Full wwPDB EM Validation Report ⓘ

Nov 4, 2024 – 03:40 PM JST

PDB ID	:	8GN7
EMDB ID	:	EMD-34156
Title	:	structure of human connexin 40.1 intercellular gap junction channel by cryoEM
Authors	:	Zhang, H.; Wang, D.P.
Deposited on	:	2022-08-23
Resolution	:	3.00 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:

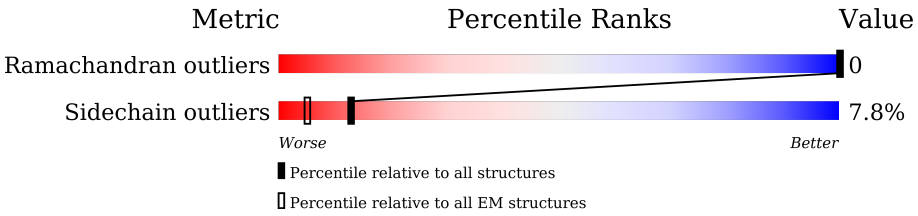
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 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)
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	233	81% 6% 13%
1	B	233	82% 5% 13%
1	G	233	81% 6% 13%
1	J	233	81% 6% 13%
1	M	233	79% 8% 13%
1	P	233	82% 5% 13%
1	S	233	81% 6% 13%
1	V	233	81% 6% 13%
1	Y	233	79% 8% 13%

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Mol	Chain	Length	Quality of chain
1	b	233	

2 Entry composition (i)

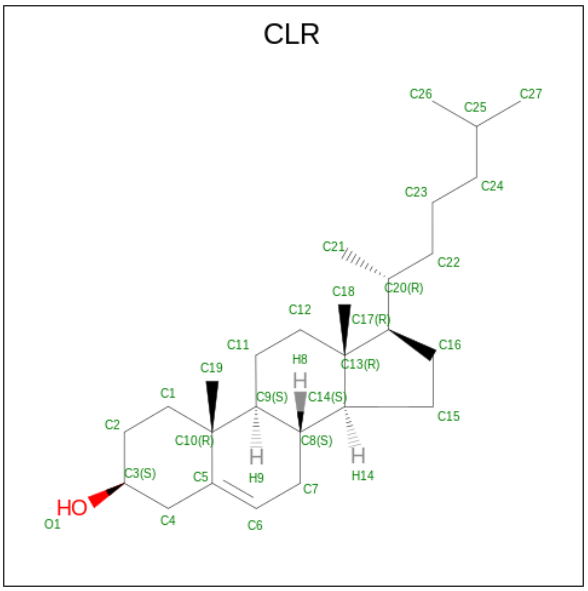
There are 4 unique types of molecules in this entry. The entry contains 17530 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Gap junction delta-4 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	203	Total	C	N	O	S	0	0
			1588	1048	269	257	14		
1	B	203	Total	C	N	O	S	0	0
			1588	1048	269	257	14		
1	G	203	Total	C	N	O	S	0	0
			1588	1048	269	257	14		
1	J	203	Total	C	N	O	S	0	0
			1588	1048	269	257	14		
1	M	203	Total	C	N	O	S	0	0
			1588	1048	269	257	14		
1	P	203	Total	C	N	O	S	0	0
			1588	1048	269	257	14		
1	S	203	Total	C	N	O	S	0	0
			1588	1048	269	257	14		
1	V	203	Total	C	N	O	S	0	0
			1588	1048	269	257	14		
1	Y	203	Total	C	N	O	S	0	0
			1588	1048	269	257	14		
1	b	203	Total	C	N	O	S	0	0
			1588	1048	269	257	14		

- Molecule 2 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
2	A	1	Total C O 28 27 1	0
2	A	1	Total C O 28 27 1	0
2	A	1	Total C O 28 27 1	0
2	B	1	Total C O 28 27 1	0
2	B	1	Total C O 28 27 1	0
2	B	1	Total C O 28 27 1	0
2	G	1	Total C O 28 27 1	0
2	G	1	Total C O 28 27 1	0
2	G	1	Total C O 28 27 1	0
2	J	1	Total C O 28 27 1	0
2	J	1	Total C O 28 27 1	0
2	M	1	Total C O 28 27 1	0
2	M	1	Total C O 28 27 1	0
2	M	1	Total C O 28 27 1	0

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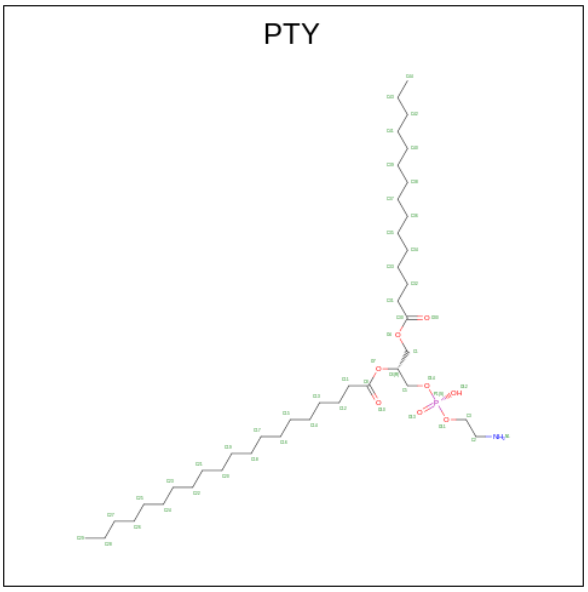
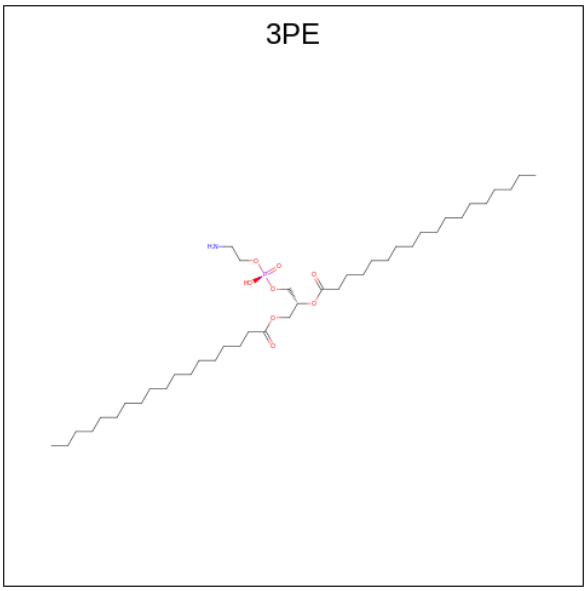
Mol	Chain	Residues	Atoms	AltConf
2	M	1	Total C O 28 27 1	0
2	P	1	Total C O 28 27 1	0
2	P	1	Total C O 28 27 1	0
2	S	1	Total C O 28 27 1	0
2	S	1	Total C O 28 27 1	0
2	S	1	Total C O 28 27 1	0
2	S	1	Total C O 28 27 1	0
2	V	1	Total C O 28 27 1	0
2	V	1	Total C O 28 27 1	0
2	Y	1	Total C O 28 27 1	0
2	Y	1	Total C O 28 27 1	0
2	Y	1	Total C O 28 27 1	0
2	Y	1	Total C O 28 27 1	0
2	b	1	Total C O 28 27 1	0
2	b	1	Total C O 28 27 1	0
2	b	1	Total C O 28 27 1	0

- Molecule 3 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: $C_{40}H_{80}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			39	29	1	8	1	
3	B	1	Total	C	N	O	P	0
			39	29	1	8	1	
3	G	1	Total	C	N	O	P	0
			39	29	1	8	1	
3	J	1	Total	C	N	O	P	0
			39	29	1	8	1	
3	M	1	Total	C	N	O	P	0
			39	29	1	8	1	
3	P	1	Total	C	N	O	P	0
			39	29	1	8	1	
3	S	1	Total	C	N	O	P	0
			39	29	1	8	1	
3	V	1	Total	C	N	O	P	0
			39	29	1	8	1	
3	Y	1	Total	C	N	O	P	0
			39	29	1	8	1	
3	b	1	Total	C	N	O	P	0
			39	29	1	8	1	

- Molecule 4 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$) (labeled as "Ligand of Interest" by depositor).



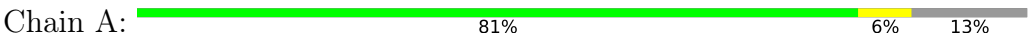
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			42	32	1	8	1	
4	B	1	Total	C	N	O	P	0
			42	32	1	8	1	
4	G	1	Total	C	N	O	P	0
			42	32	1	8	1	
4	J	1	Total	C	N	O	P	0
			42	32	1	8	1	
4	M	1	Total	C	N	O	P	0
			42	32	1	8	1	
4	P	1	Total	C	N	O	P	0
			42	32	1	8	1	
4	S	1	Total	C	N	O	P	0
			42	32	1	8	1	
4	V	1	Total	C	N	O	P	0
			42	32	1	8	1	
4	Y	1	Total	C	N	O	P	0
			42	32	1	8	1	
4	b	1	Total	C	N	O	P	0
			42	32	1	8	1	

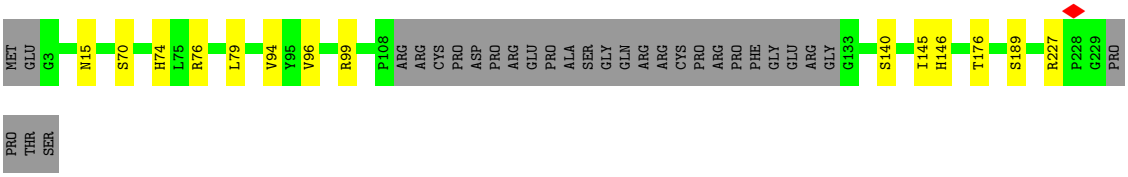
3 Residue-property plots (i)

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: Gap junction delta-4 protein

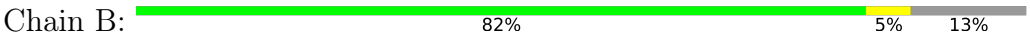
Chain A:





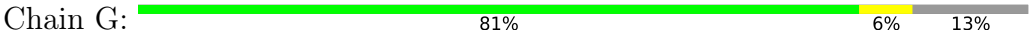
• Molecule 1: Gap junction delta-4 protein

Chain B:



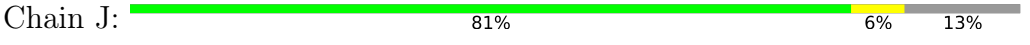
• Molecule 1: Gap junction delta-4 protein

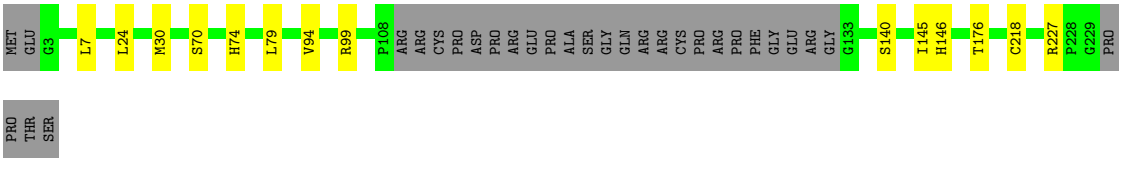
Chain G:



• Molecule 1: Gap junction delta-4 protein

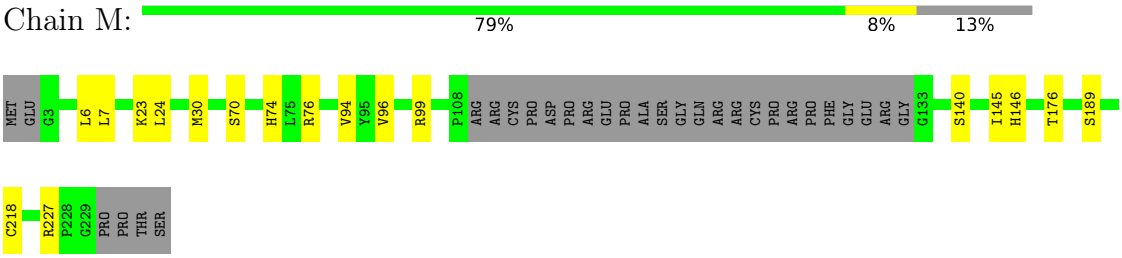
Chain J:





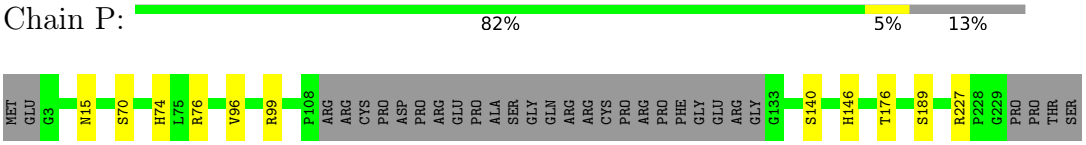
• Molecule 1: Gap junction delta-4 protein

Chain M:



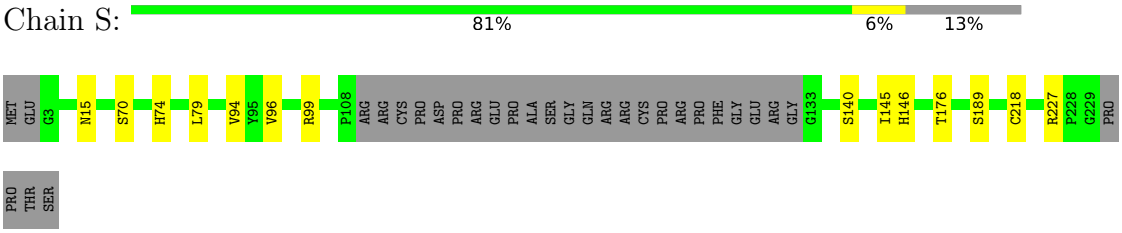
• Molecule 1: Gap junction delta-4 protein

Chain P:



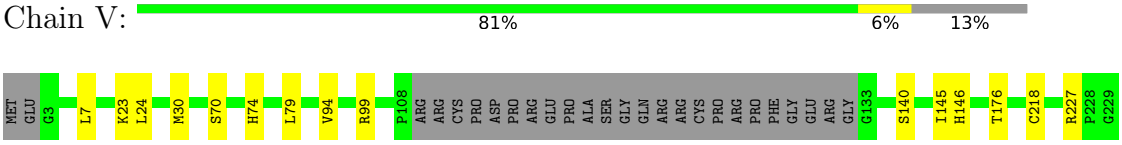
• Molecule 1: Gap junction delta-4 protein

Chain S:



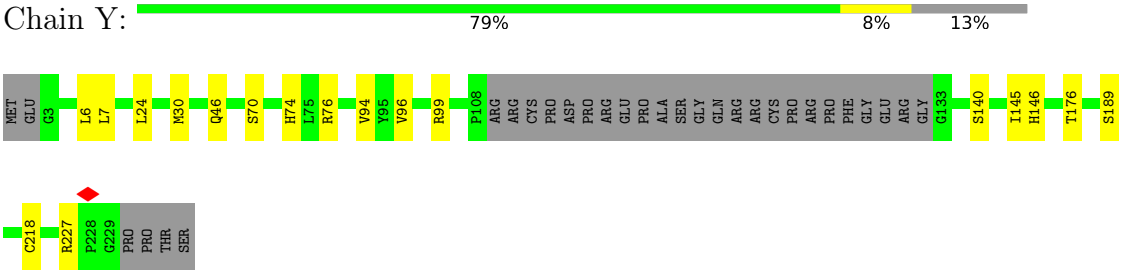
• Molecule 1: Gap junction delta-4 protein

Chain V:



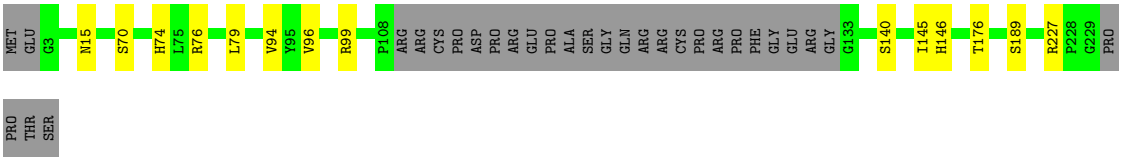
• Molecule 1: Gap junction delta-4 protein

Chain Y:



• Molecule 1: Gap junction delta-4 protein

Chain b:


MET GLU G3 N15 S70 H74 L75 R76 L79 V94 Y95 V96 R99 P108 ARG ARG CYS PRO ASP PRO ARG GLU PRO ALA SER GLY GLN ARG ARG CYS PRO ARG PRO PHE GLY GLU ARG GLY G133 S140 I145 H146 T176 S189 R227 P228 G229 PRO
PRO THR SER

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	41530	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	4.208	Depositor
Minimum map value	-2.586	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.103	Depositor
Recommended contour level	0.21	Depositor
Map size (Å)	353.28, 353.28, 353.28	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.92, 0.92, 0.92	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CLR, 3PE, PTY

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	0.25	0/1628	0.51	0/2215
1	B	0.25	0/1628	0.52	0/2215
1	G	0.25	0/1628	0.52	1/2215 (0.0%)
1	J	0.25	0/1628	0.52	1/2215 (0.0%)
1	M	0.25	0/1628	0.54	2/2215 (0.1%)
1	P	0.25	0/1628	0.53	0/2215
1	S	0.25	0/1628	0.51	0/2215
1	V	0.25	0/1628	0.52	1/2215 (0.0%)
1	Y	0.25	0/1628	0.53	2/2215 (0.1%)
1	b	0.25	0/1628	0.52	0/2215
All	All	0.25	0/16280	0.52	7/22150 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	24	LEU	CA-CB-CG	5.90	128.86	115.30
1	J	24	LEU	CA-CB-CG	5.66	128.31	115.30
1	Y	24	LEU	CA-CB-CG	5.65	128.30	115.30
1	V	24	LEU	CA-CB-CG	5.54	128.05	115.30
1	Y	6	LEU	CA-CB-CG	5.50	127.95	115.30
1	M	6	LEU	CA-CB-CG	5.44	127.82	115.30
1	G	6	LEU	CA-CB-CG	5.03	126.88	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles

5.3.1 Protein backbone

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	199/233 (85%)	193 (97%)	6 (3%)	0	100	100
1	B	199/233 (85%)	195 (98%)	4 (2%)	0	100	100
1	G	199/233 (85%)	194 (98%)	5 (2%)	0	100	100
1	J	199/233 (85%)	193 (97%)	6 (3%)	0	100	100
1	M	199/233 (85%)	193 (97%)	6 (3%)	0	100	100
1	P	199/233 (85%)	195 (98%)	4 (2%)	0	100	100
1	S	199/233 (85%)	194 (98%)	5 (2%)	0	100	100
1	V	199/233 (85%)	193 (97%)	6 (3%)	0	100	100
1	Y	199/233 (85%)	193 (97%)	6 (3%)	0	100	100
1	b	199/233 (85%)	193 (97%)	6 (3%)	0	100	100
All	All	1990/2330 (85%)	1936 (97%)	54 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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	174/200 (87%)	160 (92%)	14 (8%)	10	35
1	B	174/200 (87%)	163 (94%)	11 (6%)	15	45
1	G	174/200 (87%)	161 (92%)	13 (8%)	11	38
1	J	174/200 (87%)	161 (92%)	13 (8%)	11	38
1	M	174/200 (87%)	158 (91%)	16 (9%)	7	29
1	P	174/200 (87%)	163 (94%)	11 (6%)	15	45
1	S	174/200 (87%)	160 (92%)	14 (8%)	10	35
1	V	174/200 (87%)	160 (92%)	14 (8%)	10	35
1	Y	174/200 (87%)	158 (91%)	16 (9%)	7	29
1	b	174/200 (87%)	160 (92%)	14 (8%)	10	35
All	All	1740/2000 (87%)	1604 (92%)	136 (8%)	13	36

All (136) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	70	SER
1	A	74	HIS
1	A	76	ARG
1	A	79	LEU
1	A	94	VAL
1	A	96	VAL
1	A	99	ARG
1	A	140	SER
1	A	145	ILE
1	A	146	HIS
1	A	176	THR
1	A	189	SER
1	A	227	ARG
1	B	15	ASN
1	B	70	SER
1	B	74	HIS
1	B	76	ARG
1	B	96	VAL
1	B	99	ARG
1	B	140	SER
1	B	146	HIS
1	B	176	THR
1	B	189	SER

