33 10	0
5	A	1	Total C O 54 39 15	0
5	B	1	Total C O 54 39 15	0
5	B	1	Total C O 54 39 15	0
5	B	1	Total C O 43 33 10	0
5	B	1	Total C O 43 33 10	0
5	B	1	Total C O 43 33 10	0
5	B	1	Total C O 65 45 20	0
5	B	1	Total C O 43 33 10	0
5	B	1	Total C O 43 33 10	0
5	B	1	Total C O 43 33 10	0
5	B	1	Total C O 54 39 15	0
5	C	1	Total C O 54 39 15	0
5	C	1	Total C O 54 39 15	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
5	C	1	Total C O 43 33 10	0
5	C	1	Total C O 43 33 10	0
5	C	1	Total C O 43 33 10	0
5	C	1	Total C O 65 45 20	0
5	C	1	Total C O 43 33 10	0
5	C	1	Total C O 43 33 10	0
5	C	1	Total C O 43 33 10	0
5	C	1	Total C O 54 39 15	0
5	D	1	Total C O 54 39 15	0
5	D	1	Total C O 54 39 15	0
5	D	1	Total C O 43 33 10	0
5	D	1	Total C O 43 33 10	0
5	D	1	Total C O 43 33 10	0
5	D	1	Total C O 65 45 20	0
5	D	1	Total C O 43 33 10	0
5	D	1	Total C O 43 33 10	0
5	D	1	Total C O 43 33 10	0
5	D	1	Total C O 54 39 15	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	AltConf
6	A	2	Total O 2 2	0

Continued on next page...

Continued from previous page...

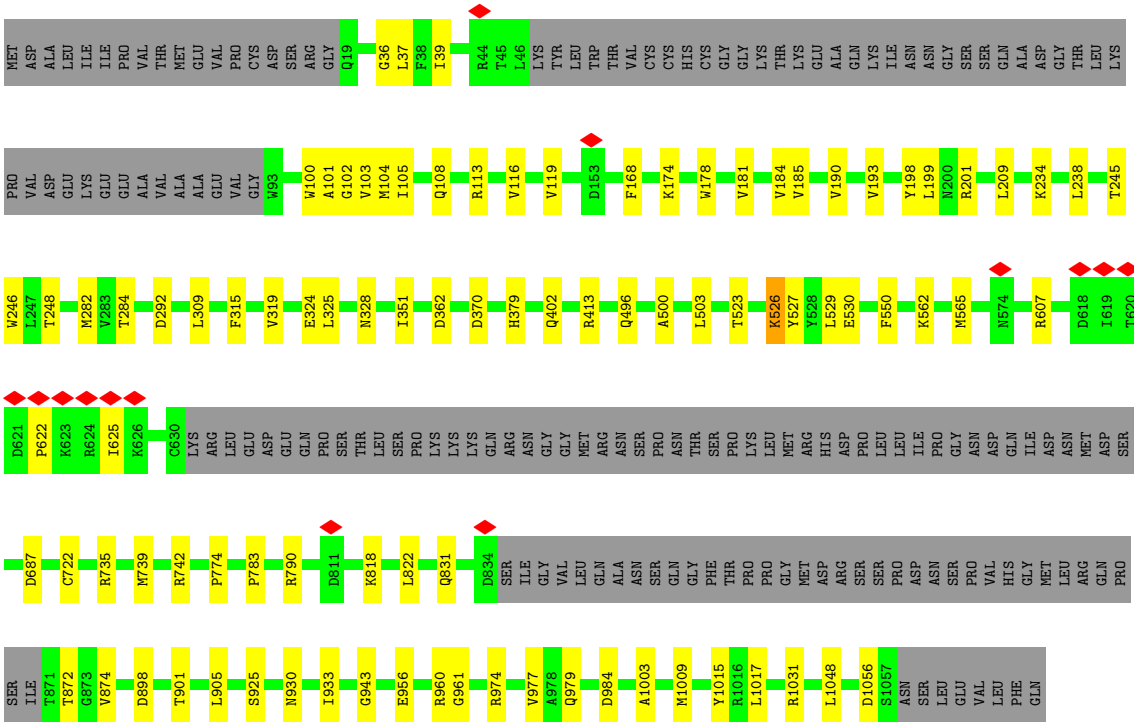
Mol	Chain	Residues	Atoms	AltConf
6	B	2	Total O 2 2	0
6	C	2	Total O 2 2	0
6	D	2	Total O 2 2	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

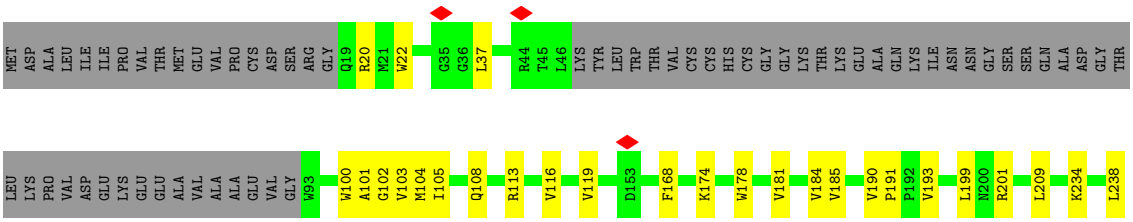
• Molecule 1: Calcium-activated potassium channel subunit alpha-1

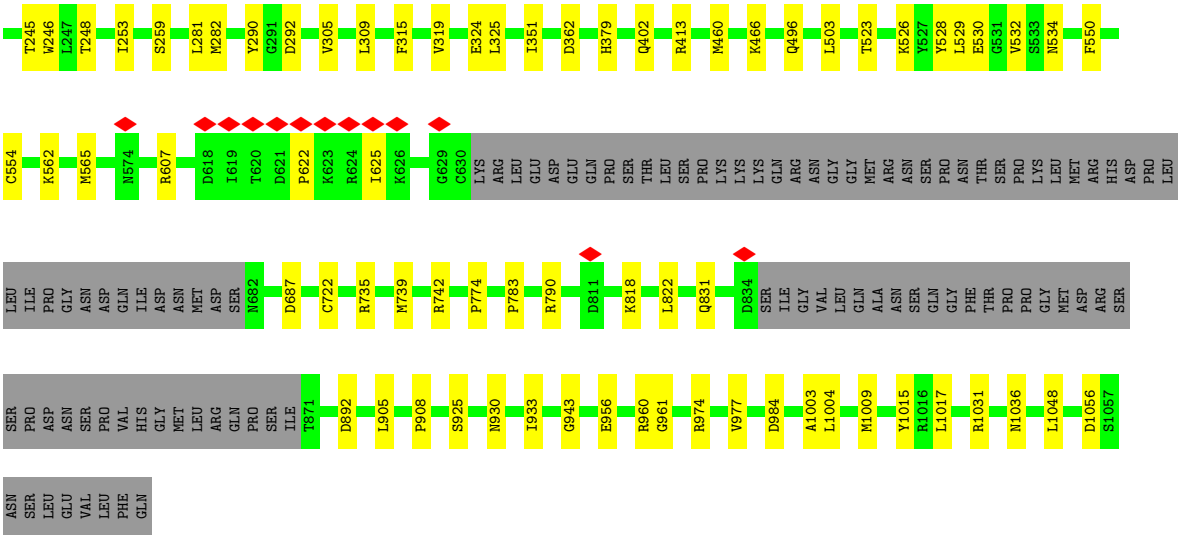
Chain A:



• Molecule 1: Calcium-activated potassium channel subunit alpha-1

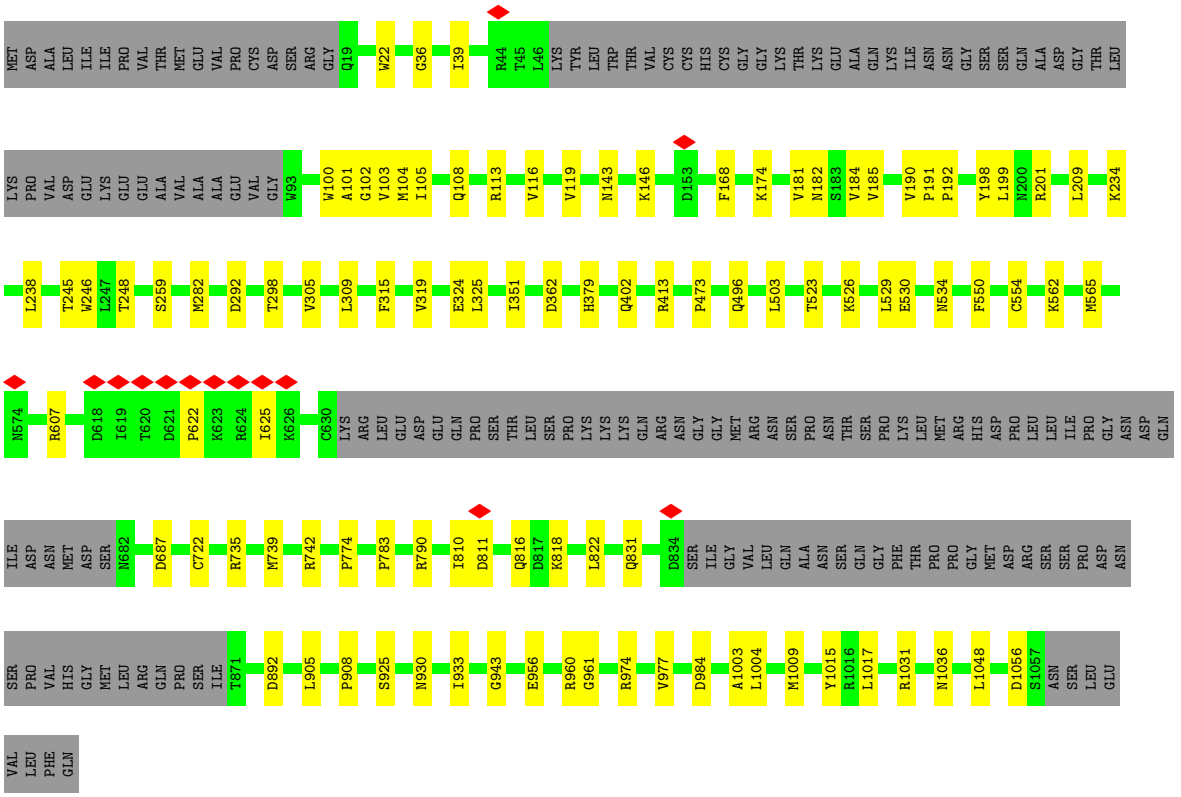
Chain B:





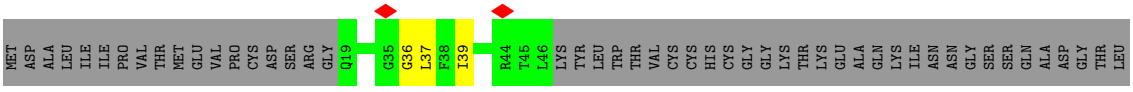
• Molecule 1: Calcium-activated potassium channel subunit alpha-1

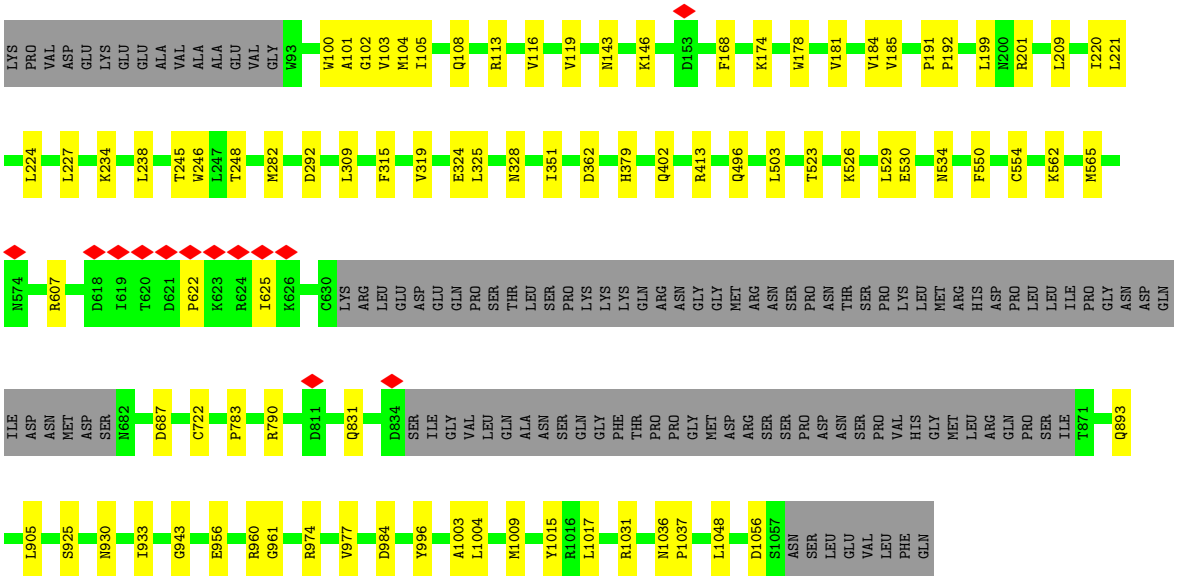
Chain C:



• Molecule 1: Calcium-activated potassium channel subunit alpha-1

Chain D:




LYS PRO VAL ASP GLU LYS GLU GLU ALA VAL ALA ALA GLU VAL GLY W93 W100 A101 G102 V103 M104 I105 Q108 R113 V116 V119 N143 K146 D153 F168 K174 W178 V181 V184 V185 P191 P192 L199 N200 R201 L209 I220 L221
L224 L227 K234 L238 T245 W246 L247 T248 M282 D292 L309 F315 V319 E324 L325 N328 I351 D362 H379 Q402 R413 Q496 L503 T523 K526 L529 E530 N534 F550 C554 K562 M565
N574 R607 D618 I619 T620 D621 P622 K623 R624 I625 K626 C630 LYS ARG LEU GLU ASP GLU GLN PRO SER THR LEU SER PRO LYS LYS LYS GLN ARG ASN GLY GLY MET ARG ASN SER PRO ASN THR SER PRO LYS LEU MET ARG HIS ASP PRO LEU LEU ILE PRO GLY ASN ASP GLN
ILE ASP ASN MET ASP SER N682 D687 C722 P783 R790 D811 Q831 D834 SER ILE GLY VAL LEU GLN ALA ASN SER GLN GLY PHE THR PRO PRO GLY MET ASP ARG SER SER PRO ASP ASN SER PRO VAL HIS GLY MET LEU ARG GLN PRO SER ILE T871 Q893
L905 S925 N930 I933 G943 E956 R960 G961 R974 V977 D984 Y996 A1003 L1004 M1009 Y1015 R1016 L1017 R1031 N1036 P1037 L1048 D1056 S1057 ASN SER LEU GLU VAL LEU PHE GLN

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	202456	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	72	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	1700	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.528	Depositor
Minimum map value	-0.207	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.085	Depositor
Map size (Å)	276.48, 276.48, 276.48	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: POV, AJP, K, CLR

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	0.15	0/7378	0.28	0/10013
1	B	0.15	0/7378	0.28	0/10013
1	C	0.15	0/7378	0.28	0/10013
1	D	0.16	0/7378	0.28	0/10013
All	All	0.15	0/29512	0.28	0/40052

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	7212	0	7198	58	0
1	B	7212	0	7198	59	0
1	C	7212	0	7198	63	0
1	D	7212	0	7198	55	0
2	A	6	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	187	0	230	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	187	0	230	4	0
3	C	224	0	275	7	0
3	D	150	0	185	3	0
4	A	28	0	46	1	0
4	B	28	0	46	3	0
4	C	28	0	46	3	0
4	D	28	0	46	0	0
5	A	485	0	0	3	0
5	B	485	0	0	2	0
5	C	485	0	0	3	0
5	D	485	0	0	3	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
6	C	2	0	0	0	0
6	D	2	0	0	0	0
All	All	31665	0	29896	247	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 4.

All (247) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:722:CYS:HB3	1:D:783:PRO:HB3	1.69	0.75
1:B:722:CYS:HB3	1:B:783:PRO:HB3	1.69	0.74
1:A:722:CYS:HB3	1:A:783:PRO:HB3	1.69	0.74
1:C:722:CYS:HB3	1:C:783:PRO:HB3	1.70	0.73
1:A:523:THR:O	1:A:526:LYS:HG2	1.91	0.70
1:B:523:THR:O	1:B:526:LYS:HG2	1.92	0.69
1:D:523:THR:O	1:D:526:LYS:HG2	1.94	0.68
1:B:790:ARG:NH2	1:B:831:GLN:O	2.28	0.66
1:C:523:THR:O	1:C:526:LYS:HG2	1.96	0.66
1:D:790:ARG:NH2	1:D:831:GLN:O	2.29	0.64
1:A:790:ARG:NH2	1:A:831:GLN:O	2.28	0.63
1:C:790:ARG:NH2	1:C:831:GLN:O	2.29	0.62
1:D:529:LEU:HD21	1:D:905:LEU:HD21	1.82	0.61
1:A:234:LYS:NZ	1:A:324:GLU:OE2	2.35	0.60
1:A:529:LEU:HD21	1:A:905:LEU:HD21	1.83	0.60
1:C:529:LEU:HD21	1:C:905:LEU:HD21	1.83	0.60
1:B:529:LEU:HD21	1:B:905:LEU:HD21	1.84	0.60
1:B:234:LYS:NZ	1:B:324:GLU:OE2	2.35	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:234:LYS:NZ	1:C:324:GLU:OE2	2.36	0.59
1:D:234:LYS:NZ	1:D:324:GLU:OE2	2.36	0.58
1:A:238:LEU:HD21	3:A:1107:POV:H31D	1.86	0.58
1:D:238:LEU:HD21	3:D:1103:POV:H31D	1.86	0.57
1:D:351:ILE:HD12	1:D:379:HIS:HB2	1.87	0.57
1:D:402:GLN:O	1:D:413:ARG:NH2	2.36	0.57
1:B:238:LEU:HD21	3:B:1102:POV:H31D	1.87	0.57
1:C:943:GLY:O	1:C:974:ARG:NH1	2.37	0.57
1:A:898:ASP:OD1	1:A:901:THR:OG1	2.22	0.56
1:C:113:ARG:NH1	5:C:1118:AJP:O78	2.40	0.55
1:A:943:GLY:O	1:A:974:ARG:NH1	2.40	0.55
1:D:526:LYS:O	1:D:530:GLU:HG3	2.06	0.55
1:A:113:ARG:NH1	5:A:1122:AJP:O78	2.39	0.55
1:C:956:GLU:OE2	1:C:960:ARG:NH2	2.34	0.55
1:C:234:LYS:HD2	1:C:325:LEU:HD11	1.87	0.55
1:D:113:ARG:NH1	5:D:1116:AJP:O78	2.40	0.55
1:B:234:LYS:HD2	1:B:325:LEU:HD11	1.88	0.54
1:B:113:ARG:NH1	5:B:1117:AJP:O78	2.40	0.54
1:B:526:LYS:O	1:B:530:GLU:HG3	2.06	0.54
1:B:402:GLN:O	1:B:413:ARG:NH2	2.37	0.54
1:B:116:VAL:HA	1:B:119:VAL:HG12	1.90	0.54
1:B:259:SER:HG	4:B:1109:CLR:H1	1.55	0.54
1:C:526:LYS:O	1:C:530:GLU:HG3	2.08	0.54
1:D:503:LEU:HD22	1:D:977:VAL:HG11	1.90	0.54
1:B:943:GLY:O	1:B:974:ARG:NH1	2.41	0.53
1:C:100:TRP:CD2	1:C:104:MET:HE1	2.44	0.53
1:D:943:GLY:O	1:D:974:ARG:NH1	2.41	0.53
1:C:238:LEU:HD21	3:C:1103:POV:H31D	1.90	0.53
1:A:956:GLU:OE2	1:A:960:ARG:NH2	2.33	0.53
1:B:100:TRP:CD2	1:B:104:MET:HE1	2.44	0.53
1:A:100:TRP:CD2	1:A:104:MET:HE1	2.44	0.53
1:D:100:TRP:CD2	1:D:104:MET:HE1	2.44	0.53
1:B:351:ILE:HD12	1:B:379:HIS:HB2	1.91	0.53
1:A:503:LEU:HD22	1:A:977:VAL:HG11	1.90	0.53
1:B:168:PHE:O	1:B:174:LYS:NZ	2.42	0.52
1:A:234:LYS:HD2	1:A:325:LEU:HD11	1.89	0.52
1:A:116:VAL:HA	1:A:119:VAL:HG12	1.92	0.52
1:C:402:GLN:O	1:C:413:ARG:NH2	2.37	0.52
1:C:503:LEU:HD22	1:C:977:VAL:HG11	1.90	0.52
1:D:234:LYS:HD2	1:D:325:LEU:HD11	1.90	0.52
1:A:309:LEU:HG	1:B:282:MET:HE2	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:503:LEU:HD22	1:B:977:VAL:HG11	1.91	0.52
1:C:562:LYS:HG3	1:C:622:PRO:HG3	1.92	0.52
1:A:351:ILE:HD12	1:A:379:HIS:HB2	1.91	0.52
1:C:309:LEU:HG	1:D:282:MET:HE2	1.92	0.52
1:A:526:LYS:O	1:A:530:GLU:HG3	2.10	0.52
1:B:309:LEU:HG	1:C:282:MET:HE2	1.92	0.51
1:C:116:VAL:HA	1:C:119:VAL:HG12	1.92	0.51
1:D:116:VAL:HA	1:D:119:VAL:HG12	1.92	0.51
1:C:810:ILE:HG12	1:C:816:GLN:HG2	1.92	0.51
1:D:221:LEU:HB3	1:D:227:LEU:HD23	1.93	0.51
1:C:185:VAL:HG23	1:C:209:LEU:HB3	1.92	0.51
1:C:351:ILE:HD12	1:C:379:HIS:HB2	1.93	0.51
1:A:185:VAL:HG23	1:A:209:LEU:HB3	1.93	0.51
1:D:562:LYS:HG3	1:D:622:PRO:HG3	1.93	0.50
1:A:282:MET:HE2	1:D:309:LEU:HG	1.94	0.50
1:A:402:GLN:O	1:A:413:ARG:NH2	2.37	0.50
1:B:185:VAL:HG23	1:B:209:LEU:HB3	1.93	0.50
1:B:534:ASN:ND2	1:B:1036:ASN:HB3	2.27	0.50
1:D:185:VAL:HG23	1:D:209:LEU:HB3	1.93	0.50
1:B:956:GLU:OE2	1:B:960:ARG:NH2	2.33	0.49
1:C:259:SER:HG	4:C:1110:CLR:H1	1.57	0.49
1:C:473:PRO:HG3	1:D:893:GLN:HB3	1.95	0.49
1:A:562:LYS:HG3	1:A:622:PRO:HG3	1.95	0.49
1:B:496:GLN:HB3	1:B:503:LEU:HD23	1.94	0.49
1:B:562:LYS:HG3	1:B:622:PRO:HG3	1.95	0.49
1:A:496:GLN:HB3	1:A:503:LEU:HD23	1.94	0.49
1:D:956:GLU:OE2	1:D:960:ARG:NH2	2.33	0.49
1:C:496:GLN:HB3	1:C:503:LEU:HD23	1.95	0.49
1:D:496:GLN:HB3	1:D:503:LEU:HD23	1.94	0.49
1:B:687:ASP:HA	1:B:961:GLY:HA2	1.96	0.47
1:B:1017:LEU:HA	1:B:1031:ARG:HG2	1.96	0.47
1:C:1056:ASP:N	1:C:1056:ASP:OD1	2.48	0.47
1:D:199:LEU:HB3	1:D:201:ARG:HG2	1.95	0.47
1:D:607:ARG:HD3	1:D:625:ILE:HB	1.97	0.47
1:A:607:ARG:HD3	1:A:625:ILE:HB	1.96	0.47
1:B:607:ARG:HD3	1:B:625:ILE:HB	1.96	0.47
1:C:1003:ALA:HB1	1:C:1009:MET:HB3	1.97	0.47
1:A:199:LEU:HB3	1:A:201:ARG:HG2	1.96	0.46
1:B:20:ARG:HB3	1:B:22:TRP:HD1	1.79	0.46
1:D:1003:ALA:HB1	1:D:1009:MET:HB3	1.97	0.46
1:D:1017:LEU:HA	1:D:1031:ARG:HG2	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:460:MET:HE3	1:B:466:LYS:HA	1.97	0.46
1:B:181:VAL:HA	1:B:184:VAL:HG12	1.98	0.46
1:B:1056:ASP:OD1	1:B:1056:ASP:N	2.48	0.46
1:C:687:ASP:HA	1:C:961:GLY:HA2	1.97	0.46
1:D:1056:ASP:OD1	1:D:1056:ASP:N	2.49	0.46
1:A:101:ALA:HA	1:A:104:MET:HE2	1.98	0.46
1:C:199:LEU:HB3	1:C:201:ARG:HG2	1.97	0.46
1:A:526:LYS:HB2	1:A:526:LYS:NZ	2.30	0.46
1:B:892:ASP:HB2	1:B:908:PRO:HG3	1.97	0.46
1:B:1003:ALA:HB1	1:B:1009:MET:HB3	1.98	0.46
1:C:1017:LEU:HA	1:C:1031:ARG:HG2	1.96	0.46
1:D:101:ALA:HA	1:D:104:MET:HE2	1.97	0.46
1:B:199:LEU:HB3	1:B:201:ARG:HG2	1.96	0.46
1:D:687:ASP:HA	1:D:961:GLY:HA2	1.98	0.46
1:A:1017:LEU:HA	1:A:1031:ARG:HG2	1.97	0.46
1:B:101:ALA:HA	1:B:104:MET:HE2	1.98	0.46
1:C:362:ASP:OD2	1:C:925:SER:OG	2.32	0.45
1:A:284:THR:OG1	1:B:290:TYR:OH	2.24	0.45
4:A:1114:CLR:H211	4:A:1114:CLR:H272	1.98	0.45
5:B:1111:AJP:O33	5:B:1111:AJP:O42	2.35	0.45
5:C:1112:AJP:O42	5:C:1112:AJP:O33	2.35	0.45
1:A:36:GLY:HA2	1:A:39:ILE:HG12	1.99	0.45
1:C:930:ASN:HB3	1:C:933:ILE:HG12	1.99	0.45
1:D:36:GLY:HA2	1:D:39:ILE:HG12	1.99	0.45
1:D:930:ASN:HB3	1:D:933:ILE:HG12	1.99	0.45
3:A:1108:POV:H32A	3:A:1108:POV:H23	1.98	0.45
5:D:1110:AJP:O42	5:D:1110:AJP:O33	2.35	0.45
1:A:687:ASP:HA	1:A:961:GLY:HA2	1.98	0.45
1:A:818:LYS:O	1:A:822:LEU:HD13	2.17	0.45
1:C:984:ASP:N	1:C:984:ASP:OD1	2.51	0.45
3:C:1104:POV:H32A	3:C:1104:POV:H23	1.99	0.44
1:D:181:VAL:HA	1:D:184:VAL:HG12	1.98	0.44
1:A:181:VAL:HA	1:A:184:VAL:HG12	2.00	0.44
1:C:607:ARG:HD3	1:C:625:ILE:HB	1.98	0.44
1:A:190:VAL:HA	1:A:193:VAL:HG12	1.98	0.44
1:C:181:VAL:HA	1:C:184:VAL:HG12	2.00	0.44
1:C:379:HIS:O	1:C:402:GLN:HA	2.18	0.44
1:D:362:ASP:OD2	1:D:925:SER:OG	2.32	0.44
5:A:1116:AJP:O42	5:A:1116:AJP:O33	2.35	0.44
1:C:36:GLY:HA2	1:C:39:ILE:HG12	2.00	0.44
3:D:1101:POV:H32A	3:D:1101:POV:H23	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:526:LYS:HG3	1:A:527:TYR:N	2.32	0.44
1:C:892:ASP:HB2	1:C:908:PRO:HG3	2.00	0.44
1:B:379:HIS:O	1:B:402:GLN:HA	2.18	0.44
1:C:818:LYS:O	1:C:822:LEU:HD13	2.18	0.44
3:B:1105:POV:H2	3:B:1105:POV:H22	1.84	0.44
1:C:101:ALA:HA	1:C:104:MET:HE2	1.98	0.44
1:D:292:ASP:N	1:D:292:ASP:OD1	2.51	0.44
4:C:1110:CLR:H162	4:C:1110:CLR:H222	1.87	0.44
1:B:362:ASP:OD2	1:B:925:SER:OG	2.32	0.43
3:B:1103:POV:H32A	3:B:1103:POV:H23	1.99	0.43
1:A:1056:ASP:N	1:A:1056:ASP:OD1	2.48	0.43
1:B:528:TYR:O	1:B:532:VAL:HG23	2.19	0.43
1:D:984:ASP:OD1	1:D:984:ASP:N	2.51	0.43
1:B:292:ASP:OD1	1:B:292:ASP:N	2.51	0.43
1:B:735:ARG:HG2	1:B:739:MET:HG3	2.00	0.43
1:D:102:GLY:HA2	1:D:105:ILE:HG12	2.01	0.43
3:D:1101:POV:H25A	3:D:1101:POV:H33	2.01	0.43
1:A:984:ASP:N	1:A:984:ASP:OD1	2.52	0.43
1:A:1003:ALA:HB1	1:A:1009:MET:HB3	2.00	0.43
1:B:190:VAL:HA	1:B:193:VAL:HG12	2.01	0.43
1:D:108:GLN:O	1:D:113:ARG:NH2	2.51	0.43
1:D:379:HIS:O	1:D:402:GLN:HA	2.19	0.43
1:B:1015:TYR:HB3	1:B:1048:LEU:HB2	2.01	0.43
1:C:292:ASP:OD1	1:C:292:ASP:N	2.51	0.43
1:D:168:PHE:O	1:D:174:LYS:NZ	2.52	0.43
1:A:379:HIS:O	1:A:402:GLN:HA	2.18	0.42
1:A:742:ARG:HD2	1:A:774:PRO:HD2	2.01	0.42
1:B:305:VAL:HG13	1:C:282:MET:HG2	2.01	0.42
1:C:1015:TYR:HB3	1:C:1048:LEU:HB2	2.01	0.42
1:C:305:VAL:HG13	1:D:282:MET:HG2	2.02	0.42
3:C:1104:POV:O22	5:C:1111:AJP:O79	2.37	0.42
3:C:1106:POV:H22	3:C:1106:POV:H2	1.84	0.42
1:A:362:ASP:OD2	1:A:925:SER:OG	2.33	0.42
1:A:1015:TYR:HB3	1:A:1048:LEU:HB2	2.01	0.42
3:B:1103:POV:H25A	3:B:1103:POV:H33	2.02	0.42
1:C:534:ASN:ND2	1:C:1036:ASN:HB3	2.34	0.42
3:C:1104:POV:H25A	3:C:1104:POV:H33	2.02	0.42
1:A:735:ARG:HG2	1:A:739:MET:HG3	2.01	0.42
1:B:818:LYS:O	1:B:822:LEU:HD13	2.19	0.42
4:B:1109:CLR:H211	4:B:1109:CLR:H272	2.01	0.42
1:C:245:THR:HA	1:C:248:THR:HG22	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1015:TYR:HB3	1:D:1048:LEU:HB2	2.01	0.42
1:A:102:GLY:HA2	1:A:105:ILE:HG12	2.01	0.42
1:B:315:PHE:O	1:B:319:VAL:HG23	2.20	0.42
1:D:534:ASN:OD1	1:D:1036:ASN:HB3	2.19	0.42
1:A:100:TRP:HA	1:A:103:VAL:HG12	2.02	0.42
1:B:102:GLY:HA2	1:B:105:ILE:HG12	2.01	0.42
1:C:735:ARG:HG2	1:C:739:MET:HG3	2.00	0.42
1:C:742:ARG:HD2	1:C:774:PRO:HD2	2.02	0.42
1:A:108:GLN:O	1:A:113:ARG:NH2	2.53	0.42
1:B:742:ARG:HD2	1:B:774:PRO:HD2	2.02	0.42
1:D:315:PHE:O	1:D:319:VAL:HG23	2.20	0.42
3:A:1108:POV:H25A	3:A:1108:POV:H33	2.01	0.42
1:A:315:PHE:O	1:A:319:VAL:HG23	2.20	0.42
1:A:550:PHE:CE1	1:A:565:MET:HE3	2.55	0.42
1:C:22:TRP:CE2	4:C:1110:CLR:H3	2.55	0.41
1:C:102:GLY:HA2	1:C:105:ILE:HG12	2.01	0.41
1:C:298:THR:HG23	3:C:1102:POV:H32A	2.01	0.41
1:D:245:THR:HA	1:D:248:THR:HG22	2.02	0.41
1:A:245:THR:HA	1:A:248:THR:HG22	2.02	0.41
1:B:100:TRP:HA	1:B:103:VAL:HG12	2.01	0.41
1:B:930:ASN:HB3	1:B:933:ILE:HG12	2.02	0.41
1:B:984:ASP:N	1:B:984:ASP:OD1	2.51	0.41
1:A:292:ASP:OD1	1:A:292:ASP:N	2.51	0.41
1:B:550:PHE:CE1	1:B:565:MET:HE3	2.55	0.41
1:C:198:TYR:HD2	1:C:199:LEU:HD22	1.86	0.41
1:C:315:PHE:O	1:C:319:VAL:HG23	2.20	0.41
1:C:550:PHE:CE1	1:C:565:MET:HE3	2.55	0.41
1:A:37:LEU:HD12	1:A:178:TRP:HD1	1.86	0.41
1:B:245:THR:HA	1:B:248:THR:HG22	2.02	0.41
1:D:100:TRP:HA	1:D:103:VAL:HG12	2.02	0.41
1:B:190:VAL:HG23	1:B:191:PRO:HD3	2.02	0.41
1:C:190:VAL:HG23	1:C:191:PRO:HD3	2.03	0.41
1:A:168:PHE:O	1:A:174:LYS:NZ	2.54	0.41
1:C:108:GLN:O	1:C:113:ARG:NH2	2.54	0.41
1:A:198:TYR:HD2	1:A:199:LEU:HD22	1.85	0.41
1:B:37:LEU:HD12	1:B:178:TRP:CD1	2.55	0.41
1:D:143:ASN:HB3	1:D:146:LYS:HB2	2.03	0.41
1:A:930:ASN:HB3	1:A:933:ILE:HG12	2.02	0.41
1:D:37:LEU:HD12	1:D:178:TRP:HD1	1.85	0.41
1:D:246:TRP:CZ2	1:D:282:MET:HB2	2.56	0.41
1:D:328:ASN:OD1	5:D:1118:AJP:O78	2.39	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:TRP:CZ2	1:A:282:MET:HB2	2.56	0.41
1:B:246:TRP:CZ2	1:B:282:MET:HB2	2.56	0.41
1:B:554:CYS:HB3	1:B:1004:LEU:HD21	2.02	0.41
1:D:550:PHE:CE1	1:D:565:MET:HE3	2.55	0.41
1:A:370:ASP:OD1	1:A:370:ASP:N	2.55	0.40
4:B:1109:CLR:H112	4:B:1109:CLR:H12	1.94	0.40
1:A:328:ASN:OD1	5:A:1124:AJP:O78	2.39	0.40
1:D:554:CYS:HB3	1:D:1004:LEU:HD21	2.02	0.40
1:A:500:ALA:HB1	1:A:979:GLN:HG3	2.03	0.40
1:A:872:THR:HG23	1:A:874:VAL:HG12	2.03	0.40
1:C:100:TRP:HA	1:C:103:VAL:HG12	2.03	0.40
1:C:191:PRO:HD2	1:C:192:PRO:HD2	2.03	0.40
1:D:191:PRO:HD2	1:D:192:PRO:HD2	2.02	0.40
1:B:108:GLN:O	1:B:113:ARG:NH2	2.55	0.40
1:B:253:ILE:HG13	1:B:281:LEU:HD21	2.04	0.40
1:C:143:ASN:HB3	1:C:146:LYS:HB2	2.03	0.40
1:C:168:PHE:O	1:C:174:LYS:NZ	2.54	0.40
1:C:182:ASN:HA	1:C:185:VAL:HG12	2.03	0.40
1:C:246:TRP:CZ2	1:C:282:MET:HB2	2.57	0.40
1:C:810:ILE:HG22	1:C:811:ASP:H	1.86	0.40
1:D:220:ILE:O	1:D:224:LEU:HG	2.22	0.40
1:D:996:TYR:CD2	1:D:1037:PRO:HG2	2.57	0.40
1:C:554:CYS:HB3	1:C:1004:LEU:HD21	2.03	0.40
3:C:1101:POV:H27A	3:C:1101:POV:H24A	2.00	0.40