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Mol	Chain	Res	Type
1	B	227	ARG
1	G	70	SER
1	G	74	HIS
1	G	79	LEU
1	G	94	VAL
1	G	96	VAL
1	G	99	ARG
1	G	140	SER
1	G	145	ILE
1	G	146	HIS
1	G	176	THR
1	G	189	SER
1	G	218	CYS
1	G	227	ARG
1	J	7	LEU
1	J	30	MET
1	J	70	SER
1	J	74	HIS
1	J	79	LEU
1	J	94	VAL
1	J	99	ARG
1	J	140	SER
1	J	145	ILE
1	J	146	HIS
1	J	176	THR
1	J	218	CYS
1	J	227	ARG
1	M	7	LEU
1	M	23	LYS
1	M	30	MET
1	M	70	SER
1	M	74	HIS
1	M	76	ARG
1	M	94	VAL
1	M	96	VAL
1	M	99	ARG
1	M	140	SER
1	M	145	ILE
1	M	146	HIS
1	M	176	THR
1	M	189	SER
1	M	218	CYS

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Mol	Chain	Res	Type
1	M	227	ARG
1	P	15	ASN
1	P	70	SER
1	P	74	HIS
1	P	76	ARG
1	P	96	VAL
1	P	99	ARG
1	P	140	SER
1	P	146	HIS
1	P	176	THR
1	P	189	SER
1	P	227	ARG
1	S	15	ASN
1	S	70	SER
1	S	74	HIS
1	S	79	LEU
1	S	94	VAL
1	S	96	VAL
1	S	99	ARG
1	S	140	SER
1	S	145	ILE
1	S	146	HIS
1	S	176	THR
1	S	189	SER
1	S	218	CYS
1	S	227	ARG
1	V	7	LEU
1	V	23	LYS
1	V	30	MET
1	V	70	SER
1	V	74	HIS
1	V	79	LEU
1	V	94	VAL
1	V	99	ARG
1	V	140	SER
1	V	145	ILE
1	V	146	HIS
1	V	176	THR
1	V	218	CYS
1	V	227	ARG
1	Y	7	LEU
1	Y	30	MET

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Mol	Chain	Res	Type
1	Y	46	GLN
1	Y	70	SER
1	Y	74	HIS
1	Y	76	ARG
1	Y	94	VAL
1	Y	96	VAL
1	Y	99	ARG
1	Y	140	SER
1	Y	145	ILE
1	Y	146	HIS
1	Y	176	THR
1	Y	189	SER
1	Y	218	CYS
1	Y	227	ARG
1	b	15	ASN
1	b	70	SER
1	b	74	HIS
1	b	76	ARG
1	b	79	LEU
1	b	94	VAL
1	b	96	VAL
1	b	99	ARG
1	b	140	SER
1	b	145	ILE
1	b	146	HIS
1	b	176	THR
1	b	189	SER
1	b	227	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

50 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	CLR	B	303	-	31,31,31	0.36	0	48,48,48	0.58	0
2	CLR	S	301	-	31,31,31	0.36	0	48,48,48	0.58	0
2	CLR	M	304	-	31,31,31	0.36	0	48,48,48	0.58	0
4	3PE	G	301	-	41,41,50	0.56	0	44,46,55	0.56	1 (2%)
4	3PE	J	301	-	41,41,50	0.56	0	44,46,55	0.56	1 (2%)
2	CLR	G	304	-	31,31,31	0.38	0	48,48,48	0.78	2 (4%)
3	PTY	b	305	-	38,38,49	0.51	0	41,43,54	0.42	0
2	CLR	Y	304	-	31,31,31	0.36	0	48,48,48	0.59	0
3	PTY	B	305	-	38,38,49	0.51	0	41,43,54	0.43	0
4	3PE	M	302	-	41,41,50	0.56	0	44,46,55	0.56	1 (2%)
2	CLR	b	304	-	31,31,31	0.38	0	48,48,48	0.78	2 (4%)
2	CLR	P	301	-	31,31,31	0.38	0	48,48,48	0.78	2 (4%)
2	CLR	J	302	-	31,31,31	0.40	0	48,48,48	0.83	1 (2%)
3	PTY	P	302	-	38,38,49	0.51	0	41,43,54	0.42	0
4	3PE	b	301	-	41,41,50	0.56	0	44,46,55	0.56	1 (2%)
2	CLR	S	305	-	31,31,31	0.38	0	48,48,48	0.77	2 (4%)
2	CLR	V	303	-	31,31,31	0.38	0	48,48,48	0.77	2 (4%)
2	CLR	M	303	-	31,31,31	0.41	0	48,48,48	0.83	1 (2%)
2	CLR	G	302	-	31,31,31	0.40	0	48,48,48	0.83	1 (2%)
2	CLR	P	304	-	31,31,31	0.40	0	48,48,48	0.83	1 (2%)
4	3PE	V	301	-	41,41,50	0.56	0	44,46,55	0.56	1 (2%)
2	CLR	B	302	-	31,31,31	0.40	0	48,48,48	0.83	1 (2%)
2	CLR	A	301	-	31,31,31	0.36	0	48,48,48	0.58	0
4	3PE	A	304	-	41,41,50	0.56	0	44,46,55	0.56	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	CLR	A	302	-	31,31,31	0.38	0	48,48,48	0.78	2 (4%)
3	PTY	J	304	-	38,38,49	0.51	0	41,43,54	0.43	0
2	CLR	M	305	-	31,31,31	0.38	0	48,48,48	0.78	2 (4%)
3	PTY	V	304	-	38,38,49	0.51	0	41,43,54	0.43	0
4	3PE	B	301	-	41,41,50	0.56	0	44,46,55	0.56	1 (2%)
2	CLR	G	303	-	31,31,31	0.36	0	48,48,48	0.58	0
2	CLR	b	302	-	31,31,31	0.40	0	48,48,48	0.83	1 (2%)
4	3PE	S	302	-	41,41,50	0.56	0	44,46,55	0.56	1 (2%)
3	PTY	A	303	-	38,38,49	0.51	0	41,43,54	0.42	0
2	CLR	J	303	-	31,31,31	0.38	0	48,48,48	0.78	2 (4%)
2	CLR	S	303	-	31,31,31	0.40	0	48,48,48	0.83	1 (2%)
4	3PE	P	303	-	41,41,50	0.56	0	44,46,55	0.56	1 (2%)
2	CLR	S	304	-	31,31,31	0.36	0	48,48,48	0.58	0
3	PTY	S	306	-	38,38,49	0.51	0	41,43,54	0.43	0
2	CLR	V	302	-	31,31,31	0.40	0	48,48,48	0.83	1 (2%)
4	3PE	Y	302	-	41,41,50	0.56	0	44,46,55	0.56	1 (2%)
3	PTY	Y	306	-	38,38,49	0.51	0	41,43,54	0.43	0
2	CLR	Y	303	-	31,31,31	0.41	0	48,48,48	0.83	1 (2%)
2	CLR	A	305	-	31,31,31	0.40	0	48,48,48	0.83	1 (2%)
2	CLR	b	303	-	31,31,31	0.36	0	48,48,48	0.58	0
3	PTY	M	306	-	38,38,49	0.51	0	41,43,54	0.43	0
3	PTY	G	305	-	38,38,49	0.51	0	41,43,54	0.43	0
2	CLR	Y	305	-	31,31,31	0.38	0	48,48,48	0.78	2 (4%)
2	CLR	B	304	-	31,31,31	0.38	0	48,48,48	0.78	2 (4%)
2	CLR	M	301	-	31,31,31	0.36	0	48,48,48	0.58	0
2	CLR	Y	301	-	31,31,31	0.36	0	48,48,48	0.58	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
2	CLR	B	303	-	-	5/10/68/68	0/4/4/4
2	CLR	S	301	-	-	5/10/68/68	0/4/4/4
2	CLR	M	304	-	-	5/10/68/68	0/4/4/4
4	3PE	G	301	-	-	15/45/45/54	-
4	3PE	J	301	-	-	15/45/45/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CLR	G	304	-	-	2/10/68/68	0/4/4/4
3	PTY	b	305	-	-	14/42/42/53	-
2	CLR	Y	304	-	-	5/10/68/68	0/4/4/4
3	PTY	B	305	-	-	14/42/42/53	-
4	3PE	M	302	-	-	15/45/45/54	-
2	CLR	b	304	-	-	2/10/68/68	0/4/4/4
2	CLR	P	301	-	-	2/10/68/68	0/4/4/4
2	CLR	J	302	-	-	4/10/68/68	0/4/4/4
3	PTY	P	302	-	-	14/42/42/53	-
4	3PE	b	301	-	-	15/45/45/54	-
2	CLR	S	305	-	-	2/10/68/68	0/4/4/4
2	CLR	V	303	-	-	2/10/68/68	0/4/4/4
2	CLR	M	303	-	-	4/10/68/68	0/4/4/4
2	CLR	G	302	-	-	4/10/68/68	0/4/4/4
2	CLR	P	304	-	-	4/10/68/68	0/4/4/4
4	3PE	V	301	-	-	15/45/45/54	-
2	CLR	B	302	-	-	4/10/68/68	0/4/4/4
2	CLR	A	301	-	-	5/10/68/68	0/4/4/4
4	3PE	A	304	-	-	15/45/45/54	-
2	CLR	A	302	-	-	2/10/68/68	0/4/4/4
3	PTY	J	304	-	-	14/42/42/53	-
2	CLR	M	305	-	-	2/10/68/68	0/4/4/4
3	PTY	V	304	-	-	15/42/42/53	-
4	3PE	B	301	-	-	15/45/45/54	-
2	CLR	G	303	-	-	5/10/68/68	0/4/4/4
2	CLR	b	302	-	-	4/10/68/68	0/4/4/4
4	3PE	S	302	-	-	15/45/45/54	-
3	PTY	A	303	-	-	14/42/42/53	-
2	CLR	J	303	-	-	2/10/68/68	0/4/4/4
2	CLR	S	303	-	-	4/10/68/68	0/4/4/4
4	3PE	P	303	-	-	15/45/45/54	-
2	CLR	S	304	-	-	5/10/68/68	0/4/4/4
3	PTY	S	306	-	-	14/42/42/53	-
2	CLR	V	302	-	-	4/10/68/68	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	3PE	Y	302	-	-	15/45/45/54	-
3	PTY	Y	306	-	-	14/42/42/53	-
2	CLR	Y	303	-	-	4/10/68/68	0/4/4/4
2	CLR	A	305	-	-	4/10/68/68	0/4/4/4
2	CLR	b	303	-	-	5/10/68/68	0/4/4/4
3	PTY	M	306	-	-	14/42/42/53	-
3	PTY	G	305	-	-	14/42/42/53	-
2	CLR	Y	305	-	-	2/10/68/68	0/4/4/4
2	CLR	B	304	-	-	2/10/68/68	0/4/4/4
2	CLR	M	301	-	-	5/10/68/68	0/4/4/4
2	CLR	Y	301	-	-	5/10/68/68	0/4/4/4

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	302	CLR	C13-C17-C20	3.50	124.97	119.49
2	J	302	CLR	C13-C17-C20	3.50	124.97	119.49
2	V	302	CLR	C13-C17-C20	3.50	124.97	119.49
2	b	302	CLR	C13-C17-C20	3.50	124.97	119.49
2	A	305	CLR	C13-C17-C20	3.50	124.97	119.49
2	S	303	CLR	C13-C17-C20	3.49	124.95	119.49
2	P	304	CLR	C13-C17-C20	3.49	124.95	119.49
2	G	302	CLR	C13-C17-C20	3.48	124.94	119.49
2	M	303	CLR	C13-C17-C20	3.47	124.92	119.49
2	Y	303	CLR	C13-C17-C20	3.46	124.91	119.49
2	Y	305	CLR	C13-C17-C20	2.33	123.13	119.49
2	B	304	CLR	C13-C17-C20	2.33	123.13	119.49
2	M	305	CLR	C13-C17-C20	2.32	123.12	119.49
2	b	304	CLR	C13-C17-C20	2.32	123.12	119.49
2	P	301	CLR	C13-C17-C20	2.32	123.11	119.49
2	A	302	CLR	C13-C17-C20	2.31	123.11	119.49
2	G	304	CLR	C13-C17-C20	2.30	123.09	119.49
4	S	302	3PE	O12-P-O14	2.30	123.61	112.24
4	G	301	3PE	O12-P-O14	2.30	123.61	112.24
4	J	301	3PE	O12-P-O14	2.30	123.60	112.24
4	b	301	3PE	O12-P-O14	2.30	123.60	112.24
4	V	301	3PE	O12-P-O14	2.30	123.60	112.24
4	A	304	3PE	O12-P-O14	2.30	123.60	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	M	302	3PE	O12-P-O14	2.30	123.60	112.24
4	P	303	3PE	O12-P-O14	2.30	123.59	112.24
4	B	301	3PE	O12-P-O14	2.30	123.59	112.24
4	Y	302	3PE	O12-P-O14	2.30	123.59	112.24
2	J	303	CLR	C13-C17-C20	2.29	123.08	119.49
2	S	305	CLR	C13-C17-C20	2.28	123.06	119.49
2	V	303	CLR	C13-C17-C20	2.28	123.05	119.49
2	Y	305	CLR	C21-C20-C17	2.09	116.11	112.92
2	M	305	CLR	C21-C20-C17	2.08	116.11	112.92
2	b	304	CLR	C21-C20-C17	2.08	116.11	112.92
2	G	304	CLR	C21-C20-C17	2.08	116.11	112.92
2	B	304	CLR	C21-C20-C17	2.08	116.10	112.92
2	P	301	CLR	C21-C20-C17	2.07	116.09	112.92
2	A	302	CLR	C21-C20-C17	2.07	116.09	112.92
2	S	305	CLR	C21-C20-C17	2.07	116.09	112.92
2	J	303	CLR	C21-C20-C17	2.05	116.06	112.92
2	V	303	CLR	C21-C20-C17	2.04	116.04	112.92

There are no chirality outliers.

All (401) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	305	CLR	C13-C17-C20-C22
2	B	302	CLR	C13-C17-C20-C22
2	G	302	CLR	C13-C17-C20-C22
2	J	302	CLR	C13-C17-C20-C22
2	M	303	CLR	C13-C17-C20-C22
2	P	304	CLR	C13-C17-C20-C22
2	S	303	CLR	C13-C17-C20-C22
2	V	302	CLR	C13-C17-C20-C22
2	Y	303	CLR	C13-C17-C20-C22
2	b	302	CLR	C13-C17-C20-C22
3	A	303	PTY	N1-C2-C3-O11
3	A	303	PTY	C2-C3-O11-P1
3	B	305	PTY	N1-C2-C3-O11
3	B	305	PTY	C2-C3-O11-P1
3	G	305	PTY	N1-C2-C3-O11
3	G	305	PTY	C2-C3-O11-P1
3	J	304	PTY	N1-C2-C3-O11
3	M	306	PTY	N1-C2-C3-O11
3	P	302	PTY	N1-C2-C3-O11
3	P	302	PTY	C2-C3-O11-P1

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Mol	Chain	Res	Type	Atoms
3	S	306	PTY	N1-C2-C3-O11
3	S	306	PTY	C2-C3-O11-P1
3	V	304	PTY	N1-C2-C3-O11
3	V	304	PTY	C2-C3-O11-P1
3	Y	306	PTY	N1-C2-C3-O11
3	b	305	PTY	N1-C2-C3-O11
3	b	305	PTY	C2-C3-O11-P1
4	A	304	3PE	C11-O13-P-O14
4	A	304	3PE	O11-C1-C2-O21
4	B	301	3PE	C11-O13-P-O14
4	B	301	3PE	O11-C1-C2-O21
4	G	301	3PE	C11-O13-P-O14
4	G	301	3PE	O11-C1-C2-O21
4	J	301	3PE	C11-O13-P-O14
4	J	301	3PE	O11-C1-C2-O21
4	M	302	3PE	C11-O13-P-O14
4	M	302	3PE	O11-C1-C2-O21
4	P	303	3PE	C11-O13-P-O14
4	P	303	3PE	O11-C1-C2-O21
4	S	302	3PE	C11-O13-P-O14
4	S	302	3PE	O11-C1-C2-O21
4	V	301	3PE	C11-O13-P-O14
4	V	301	3PE	O11-C1-C2-O21
4	Y	302	3PE	C11-O13-P-O14
4	Y	302	3PE	O11-C1-C2-O21
4	b	301	3PE	C11-O13-P-O14
4	b	301	3PE	O11-C1-C2-O21
2	A	305	CLR	C16-C17-C20-C22
2	B	302	CLR	C16-C17-C20-C22
2	G	302	CLR	C16-C17-C20-C22
2	P	304	CLR	C16-C17-C20-C22
2	S	303	CLR	C16-C17-C20-C22
2	b	302	CLR	C16-C17-C20-C22
2	M	303	CLR	C16-C17-C20-C22
2	J	302	CLR	C16-C17-C20-C22
2	V	302	CLR	C16-C17-C20-C22
2	Y	303	CLR	C16-C17-C20-C22
2	J	303	CLR	C17-C20-C22-C23
2	A	302	CLR	C21-C20-C22-C23
2	B	304	CLR	C21-C20-C22-C23
2	G	304	CLR	C21-C20-C22-C23
2	J	303	CLR	C21-C20-C22-C23

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Mol	Chain	Res	Type	Atoms
2	M	305	CLR	C21-C20-C22-C23
2	P	301	CLR	C21-C20-C22-C23
2	S	305	CLR	C21-C20-C22-C23
2	V	303	CLR	C21-C20-C22-C23
2	Y	305	CLR	C21-C20-C22-C23
2	b	304	CLR	C21-C20-C22-C23
2	A	302	CLR	C17-C20-C22-C23
2	B	304	CLR	C17-C20-C22-C23
2	G	304	CLR	C17-C20-C22-C23
2	M	305	CLR	C17-C20-C22-C23
2	P	301	CLR	C17-C20-C22-C23
2	S	305	CLR	C17-C20-C22-C23
2	V	303	CLR	C17-C20-C22-C23
2	Y	305	CLR	C17-C20-C22-C23
2	b	304	CLR	C17-C20-C22-C23
2	A	305	CLR	C16-C17-C20-C21
2	B	302	CLR	C16-C17-C20-C21
2	P	304	CLR	C16-C17-C20-C21
2	S	303	CLR	C16-C17-C20-C21
2	b	302	CLR	C16-C17-C20-C21
2	A	301	CLR	C13-C17-C20-C22
2	B	303	CLR	C13-C17-C20-C22
2	G	303	CLR	C13-C17-C20-C22
2	M	301	CLR	C13-C17-C20-C22
2	M	304	CLR	C13-C17-C20-C22
2	S	301	CLR	C13-C17-C20-C22
2	S	304	CLR	C13-C17-C20-C22
2	Y	301	CLR	C13-C17-C20-C22
2	b	303	CLR	C13-C17-C20-C22
2	A	301	CLR	C16-C17-C20-C21
2	G	302	CLR	C16-C17-C20-C21
2	G	303	CLR	C16-C17-C20-C21
2	J	302	CLR	C16-C17-C20-C21
2	M	301	CLR	C16-C17-C20-C21
2	M	303	CLR	C16-C17-C20-C21
2	S	301	CLR	C16-C17-C20-C21
2	V	302	CLR	C16-C17-C20-C21
2	Y	301	CLR	C16-C17-C20-C21
2	Y	303	CLR	C16-C17-C20-C21
2	b	303	CLR	C16-C17-C20-C21
2	Y	304	CLR	C13-C17-C20-C22
2	B	303	CLR	C16-C17-C20-C21

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Mol	Chain	Res	Type	Atoms
2	M	304	CLR	C16-C17-C20-C21
2	S	304	CLR	C16-C17-C20-C21
2	Y	304	CLR	C16-C17-C20-C21
2	G	303	CLR	C22-C23-C24-C25
2	M	301	CLR	C22-C23-C24-C25
2	S	301	CLR	C22-C23-C24-C25
2	S	304	CLR	C22-C23-C24-C25
2	Y	304	CLR	C22-C23-C24-C25
2	B	303	CLR	C22-C23-C24-C25
2	M	304	CLR	C22-C23-C24-C25
2	Y	301	CLR	C22-C23-C24-C25
2	A	301	CLR	C13-C17-C20-C21
2	B	303	CLR	C13-C17-C20-C21
2	G	303	CLR	C13-C17-C20-C21
2	M	301	CLR	C13-C17-C20-C21
2	M	304	CLR	C13-C17-C20-C21
2	S	301	CLR	C13-C17-C20-C21
2	S	304	CLR	C13-C17-C20-C21
2	Y	301	CLR	C13-C17-C20-C21
2	Y	304	CLR	C13-C17-C20-C21
2	b	303	CLR	C13-C17-C20-C21
2	A	301	CLR	C22-C23-C24-C25
2	b	303	CLR	C22-C23-C24-C25
3	A	303	PTY	C3-O11-P1-O14
3	B	305	PTY	C3-O11-P1-O14
3	G	305	PTY	C3-O11-P1-O14
3	J	304	PTY	C3-O11-P1-O14
3	M	306	PTY	C3-O11-P1-O14
3	P	302	PTY	C3-O11-P1-O14
3	S	306	PTY	C3-O11-P1-O14
3	V	304	PTY	C3-O11-P1-O14
3	Y	306	PTY	C3-O11-P1-O14
3	b	305	PTY	C3-O11-P1-O14
4	A	304	3PE	C11-O13-P-O11
4	B	301	3PE	C11-O13-P-O11
4	G	301	3PE	C11-O13-P-O11
4	J	301	3PE	C11-O13-P-O11
4	M	302	3PE	C11-O13-P-O11
4	P	303	3PE	C11-O13-P-O11
4	S	302	3PE	C11-O13-P-O11
4	V	301	3PE	C11-O13-P-O11
4	Y	302	3PE	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
4	b	301	3PE	C11-O13-P-O11
4	B	301	3PE	C35-C36-C37-C38
4	G	301	3PE	C35-C36-C37-C38
4	P	303	3PE	C35-C36-C37-C38
4	S	302	3PE	C35-C36-C37-C38
3	P	302	PTY	C35-C36-C37-C38
4	A	304	3PE	C35-C36-C37-C38
4	J	301	3PE	C35-C36-C37-C38
4	M	302	3PE	C35-C36-C37-C38
4	Y	302	3PE	C35-C36-C37-C38
4	b	301	3PE	C35-C36-C37-C38
4	V	301	3PE	C35-C36-C37-C38
3	B	305	PTY	C35-C36-C37-C38
3	b	305	PTY	C12-C13-C14-C15
3	A	303	PTY	C12-C13-C14-C15
3	B	305	PTY	C12-C13-C14-C15
3	J	304	PTY	C35-C36-C37-C38
3	V	304	PTY	C35-C36-C37-C38
3	P	302	PTY	C12-C13-C14-C15
3	J	304	PTY	C12-C13-C14-C15
3	M	306	PTY	C35-C36-C37-C38
3	Y	306	PTY	C35-C36-C37-C38
3	Y	306	PTY	C12-C13-C14-C15
3	M	306	PTY	C12-C13-C14-C15
3	G	305	PTY	C35-C36-C37-C38
3	S	306	PTY	C35-C36-C37-C38
3	A	303	PTY	C35-C36-C37-C38
3	V	304	PTY	C12-C13-C14-C15
3	b	305	PTY	C35-C36-C37-C38
3	G	305	PTY	C12-C13-C14-C15
3	S	306	PTY	C12-C13-C14-C15
2	B	303	CLR	C16-C17-C20-C22
2	G	303	CLR	C16-C17-C20-C22
2	M	301	CLR	C16-C17-C20-C22
2	S	304	CLR	C16-C17-C20-C22
2	Y	301	CLR	C16-C17-C20-C22
2	A	301	CLR	C16-C17-C20-C22
2	S	301	CLR	C16-C17-C20-C22
2	b	303	CLR	C16-C17-C20-C22
4	A	304	3PE	C22-C21-O21-C2
4	B	301	3PE	C22-C21-O21-C2
4	G	301	3PE	C22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
4	M	302	3PE	C22-C21-O21-C2
4	P	303	3PE	C22-C21-O21-C2
4	S	302	3PE	C22-C21-O21-C2
4	Y	302	3PE	C22-C21-O21-C2
4	b	301	3PE	C22-C21-O21-C2
3	G	305	PTY	C36-C37-C38-C39
3	V	304	PTY	C36-C37-C38-C39
2	M	304	CLR	C16-C17-C20-C22
3	J	304	PTY	C36-C37-C38-C39
3	S	306	PTY	C36-C37-C38-C39
3	B	305	PTY	C36-C37-C38-C39
3	P	302	PTY	C36-C37-C38-C39
4	J	301	3PE	C22-C21-O21-C2
4	V	301	3PE	C22-C21-O21-C2
3	A	303	PTY	C36-C37-C38-C39
3	b	305	PTY	C36-C37-C38-C39
4	B	301	3PE	C3C-C3D-C3E-C3F
4	A	304	3PE	O11-C1-C2-C3
4	B	301	3PE	O11-C1-C2-C3
4	G	301	3PE	O11-C1-C2-C3
4	J	301	3PE	O11-C1-C2-C3
4	M	302	3PE	O11-C1-C2-C3
4	P	303	3PE	O11-C1-C2-C3
4	S	302	3PE	O11-C1-C2-C3
4	V	301	3PE	O11-C1-C2-C3
4	Y	302	3PE	O11-C1-C2-C3
4	b	301	3PE	O11-C1-C2-C3
2	A	305	CLR	C13-C17-C20-C21
2	B	302	CLR	C13-C17-C20-C21
2	P	304	CLR	C13-C17-C20-C21
2	S	303	CLR	C13-C17-C20-C21
2	b	302	CLR	C13-C17-C20-C21
3	Y	306	PTY	C36-C37-C38-C39
4	P	303	3PE	C3C-C3D-C3E-C3F
4	A	304	3PE	C3C-C3D-C3E-C3F
4	b	301	3PE	C3C-C3D-C3E-C3F
3	M	306	PTY	C36-C37-C38-C39
3	A	303	PTY	O4-C1-C6-C5
3	B	305	PTY	O4-C1-C6-C5
3	G	305	PTY	O4-C1-C6-C5
3	J	304	PTY	O4-C1-C6-C5
3	M	306	PTY	O4-C1-C6-C5

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Mol	Chain	Res	Type	Atoms
3	S	306	PTY	O4-C1-C6-C5
3	V	304	PTY	O4-C1-C6-C5
3	Y	306	PTY	O4-C1-C6-C5
3	b	305	PTY	O4-C1-C6-C5
2	Y	304	CLR	C16-C17-C20-C22
4	Y	302	3PE	C3C-C3D-C3E-C3F
4	V	301	3PE	C3C-C3D-C3E-C3F
2	G	302	CLR	C13-C17-C20-C21
2	M	303	CLR	C13-C17-C20-C21
4	G	301	3PE	C3C-C3D-C3E-C3F
4	S	302	3PE	C3C-C3D-C3E-C3F
4	J	301	3PE	C3C-C3D-C3E-C3F
4	M	302	3PE	C3C-C3D-C3E-C3F
2	J	302	CLR	C13-C17-C20-C21
2	V	302	CLR	C13-C17-C20-C21
2	Y	303	CLR	C13-C17-C20-C21
4	G	301	3PE	O22-C21-O21-C2
4	S	302	3PE	O22-C21-O21-C2
4	A	304	3PE	O22-C21-O21-C2
4	M	302	3PE	O22-C21-O21-C2
4	Y	302	3PE	O22-C21-O21-C2
4	B	301	3PE	O22-C21-O21-C2
4	J	301	3PE	O22-C21-O21-C2
4	P	303	3PE	O22-C21-O21-C2
4	V	301	3PE	O22-C21-O21-C2
4	b	301	3PE	O22-C21-O21-C2
4	B	301	3PE	C3D-C3E-C3F-C3G
3	P	302	PTY	O4-C1-C6-C5
4	P	303	3PE	C3D-C3E-C3F-C3G
4	Y	302	3PE	C3D-C3E-C3F-C3G
4	V	301	3PE	C3D-C3E-C3F-C3G
4	b	301	3PE	C3D-C3E-C3F-C3G
4	G	301	3PE	C3D-C3E-C3F-C3G
3	A	303	PTY	O14-C5-C6-O7
4	J	301	3PE	C3D-C3E-C3F-C3G
4	A	304	3PE	C3D-C3E-C3F-C3G
4	S	302	3PE	C3D-C3E-C3F-C3G
4	M	302	3PE	C3D-C3E-C3F-C3G
3	B	305	PTY	O14-C5-C6-O7
3	G	305	PTY	O14-C5-C6-O7
3	J	304	PTY	O14-C5-C6-O7
3	M	306	PTY	O14-C5-C6-O7

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Mol	Chain	Res	Type	Atoms
3	P	302	PTY	O14-C5-C6-O7
3	S	306	PTY	O14-C5-C6-O7
3	V	304	PTY	O14-C5-C6-O7
3	Y	306	PTY	O14-C5-C6-O7
3	b	305	PTY	O14-C5-C6-O7
3	A	303	PTY	O4-C1-C6-O7
3	G	305	PTY	O4-C1-C6-O7
3	Y	306	PTY	O4-C1-C6-O7
3	b	305	PTY	O4-C1-C6-O7
3	A	303	PTY	C3-O11-P1-O13
3	B	305	PTY	C3-O11-P1-O13
3	G	305	PTY	C3-O11-P1-O13
3	J	304	PTY	C3-O11-P1-O13
3	M	306	PTY	C3-O11-P1-O13
3	P	302	PTY	C3-O11-P1-O13
3	S	306	PTY	C3-O11-P1-O13
3	V	304	PTY	C3-O11-P1-O13
3	Y	306	PTY	C3-O11-P1-O13
3	b	305	PTY	C3-O11-P1-O13
4	A	304	3PE	C11-O13-P-O12
4	B	301	3PE	C11-O13-P-O12
4	G	301	3PE	C11-O13-P-O12
4	J	301	3PE	C11-O13-P-O12
4	M	302	3PE	C11-O13-P-O12
4	P	303	3PE	C11-O13-P-O12
4	S	302	3PE	C11-O13-P-O12
4	V	301	3PE	C11-O13-P-O12
4	Y	302	3PE	C11-O13-P-O12
4	b	301	3PE	C11-O13-P-O12
3	A	303	PTY	O14-C5-C6-C1
3	B	305	PTY	O14-C5-C6-C1
3	G	305	PTY	O14-C5-C6-C1
3	J	304	PTY	O14-C5-C6-C1
3	M	306	PTY	O14-C5-C6-C1
3	P	302	PTY	O14-C5-C6-C1
3	S	306	PTY	O14-C5-C6-C1
3	V	304	PTY	O14-C5-C6-C1
3	Y	306	PTY	O14-C5-C6-C1
3	b	305	PTY	O14-C5-C6-C1
3	J	304	PTY	C2-C3-O11-P1
3	M	306	PTY	C2-C3-O11-P1
3	Y	306	PTY	C2-C3-O11-P1

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Mol	Chain	Res	Type	Atoms
3	M	306	PTY	O4-C1-C6-O7
3	S	306	PTY	O4-C1-C6-O7
4	G	301	3PE	C37-C38-C39-C3A
4	S	302	3PE	C37-C38-C39-C3A
4	Y	302	3PE	C37-C38-C39-C3A
3	J	304	PTY	O4-C1-C6-O7
3	V	304	PTY	O4-C1-C6-O7
3	S	306	PTY	C8-C11-C12-C13
4	M	302	3PE	C37-C38-C39-C3A
4	P	303	3PE	C37-C38-C39-C3A
4	B	301	3PE	C37-C38-C39-C3A
3	G	305	PTY	C8-C11-C12-C13
3	V	304	PTY	C8-C11-C12-C13
3	M	306	PTY	C8-C11-C12-C13
3	Y	306	PTY	C8-C11-C12-C13
3	B	305	PTY	O4-C1-C6-O7
3	J	304	PTY	C8-C11-C12-C13
3	G	305	PTY	C13-C14-C15-C16
3	B	305	PTY	C13-C14-C15-C16
3	P	302	PTY	C13-C14-C15-C16
3	b	305	PTY	C13-C14-C15-C16
3	A	303	PTY	C13-C14-C15-C16
4	b	301	3PE	C38-C39-C3A-C3B
3	S	306	PTY	C13-C14-C15-C16
3	J	304	PTY	C13-C14-C15-C16
3	Y	306	PTY	C13-C14-C15-C16
3	M	306	PTY	C13-C14-C15-C16
4	A	304	3PE	C38-C39-C3A-C3B
4	J	301	3PE	C38-C39-C3A-C3B
4	V	301	3PE	C38-C39-C3A-C3B
3	P	302	PTY	C8-C11-C12-C13
4	Y	302	3PE	C38-C39-C3A-C3B
3	V	304	PTY	C13-C14-C15-C16
4	M	302	3PE	C38-C39-C3A-C3B
4	A	304	3PE	C37-C38-C39-C3A
4	b	301	3PE	C37-C38-C39-C3A
4	J	301	3PE	C37-C38-C39-C3A
3	P	302	PTY	O4-C1-C6-O7
3	B	305	PTY	C8-C11-C12-C13
4	V	301	3PE	C37-C38-C39-C3A
4	B	301	3PE	C38-C39-C3A-C3B
4	P	303	3PE	C38-C39-C3A-C3B

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Mol	Chain	Res	Type	Atoms
4	G	301	3PE	C38-C39-C3A-C3B
4	G	301	3PE	C39-C3A-C3B-C3C
4	S	302	3PE	C38-C39-C3A-C3B
4	V	301	3PE	C39-C3A-C3B-C3C
4	S	302	3PE	C39-C3A-C3B-C3C
3	A	303	PTY	C8-C11-C12-C13
4	B	301	3PE	C39-C3A-C3B-C3C
4	J	301	3PE	C39-C3A-C3B-C3C
4	J	301	3PE	O21-C21-C22-C23
4	M	302	3PE	O21-C21-C22-C23
4	P	303	3PE	O21-C21-C22-C23
4	V	301	3PE	O21-C21-C22-C23
3	b	305	PTY	C8-C11-C12-C13
4	b	301	3PE	C39-C3A-C3B-C3C
4	A	304	3PE	O21-C21-C22-C23
4	B	301	3PE	O21-C21-C22-C23
4	G	301	3PE	O21-C21-C22-C23
4	S	302	3PE	O21-C21-C22-C23
4	Y	302	3PE	O21-C21-C22-C23
4	Y	302	3PE	C39-C3A-C3B-C3C
4	b	301	3PE	O21-C21-C22-C23
4	A	304	3PE	C39-C3A-C3B-C3C
4	P	303	3PE	C39-C3A-C3B-C3C
4	J	301	3PE	O22-C21-C22-C23
4	M	302	3PE	O22-C21-C22-C23
4	V	301	3PE	O22-C21-C22-C23
4	B	301	3PE	O22-C21-C22-C23
4	G	301	3PE	O22-C21-C22-C23
4	P	303	3PE	O22-C21-C22-C23
4	S	302	3PE	O22-C21-C22-C23
4	M	302	3PE	C39-C3A-C3B-C3C
4	Y	302	3PE	O22-C21-C22-C23
4	b	301	3PE	O22-C21-C22-C23
4	A	304	3PE	O22-C21-C22-C23
3	b	305	PTY	C12-C11-C8-O7
3	A	303	PTY	C12-C11-C8-O7
3	B	305	PTY	C12-C11-C8-O7
3	J	304	PTY	C12-C11-C8-O7
3	M	306	PTY	C12-C11-C8-O7
3	P	302	PTY	C12-C11-C8-O7
3	Y	306	PTY	C12-C11-C8-O7
3	V	304	PTY	C14-C15-C16-C17

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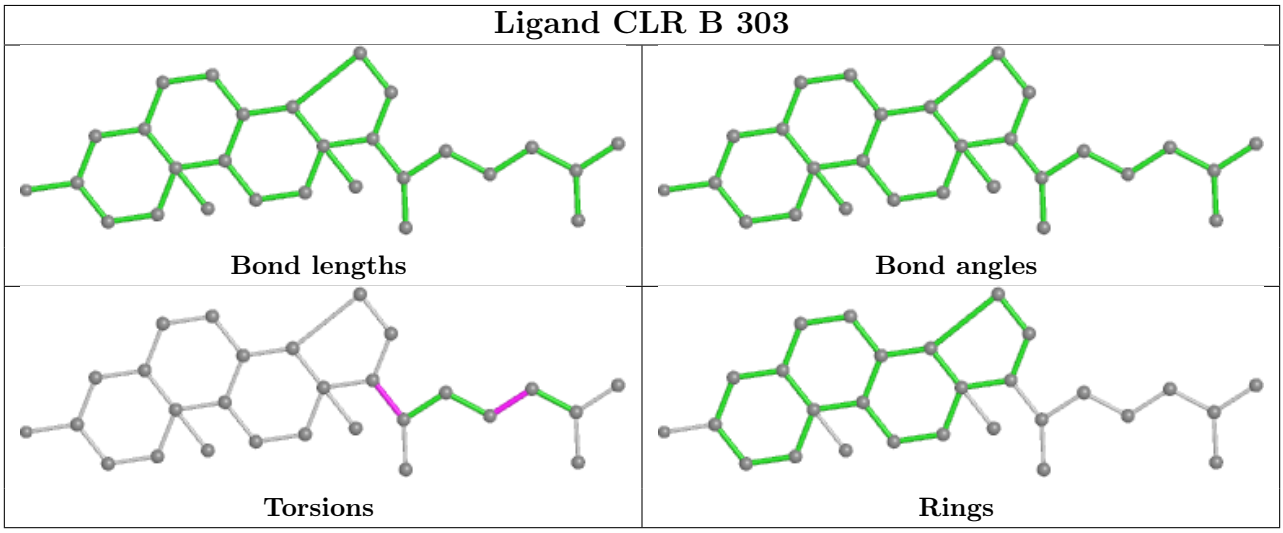
Mol	Chain	Res	Type	Atoms
3	G	305	PTY	C12-C11-C8-O7
3	S	306	PTY	C12-C11-C8-O7
3	V	304	PTY	C12-C11-C8-O7

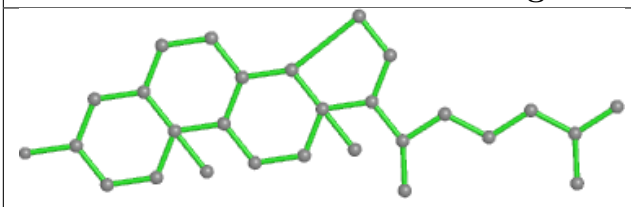
There are no ring outliers.

No monomer is involved in short contacts.