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	898/1065 (84%)	882 (98%)	16 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	898/1065 (84%)	884 (98%)	14 (2%)	0	100	100
1	C	898/1065 (84%)	885 (99%)	13 (1%)	0	100	100
1	D	898/1065 (84%)	881 (98%)	17 (2%)	0	100	100
All	All	3592/4260 (84%)	3532 (98%)	60 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	796/936 (85%)	795 (100%)	1 (0%)	92	98
1	B	796/936 (85%)	796 (100%)	0	100	100
1	C	796/936 (85%)	796 (100%)	0	100	100
1	D	796/936 (85%)	796 (100%)	0	100	100
All	All	3184/3744 (85%)	3183 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	526	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	182	ASN
1	A	270	GLN
1	A	358	ASN
1	A	379	HIS
1	A	534	ASN
1	A	807	GLN
1	A	932	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	182	ASN
1	B	270	GLN
1	B	328	ASN
1	B	358	ASN
1	B	379	HIS
1	B	807	GLN
1	B	932	ASN
1	C	182	ASN
1	C	270	GLN
1	C	328	ASN
1	C	358	ASN
1	C	932	ASN
1	D	182	ASN
1	D	270	GLN
1	D	328	ASN
1	D	358	ASN
1	D	464	HIS
1	D	534	ASN
1	D	932	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 81 ligands modelled in this entry, 9 are monoatomic - leaving 72 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	AJP	D	1109	-	61,61,95	0.15	0	93,98,149	0.45	0
3	POV	A	1111	-	14,14,51	1.23	2 (14%)	14,14,59	1.42	2 (14%)
3	POV	B	1101	-	36,36,51	0.71	1 (2%)	39,41,59	0.90	2 (5%)
3	POV	B	1103	-	38,38,51	0.69	1 (2%)	41,43,59	0.84	2 (4%)
3	POV	A	1109	-	9,9,51	0.59	0	8,8,59	0.28	0
3	POV	A	1112	-	27,27,51	0.80	1 (3%)	30,32,59	0.94	2 (6%)
3	POV	C	1102	-	36,36,51	0.71	1 (2%)	39,41,59	0.89	2 (5%)
5	AJP	C	1114	-	49,49,95	0.16	0	75,80,149	0.44	0
3	POV	D	1102	-	9,9,51	0.59	0	8,8,59	0.28	0
5	AJP	B	1113	-	49,49,95	0.16	0	75,80,149	0.45	0
3	POV	C	1106	-	31,31,51	0.76	1 (3%)	34,36,59	0.91	2 (5%)
5	AJP	B	1118	-	49,49,95	0.15	0	75,80,149	0.42	0
3	POV	B	1102	-	25,25,51	0.77	1 (4%)	28,28,59	0.95	2 (7%)
3	POV	B	1105	-	31,31,51	0.75	1 (3%)	34,36,59	0.92	2 (5%)
3	POV	D	1101	-	38,38,51	0.69	1 (2%)	41,43,59	0.84	2 (4%)
5	AJP	A	1124	-	61,61,95	0.14	0	93,98,149	0.35	0
5	AJP	A	1120	-	73,73,95	0.15	0	111,116,149	0.42	0
3	POV	A	1108	-	38,38,51	0.69	1 (2%)	41,43,59	0.84	2 (4%)
4	CLR	A	1114	-	31,31,31	0.39	0	48,48,48	0.57	0
3	POV	C	1104	-	38,38,51	0.69	1 (2%)	41,43,59	0.83	2 (4%)
5	AJP	A	1117	-	49,49,95	0.14	0	75,80,149	0.33	0
5	AJP	D	1116	-	49,49,95	0.14	0	75,80,149	0.33	0
5	AJP	D	1114	-	73,73,95	0.14	0	111,116,149	0.42	0
3	POV	B	1104	-	9,9,51	0.59	0	8,8,59	0.28	0
3	POV	D	1103	-	25,25,51	0.76	1 (4%)	28,28,59	0.95	2 (7%)
4	CLR	B	1109	-	31,31,31	0.39	0	48,48,48	0.62	0
5	AJP	C	1119	-	49,49,95	0.15	0	75,80,149	0.42	0
5	AJP	A	1121	-	49,49,95	0.16	0	75,80,149	0.37	0
5	AJP	A	1119	-	49,49,95	0.15	0	75,80,149	0.35	0
5	AJP	C	1111	-	61,61,95	0.15	0	93,98,149	0.45	0
3	POV	C	1105	-	9,9,51	0.58	0	8,8,59	0.28	0
5	AJP	A	1116	-	61,61,95	0.15	0	93,98,149	0.46	0
3	POV	B	1107	-	27,27,51	0.80	1 (3%)	30,32,59	0.94	2 (6%)
5	AJP	B	1110	-	61,61,95	0.15	0	93,98,149	0.45	0
3	POV	C	1108	-	27,27,51	0.81	1 (3%)	30,32,59	0.95	2 (6%)
3	POV	A	1106	-	36,36,51	0.70	1 (2%)	39,41,59	0.90	2 (5%)
5	AJP	D	1115	-	49,49,95	0.15	0	75,80,149	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	POV	A	1107	-	25,25,51	0.76	1 (4%)	28,28,59	0.95	2 (7%)
5	AJP	C	1115	-	49,49,95	0.15	0	75,80,149	0.35	0
5	AJP	C	1113	-	49,49,95	0.14	0	75,80,149	0.33	0
5	AJP	B	1115	-	73,73,95	0.14	0	111,116,149	0.42	0
5	AJP	A	1118	-	49,49,95	0.16	0	75,80,149	0.44	0
5	AJP	D	1110	-	61,61,95	0.15	0	93,98,149	0.47	0
3	POV	D	1106	-	27,27,51	0.81	1 (3%)	30,32,59	0.94	2 (6%)
5	AJP	D	1118	-	61,61,95	0.14	0	93,98,149	0.35	0
3	POV	D	1104	-	31,31,51	0.76	1 (3%)	34,36,59	0.92	2 (5%)
5	AJP	D	1112	-	49,49,95	0.16	0	75,80,149	0.44	0
5	AJP	B	1111	-	61,61,95	0.15	0	93,98,149	0.46	0
5	AJP	D	1117	-	49,49,95	0.15	0	75,80,149	0.42	0
5	AJP	D	1113	-	49,49,95	0.15	0	75,80,149	0.35	0
5	AJP	A	1115	-	61,61,95	0.16	0	93,98,149	0.46	0
5	AJP	B	1114	-	49,49,95	0.15	0	75,80,149	0.35	0
3	POV	C	1101	-	36,36,51	0.70	1 (2%)	39,41,59	0.90	2 (5%)
5	AJP	C	1112	-	61,61,95	0.15	0	93,98,149	0.47	0
3	POV	B	1106	-	14,14,51	1.25	2 (14%)	14,14,59	1.43	2 (14%)
4	CLR	D	1108	-	31,31,31	0.40	0	48,48,48	0.57	0
3	POV	D	1105	-	14,14,51	1.24	2 (14%)	14,14,59	1.42	2 (14%)
5	AJP	B	1119	-	61,61,95	0.14	0	93,98,149	0.35	0
5	AJP	C	1117	-	49,49,95	0.16	0	75,80,149	0.36	0
3	POV	A	1110	-	31,31,51	0.76	1 (3%)	34,36,59	0.92	2 (5%)
4	CLR	C	1110	-	31,31,31	0.40	0	48,48,48	0.55	0
5	AJP	B	1112	-	49,49,95	0.14	0	75,80,149	0.33	0
5	AJP	C	1118	-	49,49,95	0.14	0	75,80,149	0.33	0
5	AJP	B	1116	-	49,49,95	0.16	0	75,80,149	0.37	0
5	AJP	B	1117	-	49,49,95	0.14	0	75,80,149	0.33	0
5	AJP	D	1111	-	49,49,95	0.15	0	75,80,149	0.33	0
5	AJP	C	1120	-	61,61,95	0.14	0	93,98,149	0.35	0
5	AJP	C	1116	-	73,73,95	0.14	0	111,116,149	0.42	0
5	AJP	A	1122	-	49,49,95	0.15	0	75,80,149	0.33	0
3	POV	C	1103	-	25,25,51	0.76	1 (4%)	28,28,59	0.94	2 (7%)
3	POV	C	1107	-	14,14,51	1.24	2 (14%)	14,14,59	1.42	2 (14%)
5	AJP	A	1123	-	49,49,95	0.14	0	75,80,149	0.42	0

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
5	AJP	D	1109	-	-	4/12/147/220	1/8/8/11
3	POV	A	1111	-	-	2/12/12/55	-
3	POV	B	1101	-	-	14/38/38/55	-
3	POV	B	1103	-	-	4/40/40/55	-
3	POV	A	1109	-	-	1/7/7/55	-
3	POV	A	1112	-	-	5/29/29/55	-
3	POV	C	1102	-	-	14/38/38/55	-
5	AJP	C	1114	-	-	1/6/121/220	0/7/7/11
3	POV	D	1102	-	-	1/7/7/55	-
5	AJP	B	1113	-	-	1/6/121/220	0/7/7/11
3	POV	C	1106	-	-	5/33/33/55	-
5	AJP	B	1118	-	-	2/6/121/220	0/7/7/11
3	POV	B	1102	-	-	4/24/24/55	-
3	POV	B	1105	-	-	5/33/33/55	-
3	POV	D	1101	-	-	4/40/40/55	-
5	AJP	A	1124	-	-	1/12/147/220	0/8/8/11
5	AJP	A	1120	-	-	5/18/173/220	0/9/9/11
3	POV	A	1108	-	-	4/40/40/55	-
4	CLR	A	1114	-	-	8/10/68/68	0/4/4/4
3	POV	C	1104	-	-	4/40/40/55	-
5	AJP	A	1117	-	-	1/6/121/220	0/7/7/11
5	AJP	D	1116	-	-	3/6/121/220	0/7/7/11
5	AJP	D	1114	-	-	5/18/173/220	0/9/9/11
3	POV	B	1104	-	-	1/7/7/55	-
3	POV	D	1103	-	-	4/24/24/55	-
4	CLR	B	1109	-	-	8/10/68/68	0/4/4/4
5	AJP	C	1119	-	-	2/6/121/220	0/7/7/11
5	AJP	A	1121	-	-	1/6/121/220	0/7/7/11
5	AJP	A	1119	-	-	0/6/121/220	0/7/7/11
5	AJP	C	1111	-	-	4/12/147/220	1/8/8/11
3	POV	C	1105	-	-	1/7/7/55	-
5	AJP	A	1116	-	-	0/12/147/220	0/8/8/11
3	POV	B	1107	-	-	5/29/29/55	-
5	AJP	B	1110	-	-	4/12/147/220	1/8/8/11
3	POV	C	1108	-	-	5/29/29/55	-
3	POV	A	1106	-	-	14/38/38/55	-
5	AJP	D	1115	-	-	1/6/121/220	0/7/7/11

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	POV	A	1107	-	-	4/24/24/55	-
5	AJP	C	1115	-	-	0/6/121/220	0/7/7/11
5	AJP	C	1113	-	-	1/6/121/220	0/7/7/11
5	AJP	B	1115	-	-	5/18/173/220	0/9/9/11
5	AJP	A	1118	-	-	1/6/121/220	0/7/7/11
5	AJP	D	1110	-	-	0/12/147/220	0/8/8/11
3	POV	D	1106	-	-	5/29/29/55	-
5	AJP	D	1118	-	-	1/12/147/220	0/8/8/11
3	POV	D	1104	-	-	5/33/33/55	-
5	AJP	D	1112	-	-	1/6/121/220	0/7/7/11
5	AJP	B	1111	-	-	0/12/147/220	0/8/8/11
5	AJP	D	1117	-	-	2/6/121/220	0/7/7/11
5	AJP	D	1113	-	-	0/6/121/220	0/7/7/11
5	AJP	A	1115	-	-	4/12/147/220	1/8/8/11
5	AJP	B	1114	-	-	0/6/121/220	0/7/7/11
3	POV	C	1101	-	-	14/38/38/55	-
5	AJP	C	1112	-	-	0/12/147/220	0/8/8/11
3	POV	B	1106	-	-	2/12/12/55	-
4	CLR	D	1108	-	-	7/10/68/68	0/4/4/4
3	POV	D	1105	-	-	2/12/12/55	-
5	AJP	B	1119	-	-	1/12/147/220	0/8/8/11
5	AJP	C	1117	-	-	1/6/121/220	0/7/7/11
3	POV	A	1110	-	-	5/33/33/55	-
4	CLR	C	1110	-	-	8/10/68/68	0/4/4/4
5	AJP	B	1112	-	-	1/6/121/220	0/7/7/11
5	AJP	C	1118	-	-	3/6/121/220	0/7/7/11
5	AJP	B	1116	-	-	1/6/121/220	0/7/7/11
5	AJP	B	1117	-	-	3/6/121/220	0/7/7/11
5	AJP	D	1111	-	-	1/6/121/220	0/7/7/11
5	AJP	C	1120	-	-	1/12/147/220	0/8/8/11
5	AJP	C	1116	-	-	5/18/173/220	0/9/9/11
5	AJP	A	1122	-	-	3/6/121/220	0/7/7/11
3	POV	C	1103	-	-	4/24/24/55	-
3	POV	C	1107	-	-	2/12/12/55	-
5	AJP	A	1123	-	-	2/6/121/220	0/7/7/11

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1106	POV	O22-C21	3.49	1.33	1.22
3	A	1111	POV	O22-C21	3.48	1.33	1.22
3	C	1107	POV	O22-C21	3.47	1.33	1.22
3	D	1105	POV	O22-C21	3.46	1.33	1.22
3	B	1102	POV	P-O12	3.07	1.66	1.54
3	C	1103	POV	P-O12	3.06	1.66	1.54
3	D	1103	POV	P-O12	3.05	1.66	1.54
3	B	1103	POV	P-O12	3.05	1.66	1.54
3	C	1108	POV	P-O12	3.05	1.66	1.54
3	D	1106	POV	P-O12	3.05	1.66	1.54
3	C	1104	POV	P-O12	3.05	1.66	1.54
3	A	1107	POV	P-O12	3.05	1.66	1.54
3	A	1108	POV	P-O12	3.04	1.66	1.54
3	C	1102	POV	P-O12	3.04	1.66	1.54
3	D	1104	POV	P-O12	3.04	1.66	1.54
3	D	1101	POV	P-O12	3.04	1.66	1.54
3	B	1105	POV	P-O12	3.04	1.66	1.54
3	B	1101	POV	P-O12	3.04	1.66	1.54
3	B	1107	POV	P-O12	3.03	1.66	1.54
3	C	1101	POV	P-O12	3.03	1.66	1.54
3	A	1106	POV	P-O12	3.03	1.66	1.54
3	C	1106	POV	P-O12	3.03	1.66	1.54
3	A	1110	POV	P-O12	3.03	1.66	1.54
3	B	1106	POV	O21-C21	-3.02	1.20	1.30
3	A	1112	POV	P-O12	3.02	1.66	1.54
3	C	1107	POV	O21-C21	-3.00	1.20	1.30
3	D	1105	POV	O21-C21	-3.00	1.20	1.30
3	A	1111	POV	O21-C21	-2.97	1.21	1.30

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1106	POV	O22-C21-C22	-3.81	111.00	123.09
3	D	1105	POV	O22-C21-C22	-3.81	111.00	123.09
3	C	1107	POV	O22-C21-C22	-3.79	111.07	123.09
3	A	1111	POV	O22-C21-C22	-3.79	111.09	123.09
3	D	1104	POV	O12-P-O11	-3.63	97.21	106.67
3	A	1111	POV	O21-C21-C22	3.63	125.46	114.00
3	B	1106	POV	O21-C21-C22	3.62	125.45	114.00
3	A	1110	POV	O12-P-O11	-3.62	97.24	106.67
3	D	1105	POV	O21-C21-C22	3.61	125.42	114.00
3	B	1105	POV	O12-P-O11	-3.61	97.25	106.67
3	C	1107	POV	O21-C21-C22	3.61	125.40	114.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1106	POV	O12-P-O11	-3.61	97.27	106.67
3	B	1103	POV	O12-P-O11	-3.54	97.44	106.67
3	D	1101	POV	O12-P-O11	-3.53	97.46	106.67
3	A	1108	POV	O12-P-O11	-3.53	97.46	106.67
3	C	1104	POV	O12-P-O11	-3.51	97.52	106.67
3	B	1102	POV	O12-P-O11	-3.47	97.62	106.67
3	A	1107	POV	O12-P-O11	-3.46	97.64	106.67
3	D	1103	POV	O12-P-O11	-3.45	97.66	106.67
3	C	1103	POV	O12-P-O11	-3.45	97.67	106.67
3	C	1108	POV	O12-P-O11	-3.42	97.76	106.67
3	D	1106	POV	O12-P-O11	-3.41	97.78	106.67
3	A	1112	POV	O12-P-O11	-3.41	97.78	106.67
3	B	1107	POV	O12-P-O11	-3.40	97.81	106.67
3	A	1106	POV	O12-P-O11	-3.39	97.84	106.67
3	B	1101	POV	O12-P-O11	-3.38	97.86	106.67
3	C	1102	POV	O12-P-O11	-3.38	97.86	106.67
3	C	1101	POV	O12-P-O11	-3.37	97.89	106.67
3	D	1104	POV	O13-P-O14	2.67	121.24	110.83
3	B	1105	POV	O13-P-O14	2.67	121.22	110.83
3	A	1110	POV	O13-P-O14	2.66	121.21	110.83
3	C	1106	POV	O13-P-O14	2.65	121.17	110.83
3	C	1108	POV	O13-P-O14	2.65	121.16	110.83
3	A	1112	POV	O13-P-O14	2.65	121.14	110.83
3	B	1102	POV	O13-P-O14	2.64	121.14	110.83
3	A	1107	POV	O13-P-O14	2.64	121.13	110.83
3	C	1103	POV	O13-P-O14	2.64	121.12	110.83
3	B	1107	POV	O13-P-O14	2.64	121.11	110.83
3	D	1103	POV	O13-P-O14	2.63	121.09	110.83
3	D	1106	POV	O13-P-O14	2.63	121.09	110.83
3	B	1101	POV	O13-P-O14	2.63	121.08	110.83
3	A	1106	POV	O13-P-O14	2.62	121.06	110.83
3	D	1101	POV	O13-P-O14	2.62	121.04	110.83
3	B	1103	POV	O13-P-O14	2.62	121.03	110.83
3	A	1108	POV	O13-P-O14	2.61	121.02	110.83
3	C	1101	POV	O13-P-O14	2.61	121.00	110.83
3	C	1104	POV	O13-P-O14	2.60	120.98	110.83
3	C	1102	POV	O13-P-O14	2.60	120.95	110.83

There are no chirality outliers.

All (243) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1106	POV	C1-O11-P-O12
3	A	1106	POV	C1-O11-P-O13
3	A	1106	POV	C1-O11-P-O14
3	A	1107	POV	C1-O11-P-O13
3	A	1108	POV	O21-C2-C3-O31
3	A	1110	POV	O22-C21-O21-C2
3	A	1112	POV	C1-O11-P-O13
3	B	1101	POV	C1-O11-P-O12
3	B	1101	POV	C1-O11-P-O13
3	B	1101	POV	C1-O11-P-O14
3	B	1102	POV	C1-O11-P-O12
3	B	1102	POV	C1-O11-P-O13
3	B	1103	POV	O21-C2-C3-O31
3	B	1105	POV	O22-C21-O21-C2
3	B	1107	POV	C1-O11-P-O13
3	C	1101	POV	C1-O11-P-O12
3	C	1101	POV	C1-O11-P-O13
3	C	1101	POV	C1-O11-P-O14
3	C	1102	POV	C1-O11-P-O12
3	C	1102	POV	C1-O11-P-O13
3	C	1102	POV	C1-O11-P-O14
3	C	1103	POV	C1-O11-P-O12
3	C	1103	POV	C1-O11-P-O13
3	C	1104	POV	O21-C2-C3-O31
3	C	1106	POV	O22-C21-O21-C2
3	C	1108	POV	C1-O11-P-O13
3	D	1101	POV	O21-C2-C3-O31
3	D	1103	POV	C1-O11-P-O13
3	D	1104	POV	O22-C21-O21-C2
3	D	1106	POV	C1-O11-P-O13
5	A	1117	AJP	C22-C23-O25-C26
5	A	1118	AJP	C22-C23-O25-C26
5	A	1121	AJP	C22-C23-O25-C26
5	B	1112	AJP	C22-C23-O25-C26
5	B	1116	AJP	C22-C23-O25-C26
5	C	1113	AJP	C22-C23-O25-C26
5	C	1114	AJP	C22-C23-O25-C26
5	C	1117	AJP	C22-C23-O25-C26
5	D	1111	AJP	C22-C23-O25-C26
5	D	1112	AJP	C22-C23-O25-C26
5	D	1115	AJP	C22-C23-O25-C26
5	A	1115	AJP	O31-C26-O25-C23
5	A	1122	AJP	O31-C26-O25-C23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	C	1118	AJP	O31-C26-O25-C23
5	D	1116	AJP	O31-C26-O25-C23
5	A	1115	AJP	O40-C35-O34-C29
5	A	1123	AJP	O31-C26-O25-C23
5	B	1110	AJP	O31-C26-O25-C23
5	B	1110	AJP	O40-C35-O34-C29
5	B	1117	AJP	O31-C26-O25-C23
5	B	1118	AJP	O31-C26-O25-C23
5	C	1111	AJP	O40-C35-O34-C29
5	C	1119	AJP	O31-C26-O25-C23
5	D	1109	AJP	O31-C26-O25-C23
5	D	1109	AJP	O40-C35-O34-C29
5	D	1117	AJP	O31-C26-O25-C23
5	A	1120	AJP	O60-C55-O54-C36
5	B	1115	AJP	O60-C55-O54-C36
5	C	1116	AJP	O60-C55-O54-C36
5	D	1114	AJP	O60-C55-O54-C36
5	A	1122	AJP	C27-C26-O25-C23
5	A	1123	AJP	C27-C26-O25-C23
5	B	1117	AJP	C27-C26-O25-C23
5	B	1118	AJP	C27-C26-O25-C23
5	C	1118	AJP	C27-C26-O25-C23
5	C	1119	AJP	C27-C26-O25-C23
5	D	1116	AJP	C27-C26-O25-C23
5	D	1117	AJP	C27-C26-O25-C23
5	A	1120	AJP	C56-C55-O54-C36
5	B	1115	AJP	C56-C55-O54-C36
5	C	1116	AJP	C56-C55-O54-C36
5	D	1114	AJP	C56-C55-O54-C36
3	A	1110	POV	C22-C21-O21-C2
3	B	1105	POV	C22-C21-O21-C2
3	C	1106	POV	C22-C21-O21-C2
3	D	1104	POV	C22-C21-O21-C2
5	C	1111	AJP	O31-C26-O25-C23
5	C	1116	AJP	C58-C59-C61-O62
5	D	1114	AJP	C58-C59-C61-O62
5	A	1120	AJP	C58-C59-C61-O62
5	B	1115	AJP	C58-C59-C61-O62
3	A	1112	POV	O21-C2-C3-O31
3	B	1107	POV	O21-C2-C3-O31
3	C	1108	POV	O21-C2-C3-O31
3	D	1106	POV	O21-C2-C3-O31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	C	1116	AJP	O60-C59-C61-O62
5	D	1114	AJP	O60-C59-C61-O62
5	A	1120	AJP	O60-C59-C61-O62
5	A	1115	AJP	C36-C35-O34-C29
5	B	1110	AJP	C36-C35-O34-C29
5	D	1109	AJP	C36-C35-O34-C29
4	C	1110	CLR	C20-C22-C23-C24
5	B	1115	AJP	O60-C59-C61-O62
5	C	1111	AJP	C36-C35-O34-C29
4	A	1114	CLR	C20-C22-C23-C24
4	D	1108	CLR	C20-C22-C23-C24
4	B	1109	CLR	C20-C22-C23-C24
4	C	1110	CLR	C22-C23-C24-C25
4	A	1114	CLR	C22-C23-C24-C25
4	D	1108	CLR	C22-C23-C24-C25
4	B	1109	CLR	C22-C23-C24-C25
3	A	1106	POV	C22-C21-O21-C2
3	B	1101	POV	C22-C21-O21-C2
3	C	1101	POV	C22-C21-O21-C2
3	C	1102	POV	C22-C21-O21-C2
3	A	1106	POV	O22-C21-O21-C2
3	B	1101	POV	O22-C21-O21-C2
3	C	1101	POV	O22-C21-O21-C2
3	C	1102	POV	O22-C21-O21-C2
3	A	1107	POV	O11-C1-C2-C3
3	B	1102	POV	O11-C1-C2-C3
3	C	1103	POV	O11-C1-C2-C3
3	D	1103	POV	O11-C1-C2-C3
4	A	1114	CLR	C23-C24-C25-C26
4	B	1109	CLR	C23-C24-C25-C26
4	C	1110	CLR	C23-C24-C25-C26
4	D	1108	CLR	C23-C24-C25-C26
4	C	1110	CLR	C23-C24-C25-C27
4	D	1108	CLR	C23-C24-C25-C27
3	C	1103	POV	C1-C2-C3-O31
3	B	1101	POV	C35-C36-C37-C38
3	C	1101	POV	C35-C36-C37-C38
3	A	1106	POV	C35-C36-C37-C38
3	C	1102	POV	C23-C24-C25-C26
3	B	1101	POV	C23-C24-C25-C26
3	A	1107	POV	C1-C2-C3-O31
3	B	1102	POV	C1-C2-C3-O31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	D	1103	POV	C1-C2-C3-O31
3	C	1102	POV	C35-C36-C37-C38
3	A	1106	POV	C23-C24-C25-C26
3	C	1102	POV	C37-C38-C39-C310
4	B	1109	CLR	C23-C24-C25-C27
3	A	1106	POV	C37-C38-C39-C310
3	B	1101	POV	C37-C38-C39-C310
3	C	1101	POV	C23-C24-C25-C26
3	C	1101	POV	C37-C38-C39-C310
4	A	1114	CLR	C23-C24-C25-C27
5	C	1111	AJP	O40-C39-C41-O42
5	A	1115	AJP	O40-C39-C41-O42
5	A	1122	AJP	O31-C30-C32-O33
5	B	1110	AJP	O40-C39-C41-O42
5	B	1117	AJP	O31-C30-C32-O33
5	C	1118	AJP	O31-C30-C32-O33
5	D	1109	AJP	O40-C39-C41-O42
5	D	1116	AJP	O31-C30-C32-O33
5	A	1120	AJP	O31-C30-C32-O33
5	A	1124	AJP	O31-C30-C32-O33
5	B	1115	AJP	O31-C30-C32-O33
5	B	1119	AJP	O31-C30-C32-O33
5	C	1116	AJP	O31-C30-C32-O33
5	C	1120	AJP	O31-C30-C32-O33
5	D	1114	AJP	O31-C30-C32-O33
5	D	1118	AJP	O31-C30-C32-O33
3	C	1102	POV	C311-C310-C39-C38
3	C	1101	POV	C311-C310-C39-C38
3	C	1102	POV	C36-C37-C38-C39
5	B	1113	AJP	C22-C23-O25-C26
3	D	1104	POV	C25-C26-C27-C28
3	B	1101	POV	C311-C310-C39-C38
3	A	1108	POV	C1-C2-C3-O31
3	A	1112	POV	C1-C2-C3-O31
3	B	1103	POV	C1-C2-C3-O31
3	B	1107	POV	C1-C2-C3-O31
3	C	1104	POV	C1-C2-C3-O31
3	C	1108	POV	C1-C2-C3-O31
3	D	1101	POV	C1-C2-C3-O31
3	D	1106	POV	C1-C2-C3-O31
3	A	1106	POV	C311-C310-C39-C38
3	C	1106	POV	C25-C26-C27-C28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	1105	POV	C25-C26-C27-C28
3	A	1110	POV	C25-C26-C27-C28
4	B	1109	CLR	C13-C17-C20-C22
4	A	1114	CLR	C13-C17-C20-C22
3	A	1107	POV	C1-O11-P-O12
3	A	1108	POV	C1-O11-P-O13
3	B	1103	POV	C1-O11-P-O13
3	C	1104	POV	C1-O11-P-O13
3	D	1101	POV	C1-O11-P-O13
3	D	1103	POV	C1-O11-P-O12
4	A	1114	CLR	C13-C17-C20-C21
4	B	1109	CLR	C13-C17-C20-C21
4	C	1110	CLR	C13-C17-C20-C21
4	C	1110	CLR	C13-C17-C20-C22
3	C	1101	POV	C36-C37-C38-C39
3	B	1101	POV	C36-C37-C38-C39
3	A	1106	POV	C36-C37-C38-C39
4	A	1114	CLR	C16-C17-C20-C22
4	B	1109	CLR	C16-C17-C20-C22
4	C	1110	CLR	C16-C17-C20-C22
4	A	1114	CLR	C16-C17-C20-C21
4	B	1109	CLR	C16-C17-C20-C21
3	A	1106	POV	C3-C2-O21-C21
3	B	1101	POV	C3-C2-O21-C21
3	C	1101	POV	C3-C2-O21-C21
3	C	1102	POV	C3-C2-O21-C21
4	C	1110	CLR	C16-C17-C20-C21
3	A	1110	POV	C27-C28-C29-C210
3	B	1105	POV	C27-C28-C29-C210
3	C	1106	POV	C27-C28-C29-C210
3	D	1104	POV	C27-C28-C29-C210
4	D	1108	CLR	C13-C17-C20-C21
3	A	1106	POV	O21-C2-C3-O31
3	B	1101	POV	O21-C2-C3-O31
3	C	1101	POV	O21-C2-C3-O31
4	D	1108	CLR	C16-C17-C20-C22
4	D	1108	CLR	C13-C17-C20-C22
3	C	1108	POV	O22-C21-O21-C2
3	A	1111	POV	O21-C21-C22-C23
3	D	1105	POV	O21-C21-C22-C23
3	B	1106	POV	O21-C21-C22-C23
3	C	1107	POV	O21-C21-C22-C23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	1106	POV	C27-C28-C29-C210
3	B	1101	POV	C27-C28-C29-C210
3	C	1101	POV	C27-C28-C29-C210
3	C	1102	POV	C27-C28-C29-C210
3	C	1102	POV	O21-C2-C3-O31
3	C	1104	POV	C24-C25-C26-C27
3	B	1103	POV	C24-C25-C26-C27
3	C	1106	POV	C29-C210-C211-C212
3	D	1104	POV	C29-C210-C211-C212
3	A	1111	POV	O22-C21-C22-C23
3	B	1106	POV	O22-C21-C22-C23
3	C	1107	POV	O22-C21-C22-C23
3	D	1105	POV	O22-C21-C22-C23
3	A	1108	POV	C24-C25-C26-C27
3	A	1110	POV	C29-C210-C211-C212
3	B	1105	POV	C29-C210-C211-C212
3	D	1101	POV	C24-C25-C26-C27
3	C	1108	POV	C22-C21-O21-C2
3	A	1112	POV	O22-C21-O21-C2
3	B	1107	POV	O22-C21-O21-C2
3	D	1106	POV	O22-C21-O21-C2
3	D	1102	POV	C25-C26-C27-C28
3	C	1105	POV	C25-C26-C27-C28
3	D	1106	POV	C22-C21-O21-C2
3	A	1109	POV	C25-C26-C27-C28
3	B	1104	POV	C25-C26-C27-C28
3	A	1112	POV	C22-C21-O21-C2
3	B	1107	POV	C22-C21-O21-C2
3	C	1101	POV	C24-C25-C26-C27
3	C	1102	POV	C24-C25-C26-C27
3	B	1101	POV	C24-C25-C26-C27
3	A	1106	POV	C24-C25-C26-C27