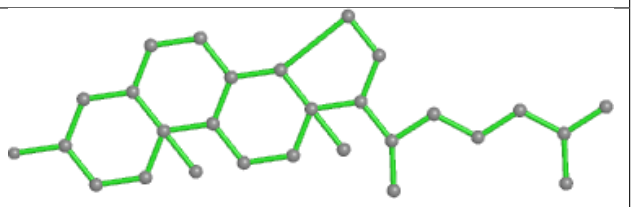
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



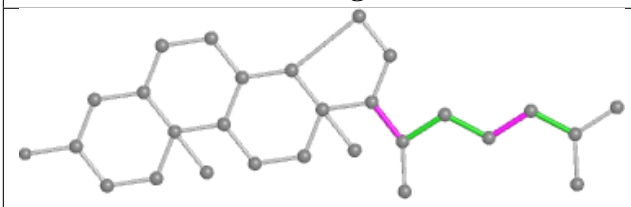
Ligand CLR S 301



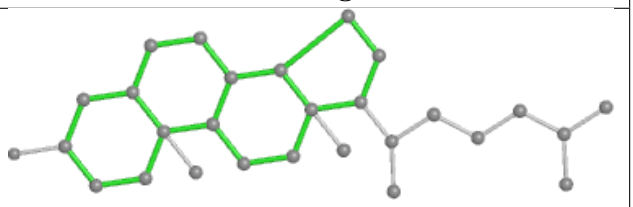
Bond lengths



Bond angles

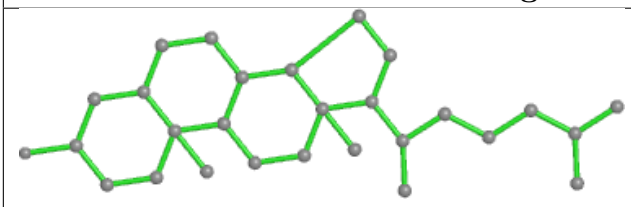


Torsions

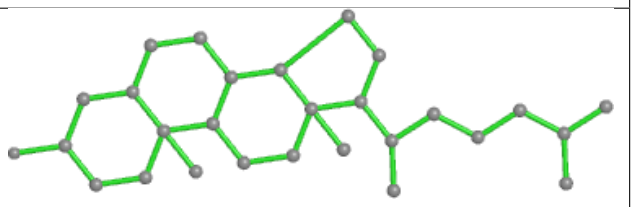


Rings

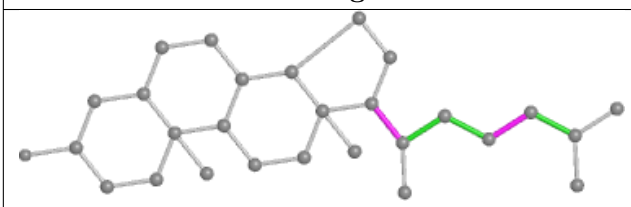
Ligand CLR M 304



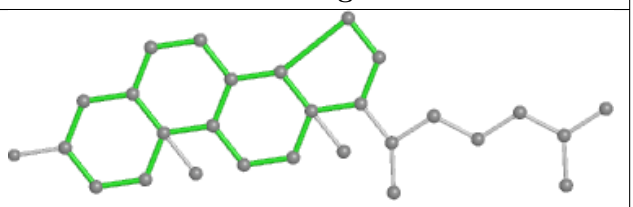
Bond lengths



Bond angles

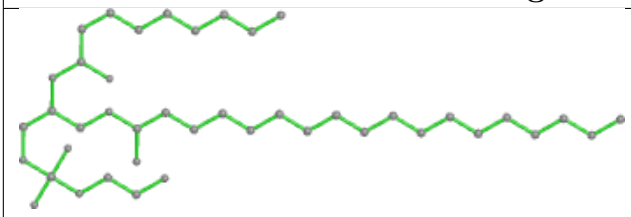


Torsions

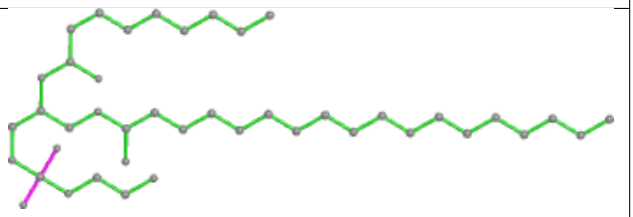


Rings

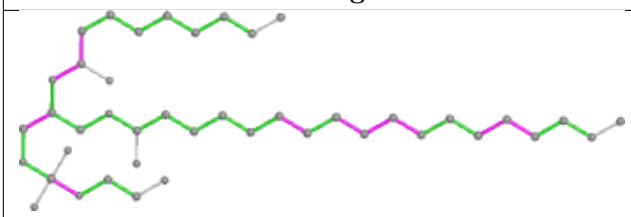
Ligand 3PE G 301



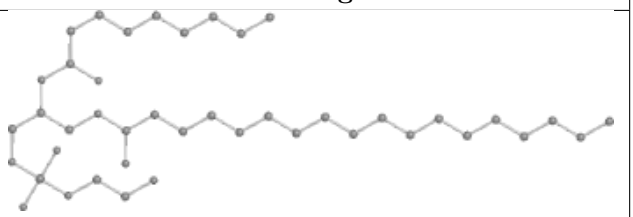
Bond lengths



Bond angles

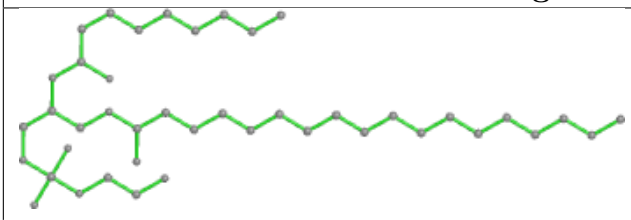


Torsions

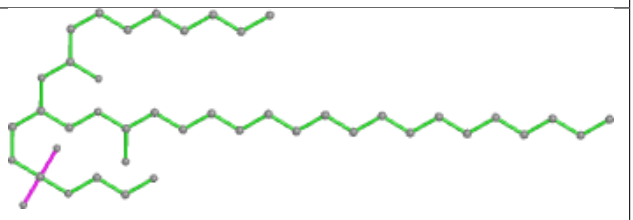


Rings

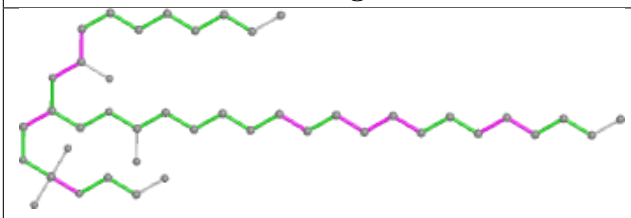
Ligand 3PE J 301



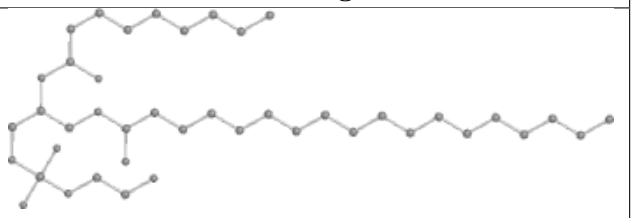
Bond lengths



Bond angles

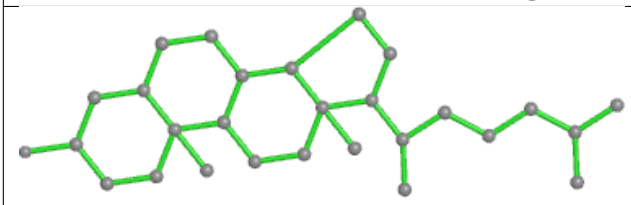


Torsions

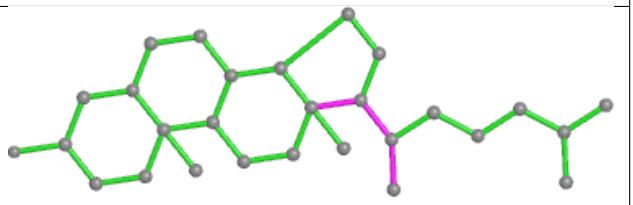


Rings

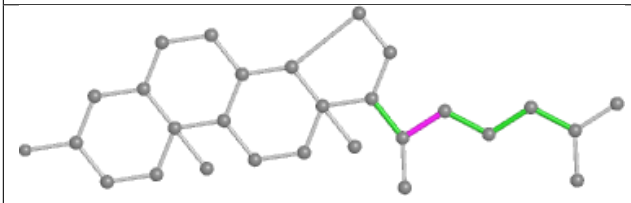
Ligand CLR G 304



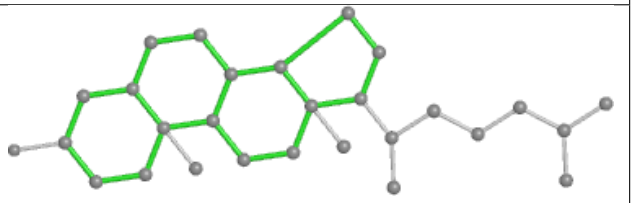
Bond lengths



Bond angles

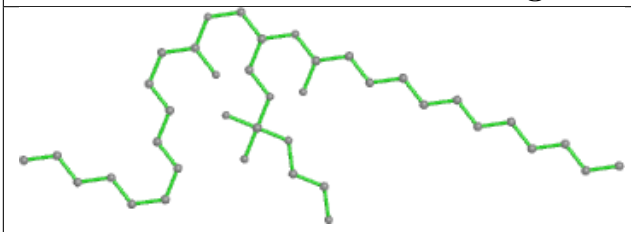


Torsions

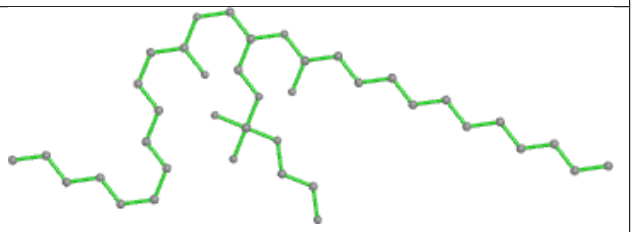


Rings

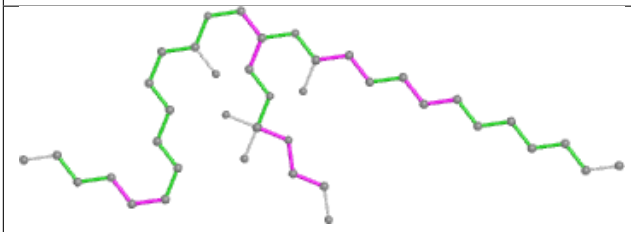
Ligand PTY b 305



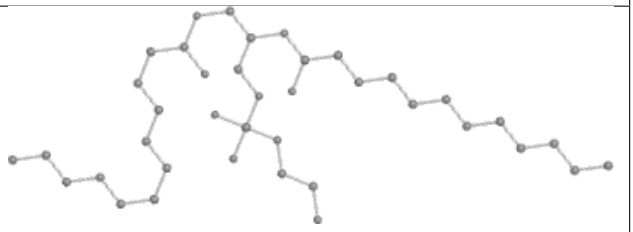
Bond lengths



Bond angles

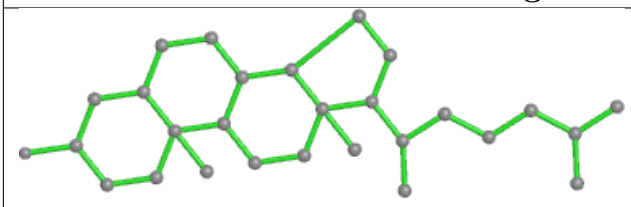


Torsions

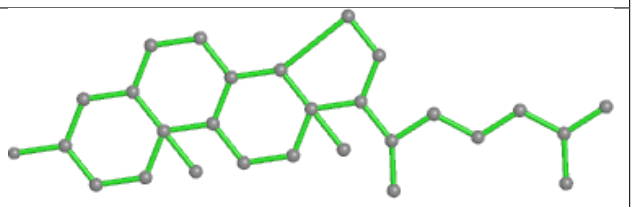


Rings

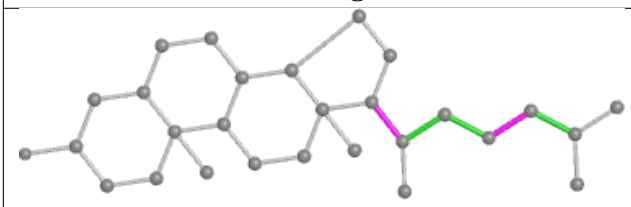
Ligand CLR Y 304



Bond lengths



Bond angles



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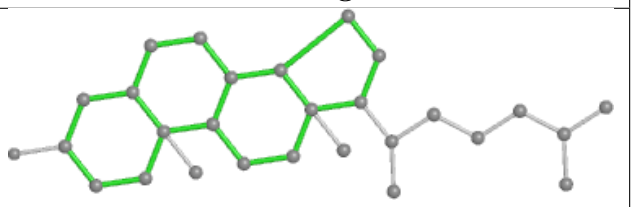
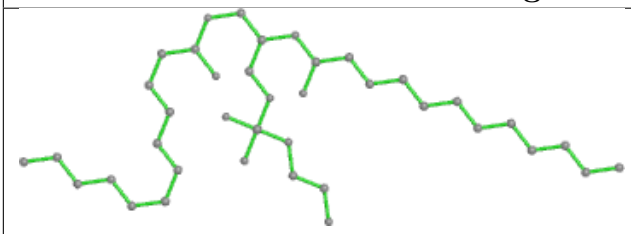


Rings

Ligand PTY B 305



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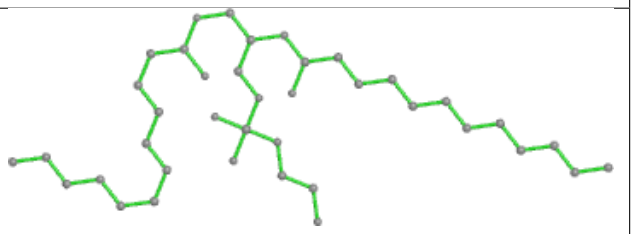
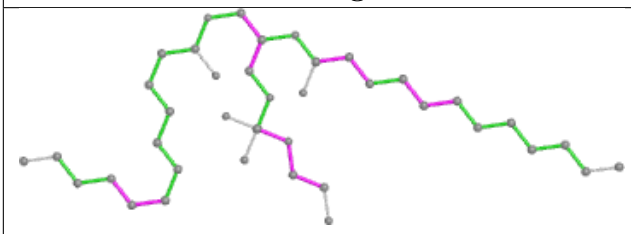
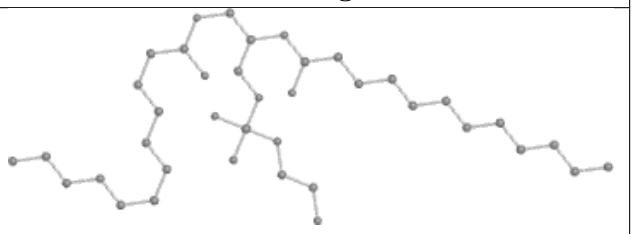


Bond angles

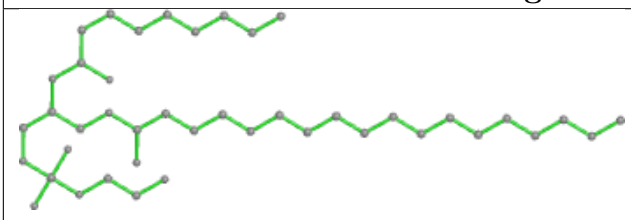


Torsions

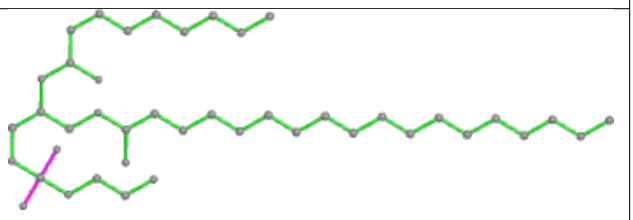


Rings

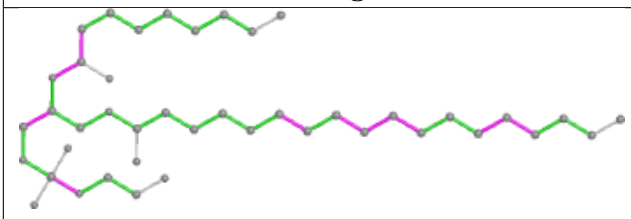
Ligand 3PE M 302



Bond lengths



Bond angles



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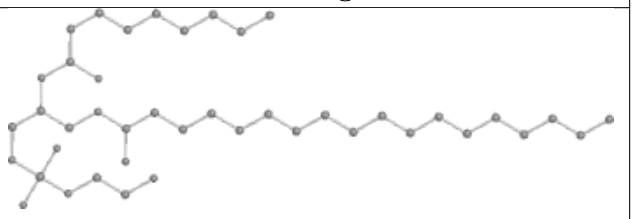
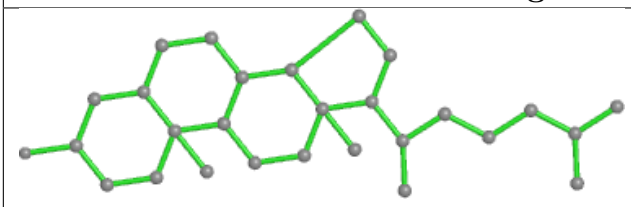
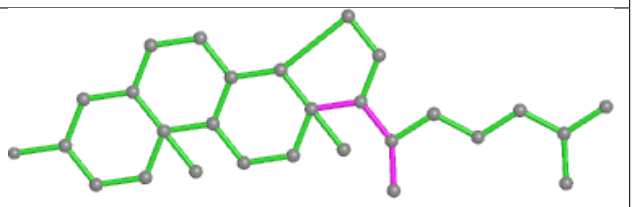