All (4) ring outliers are listed below:

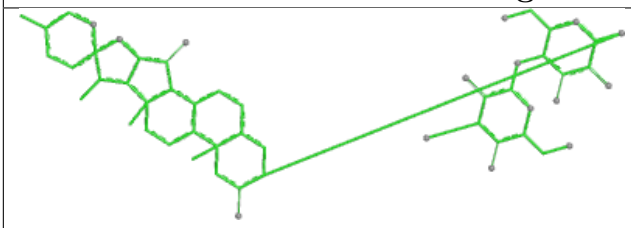
Mol	Chain	Res	Type	Atoms
5	C	1111	AJP	C19-C20-C21-C22-C23-C24
5	D	1109	AJP	C19-C20-C21-C22-C23-C24
5	B	1110	AJP	C19-C20-C21-C22-C23-C24
5	A	1115	AJP	C19-C20-C21-C22-C23-C24

26 monomers are involved in 34 short contacts:

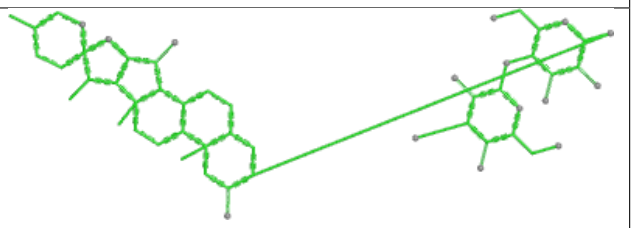
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1103	POV	2	0
3	C	1102	POV	1	0
3	C	1106	POV	1	0
3	B	1102	POV	1	0
3	B	1105	POV	1	0
3	D	1101	POV	2	0
5	A	1124	AJP	1	0
3	A	1108	POV	2	0
4	A	1114	CLR	1	0
3	C	1104	POV	3	0
5	D	1116	AJP	1	0
3	D	1103	POV	1	0
4	B	1109	CLR	3	0
5	C	1111	AJP	1	0
5	A	1116	AJP	1	0
3	A	1107	POV	1	0
5	D	1110	AJP	1	0
5	D	1118	AJP	1	0
5	B	1111	AJP	1	0
3	C	1101	POV	1	0
5	C	1112	AJP	1	0
4	C	1110	CLR	3	0
5	C	1118	AJP	1	0
5	B	1117	AJP	1	0
5	A	1122	AJP	1	0
3	C	1103	POV	1	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.

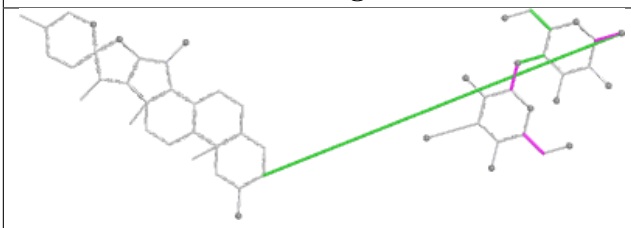
Ligand AJP D 1109



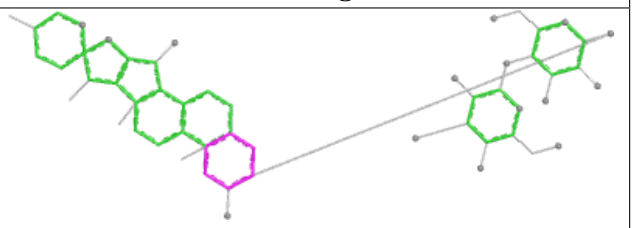
Bond lengths



Bond angles

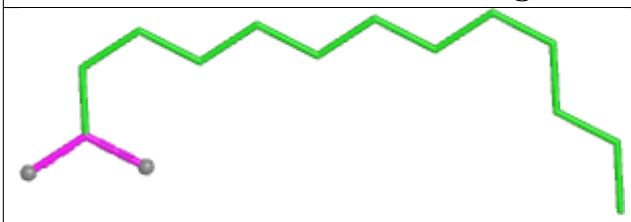


Torsions

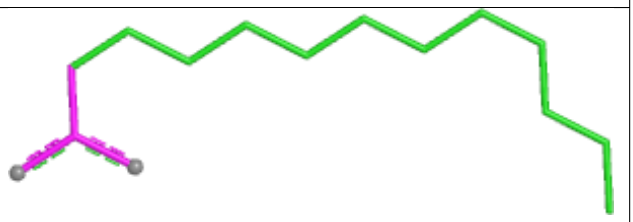


Rings

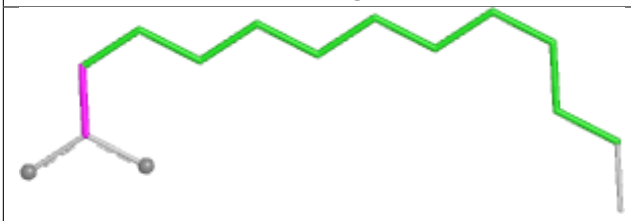
Ligand POV A 1111



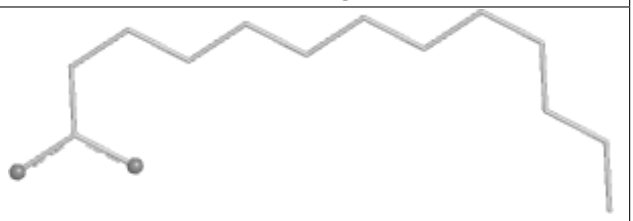
Bond lengths



Bond angles

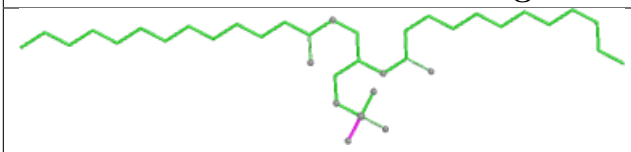


Torsions

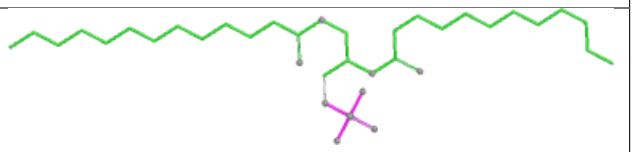


Rings

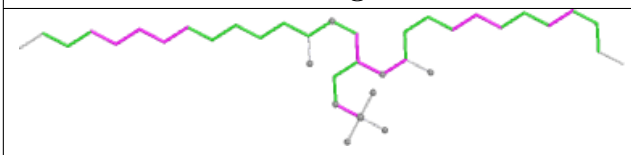
Ligand POV B 1101



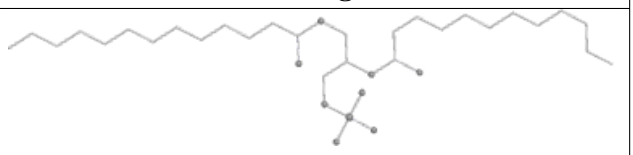
Bond lengths



Bond angles

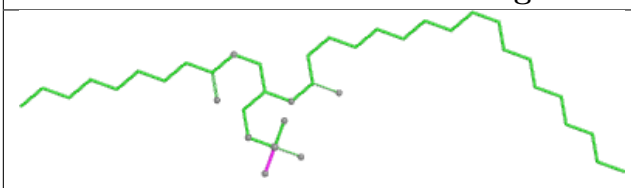


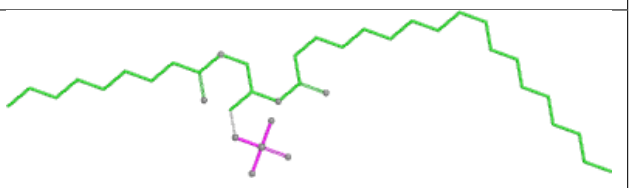
Torsions

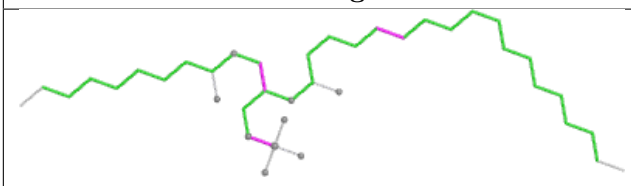


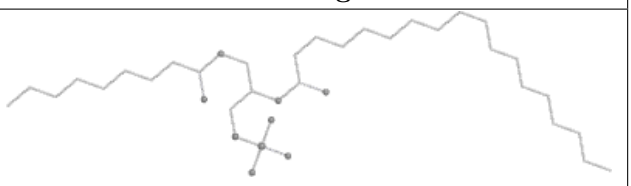
Rings

Ligand POV B 1103


Bond lengths

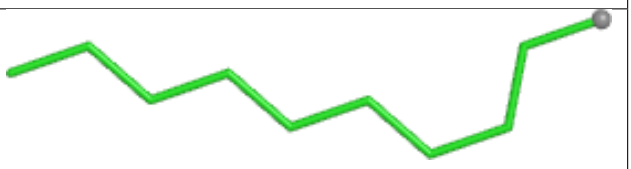

Bond angles

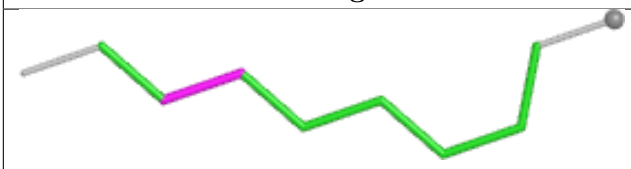

Torsions

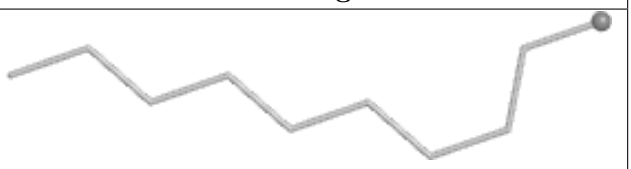

Rings

Ligand POV A 1109

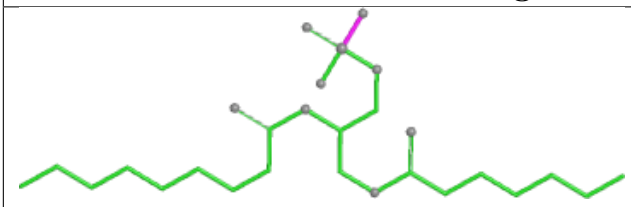

Bond lengths

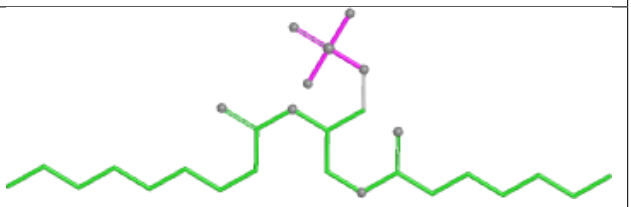

Bond angles

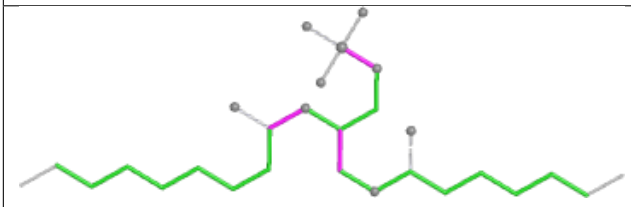

Torsions

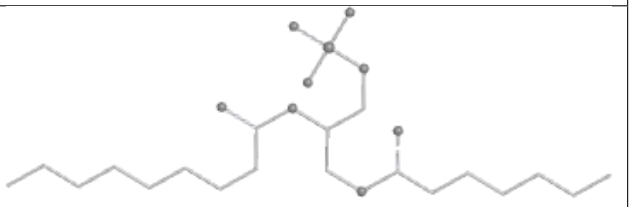

Rings

Ligand POV A 1112

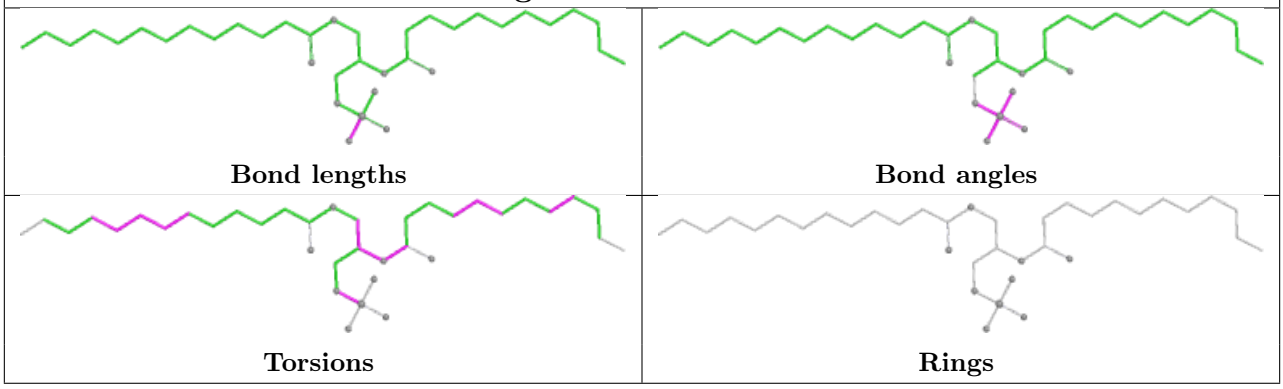

Bond lengths


Bond angles

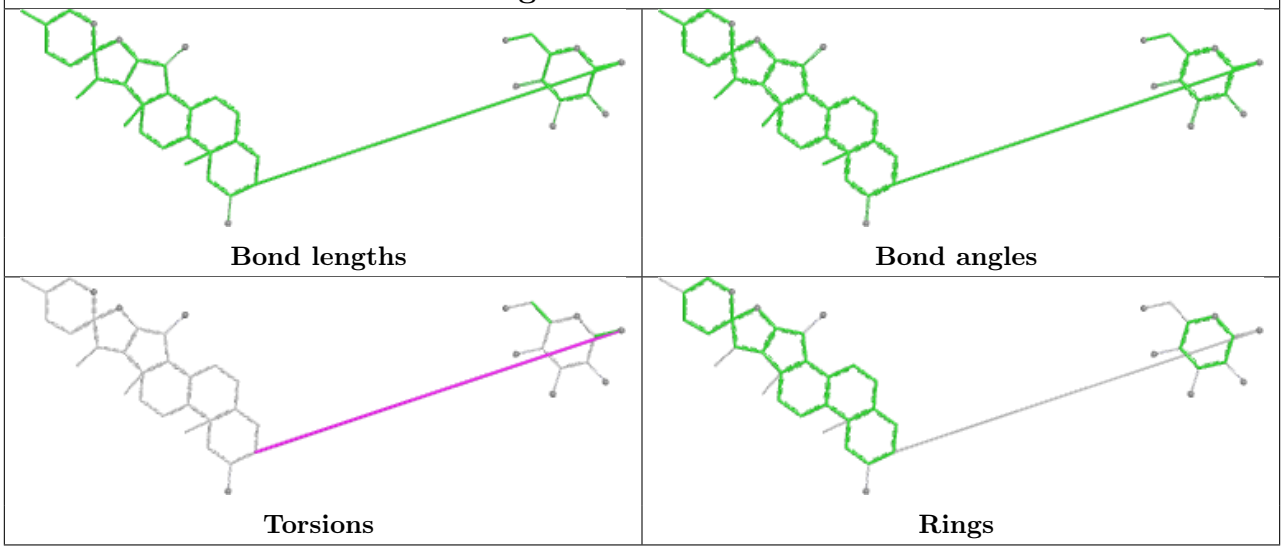

Torsions


Rings

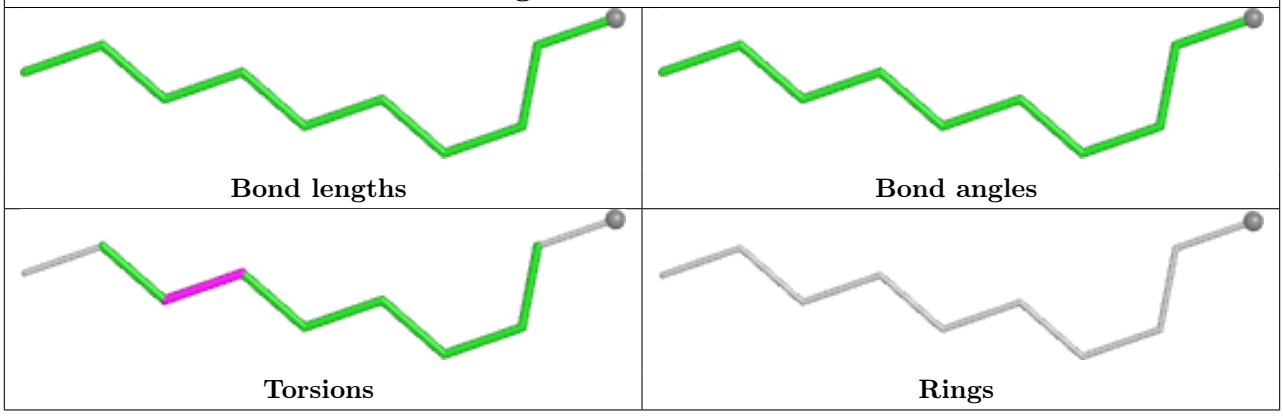
Ligand POV C 1102



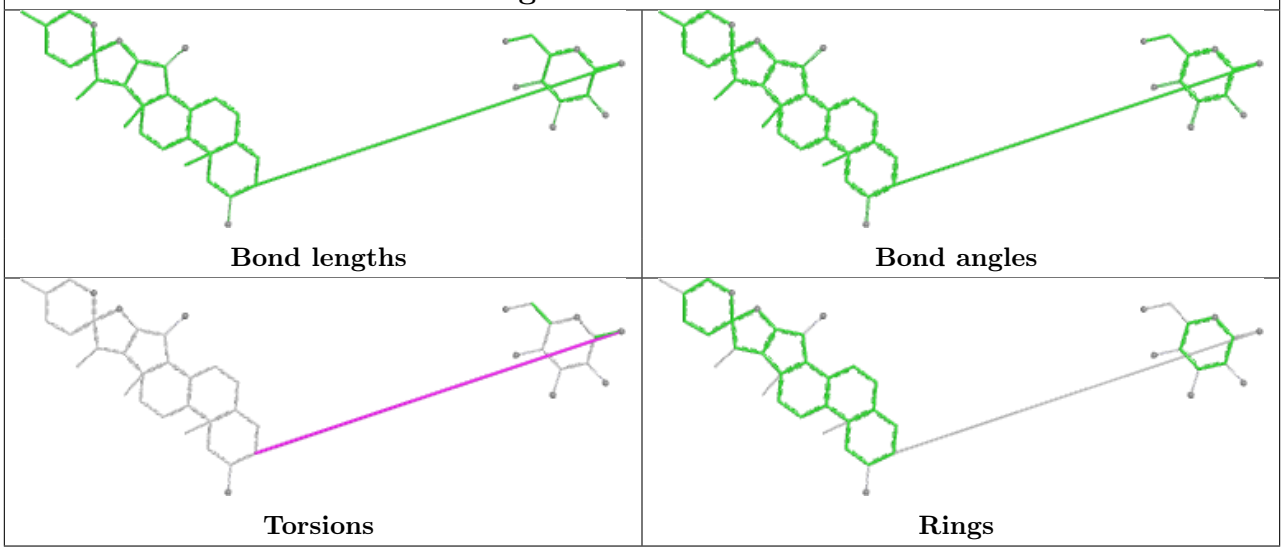
Ligand AJP C 1114



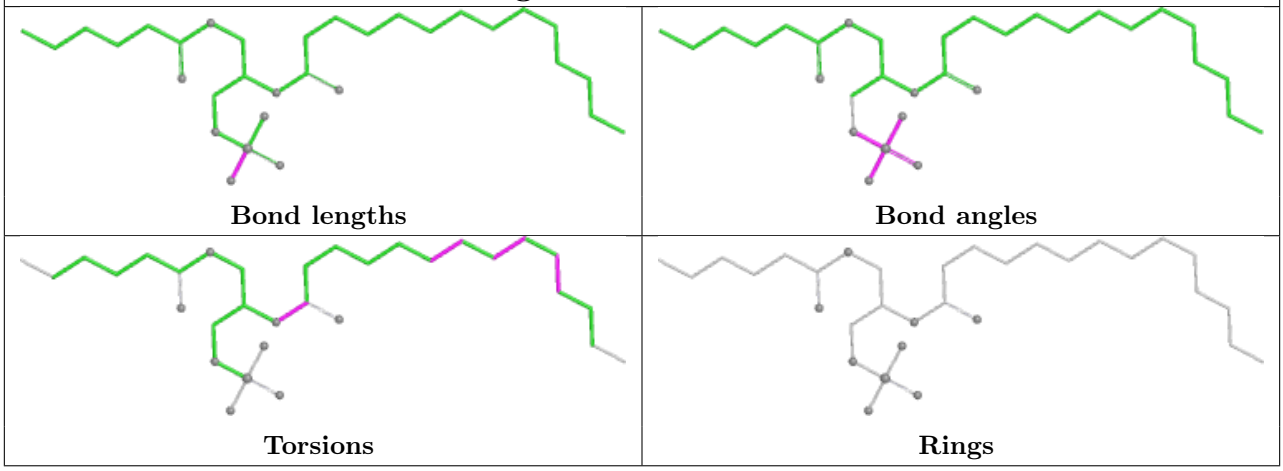
Ligand POV D 1102



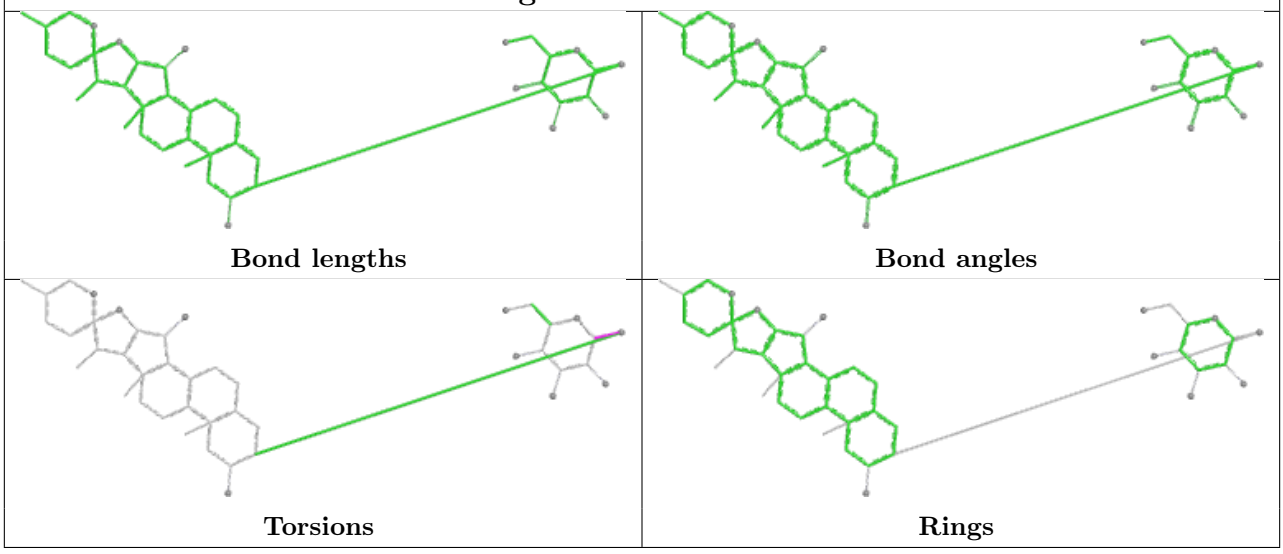
Ligand AJP B 1113



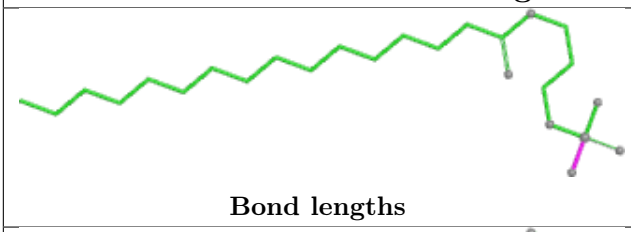
Ligand POV C 1106

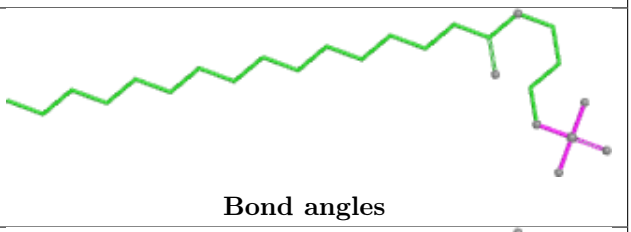


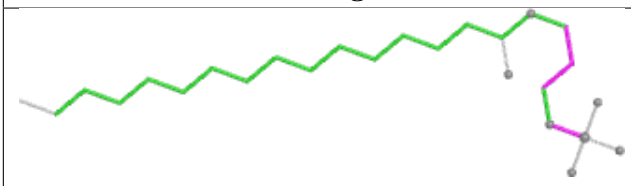
Ligand AJP B 1118



Ligand POV B 1102

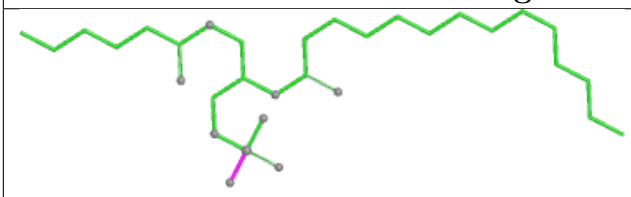

Bond lengths

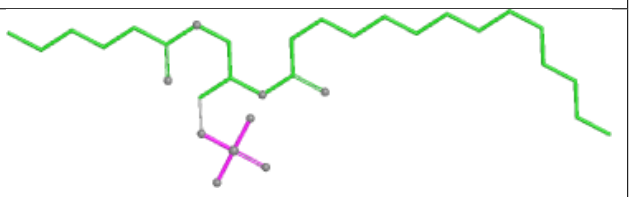

Bond angles

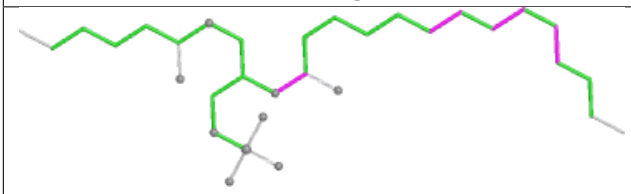

Torsions

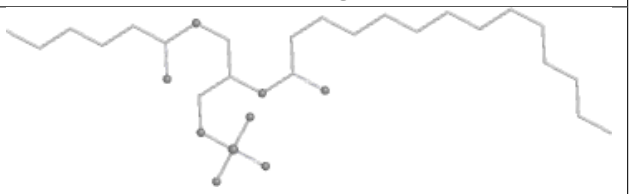

Rings

Ligand POV B 1105

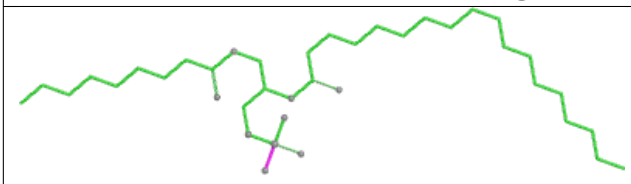

Bond lengths

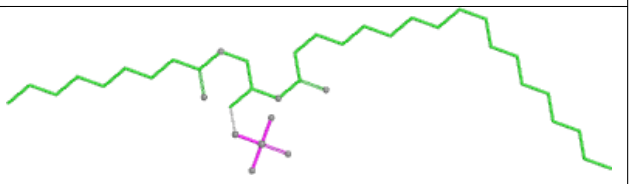

Bond angles

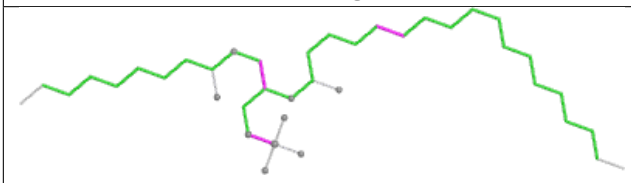

Torsions

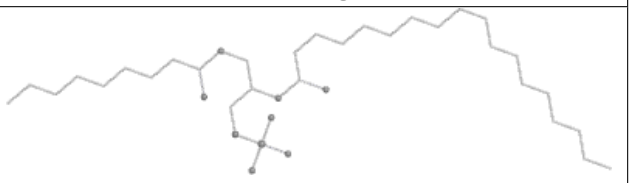

Rings

Ligand POV D 1101

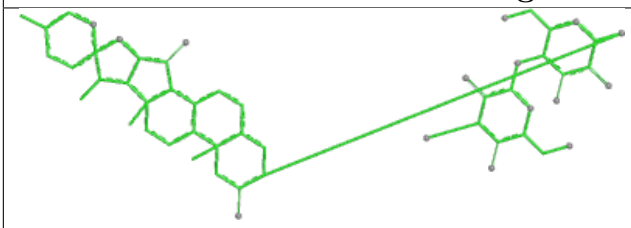

Bond lengths


Bond angles

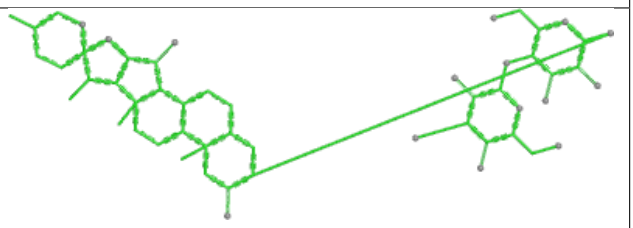

Torsions


Rings

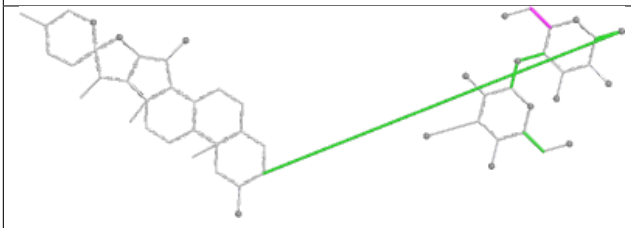
Ligand AJP A 1124



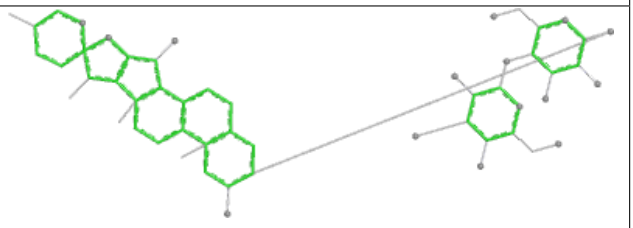
Bond lengths



Bond angles

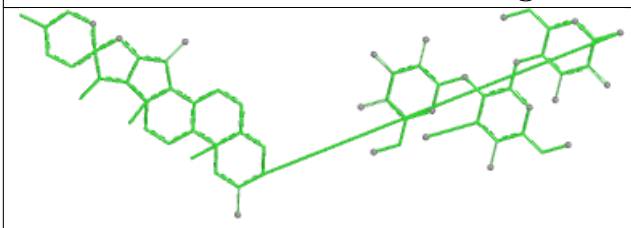


Torsions

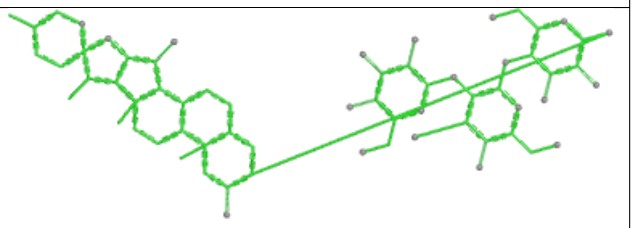


Rings

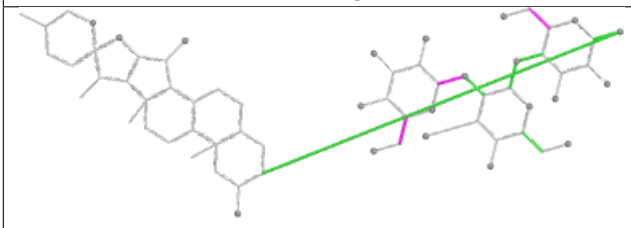
Ligand AJP A 1120



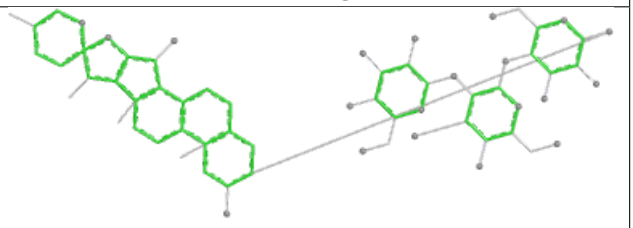
Bond lengths



Bond angles

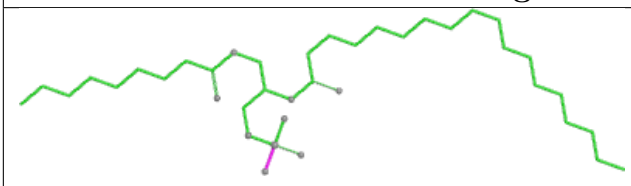


Torsions

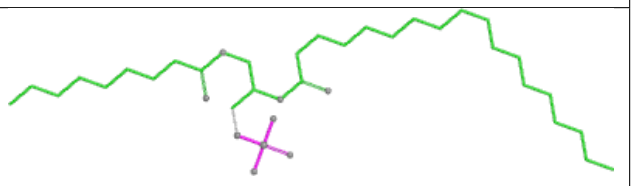


Rings

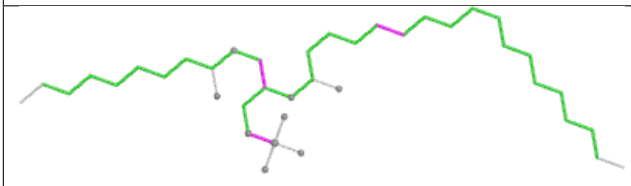
Ligand POV A 1108



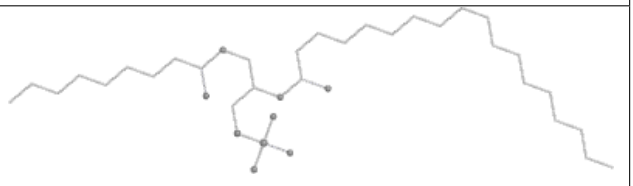
Bond lengths



Bond angles

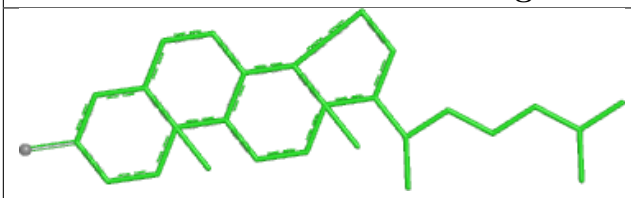


Torsions

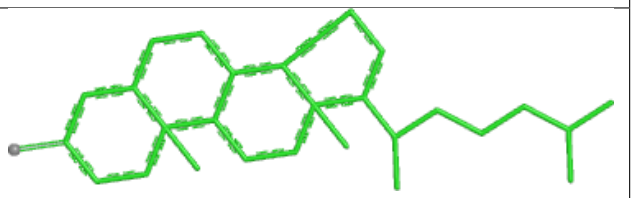


Rings

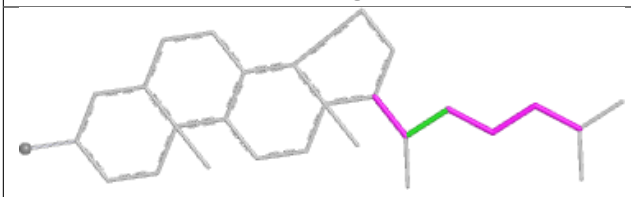
Ligand CLR A 1114



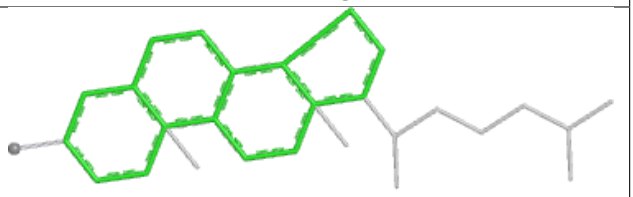
Bond lengths



Bond angles

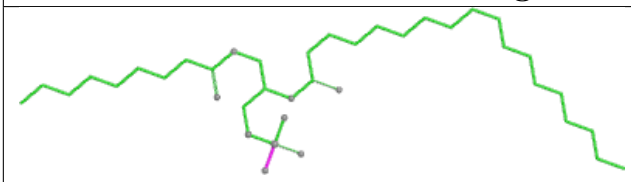


Torsions

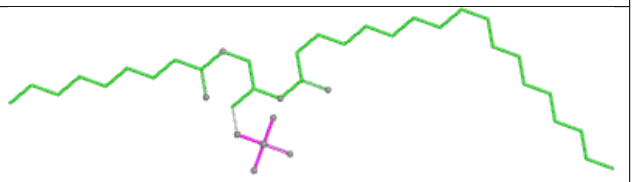


Rings

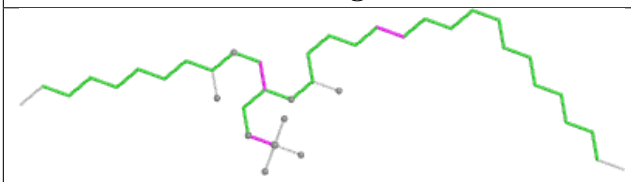
Ligand POV C 1104



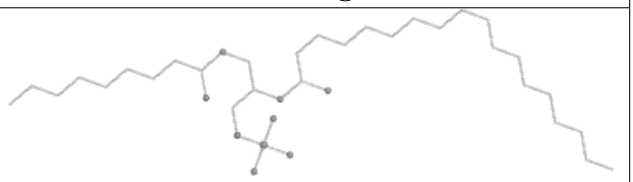
Bond lengths



Bond angles

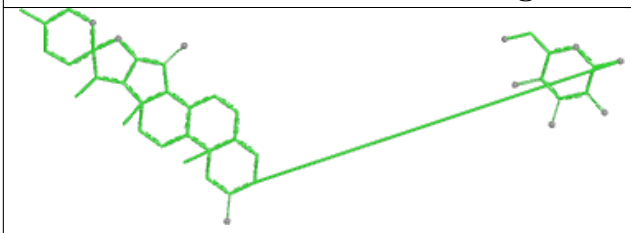


Torsions

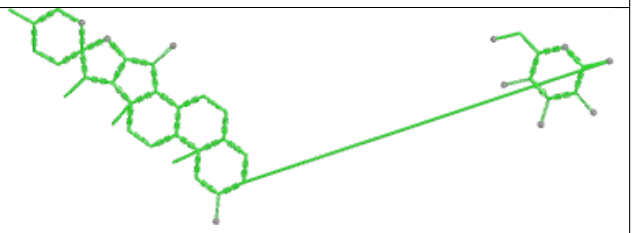


Rings

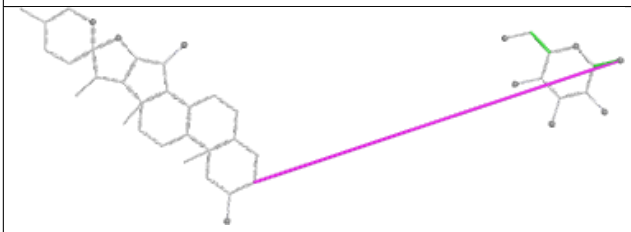
Ligand AJP A 1117



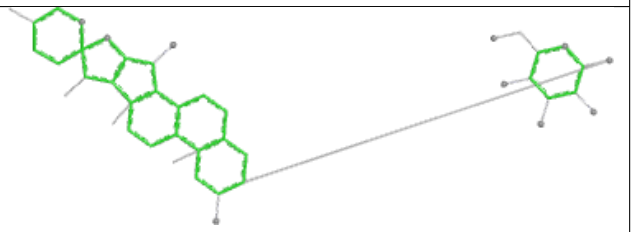