Rings

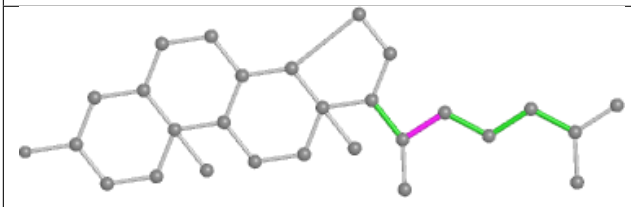
Ligand CLR b 304



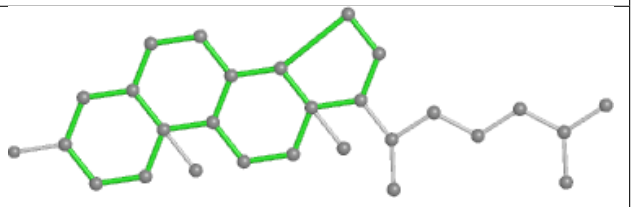
Bond lengths



Bond angles

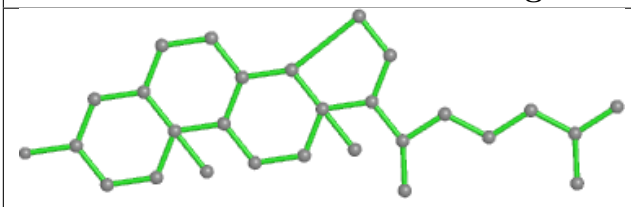


Torsions

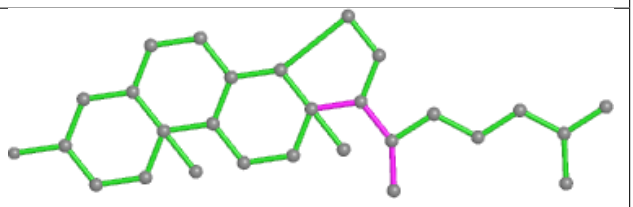


Rings

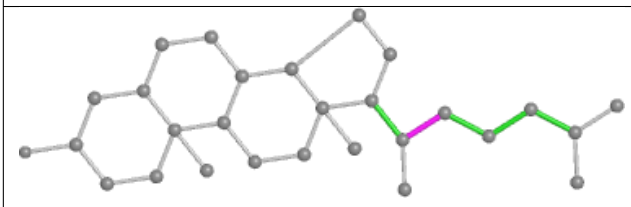
Ligand CLR P 301



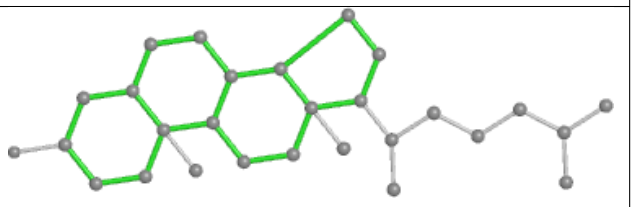
Bond lengths



Bond angles

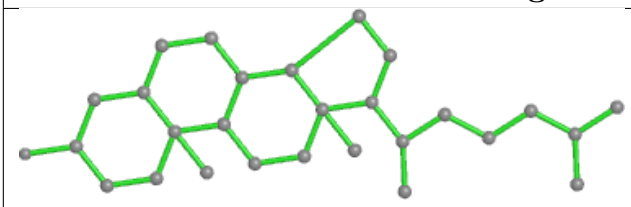


Torsions

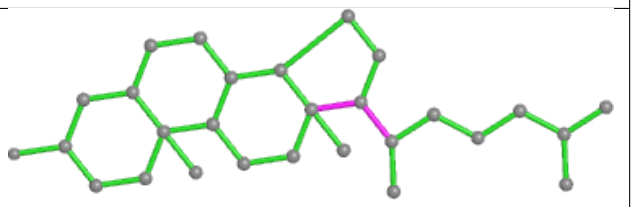


Rings

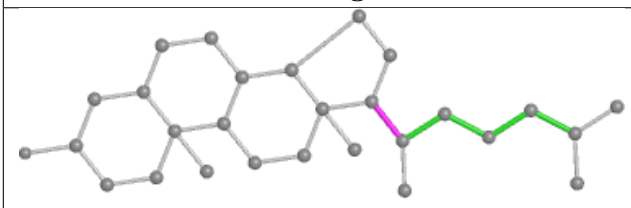
Ligand CLR J 302



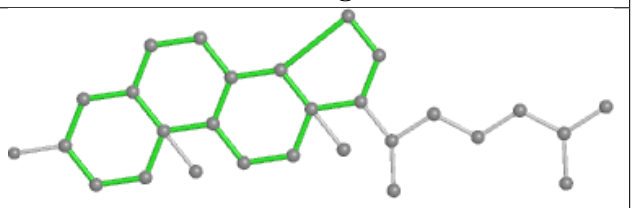
Bond lengths



Bond angles

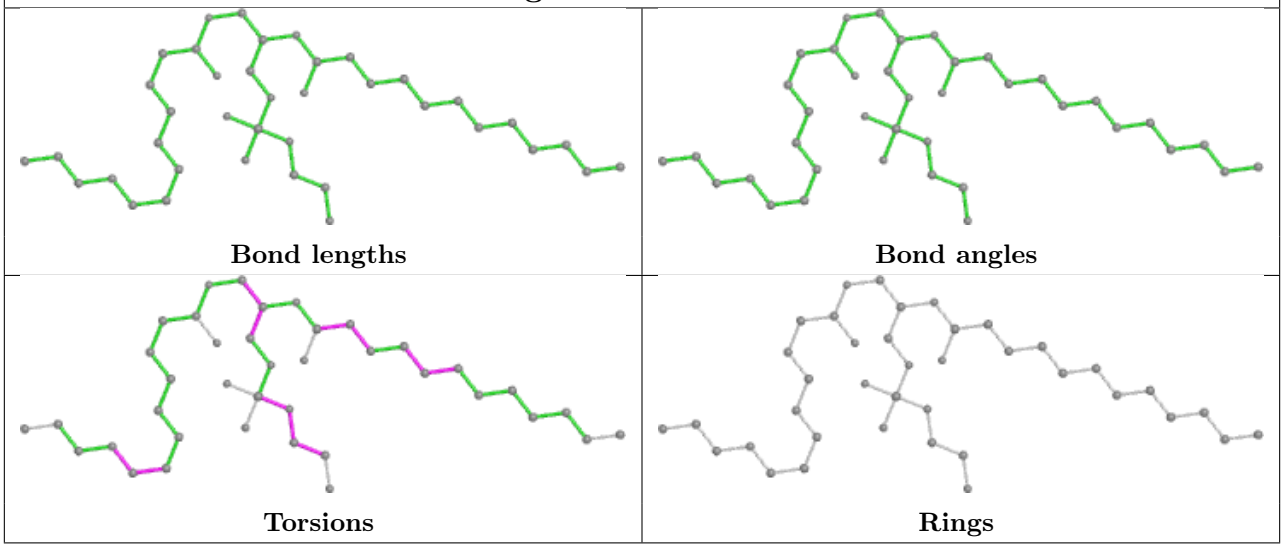


Torsions

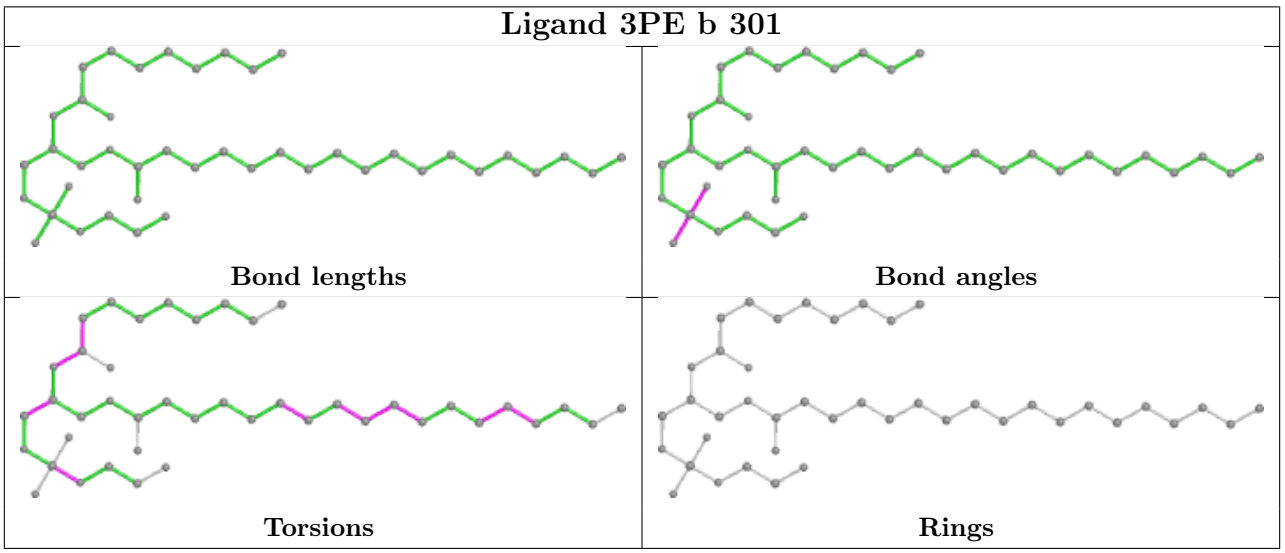


Rings

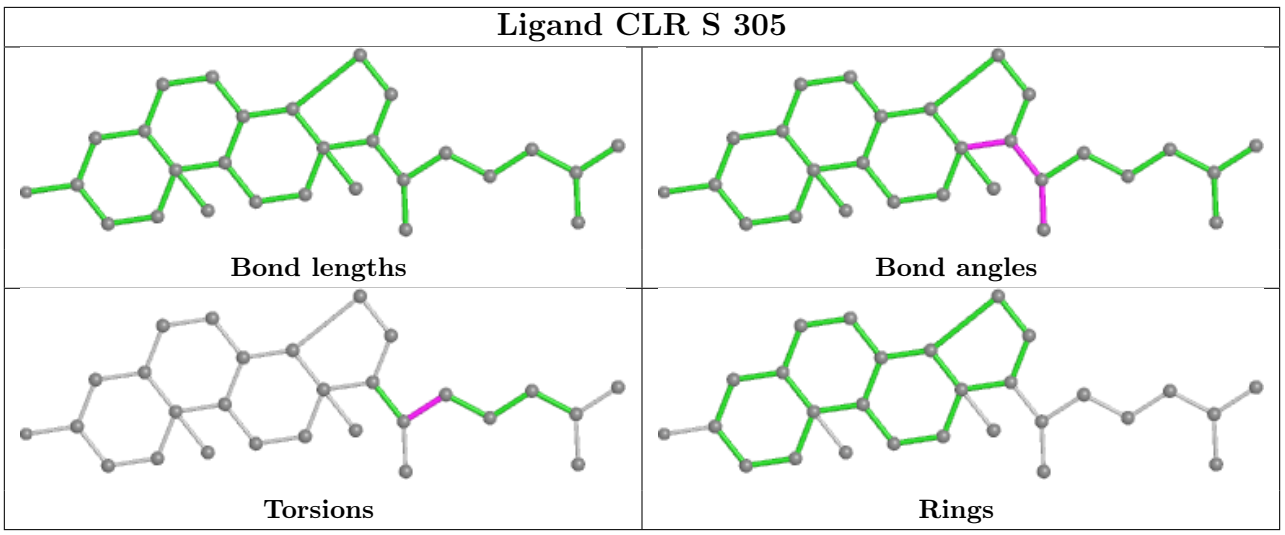
Ligand PTY P 302



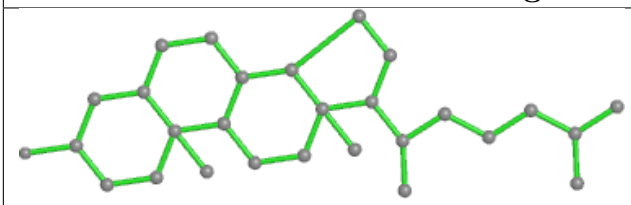
Ligand 3PE b 301



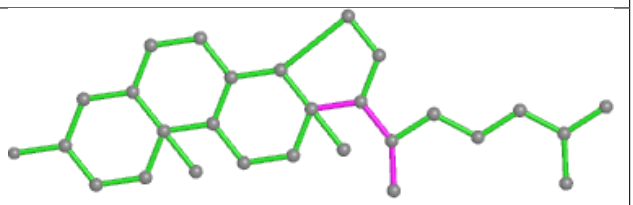
Ligand CLR S 305



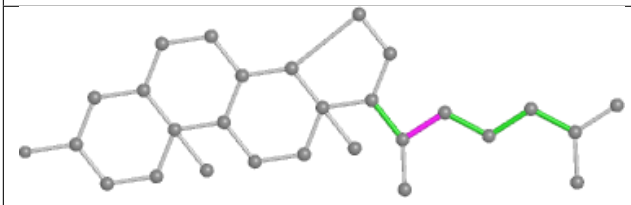
Ligand CLR V 303



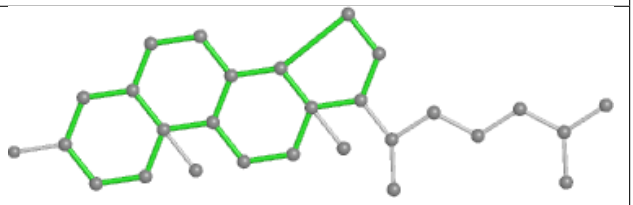
Bond lengths



Bond angles

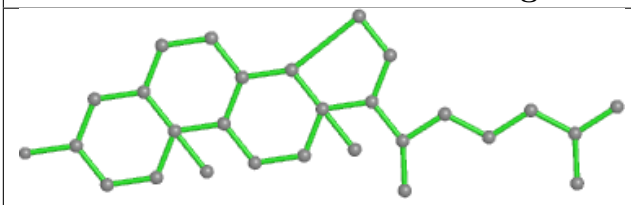


Torsions

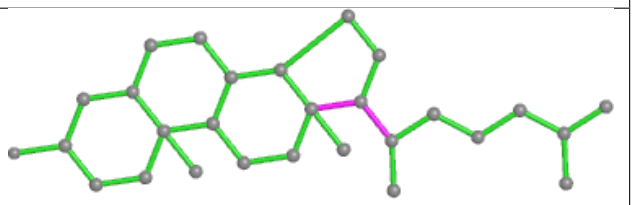


Rings

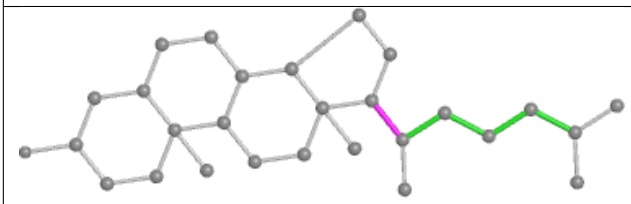
Ligand CLR M 303



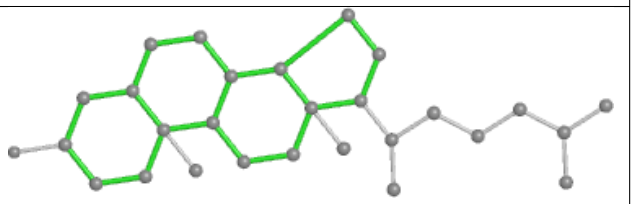
Bond lengths



Bond angles

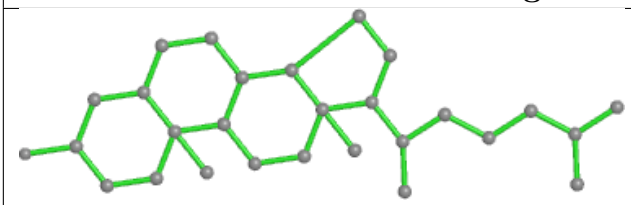


Torsions

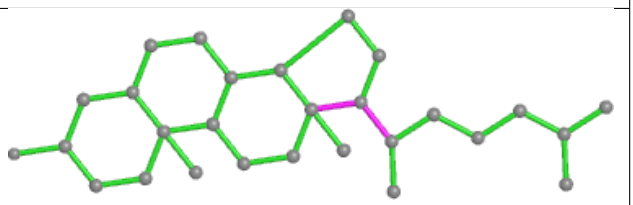


Rings

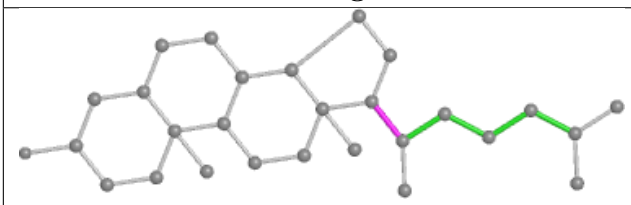
Ligand CLR G 302



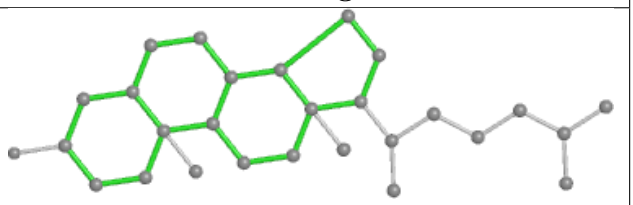
Bond lengths



Bond angles

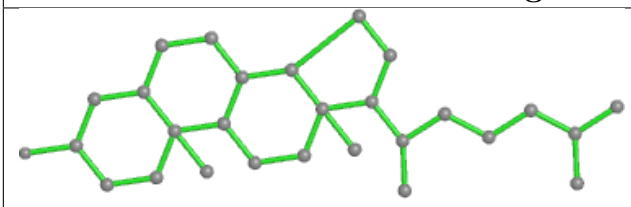


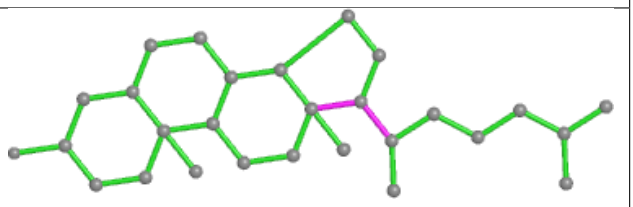
Torsions

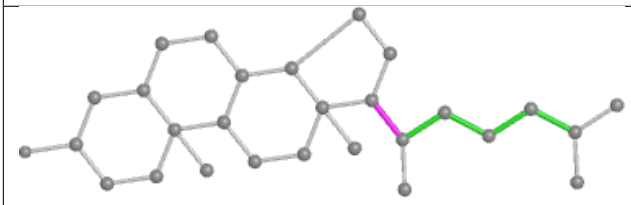


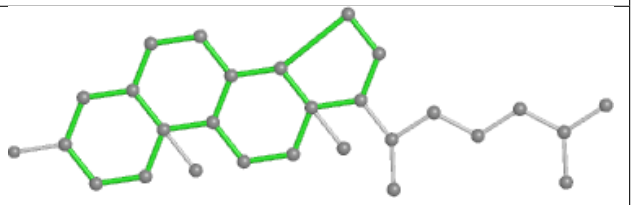
Rings

Ligand CLR P 304

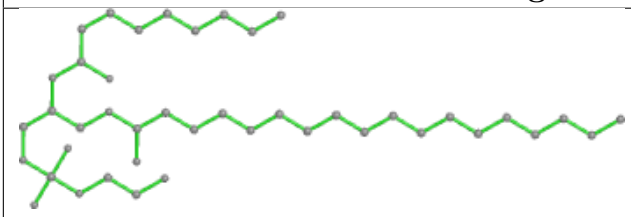

Bond lengths


Bond angles


Torsions


Rings

Ligand 3PE V 301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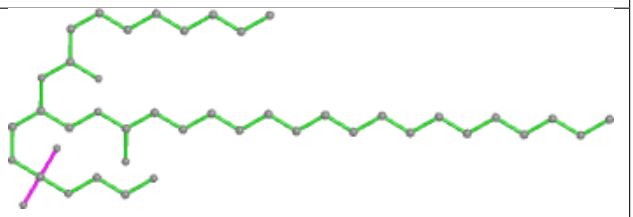
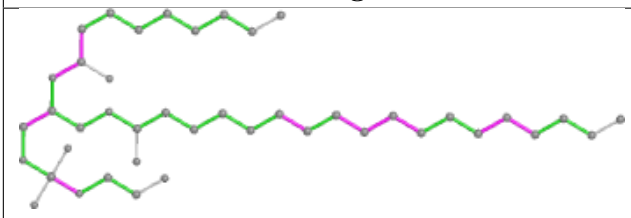
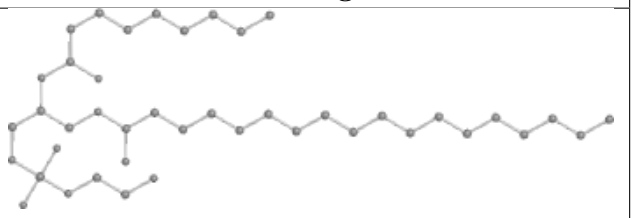
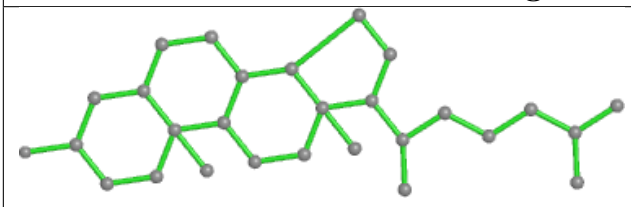

Bond angles


Torsions


Rings

Ligand CLR B 302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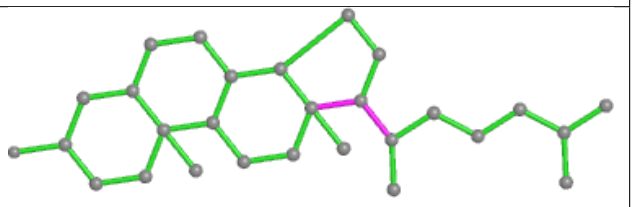
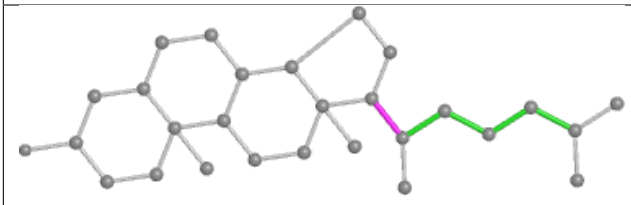
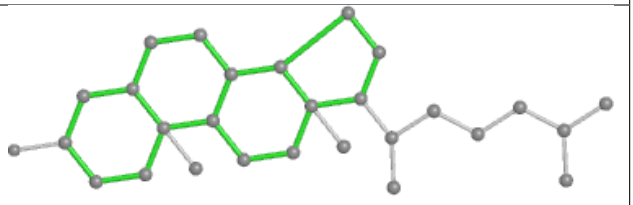
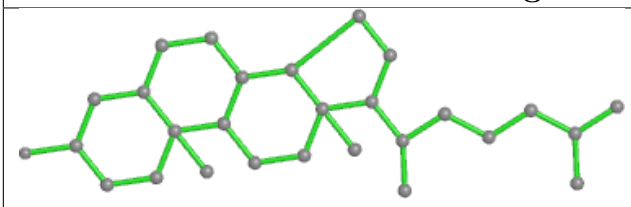

Bond angles


Torsions


Rings

Ligand CLR A 301



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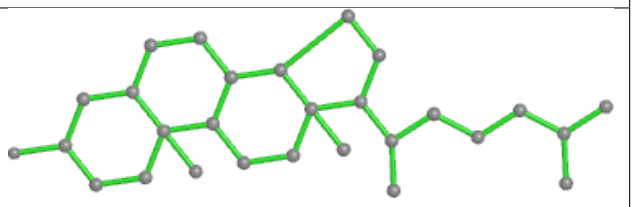
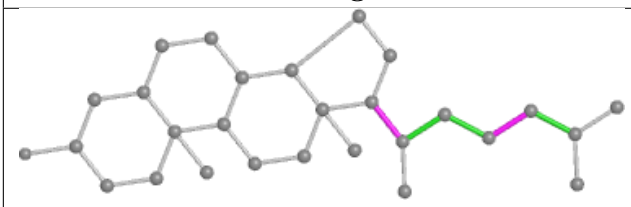
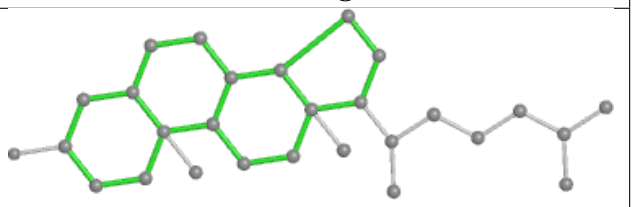


Bond angles

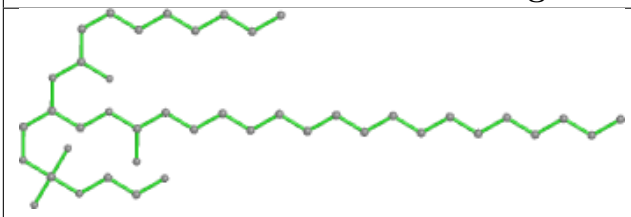


Torsions



Rings

Ligand 3PE A 304



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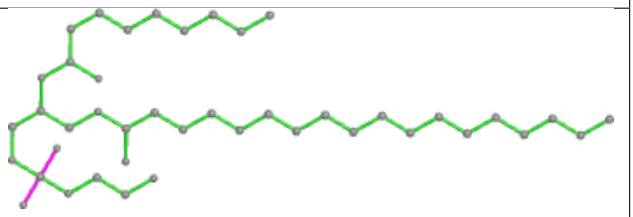
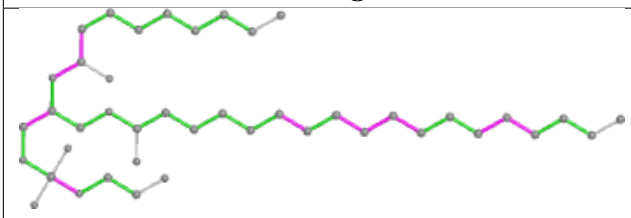
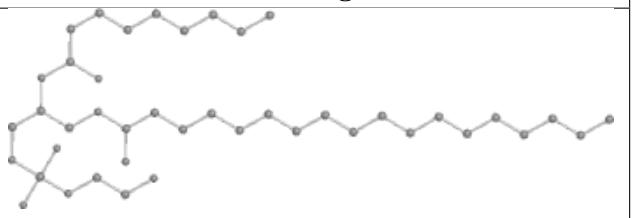