Bond lengths



Bond angles

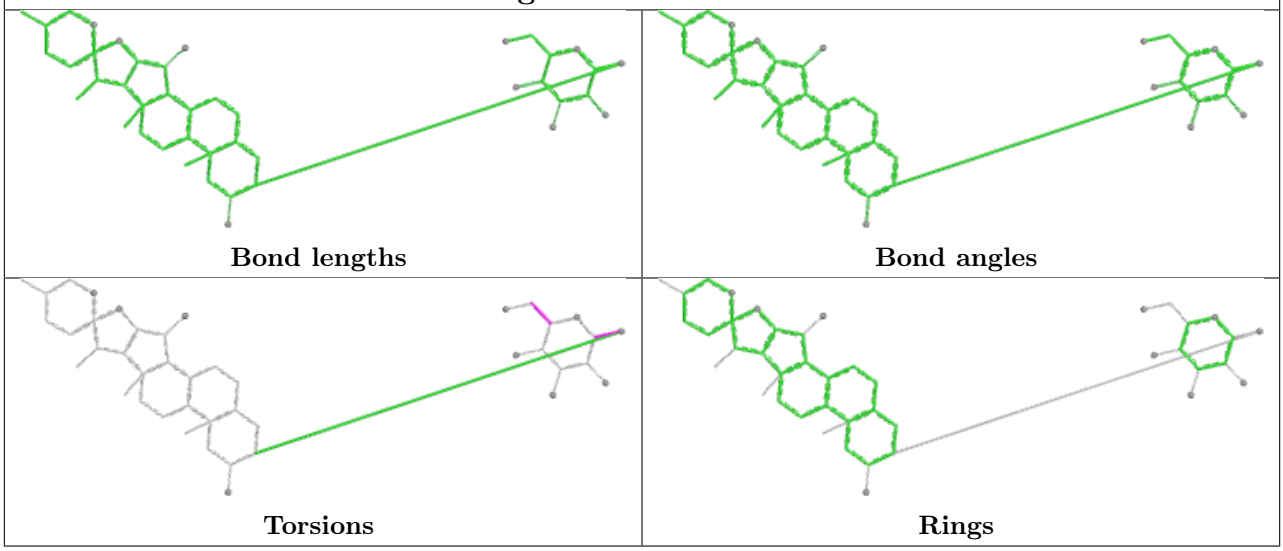


Torsions

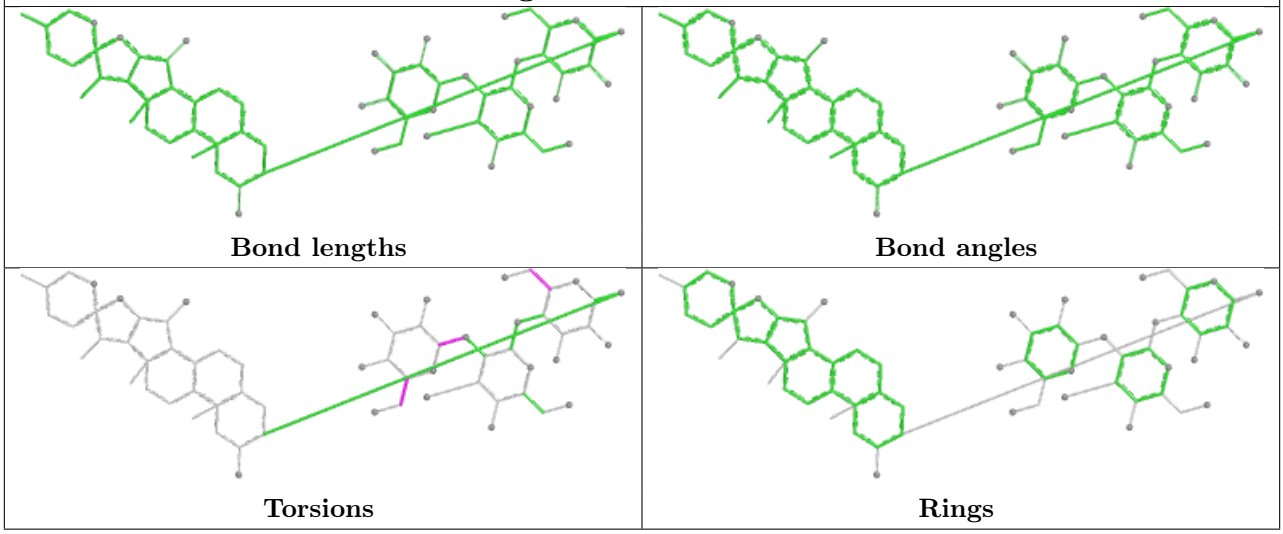


Rings

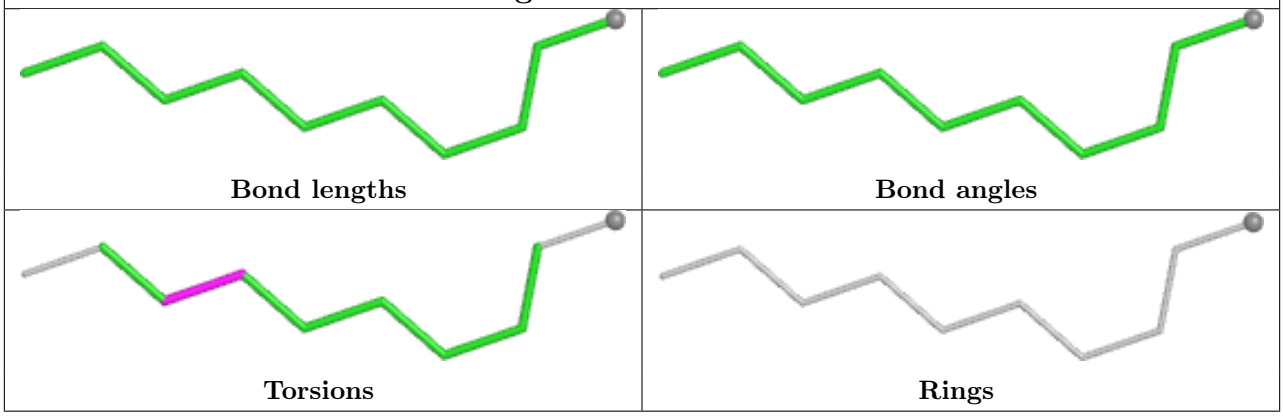
Ligand AJP D 1116



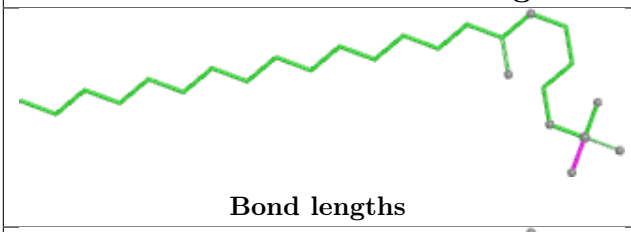
Ligand AJP D 1114



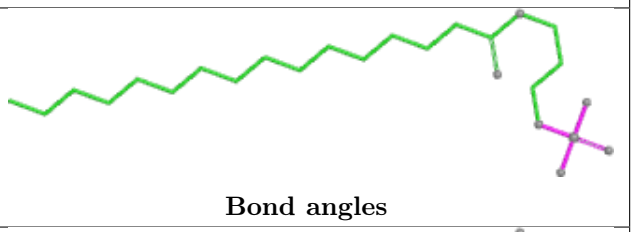
Ligand POV B 1104



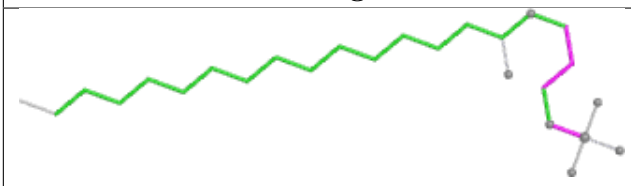
Ligand POV D 1103



Bond lengths



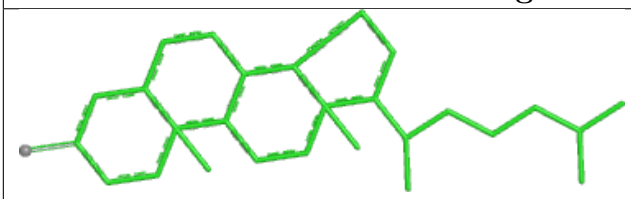
Bond angles



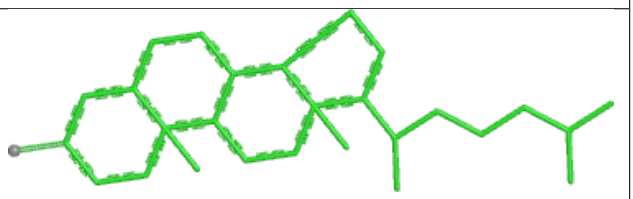
Torsions

Rings

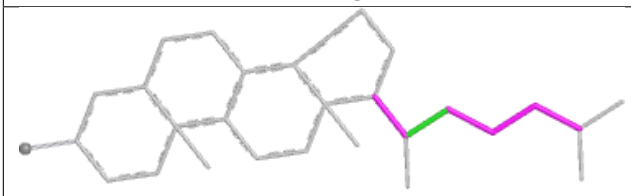
Ligand CLR B 1109



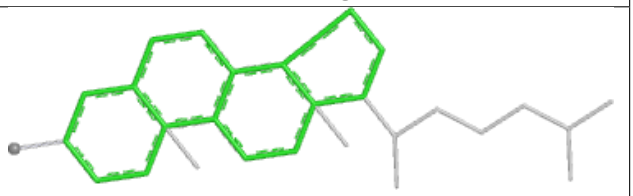
Bond lengths



Bond angles

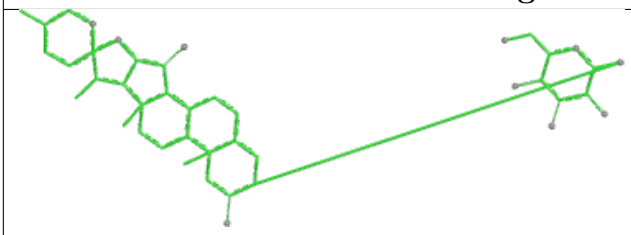


Torsions

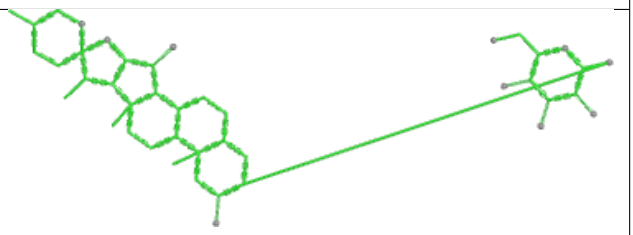


Rings

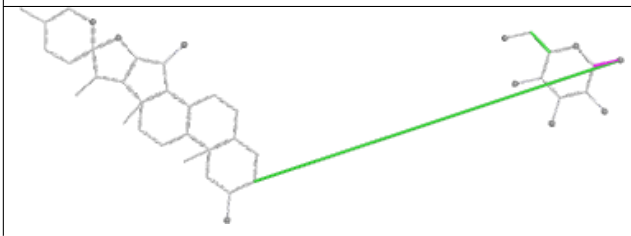
Ligand AJP C 1119



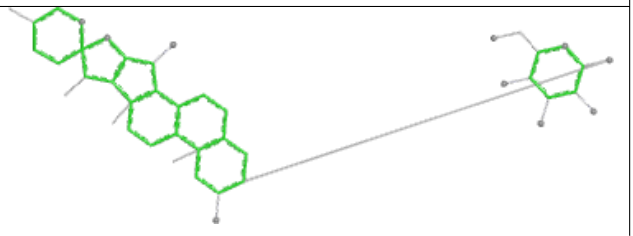
Bond lengths



Bond angles

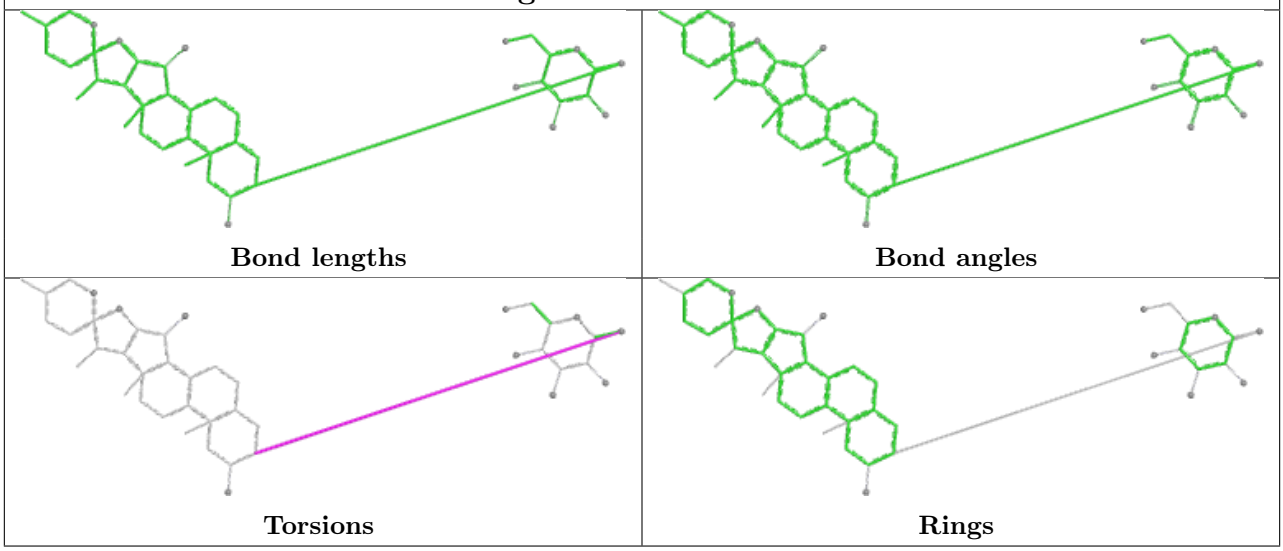


Torsions

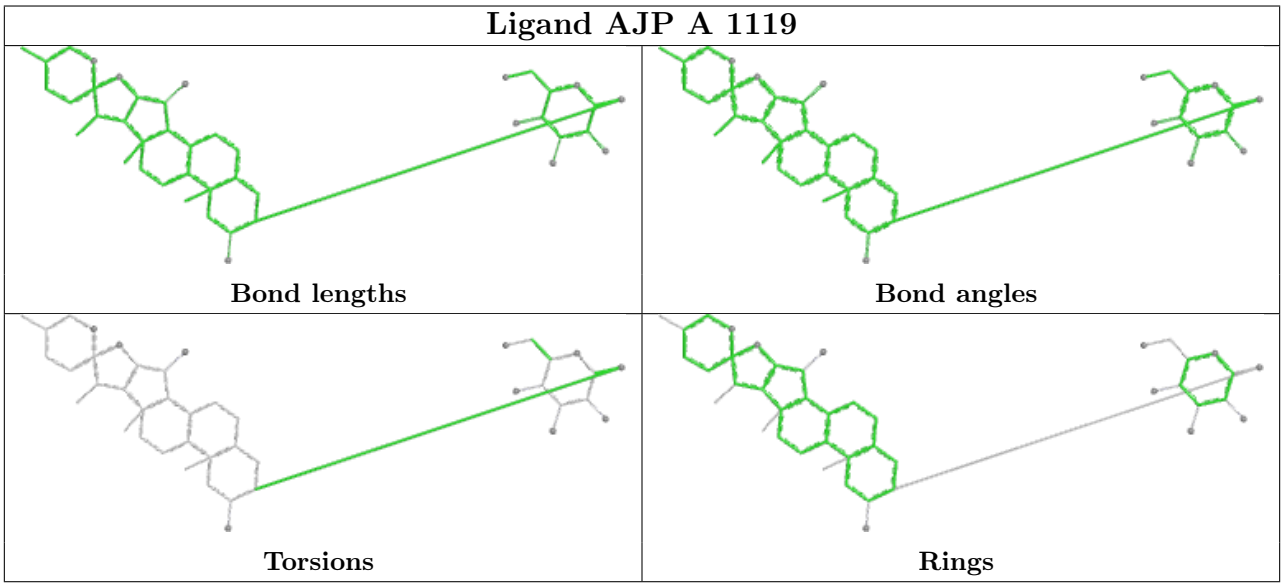


Rings

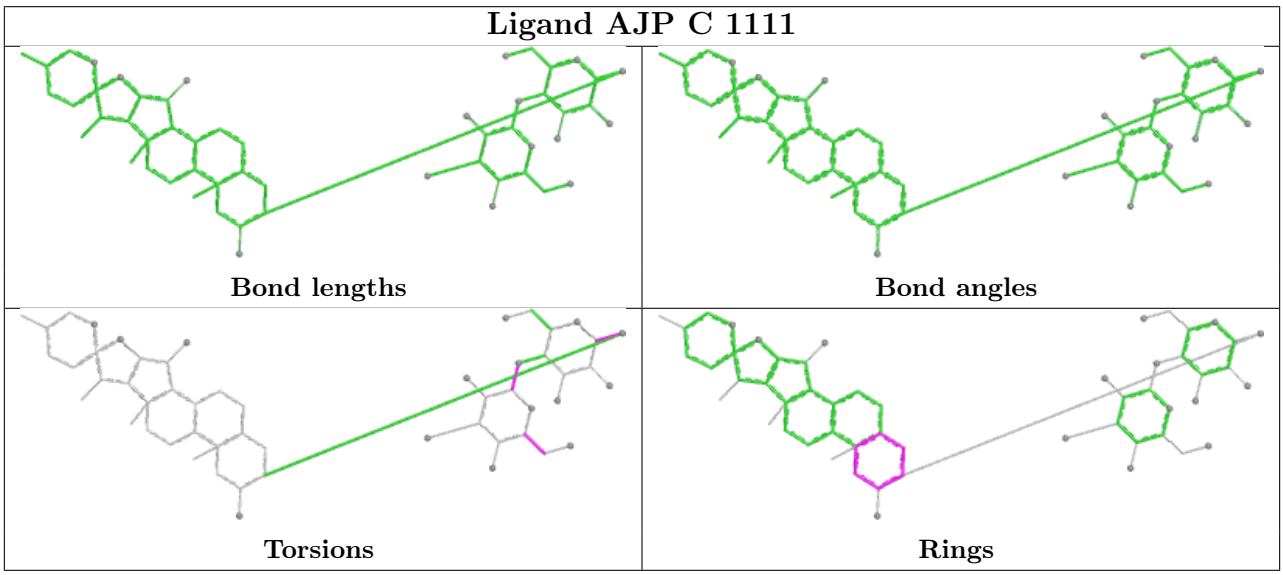
Ligand AJP A 1121



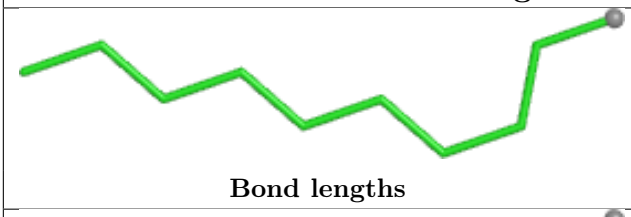
Ligand AJP A 1119



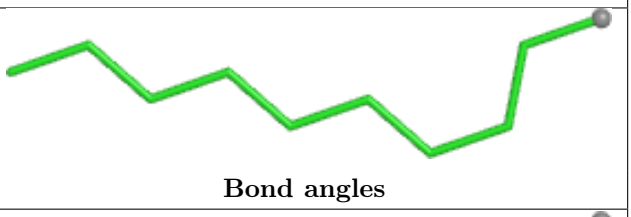
Ligand AJP C 1111



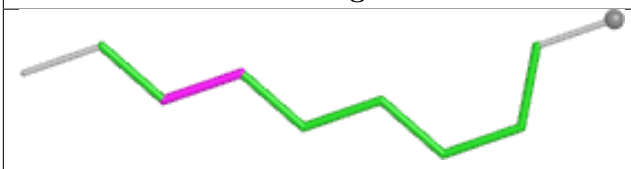
Ligand POV C 1105



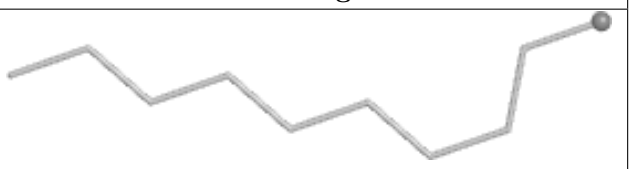
Bond lengths



Bond angles

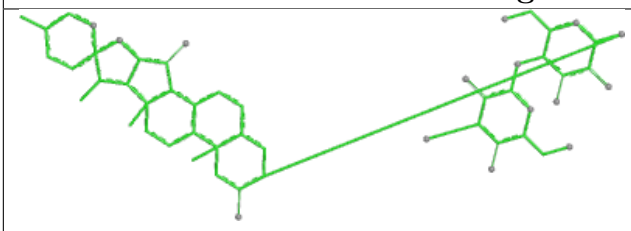


Torsions

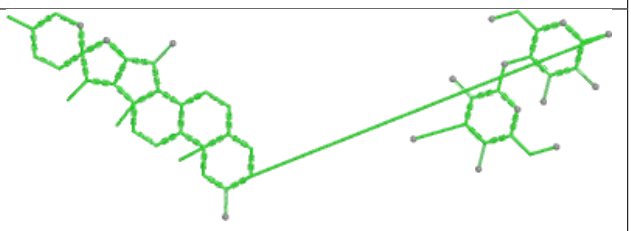


Rings

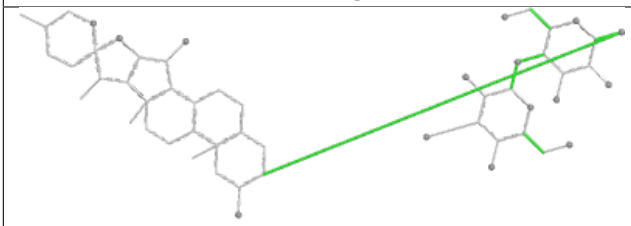
Ligand AJP A 1116



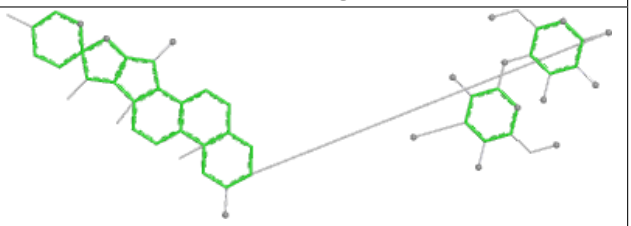
Bond lengths



Bond angles

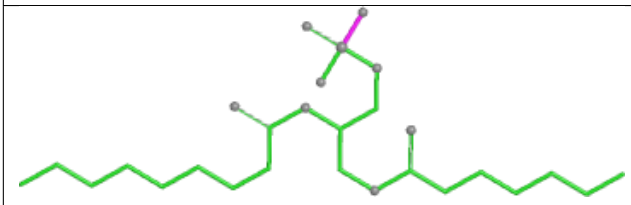


Torsions

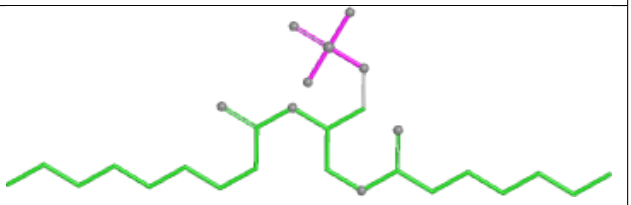


Rings

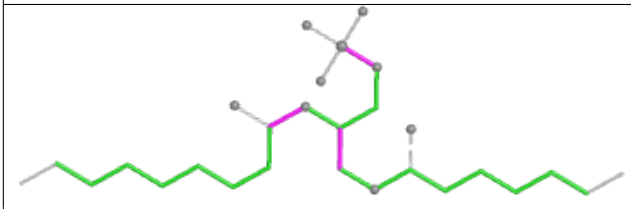
Ligand POV B 1107



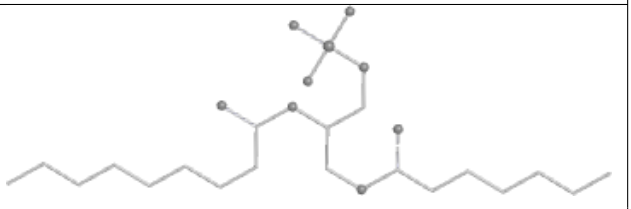
Bond lengths



Bond angles

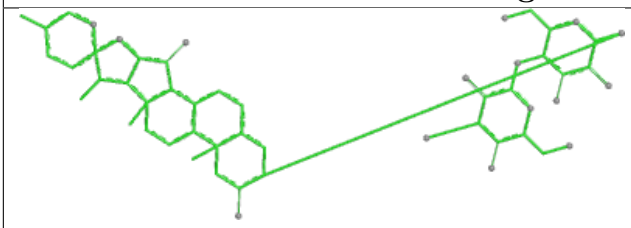


Torsions

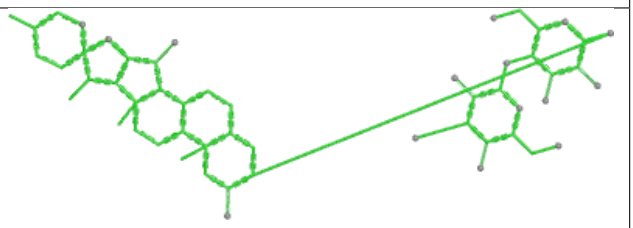


Rings

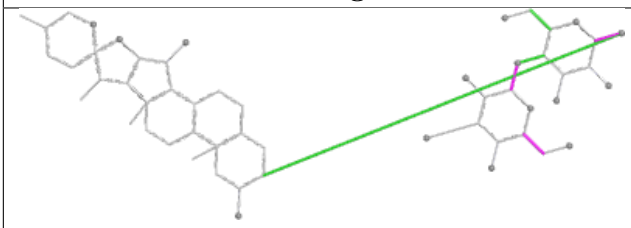
Ligand AJP B 1110



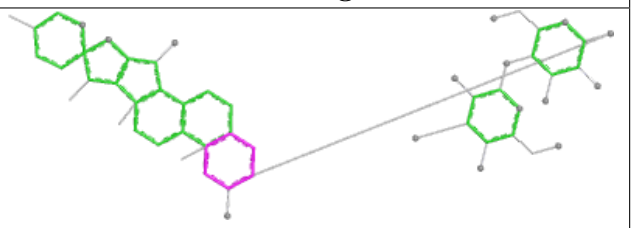
Bond lengths



Bond angles

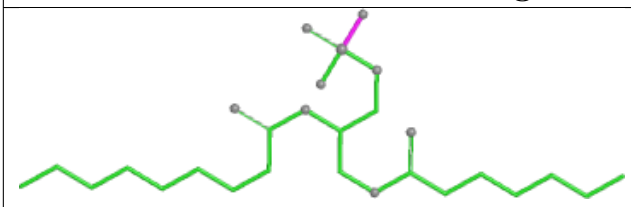


Torsions

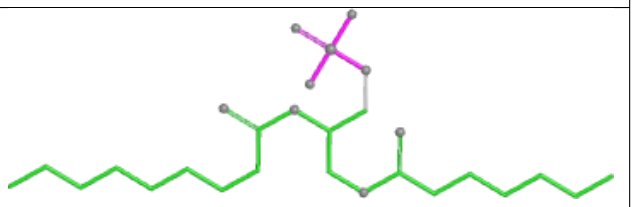


Rings

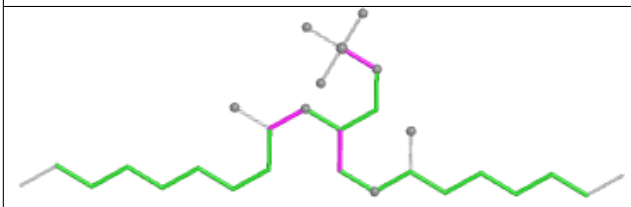
Ligand POV C 1108



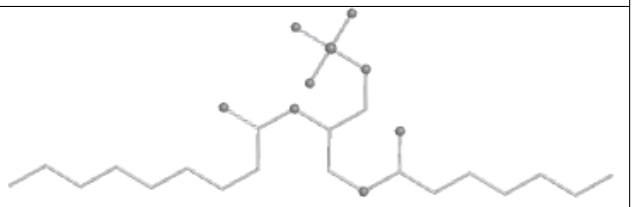
Bond lengths



Bond angles

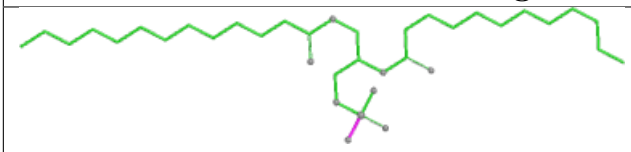


Torsions

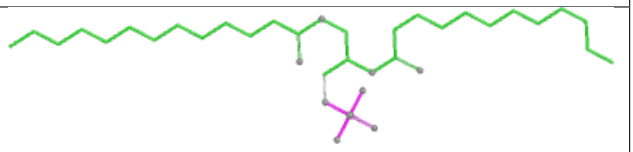


Rings

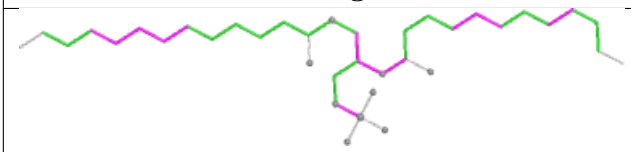
Ligand POV A 1106



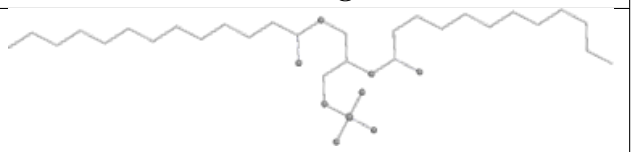
Bond lengths



Bond angles

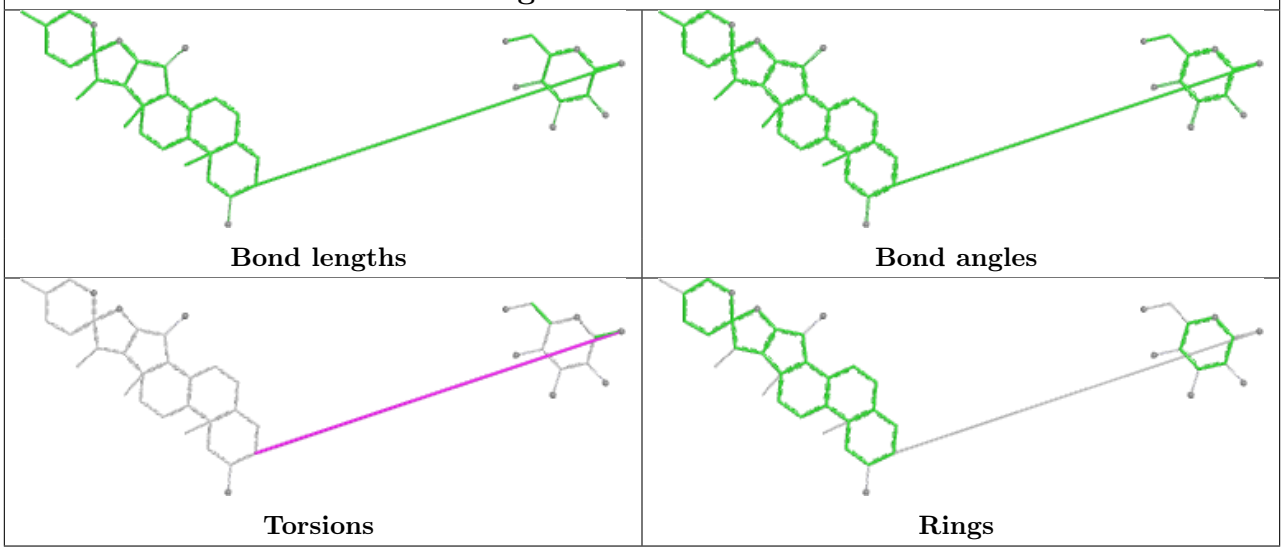


Torsions

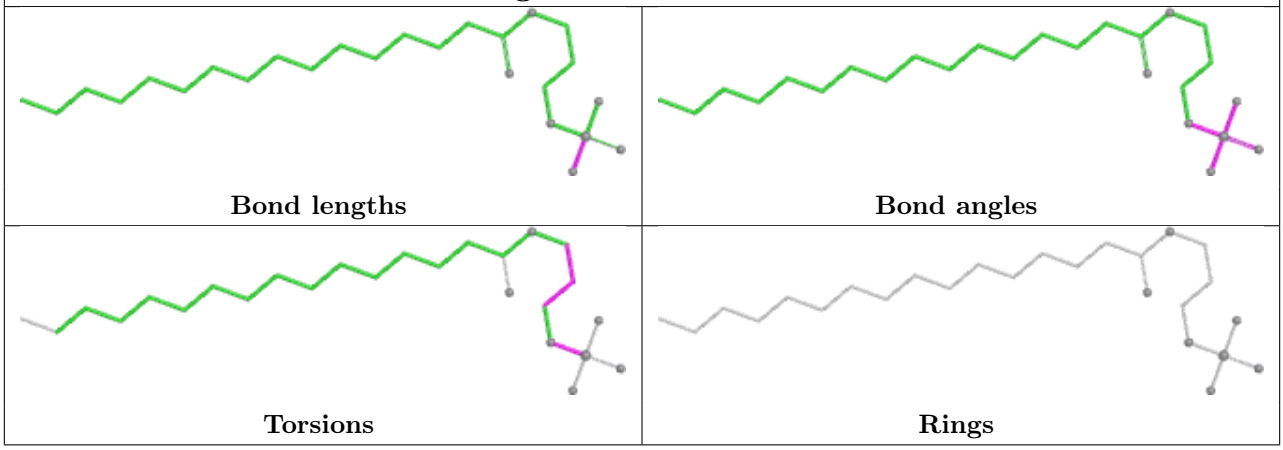


Rings

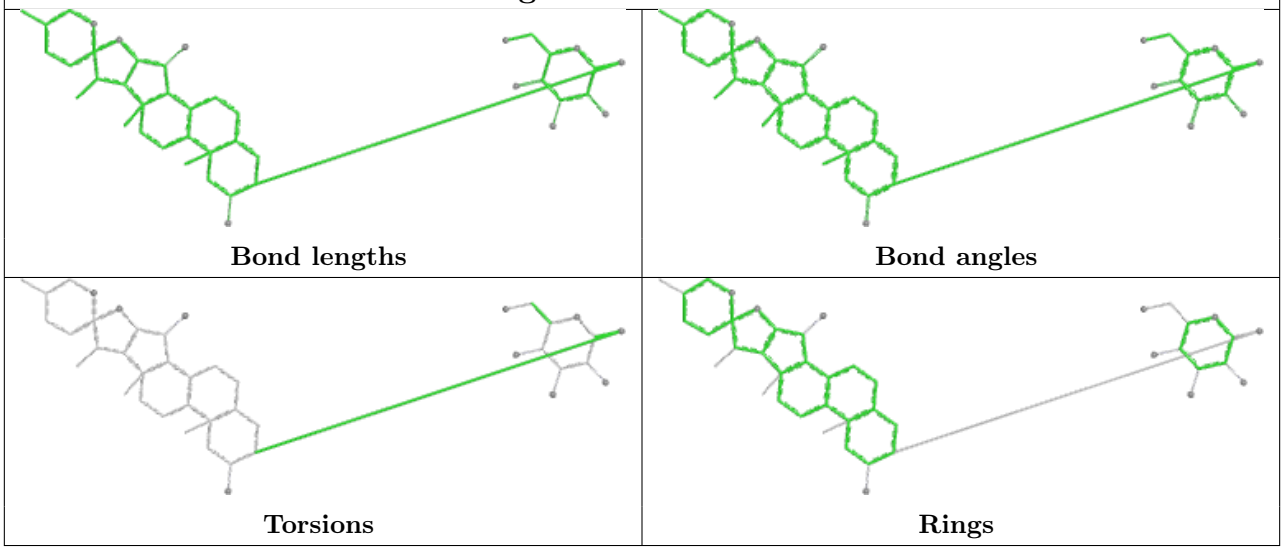
Ligand AJP D 1115



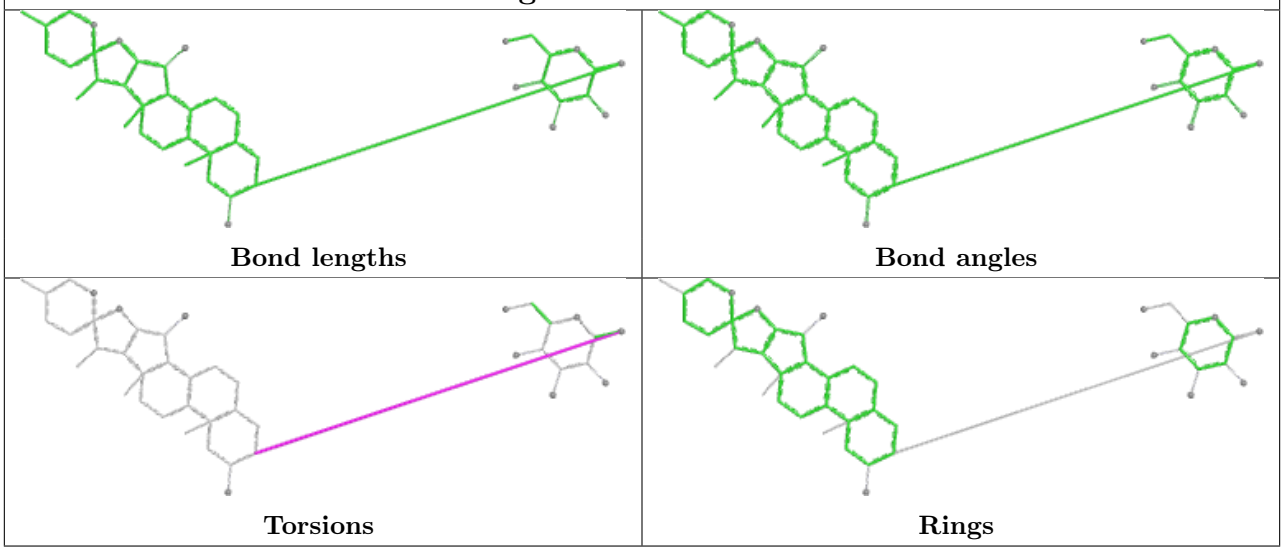
Ligand POV A 1107



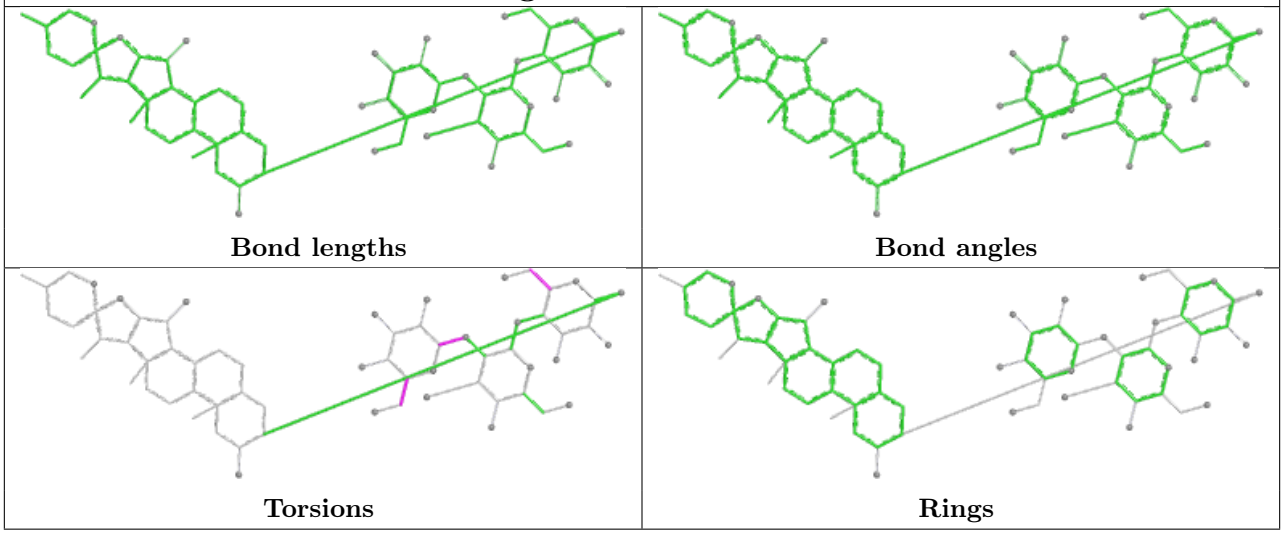
Ligand AJP C 1115



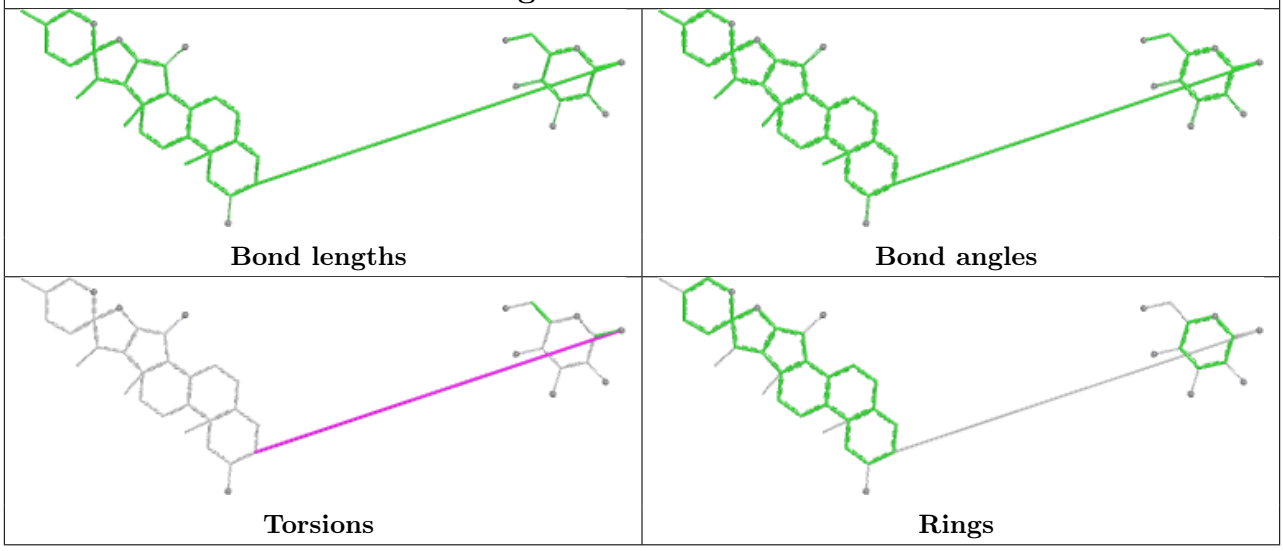
Ligand AJP C 1113



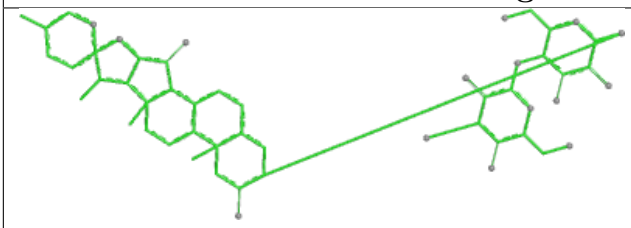
Ligand AJP B 1115



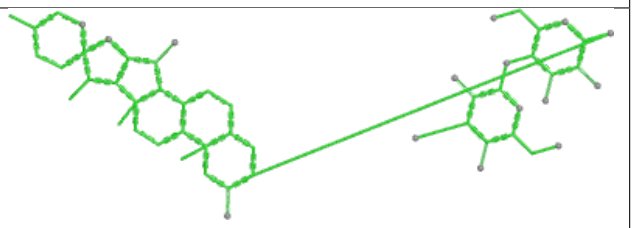
Ligand AJP A 1118



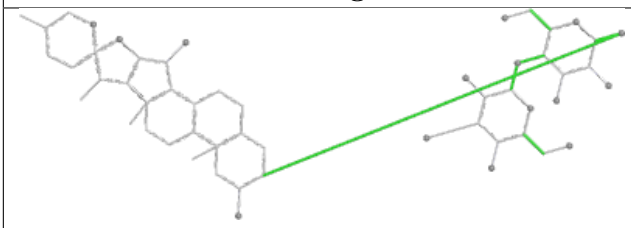
Ligand AJP D 1110



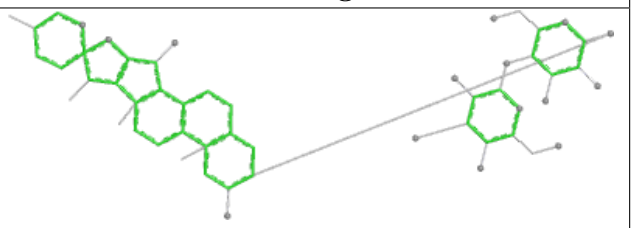
Bond lengths



Bond angles

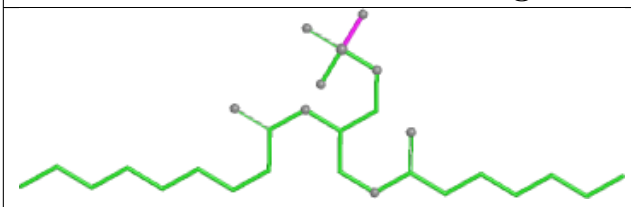


Torsions

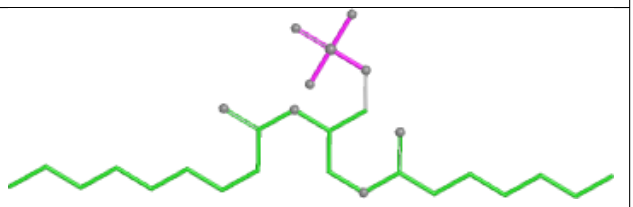


Rings

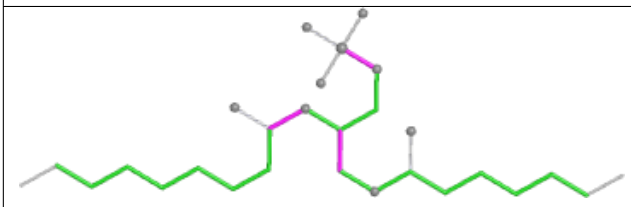
Ligand POV D 1106



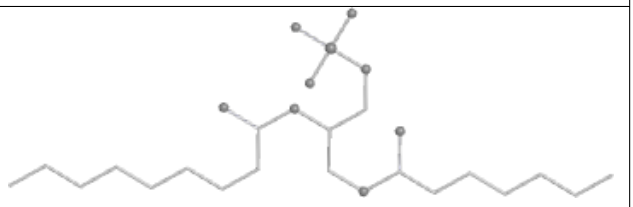
Bond lengths



Bond angles

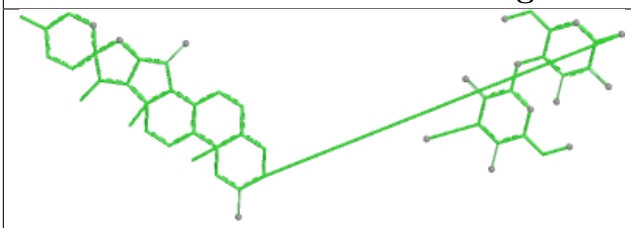


Torsions

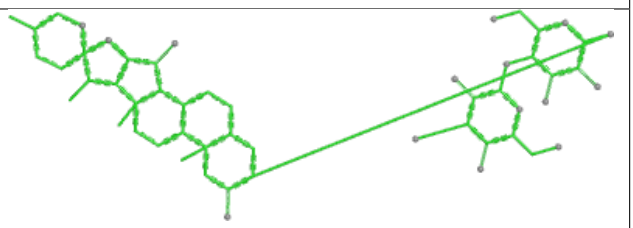


Rings

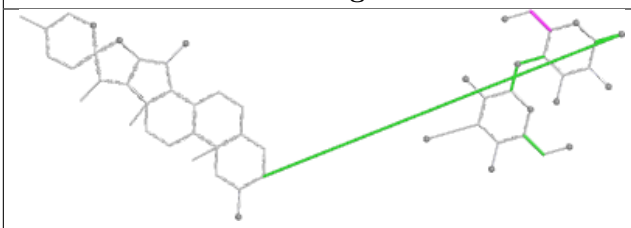
Ligand AJP D 1118



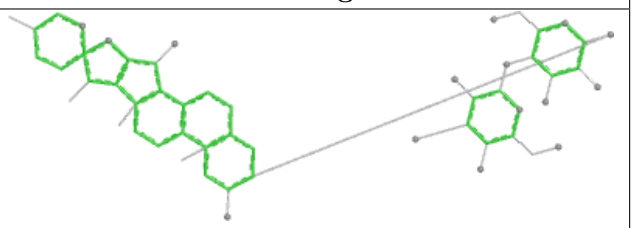
Bond lengths



Bond angles

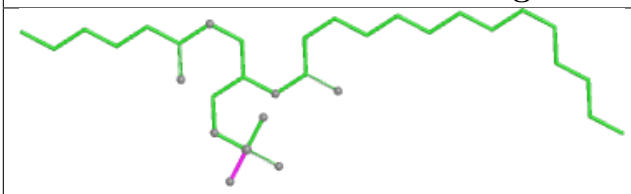


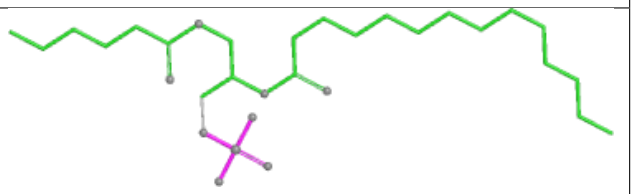