Bond angles

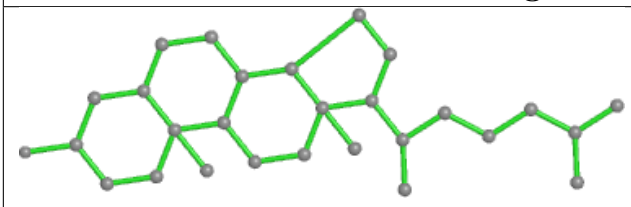


Torsions



Rings

Ligand CLR A 302



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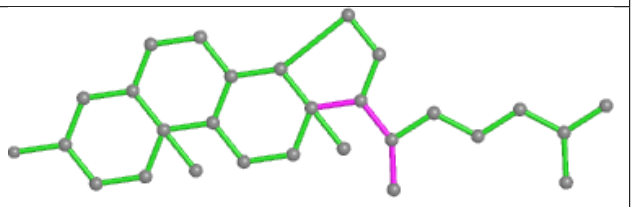

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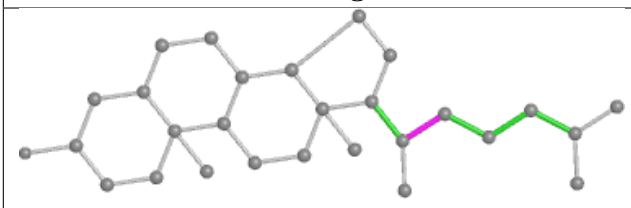
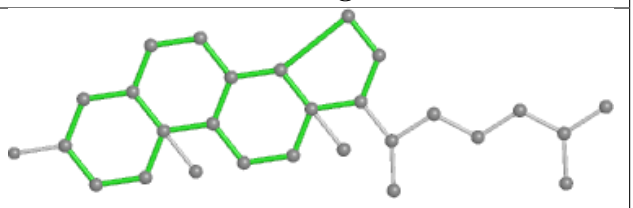
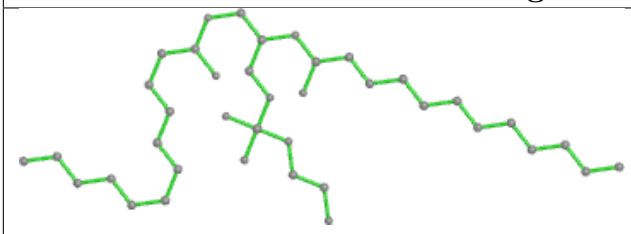


Torsions

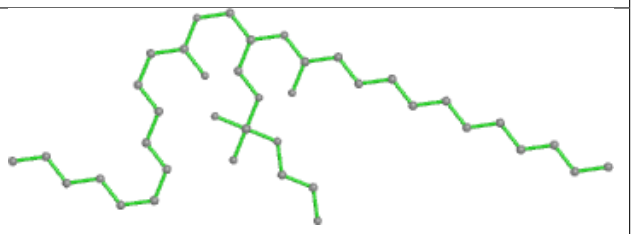


Rings

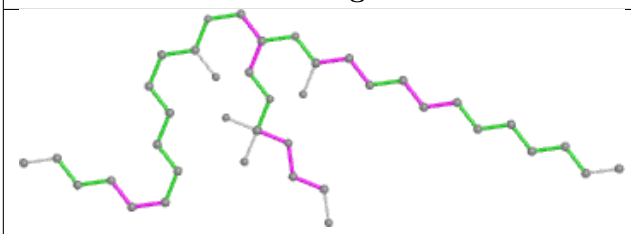
Ligand PTY J 304



Bond lengths



Bond angles



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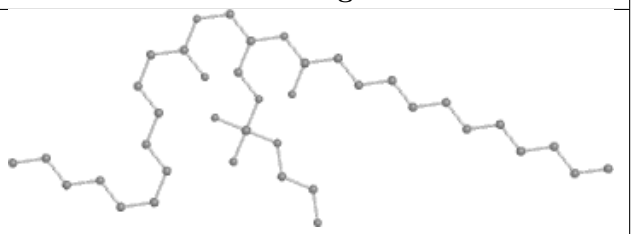
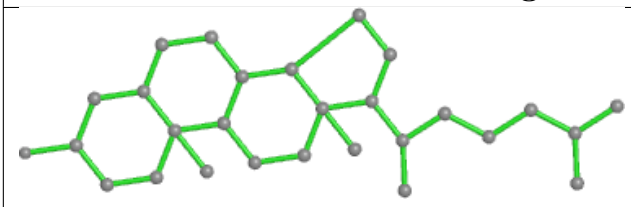
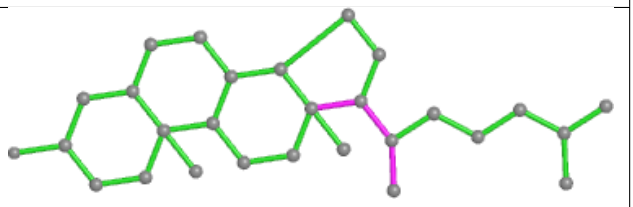


Rings

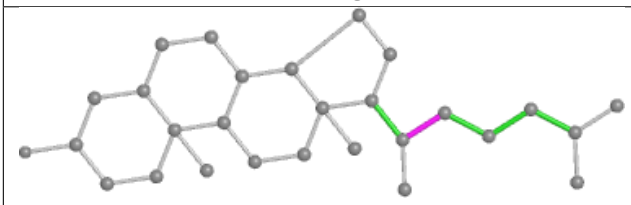
Ligand CLR M 305



Bond lengths



Bond angles



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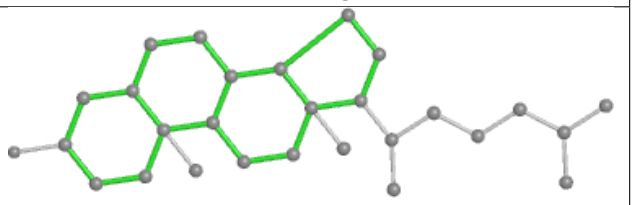
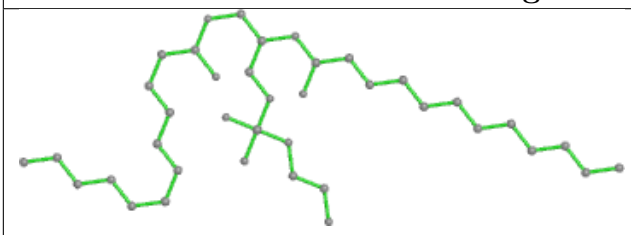


Rings

Ligand PTY V 304



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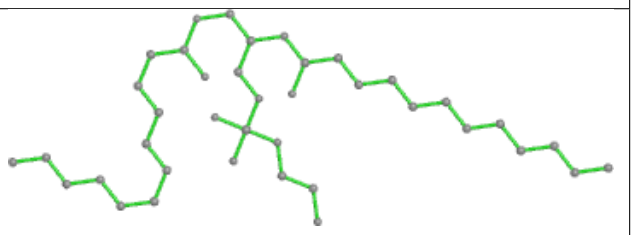
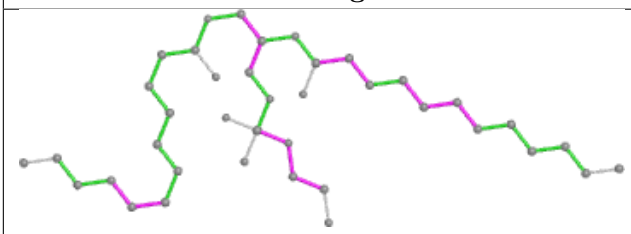


Bond angles



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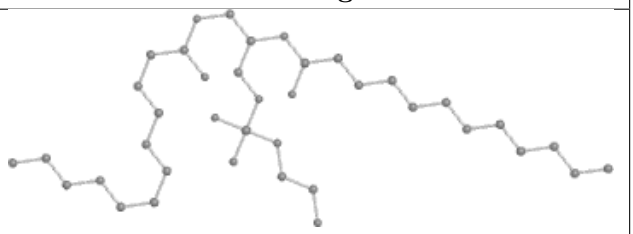
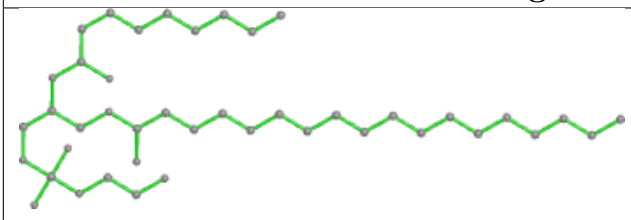
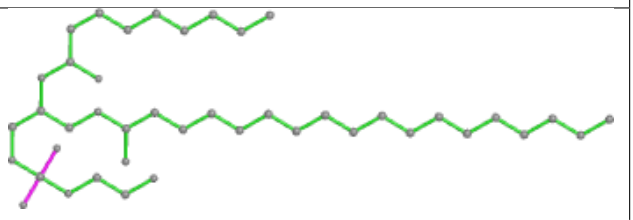


Rings

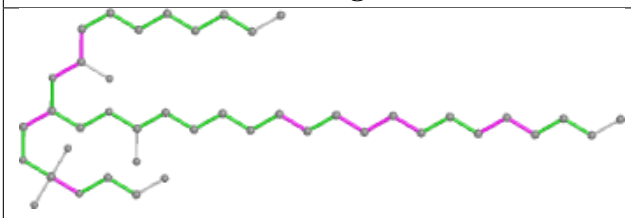
Ligand 3PE B 301



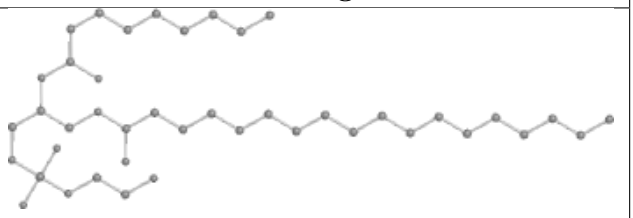
Bond lengths



Bond angles

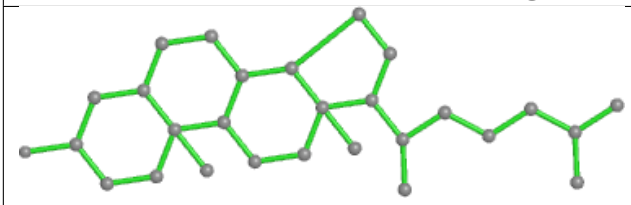


Torsions

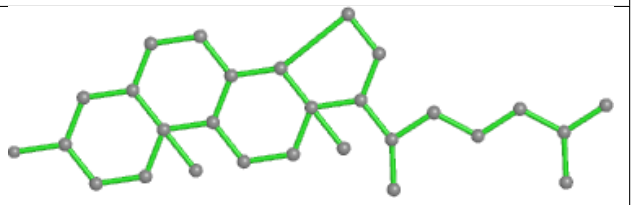


Rings

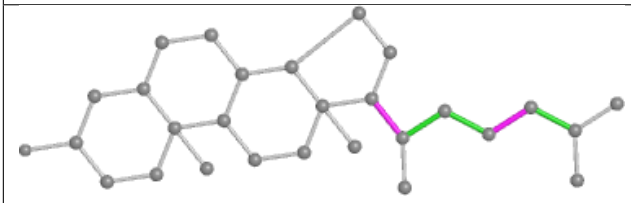
Ligand CLR G 303



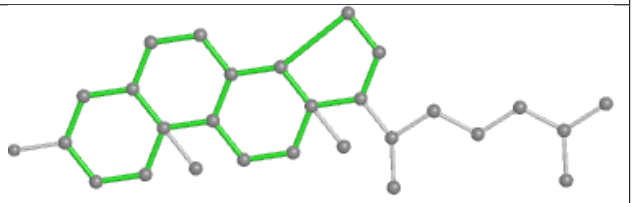
Bond lengths



Bond angles

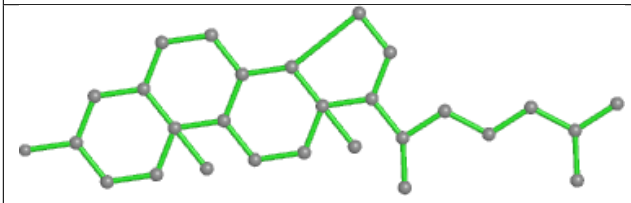


Torsions

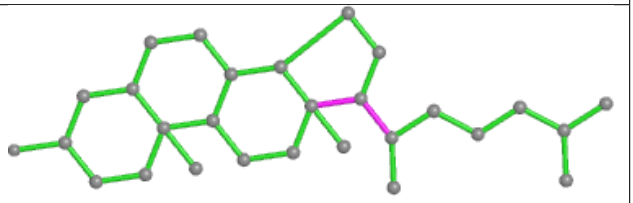


Rings

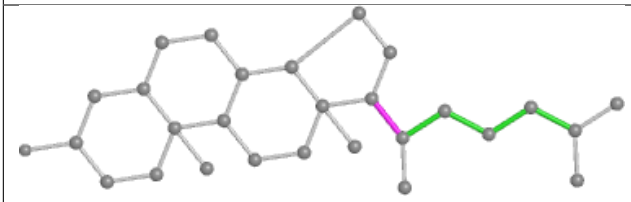
Ligand CLR b 302



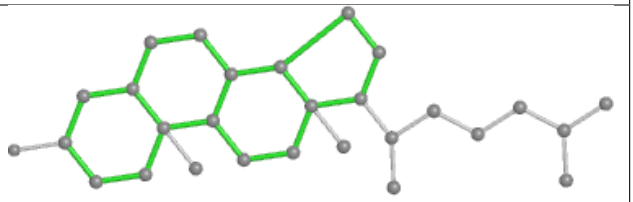
Bond lengths



Bond angles

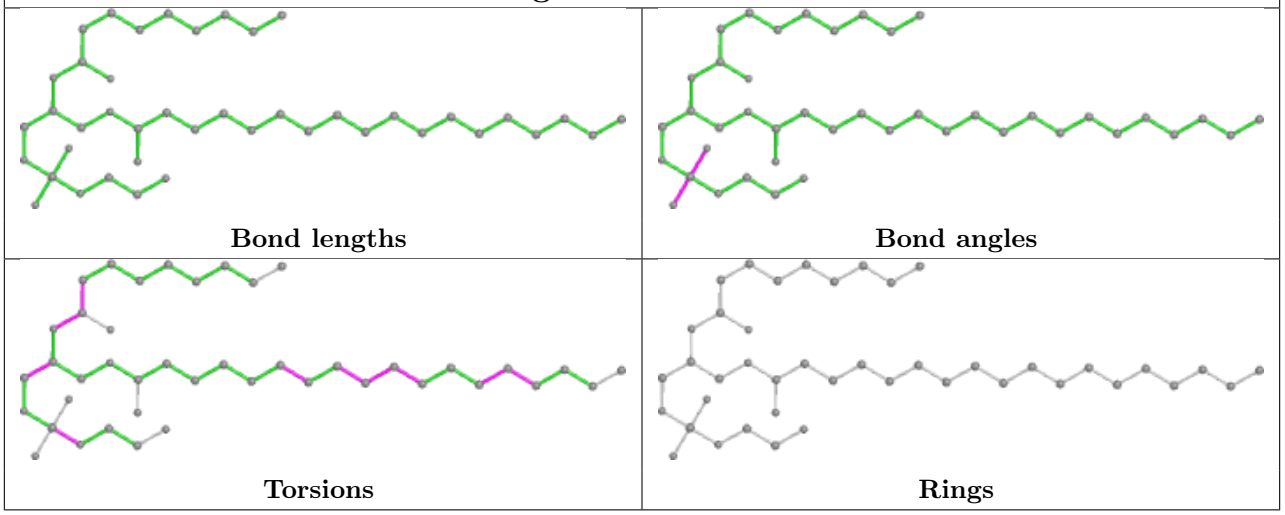


Torsions

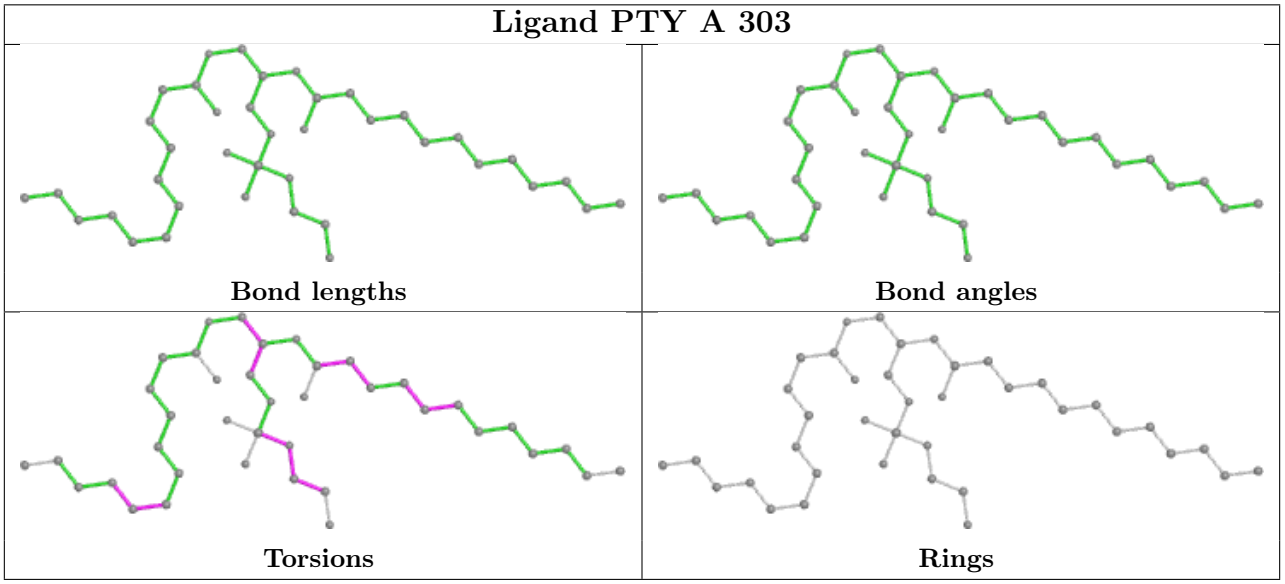


Rings

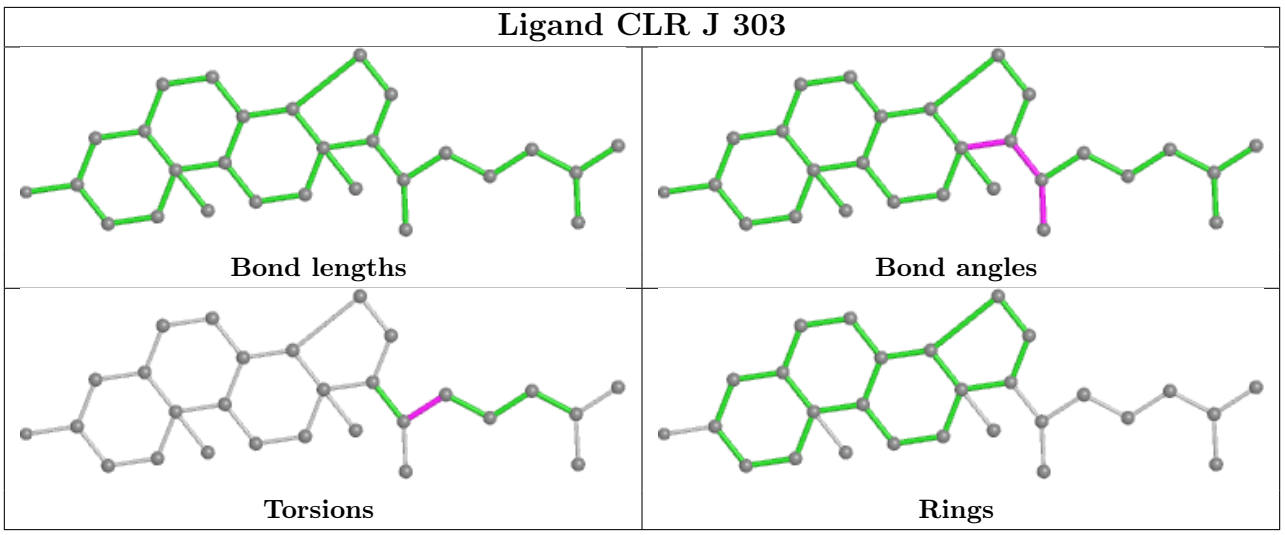
Ligand 3PE S 302



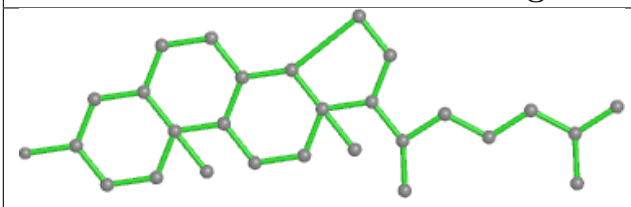
Ligand PTY A 303



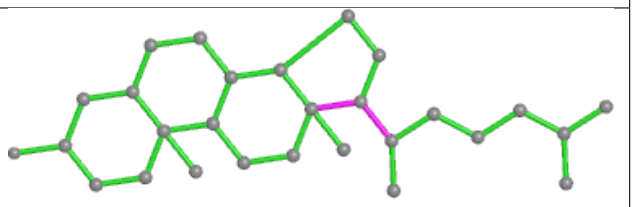
Ligand CLR J 303



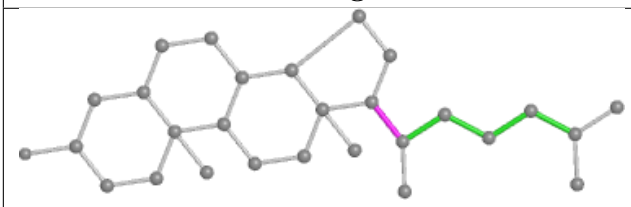
Ligand CLR S 303



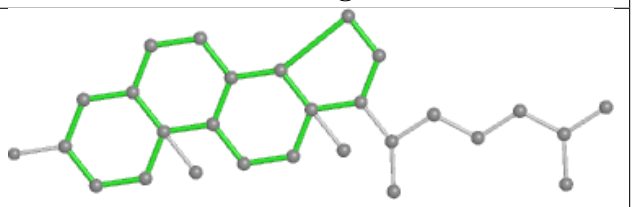
Bond lengths



Bond angles

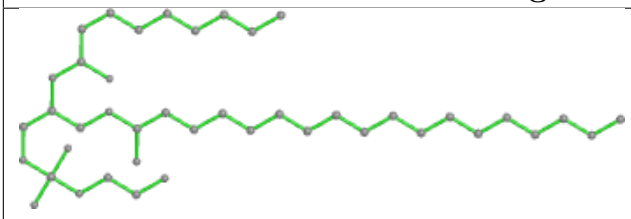


Torsions

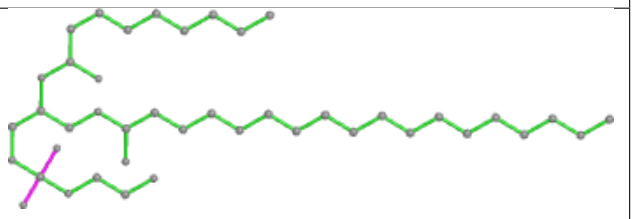


Rings

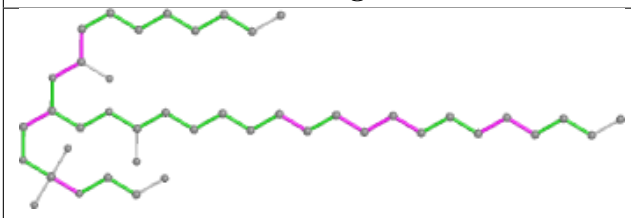
Ligand 3PE P 303



Bond lengths



Bond angles



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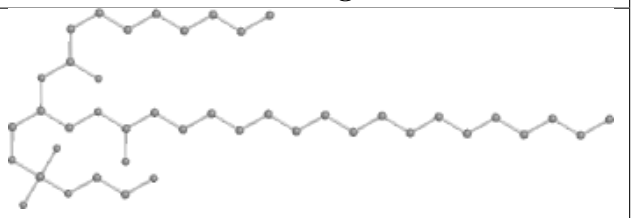
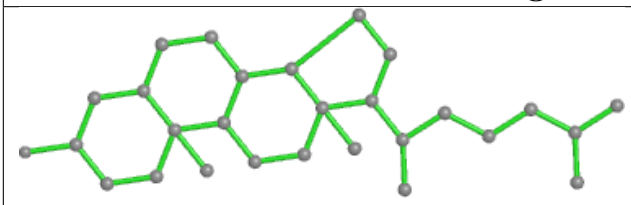
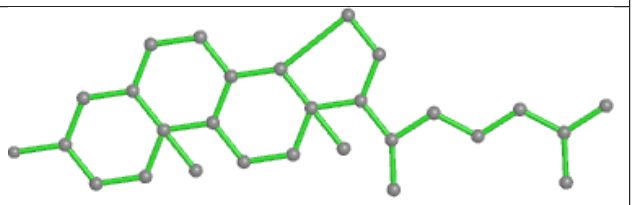