Torsions

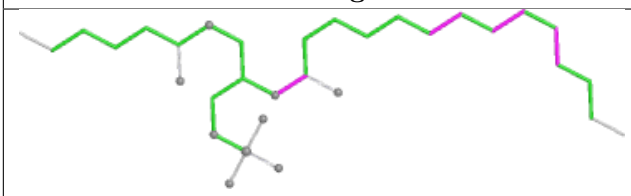


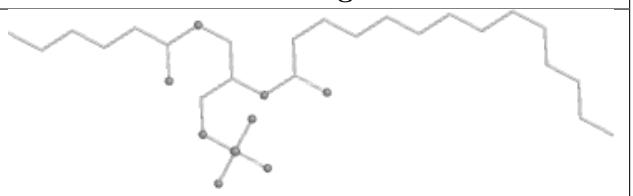
Rings

Ligand POV D 1104

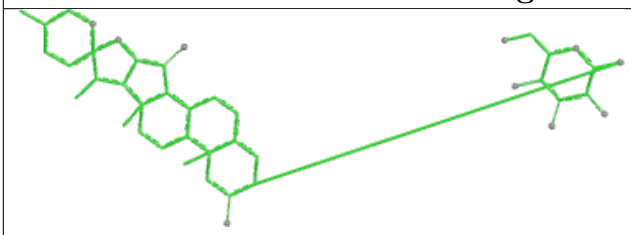

Bond lengths

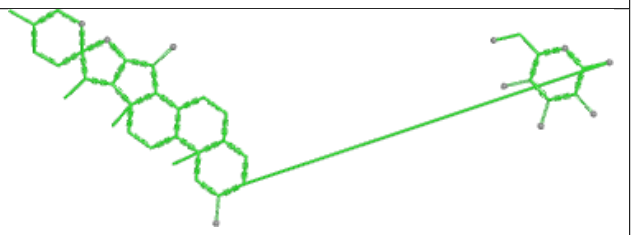

Bond angles

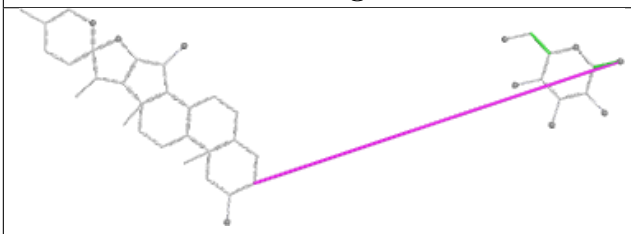

Torsions

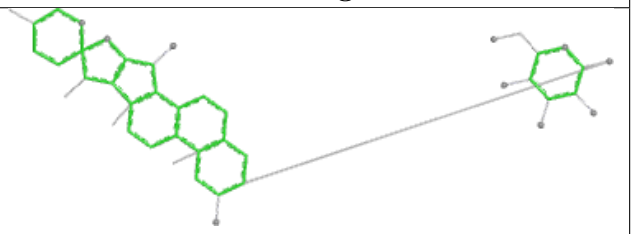

Rings

Ligand AJP D 1112

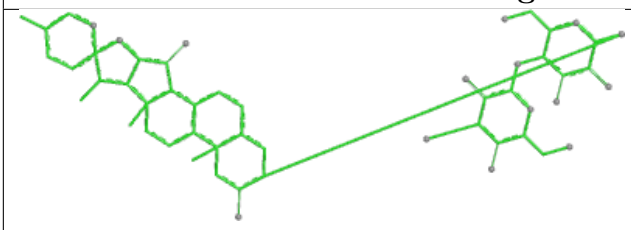

Bond lengths

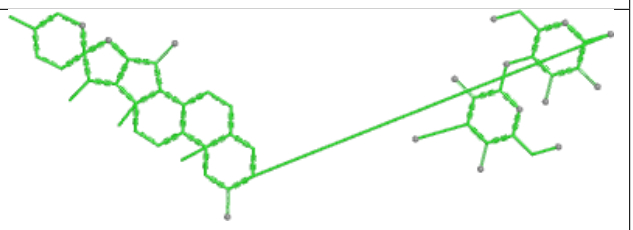

Bond angles

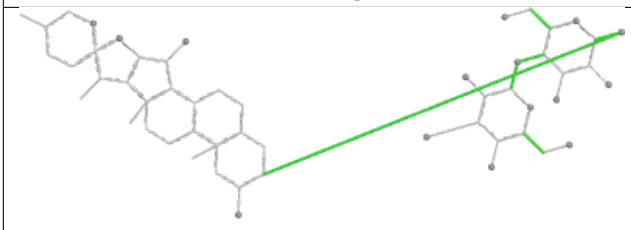

Torsions

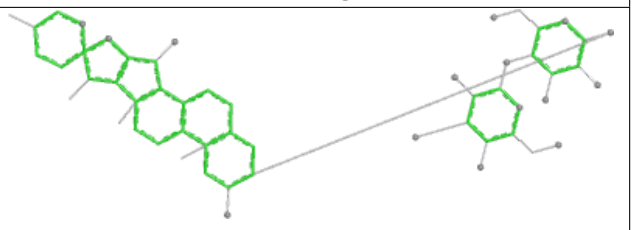

Rings

Ligand AJP B 1111

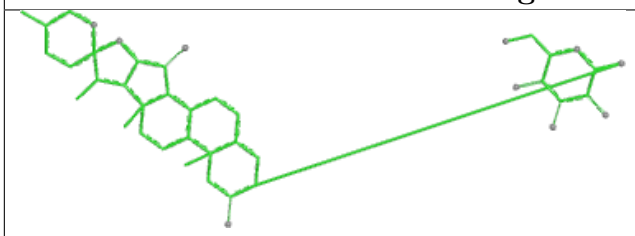

Bond lengths


Bond angles

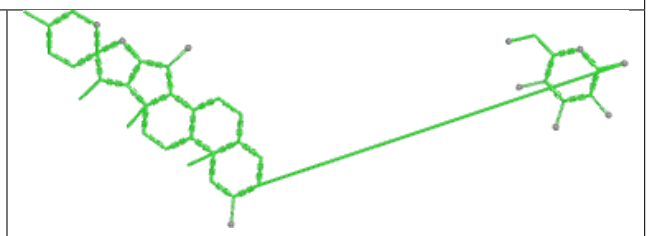

Torsions


Rings

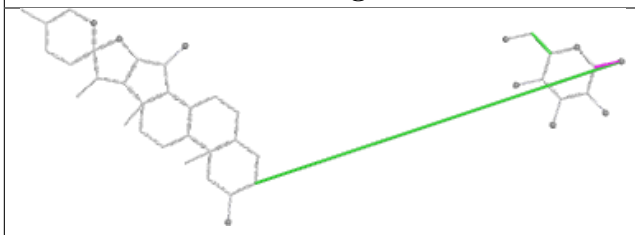
Ligand AJP D 1117



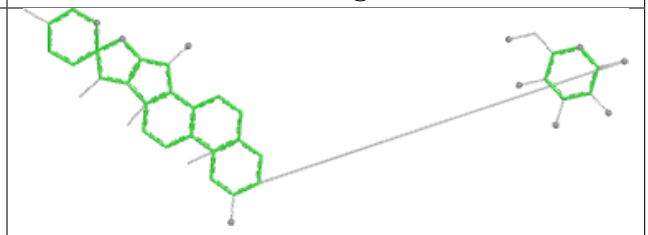
Bond lengths



Bond angles

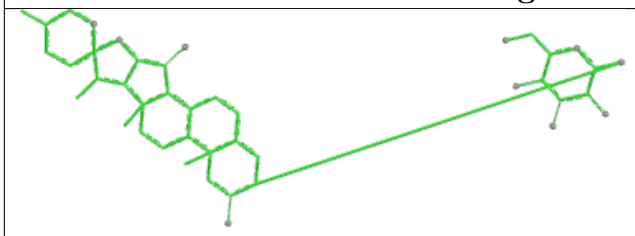


Torsions

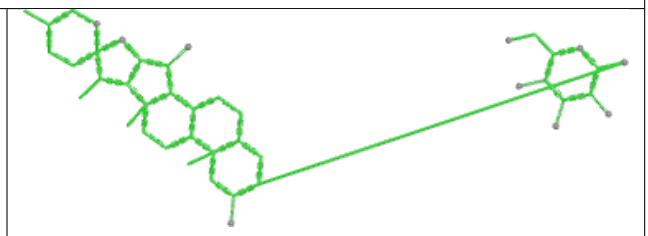


Rings

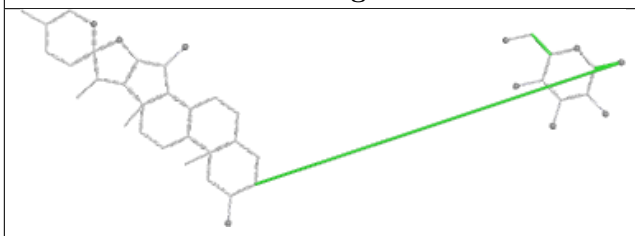
Ligand AJP D 1113



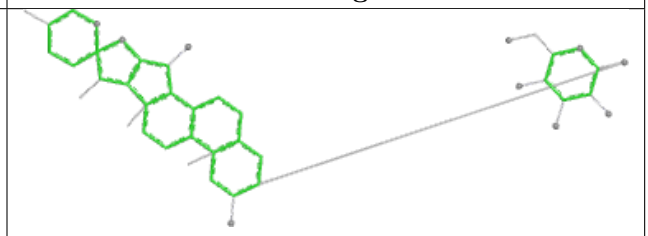
Bond lengths



Bond angles

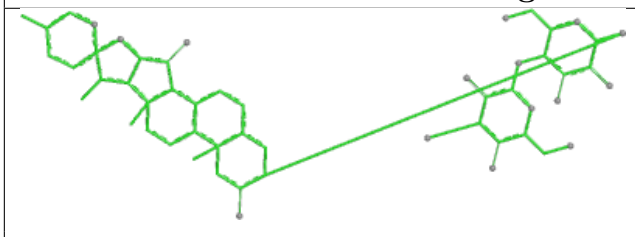


Torsions

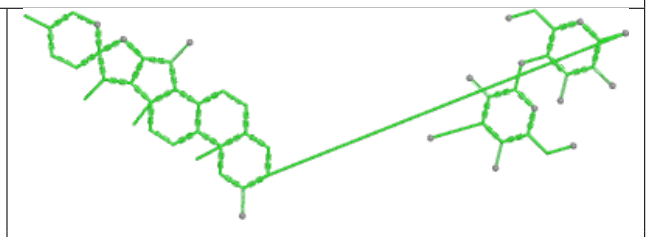


Rings

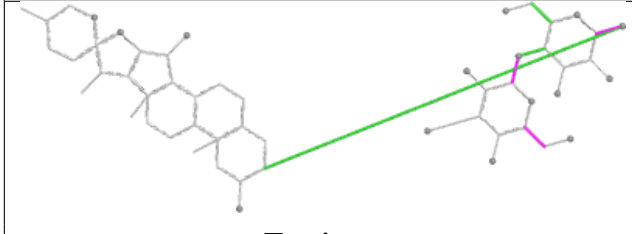
Ligand AJP A 1115



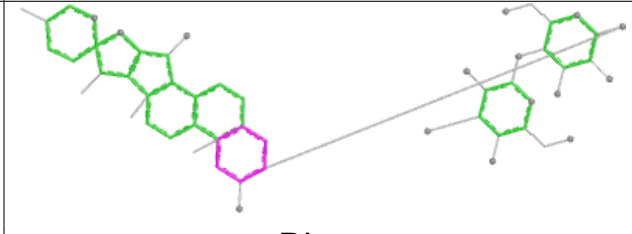
Bond lengths



Bond angles

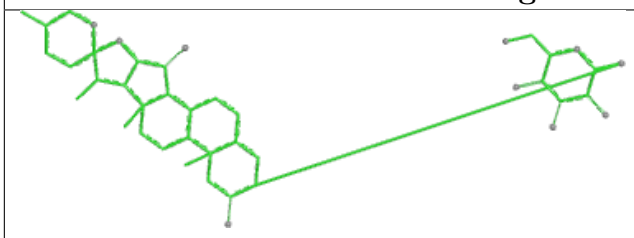


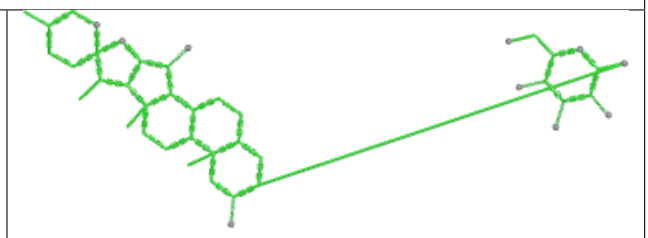
Torsions

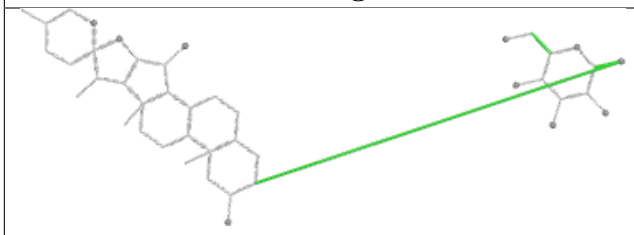


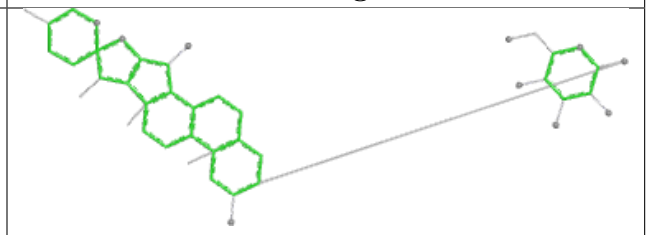
Rings

Ligand AJP B 1114

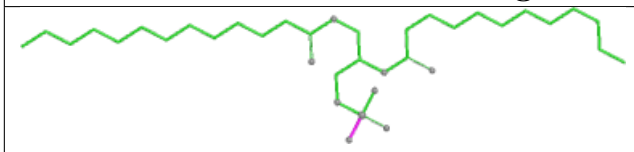

Bond lengths

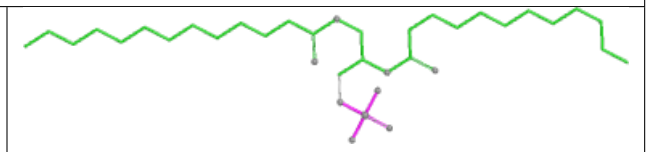

Bond angles

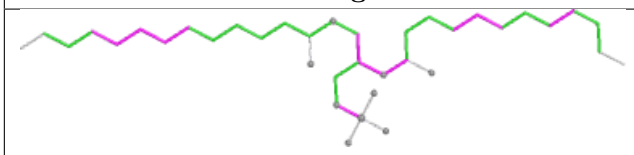

Torsions

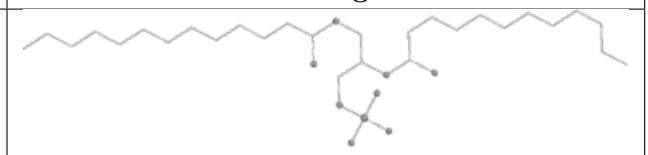

Rings

Ligand POV C 1101

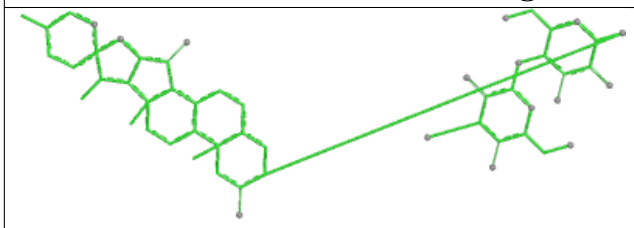

Bond lengths

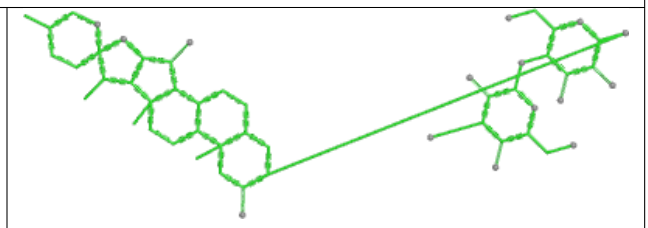

Bond angles

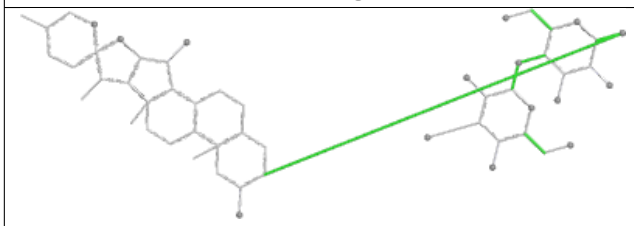

Torsions

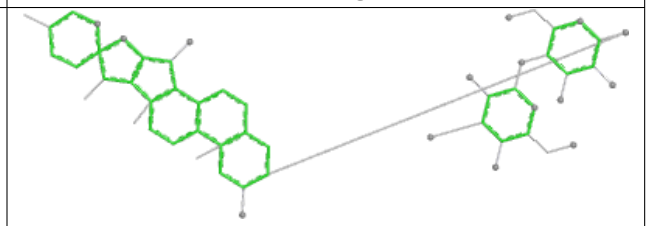

Rings

Ligand AJP C 1112

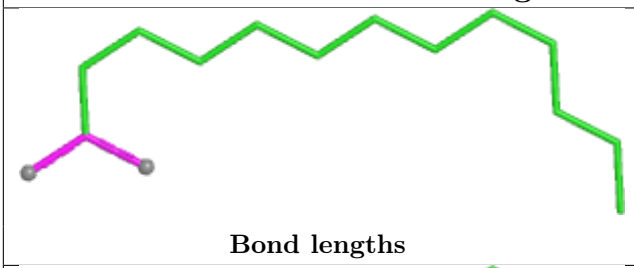

Bond lengths


Bond angles

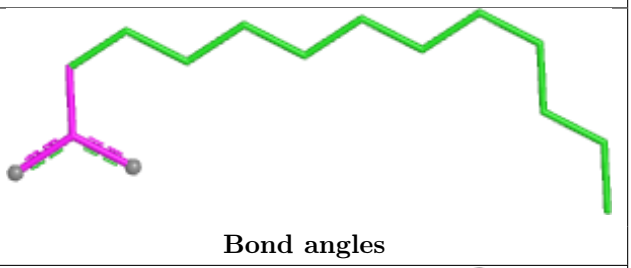

Torsions


Rings

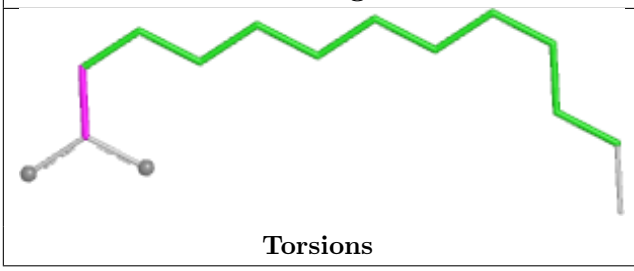
Ligand POV B 1106



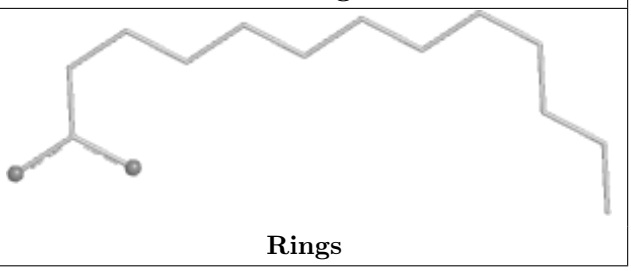
Bond lengths



Bond angles

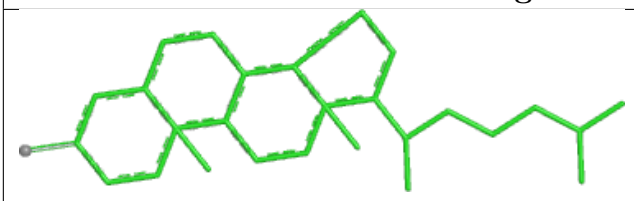


Torsions

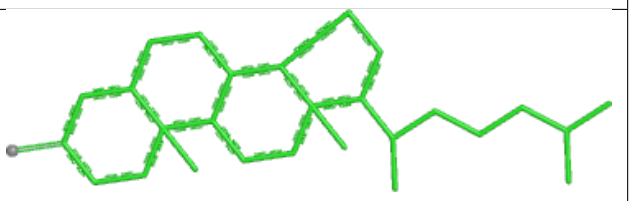


Rings

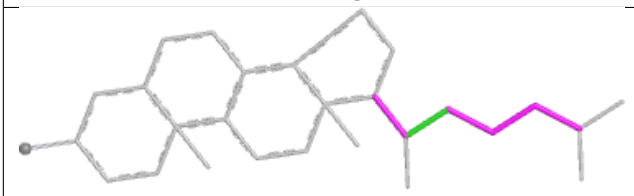
Ligand CLR D 1108



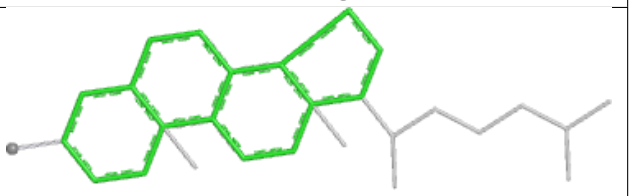
Bond lengths



Bond angles

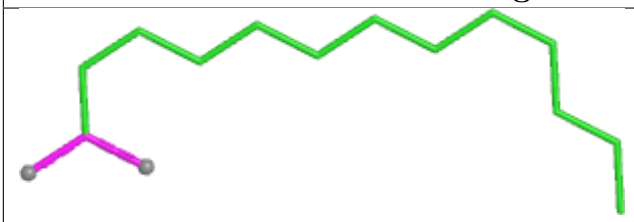


Torsions

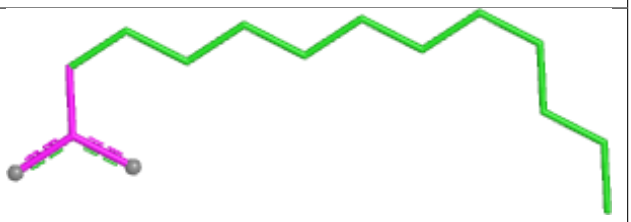


Rings

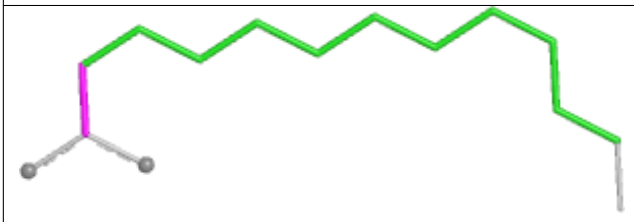
Ligand POV D 1105



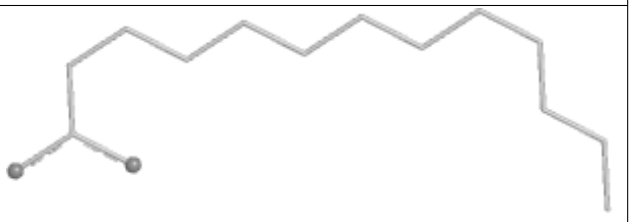
Bond lengths



Bond angles

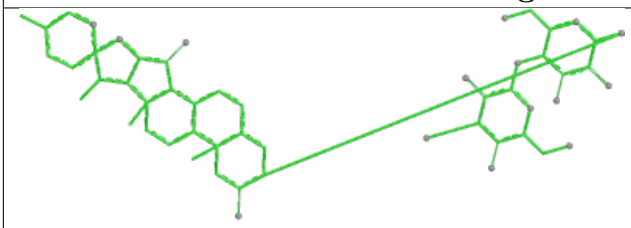


Torsions

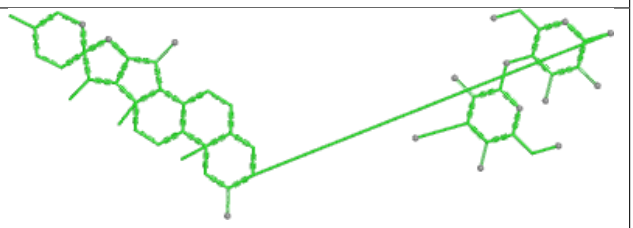


Rings

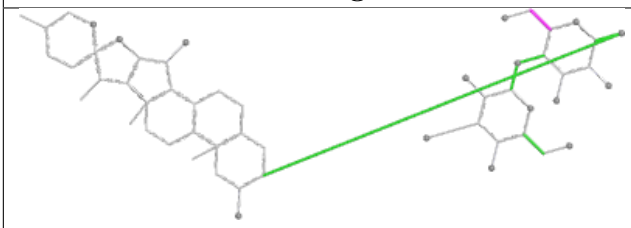
Ligand AJP B 1119



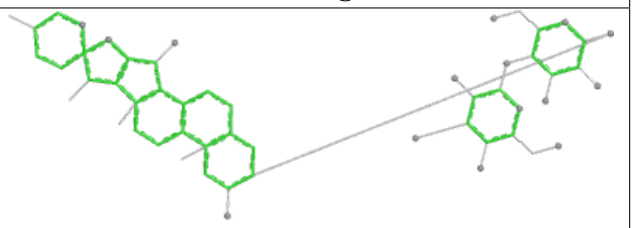
Bond lengths



Bond angles

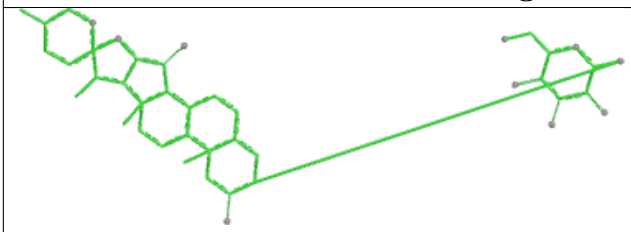


Torsions

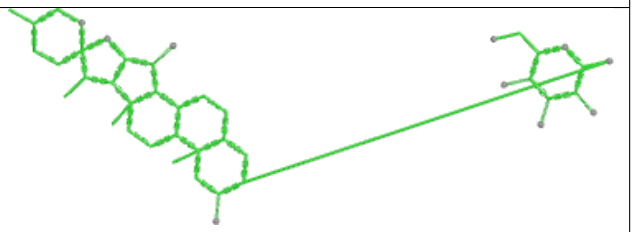


Rings

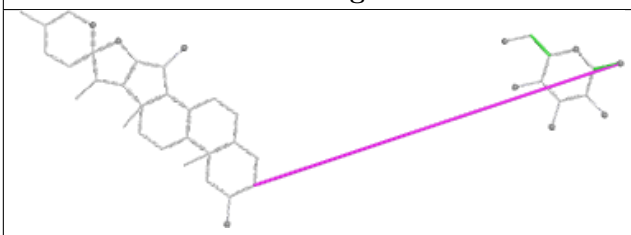
Ligand AJP C 1117



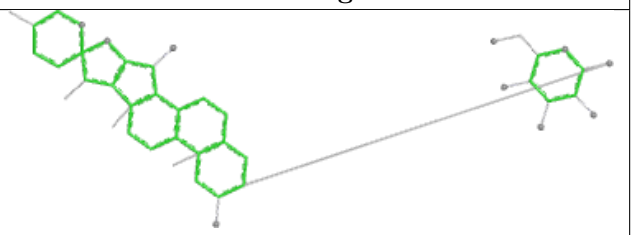
Bond lengths



Bond angles

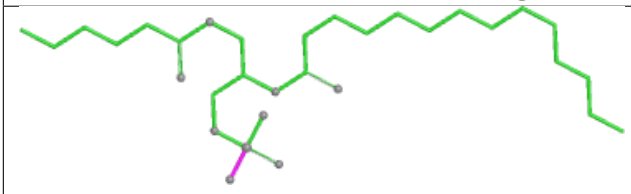


Torsions

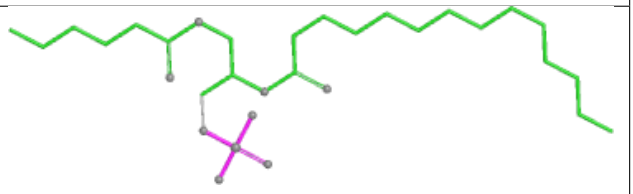


Rings

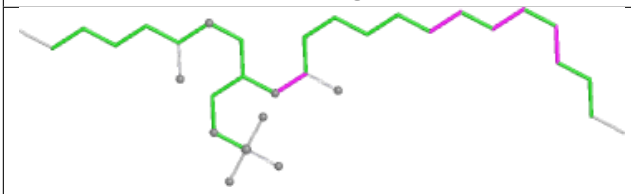
Ligand POV A 1110



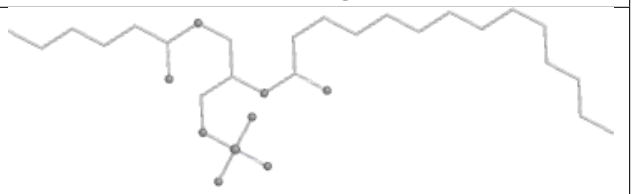
Bond lengths



Bond angles

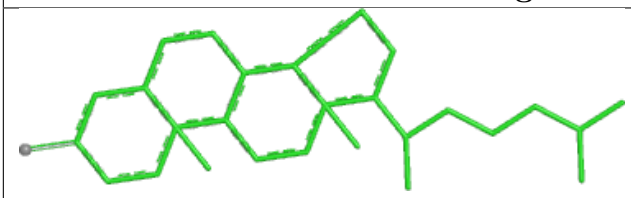


Torsions

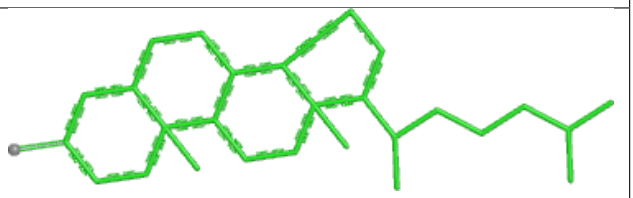


Rings

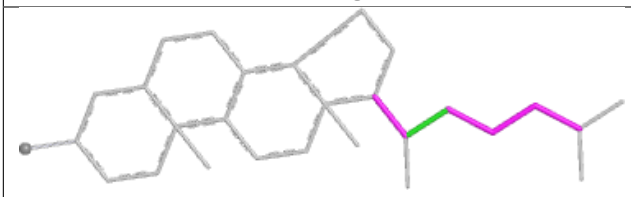
Ligand CLR C 1110



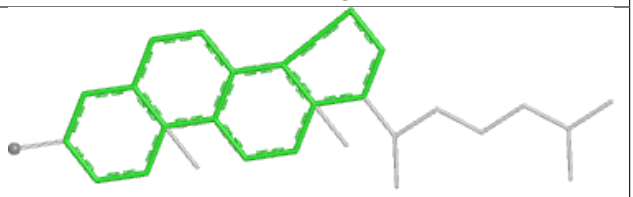
Bond lengths



Bond angles

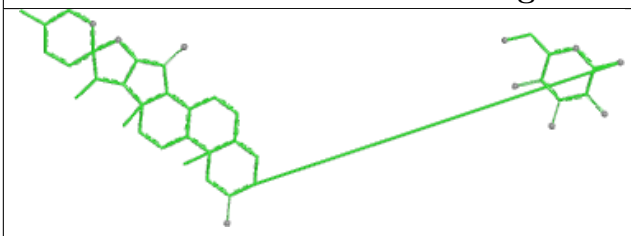


Torsions

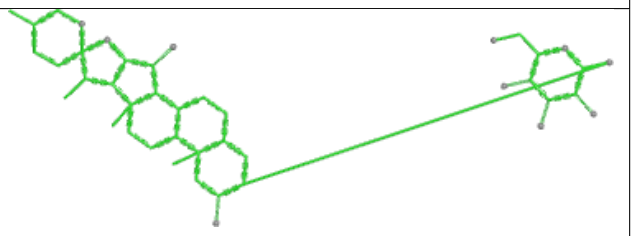


Rings

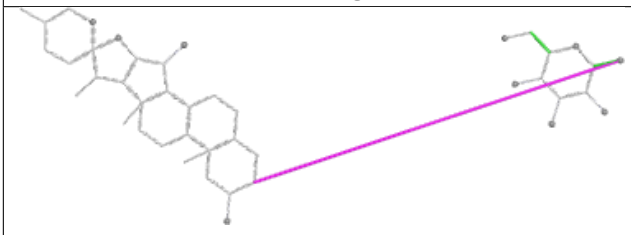
Ligand AJP B 1112



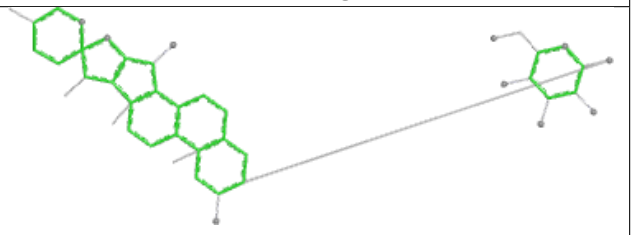
Bond lengths



Bond angles

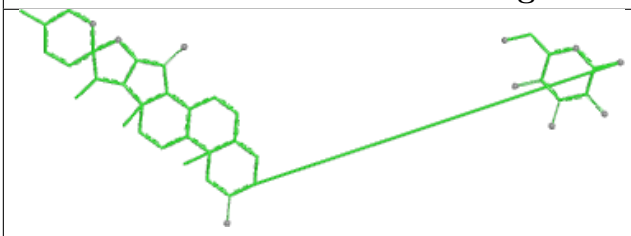


Torsions

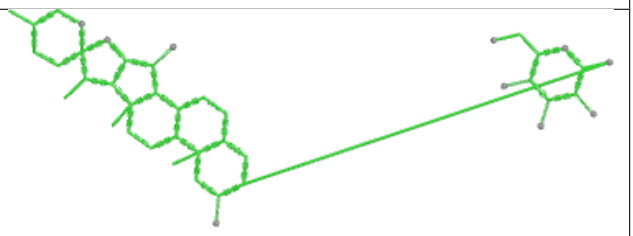


Rings

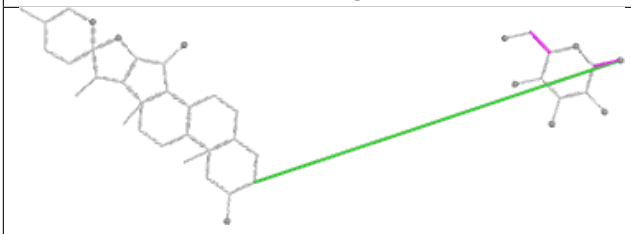
Ligand AJP C 1118



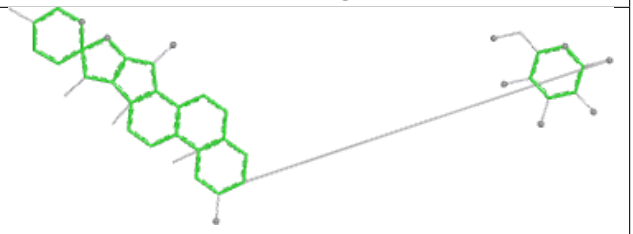
Bond lengths



Bond angles

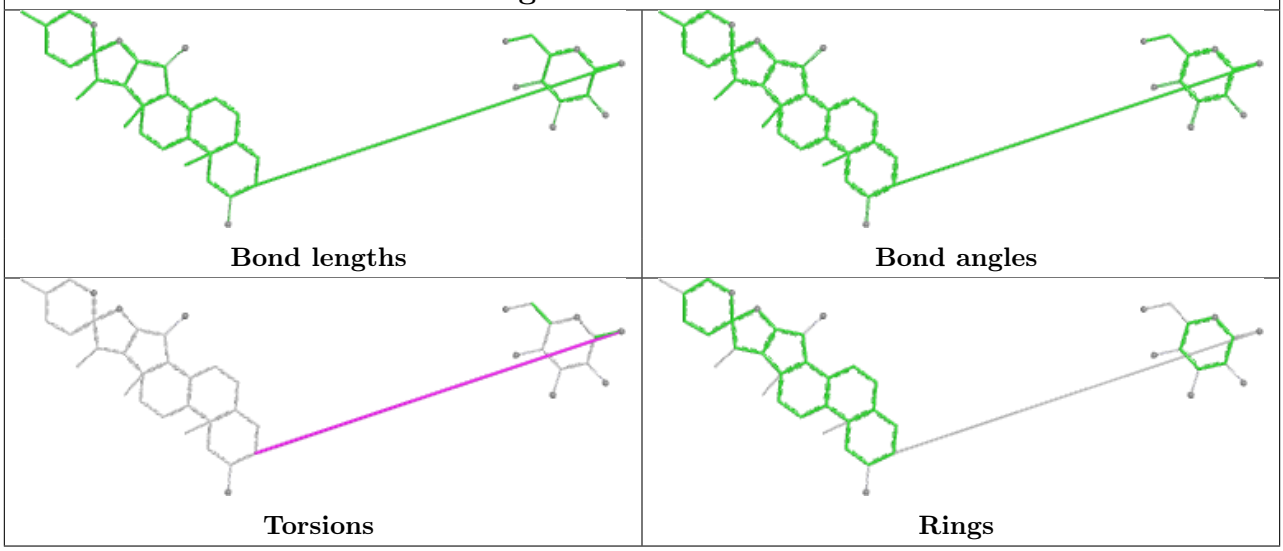


Torsions

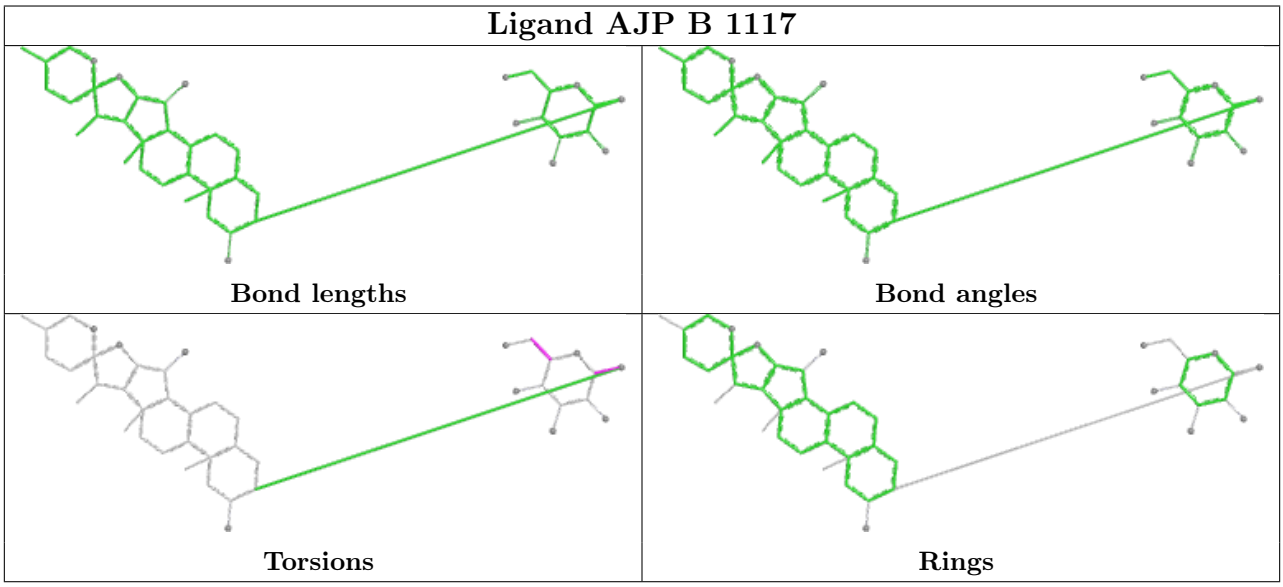


Rings

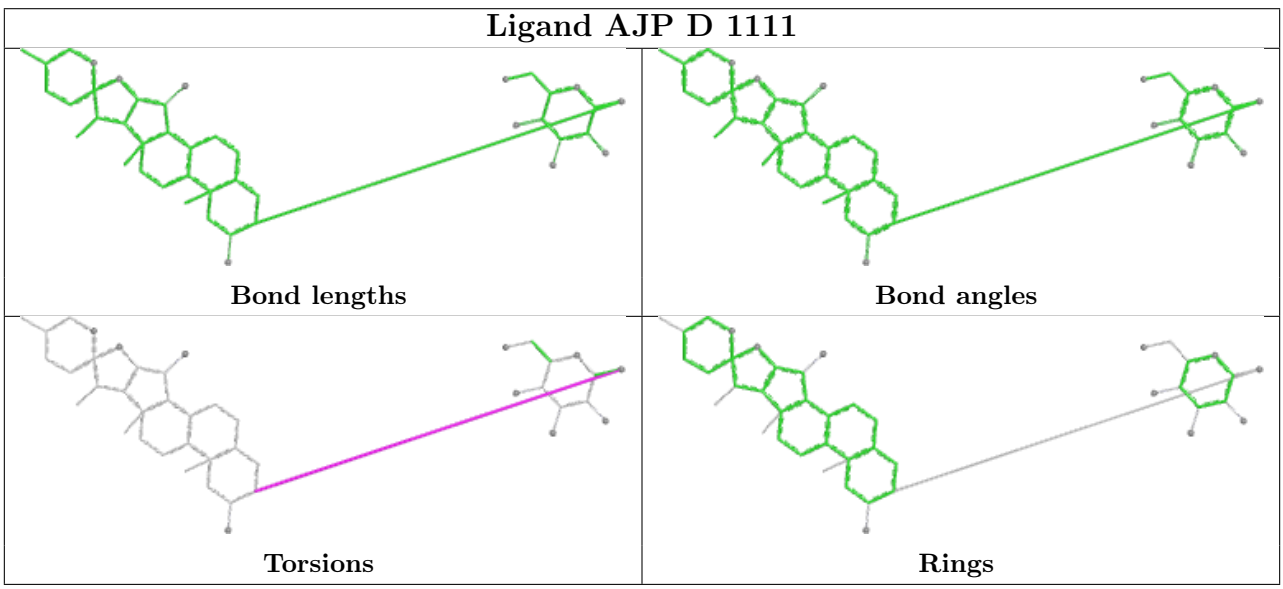
Ligand AJP B 1116



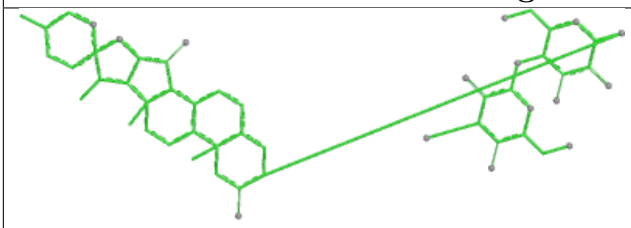
Ligand AJP B 1117



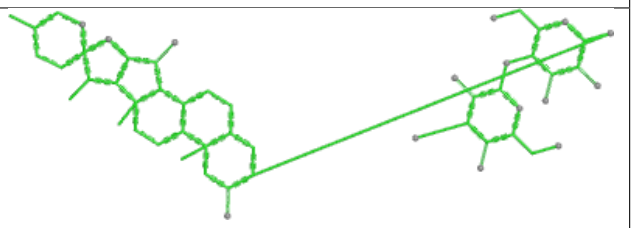
Ligand AJP D 1111



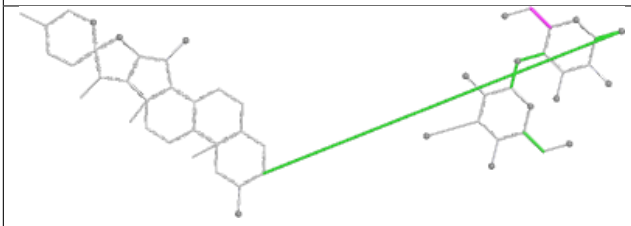
Ligand AJP C 1120



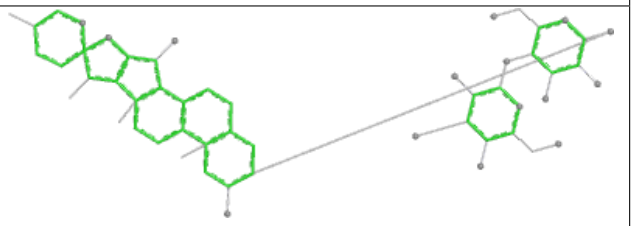
Bond lengths



Bond angles

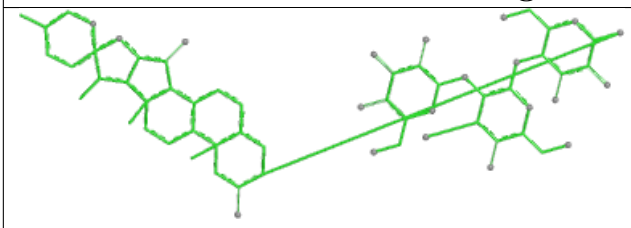


Torsions

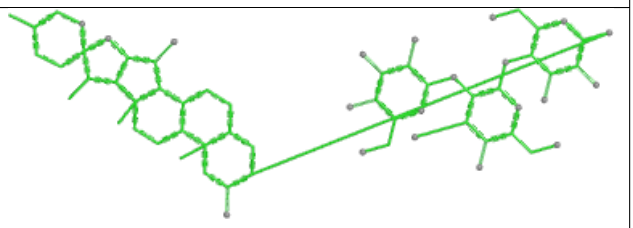


Rings

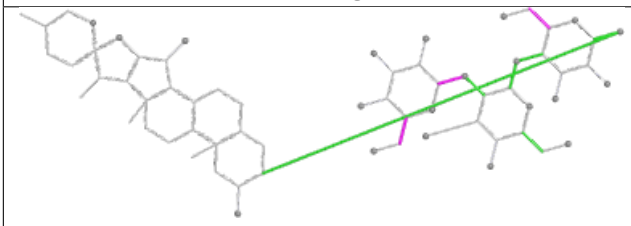
Ligand AJP C 1116



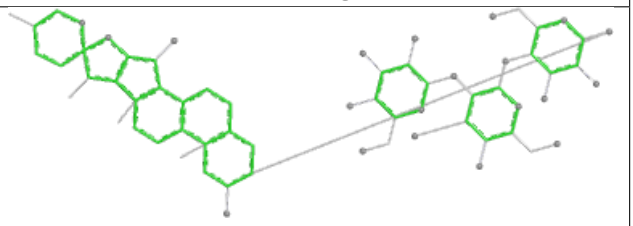
Bond lengths



Bond angles

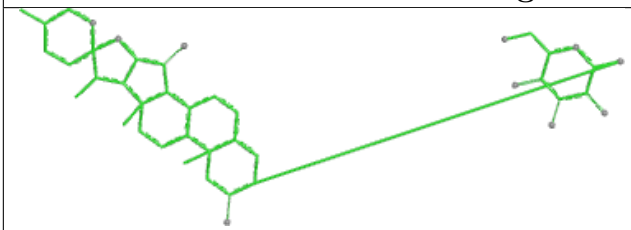


Torsions

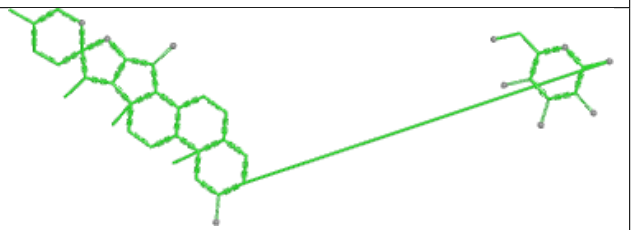


Rings

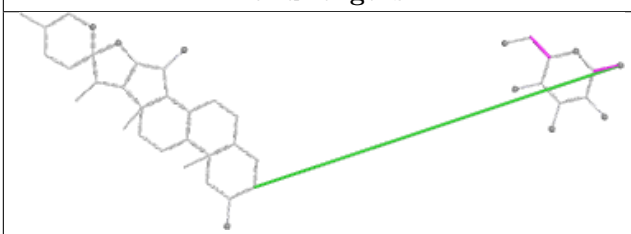
Ligand AJP A 1122



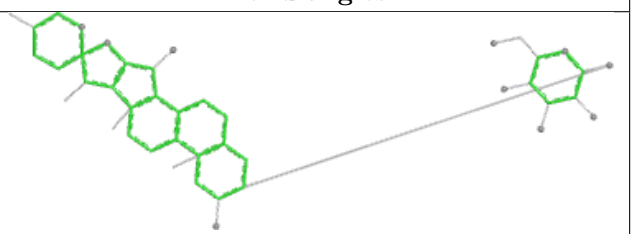
Bond lengths



Bond angles

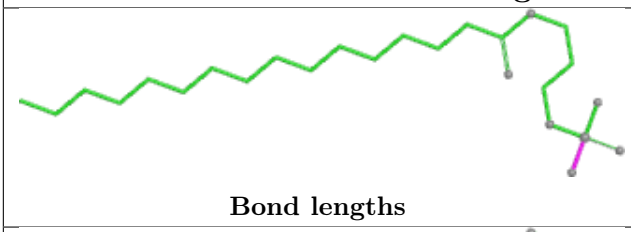


Torsions

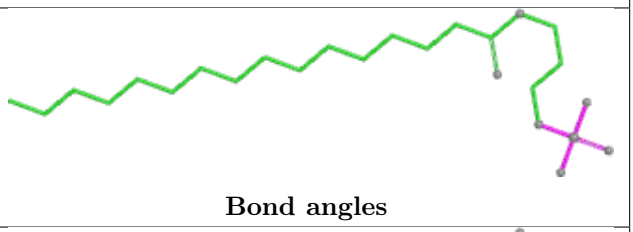


Rings

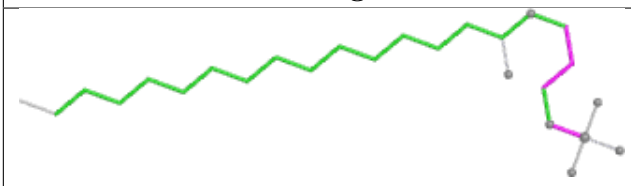
Ligand POV C 1103



Bond lengths



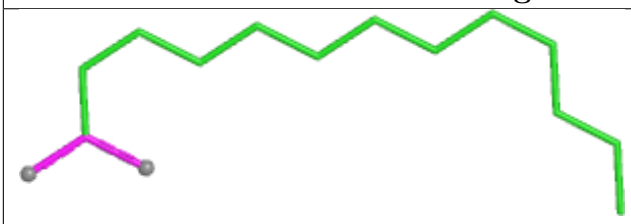
Bond angles



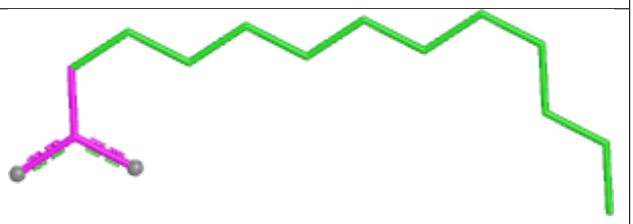
Torsions

Rings

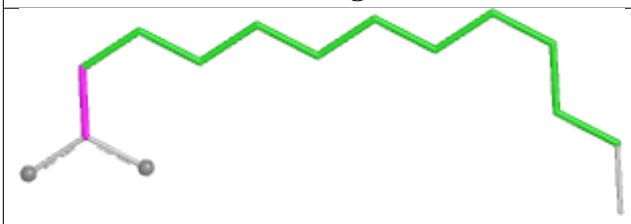
Ligand POV C 1107



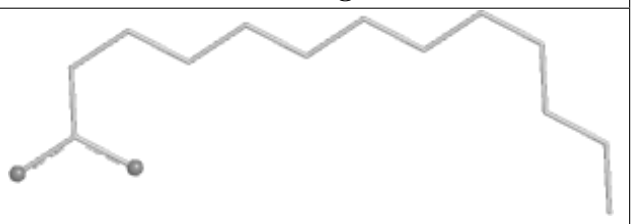
Bond lengths



Bond angles

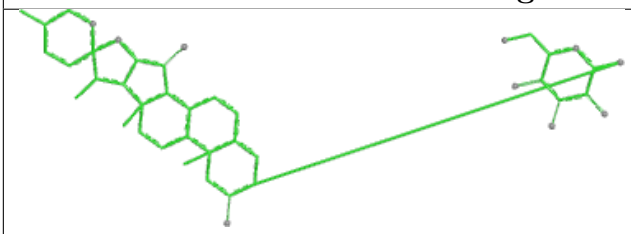


Torsions

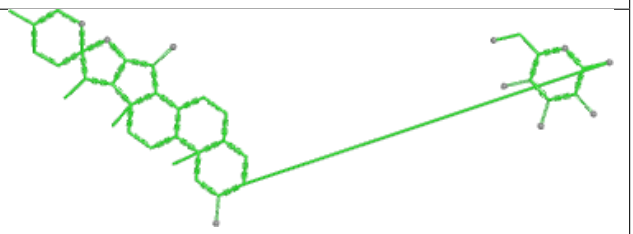


Rings

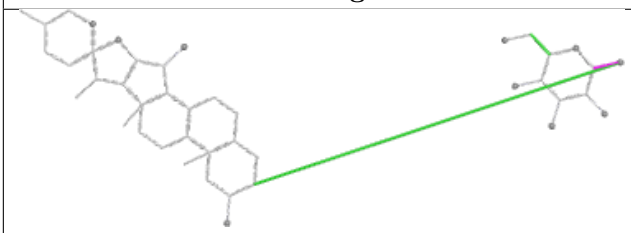
Ligand AJP A 1123



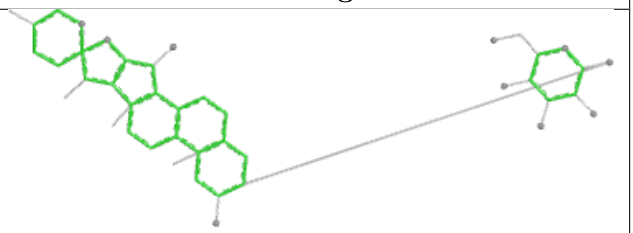
Bond lengths



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.

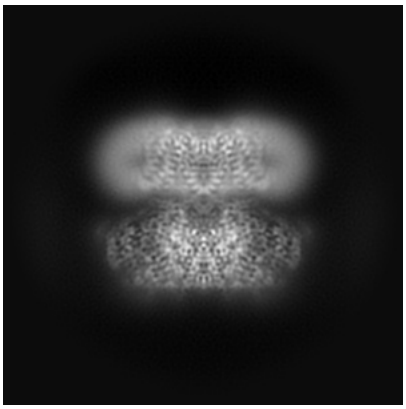
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-42988. These allow visual inspection of the internal detail of the map and identification of artifacts.

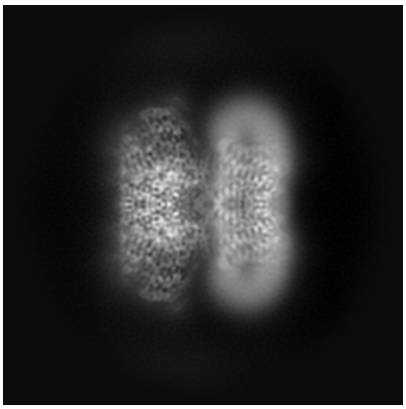
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

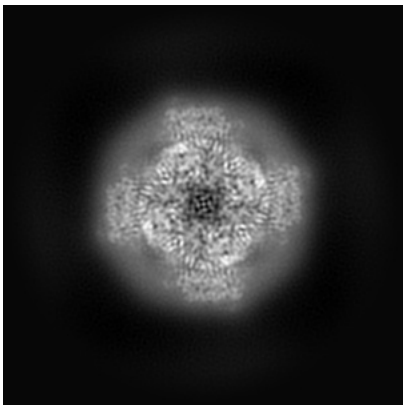
6.1.1 Primary map



X

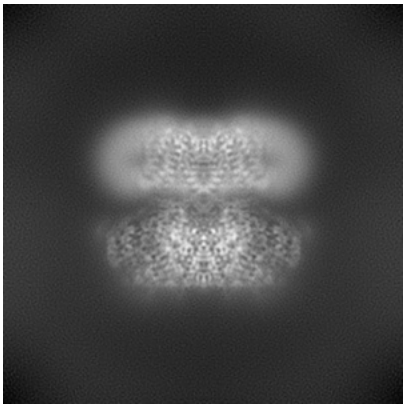


Y

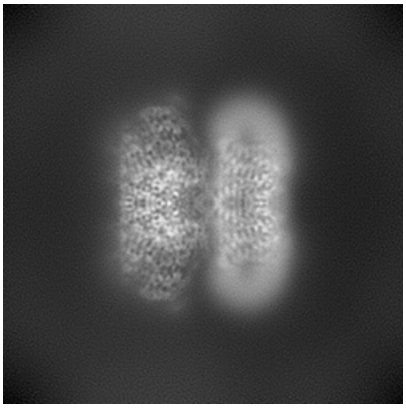


Z

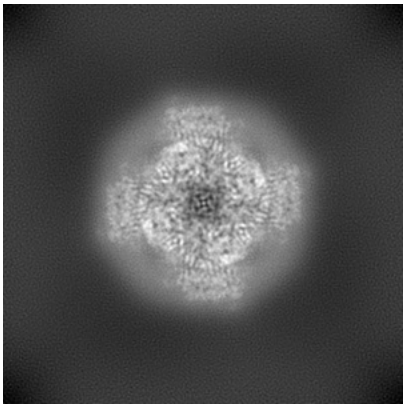
6.1.2 Raw map



X



Y

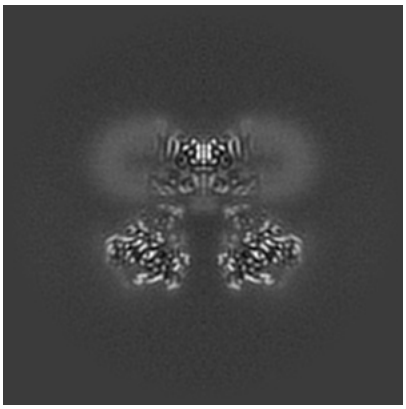


Z

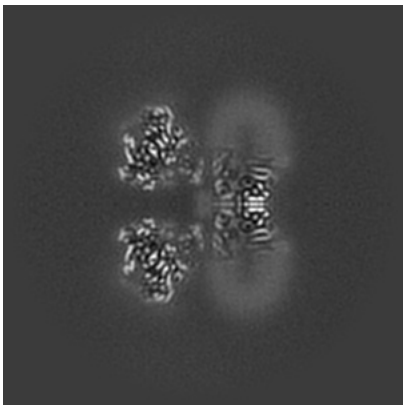
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

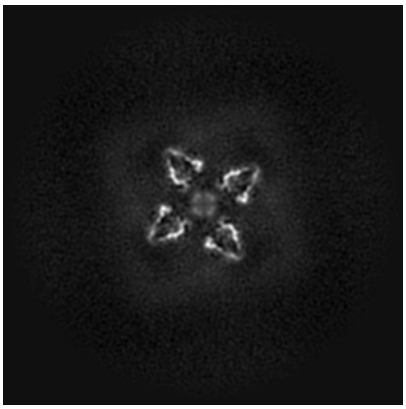
6.2.1 Primary map



X Index: 128

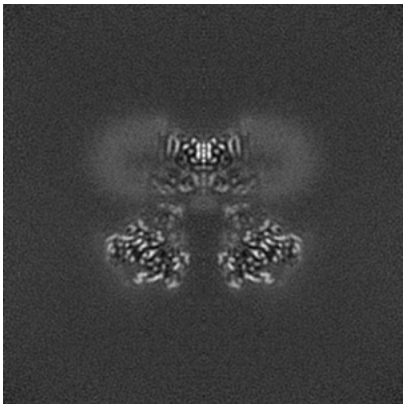


Y Index: 128

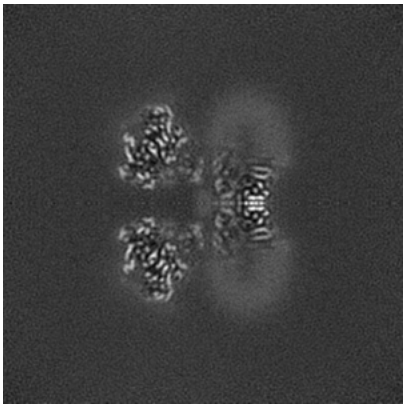


Z Index: 128

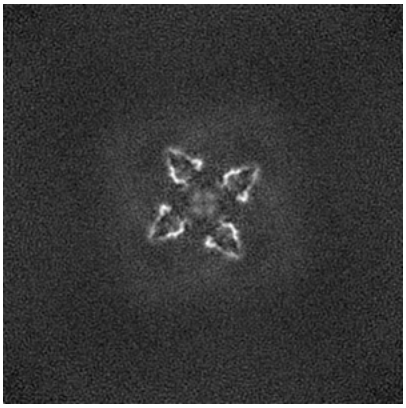
6.2.2 Raw map



X Index: 128



Y Index: 128

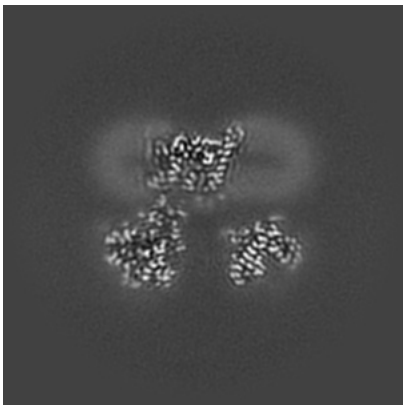


Z Index: 128

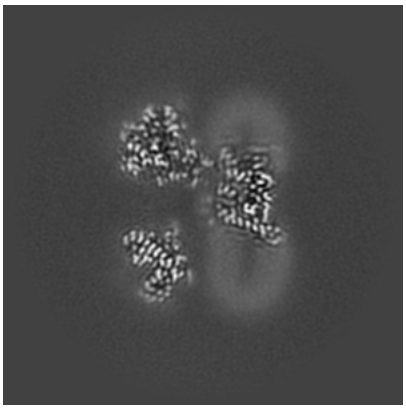
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

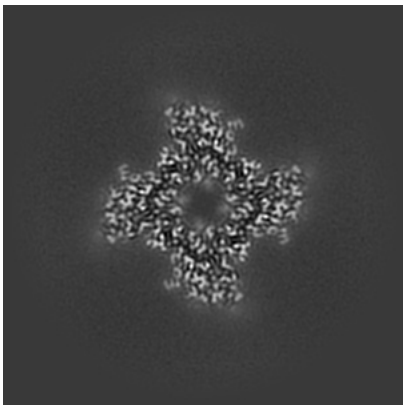
6.3.1 Primary map



X Index: 135

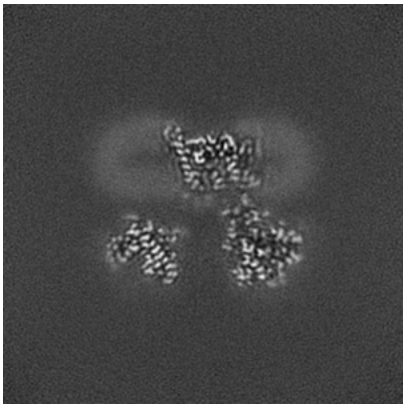


Y Index: 135

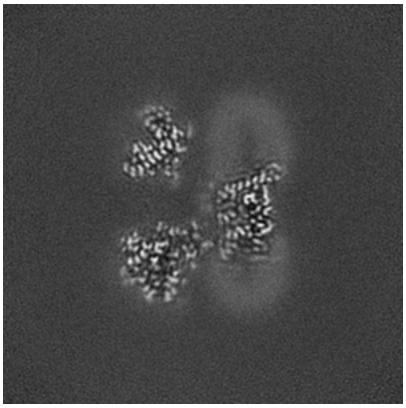


Z Index: 105

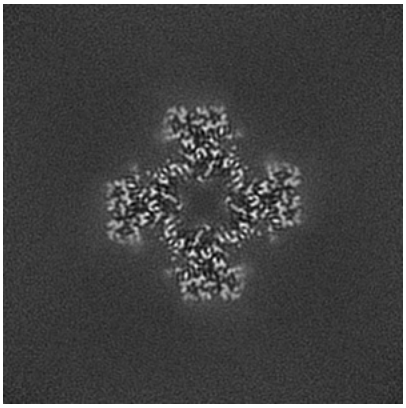
6.3.2 Raw map



X Index: 121



Y Index: 121

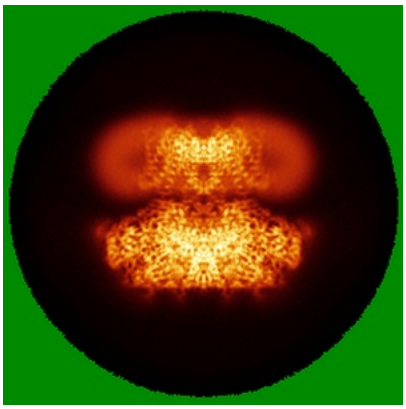


Z Index: 97

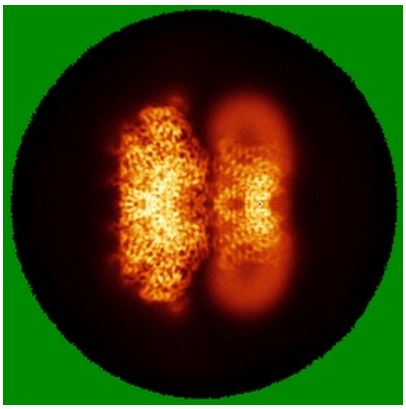
The images above show the largest variance slices of the map in three orthogonal directions.

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

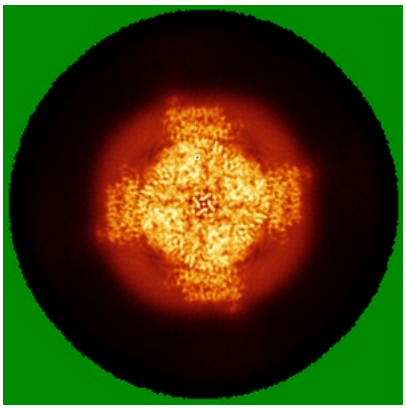
6.4.1 Primary map



X

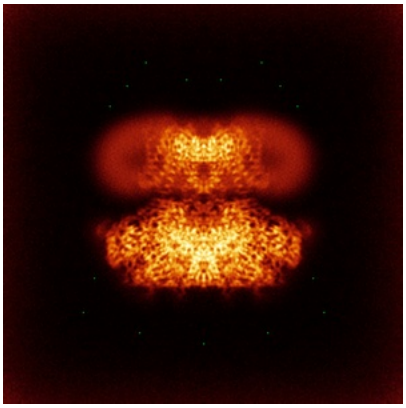


Y

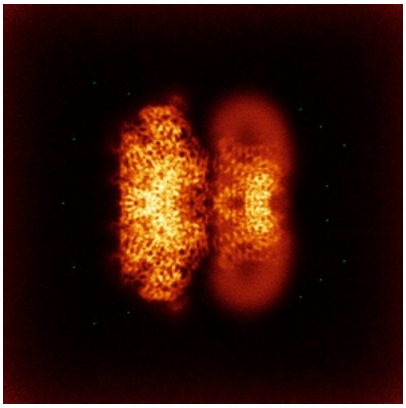


Z

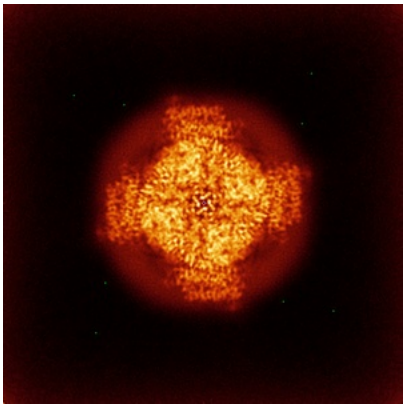
6.4.2 Raw map



X



Y

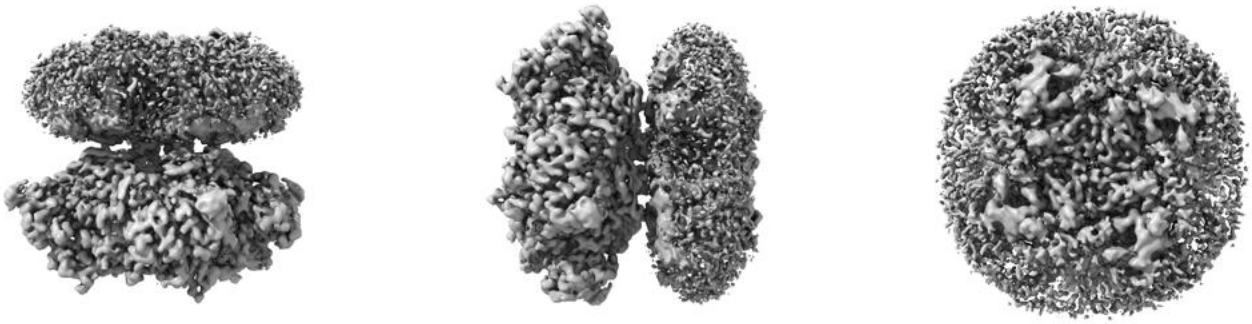


Z

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

6.5 Orthogonal surface views (i)

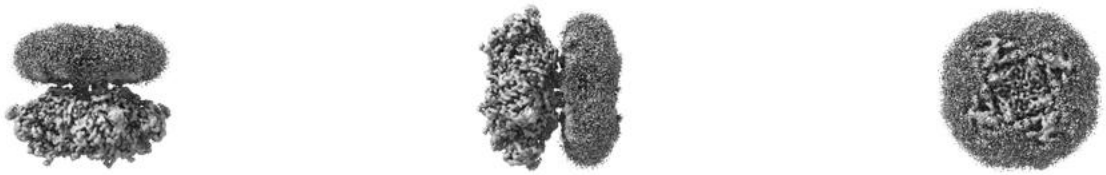
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.085. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

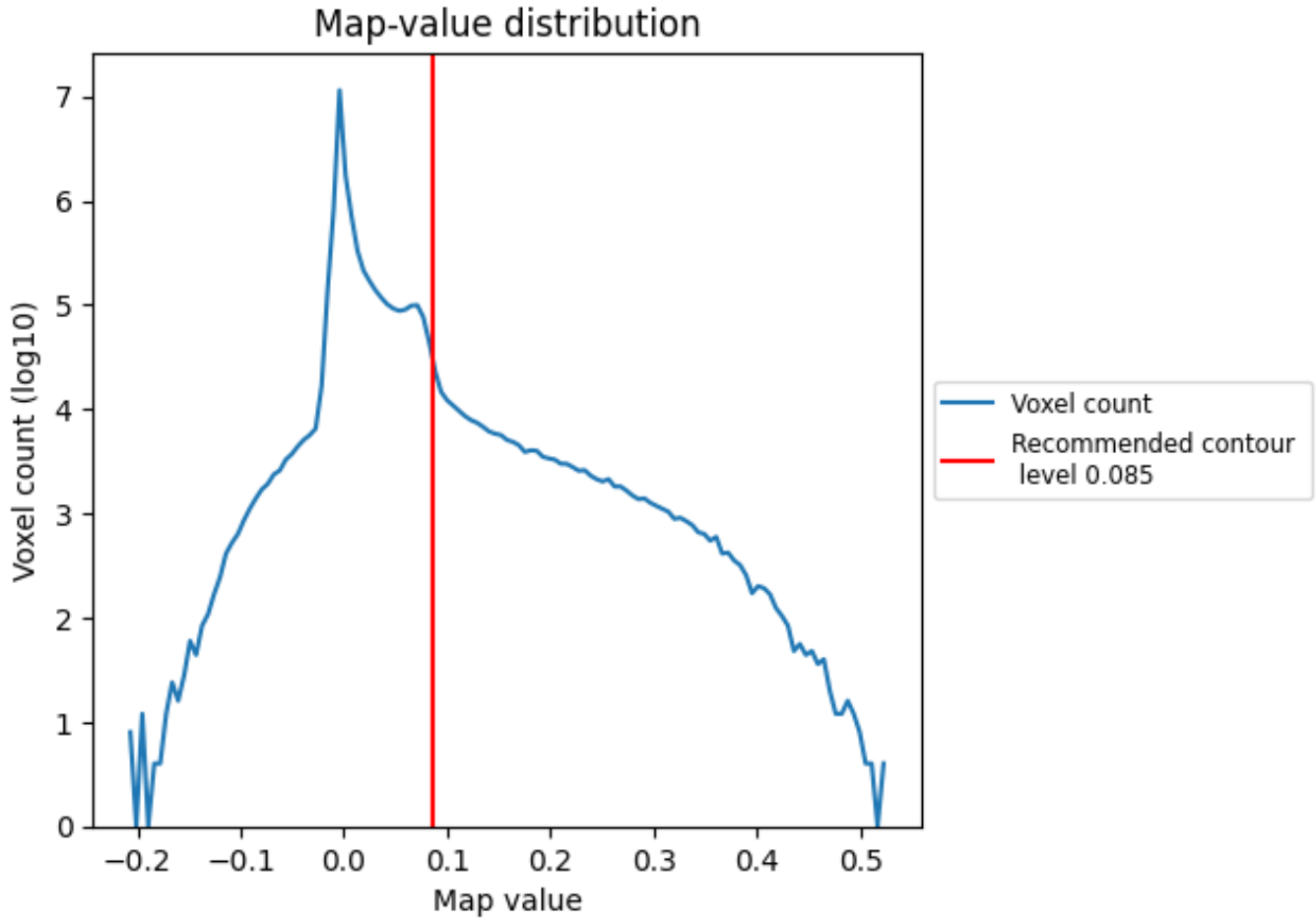
6.6 Mask visualisation (i)

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

7 Map analysis

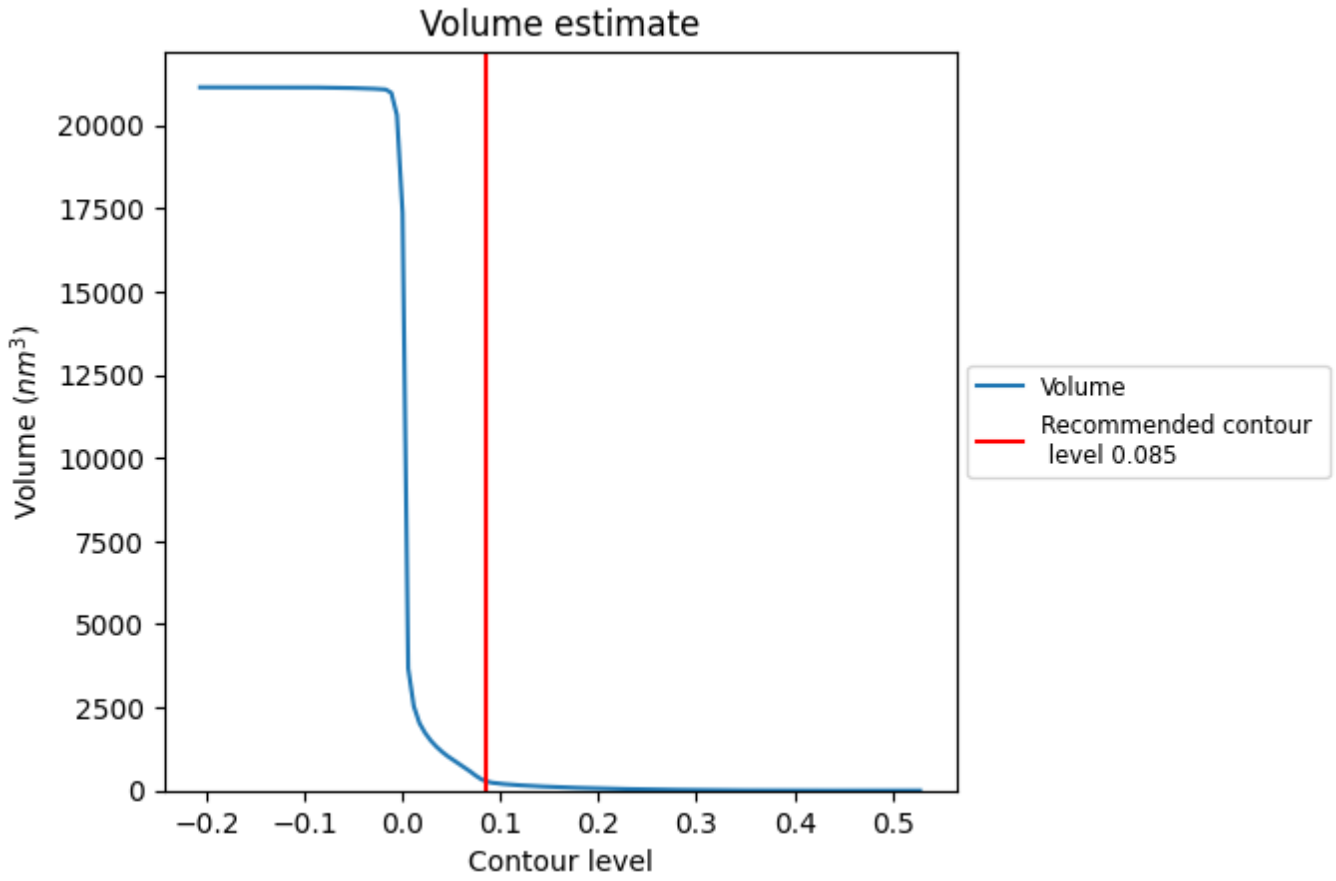
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

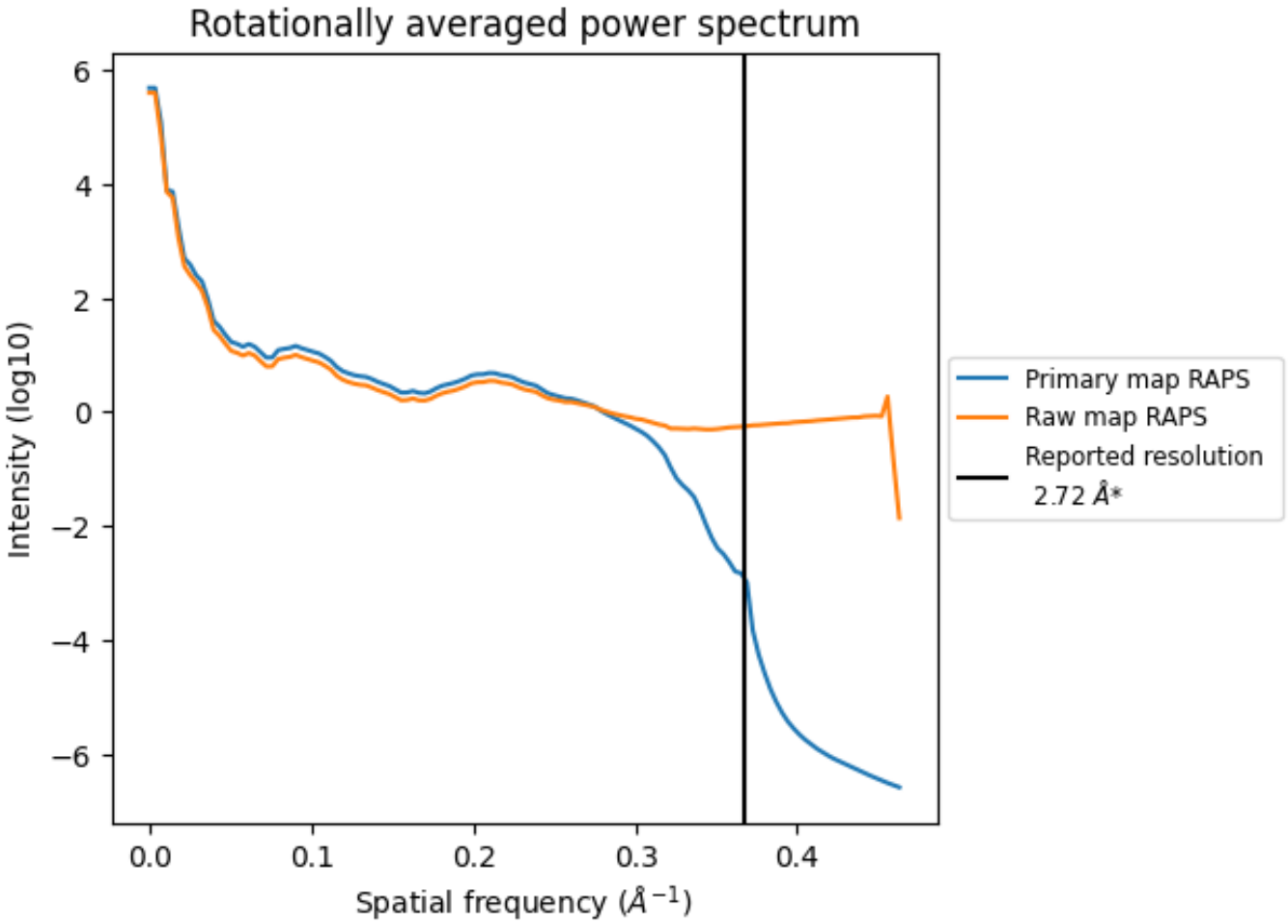
7.2 Volume estimate



The volume at the recommended contour level is 284 nm^3; this corresponds to an approximate mass of 256 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)

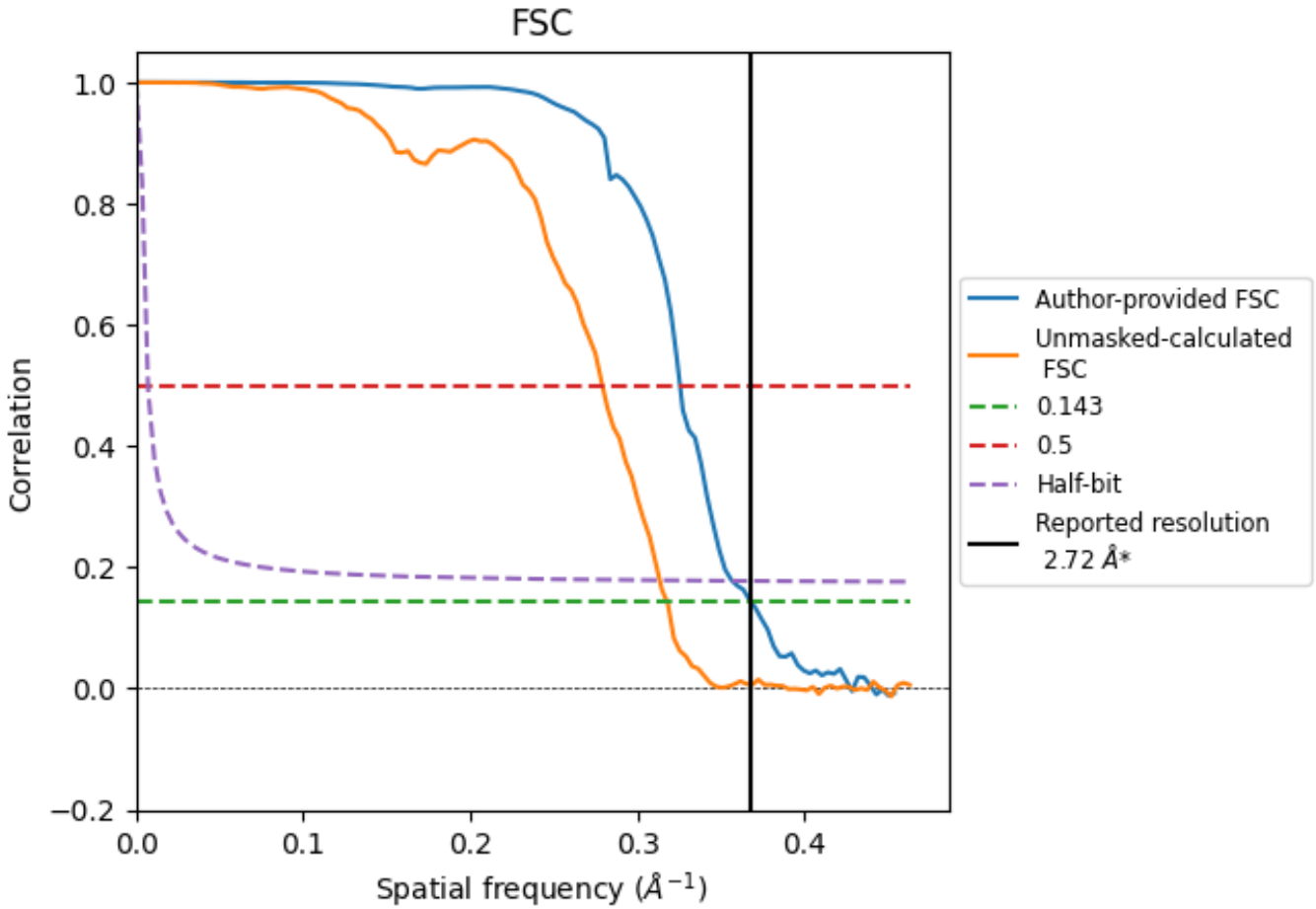


*Reported resolution corresponds to spatial frequency of 0.368 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.368 Å^{-1}

8.2 Resolution estimates (i)

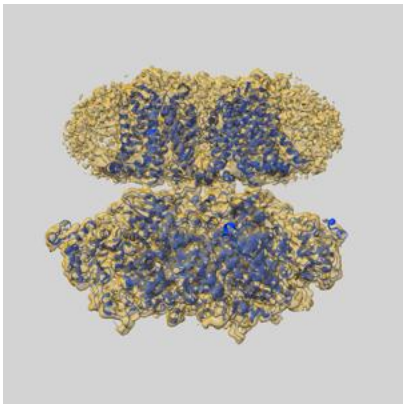
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.72	-	-
Author-provided FSC curve	2.72	3.07	2.80
Unmasked-calculated*	3.15	3.58	3.19

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.15 differs from the reported value 2.72 by more than 10 %

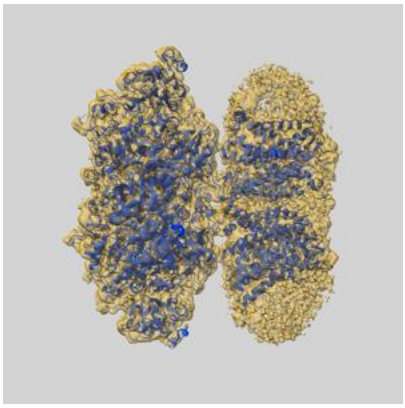
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-42988 and PDB model 8V63. Per-residue inclusion information can be found in section 3 on page 11.

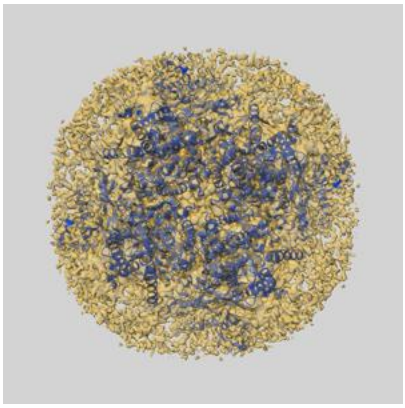
9.1 Map-model overlay



X



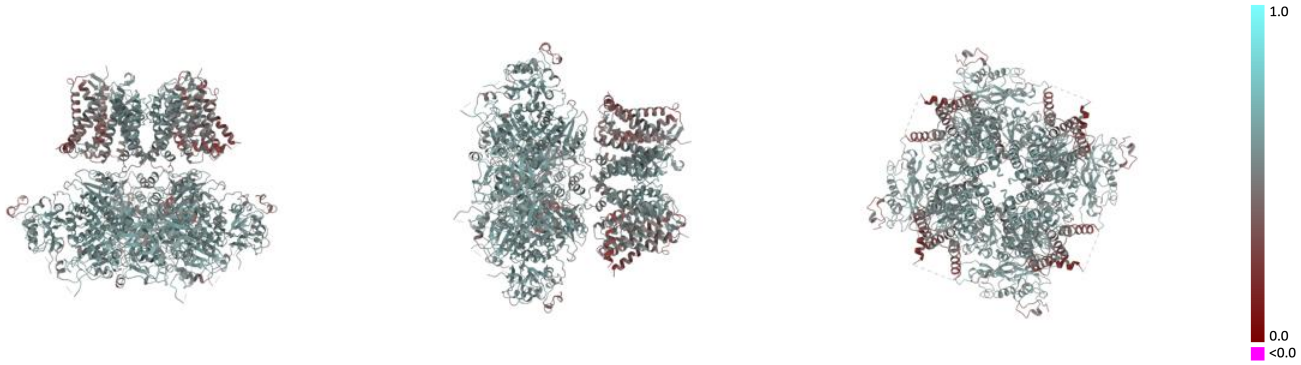
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.085 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.

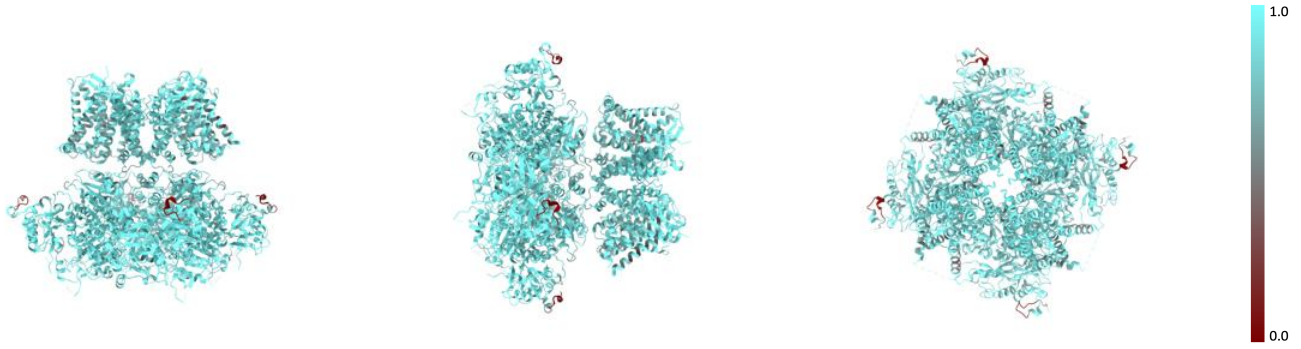
9.2 Q-score mapped to coordinate model (i)



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.

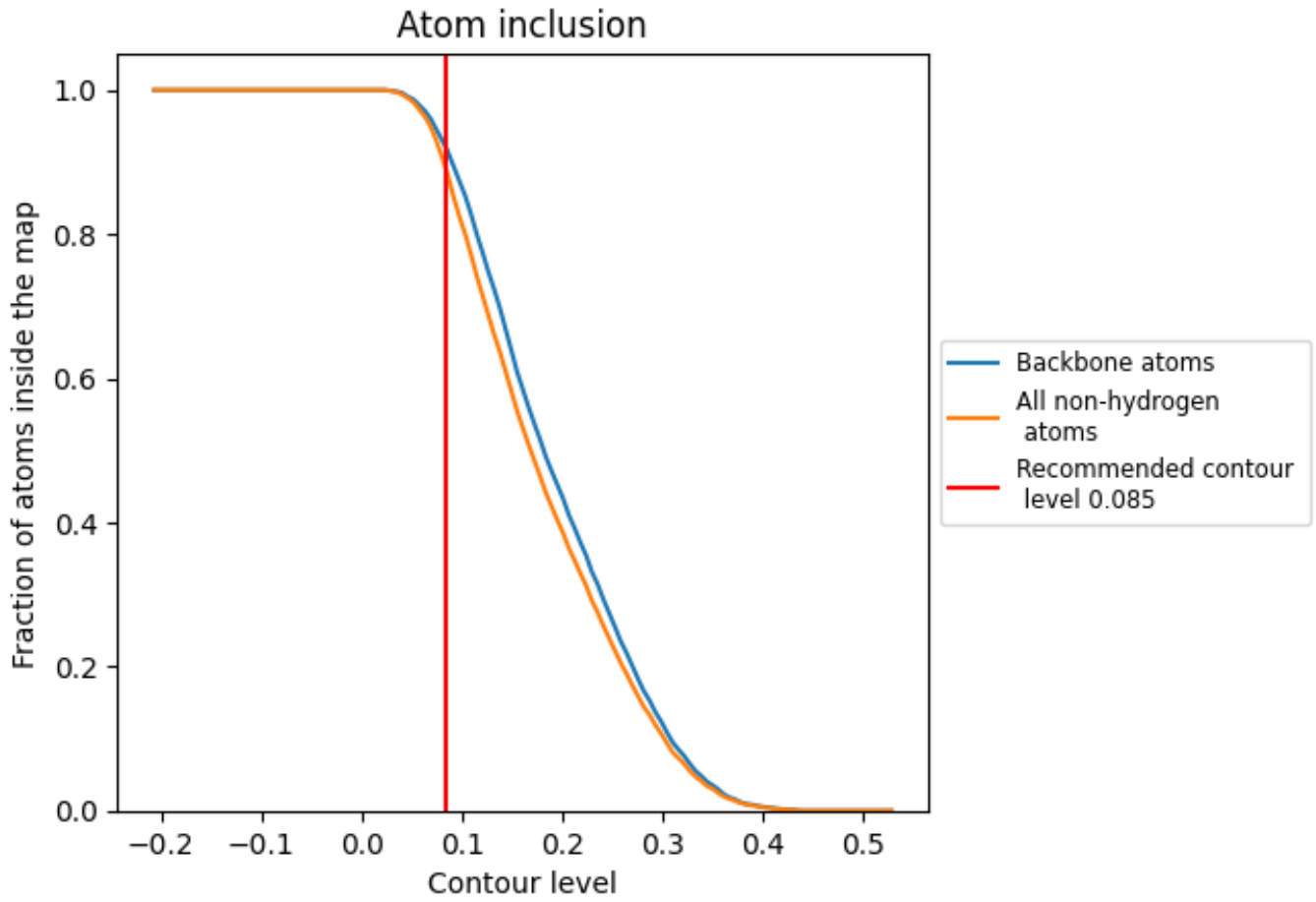
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.085).

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 89% 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 (0.085) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8870	0.5250
A	0.8890	0.5250
B	0.8900	0.5250
C	0.8890	0.5260
D	0.8880	0.5240