Rings

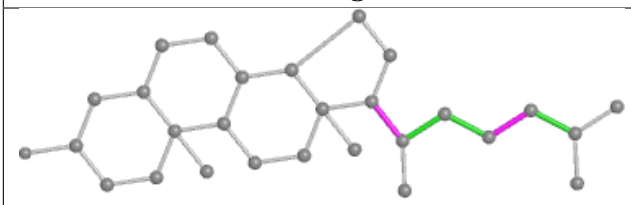
Ligand CLR S 304



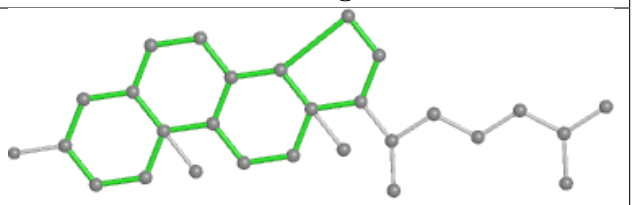
Bond lengths



Bond angles

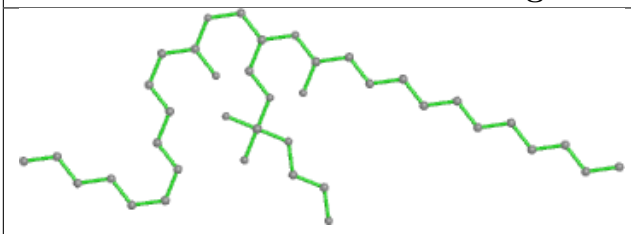


Torsions

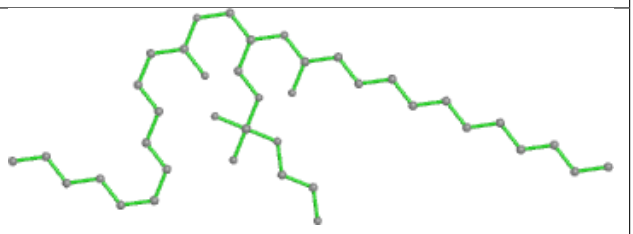


Rings

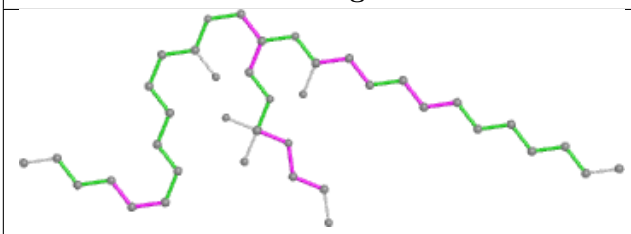
Ligand PTY S 306



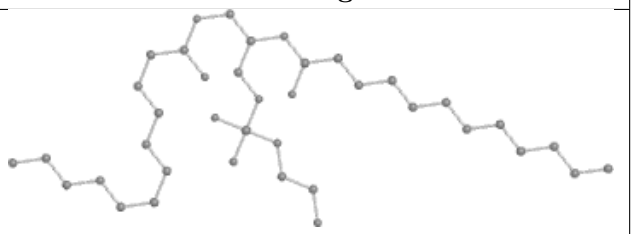
Bond lengths



Bond angles

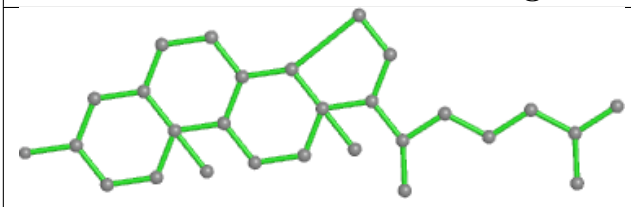


Torsions

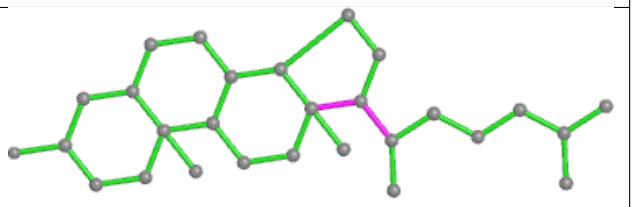


Rings

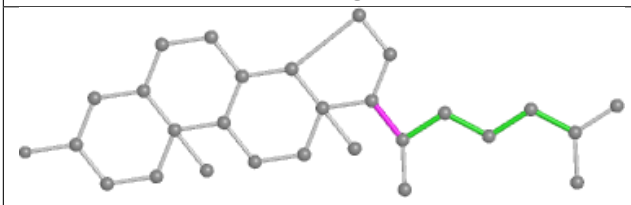
Ligand CLR V 302



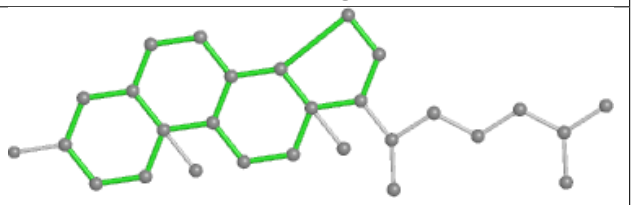
Bond lengths



Bond angles

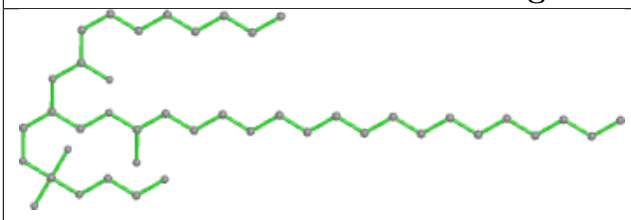


Torsions

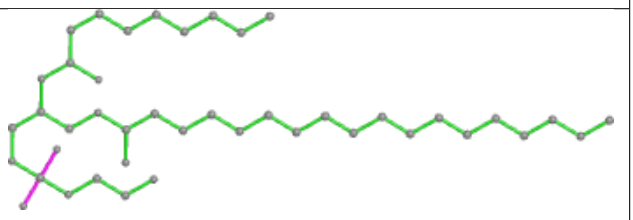


Rings

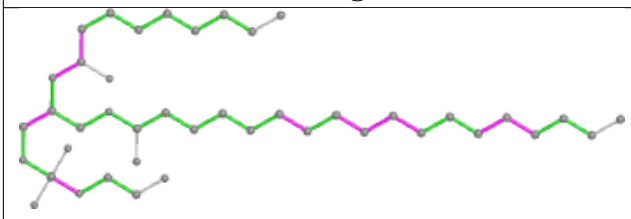
Ligand 3PE Y 302



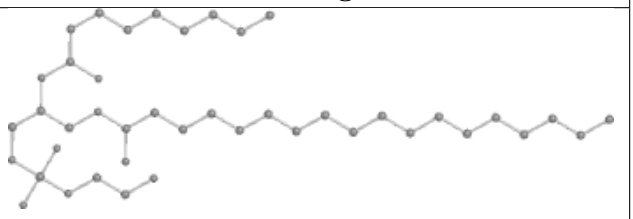
Bond lengths



Bond angles

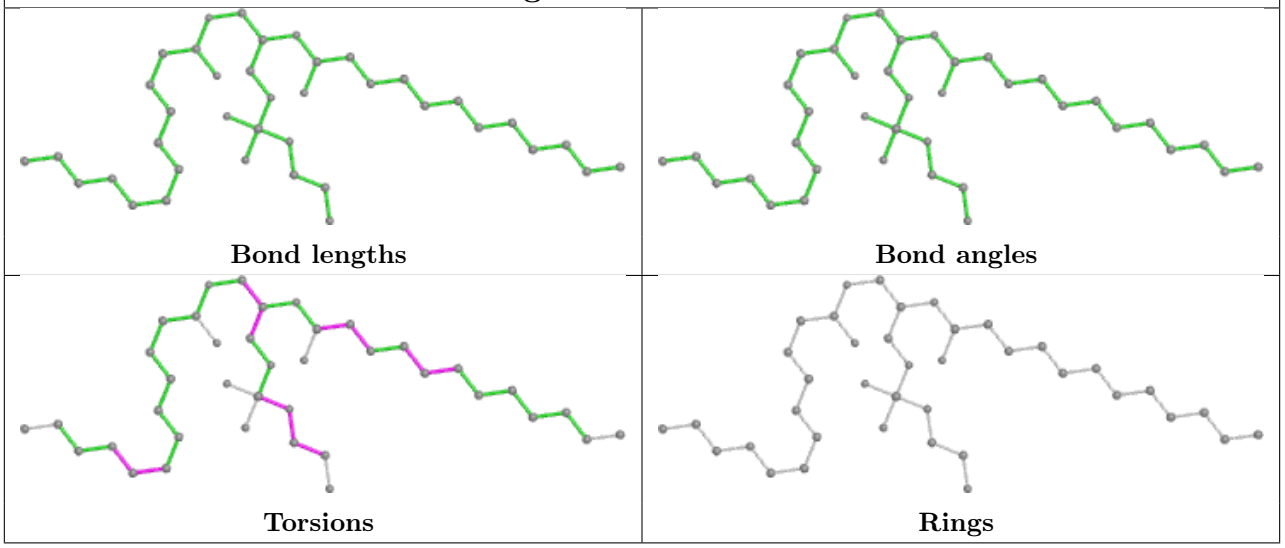


Torsions

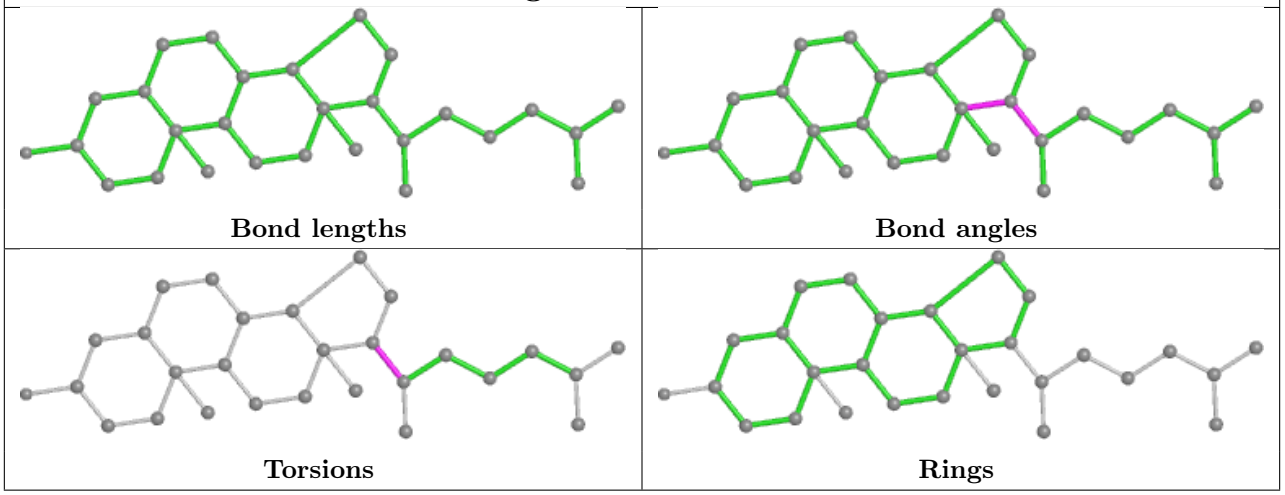


Rings

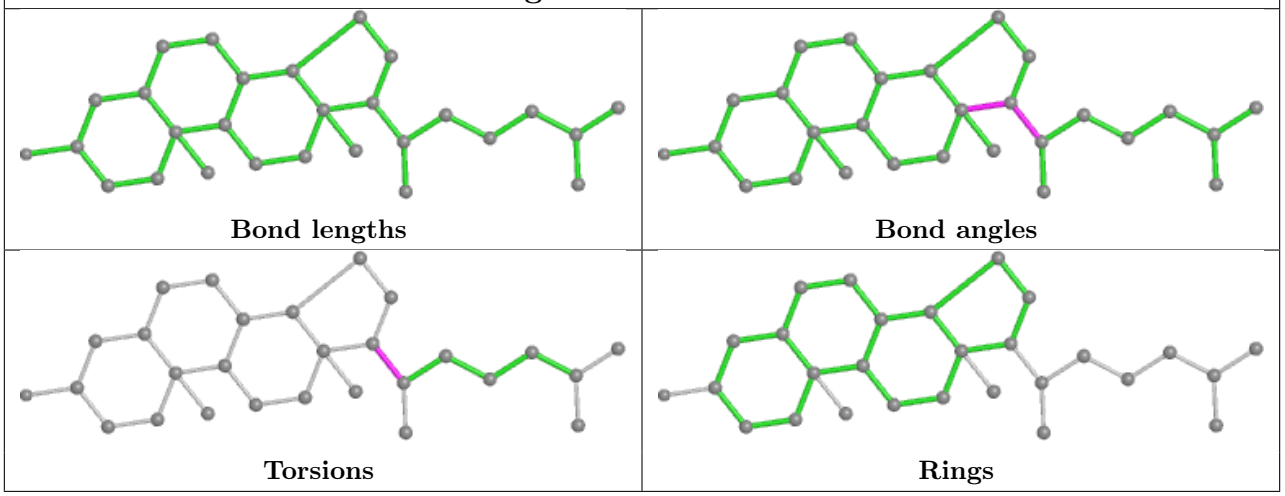
Ligand PTY Y 306



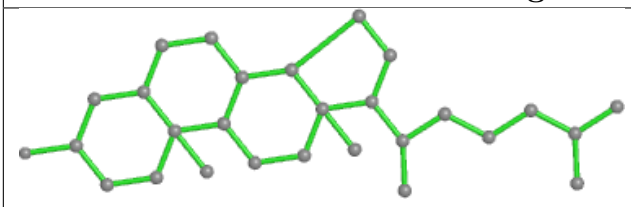
Ligand CLR Y 303

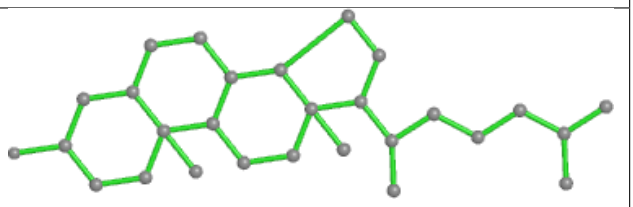


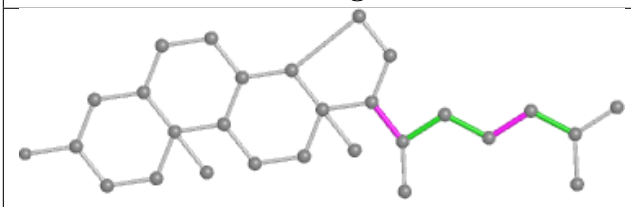
Ligand CLR A 305

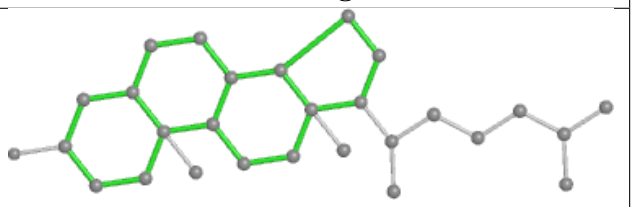


Ligand CLR b 303

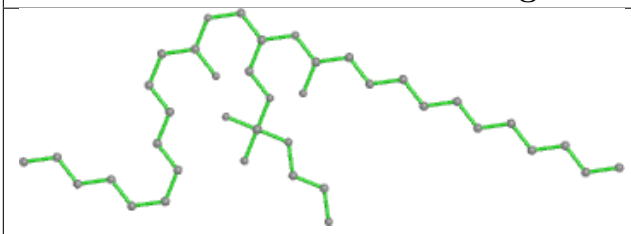

Bond lengths

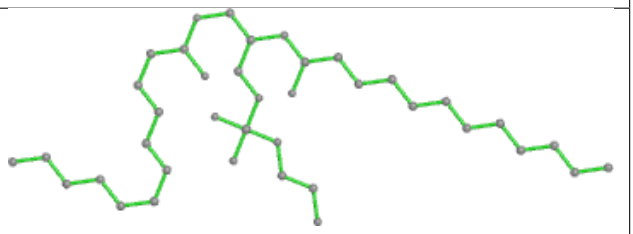

Bond angles

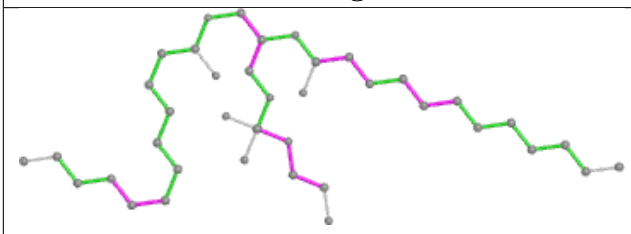

Torsions

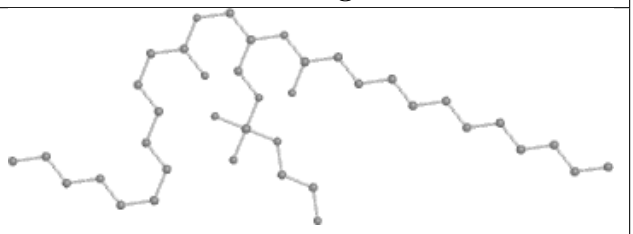

Rings

Ligand PTY M 306

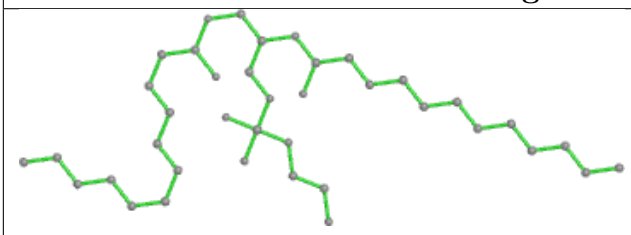

Bond lengths

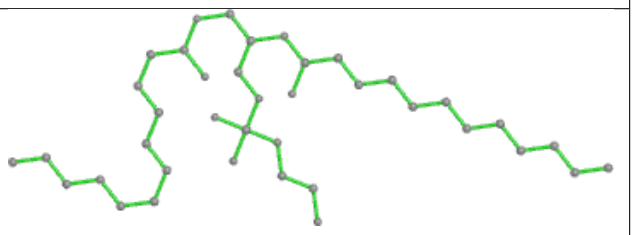

Bond angles

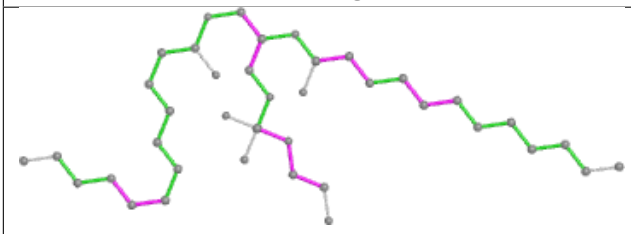

Torsions

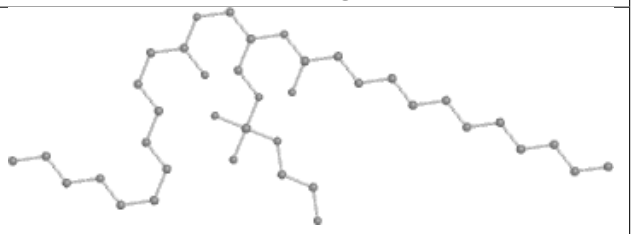

Rings

Ligand PTY G 305

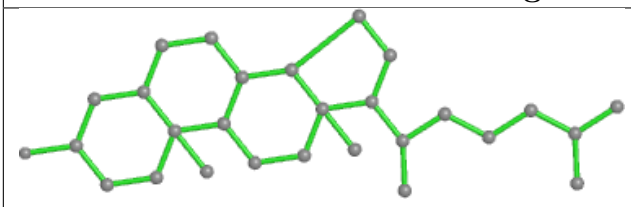

Bond lengths

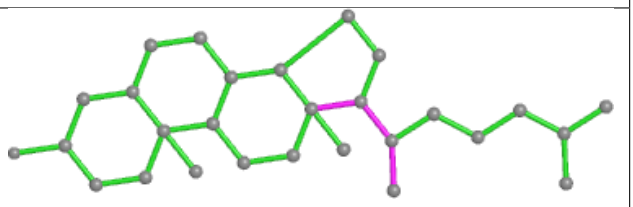

Bond angles

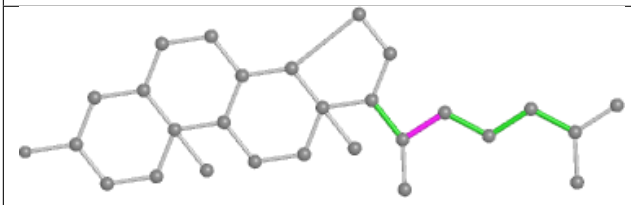

Torsions

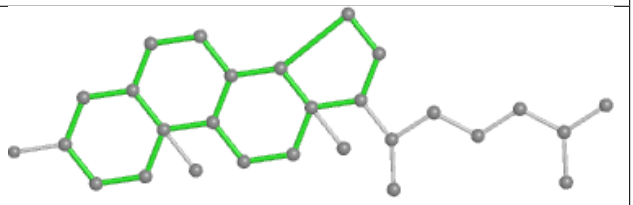

Rings

Ligand CLR Y 305

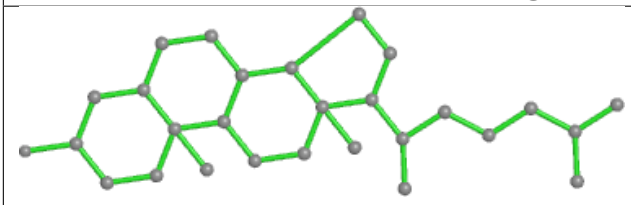

Bond lengths

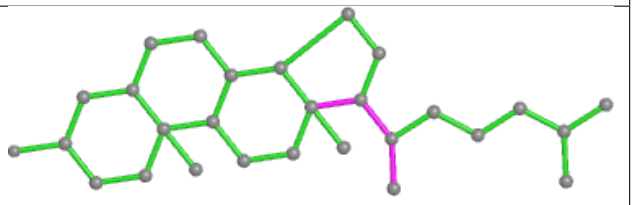

Bond angles

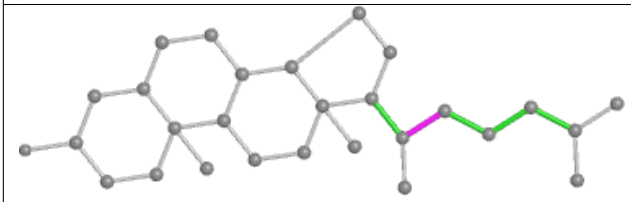

Torsions

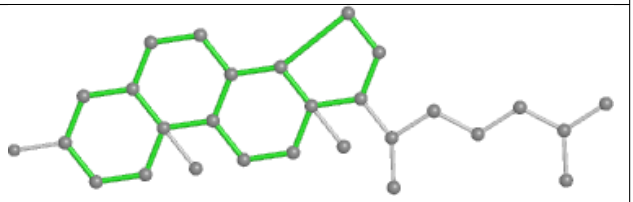

Rings

Ligand CLR B 304

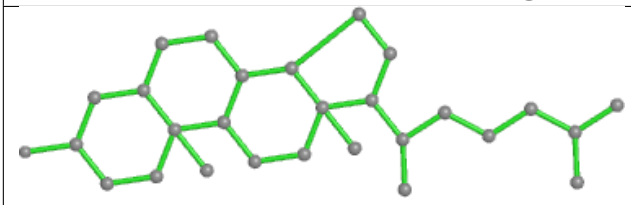

Bond lengths

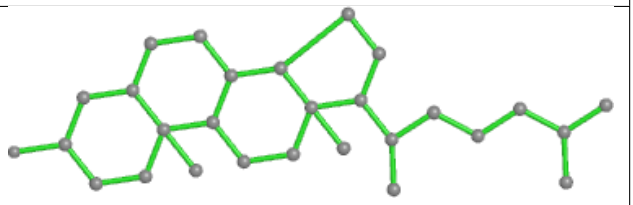

Bond angles

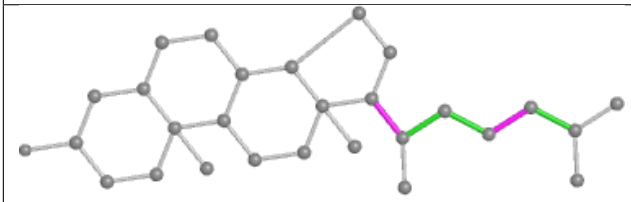

Torsions

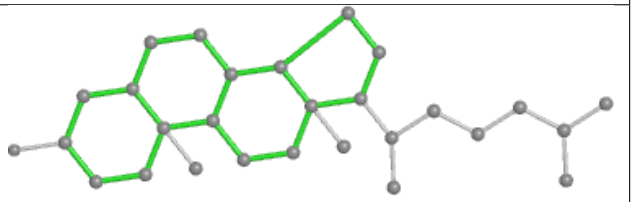

Rings

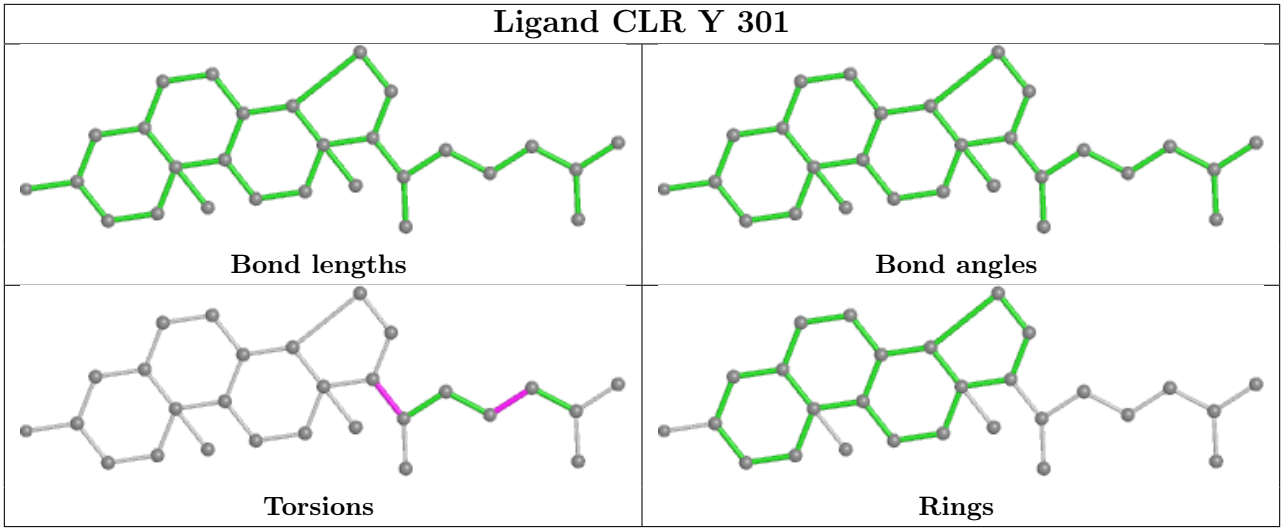
Ligand CLR M 301


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.

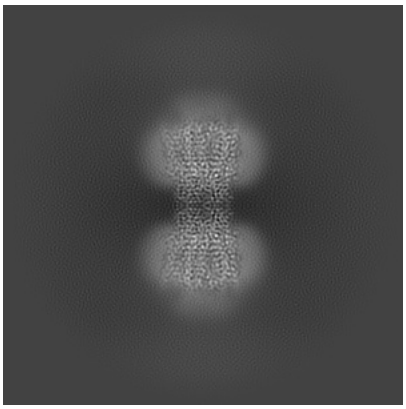
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-34156. These allow visual inspection of the internal detail of the map and identification of artifacts.

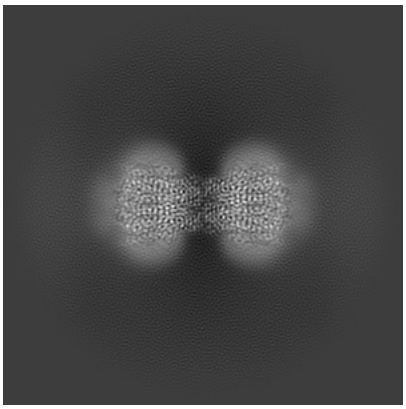
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

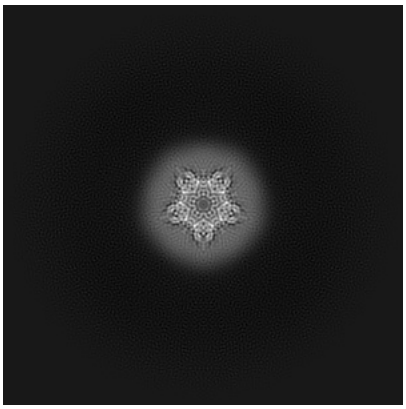
6.1.1 Primary map



X

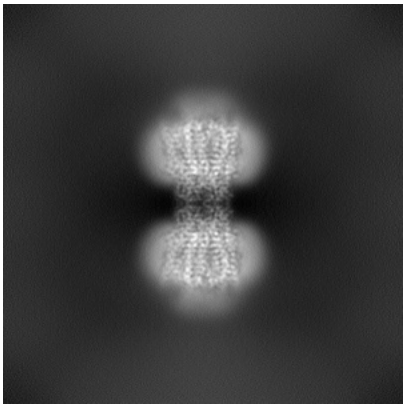


Y

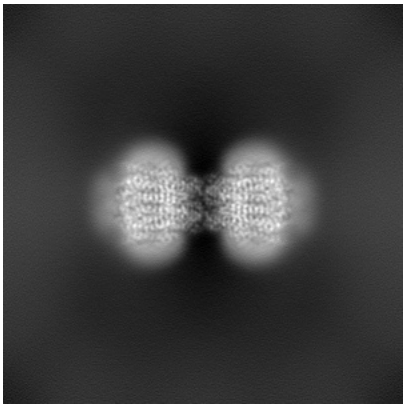


Z

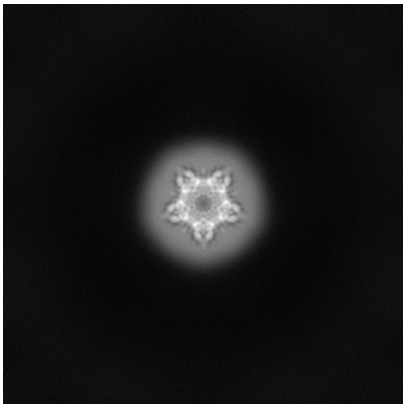
6.1.2 Raw map



X



Y

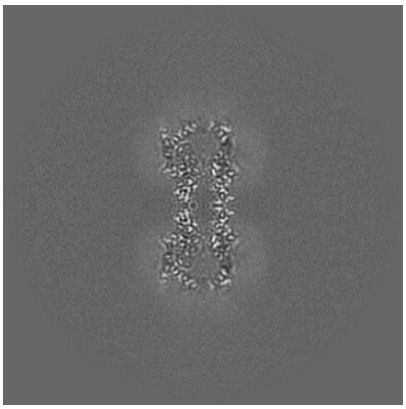


Z

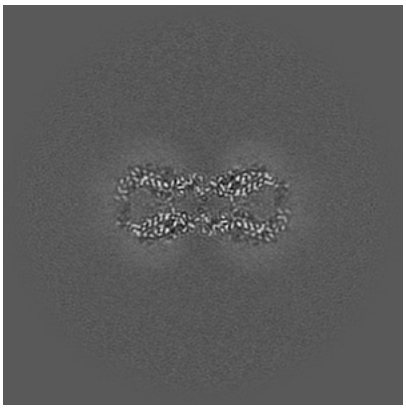
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

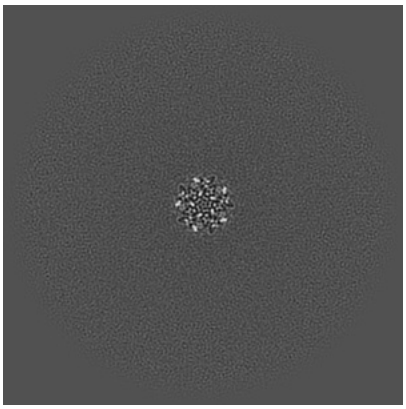
6.2.1 Primary map



X Index: 192

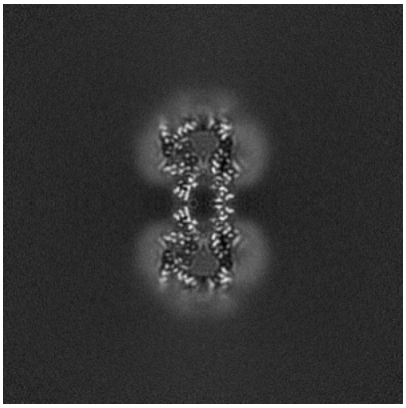


Y Index: 192

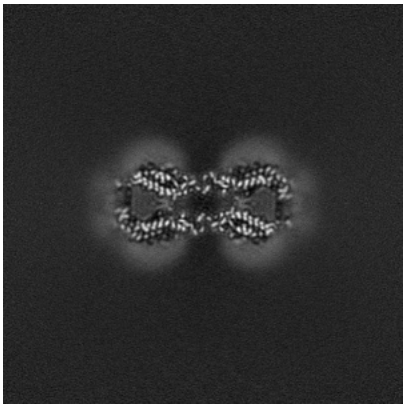


Z Index: 192

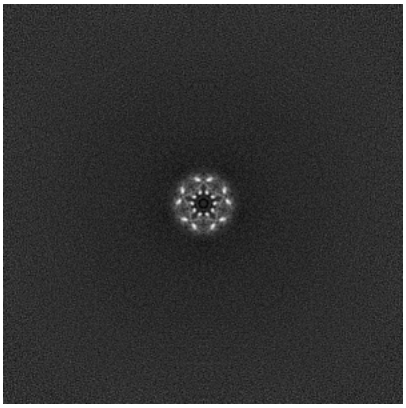
6.2.2 Raw map



X Index: 192



Y Index: 192

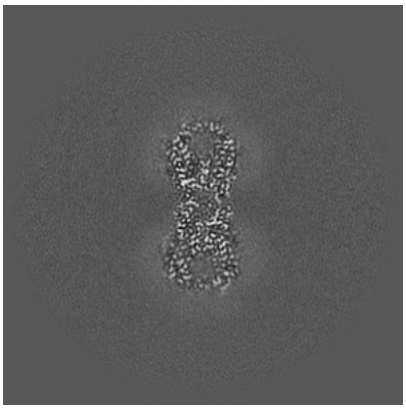


Z Index: 192

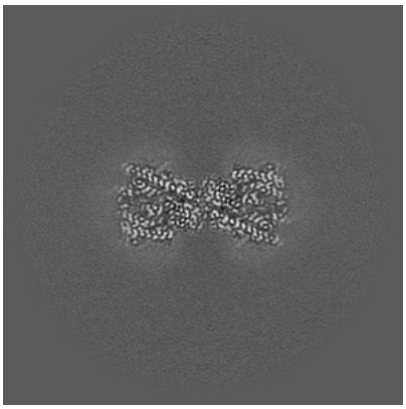
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

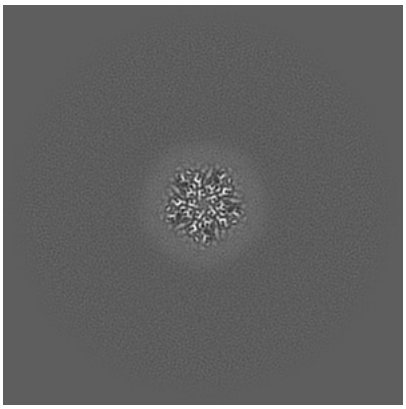
6.3.1 Primary map



X Index: 201

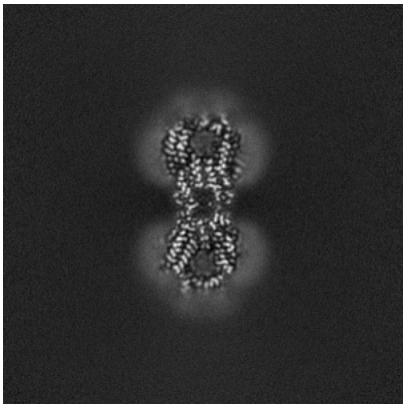


Y Index: 178

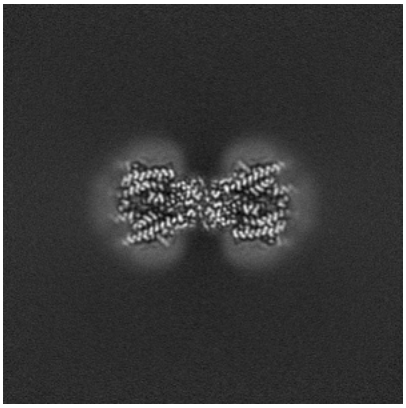


Z Index: 157

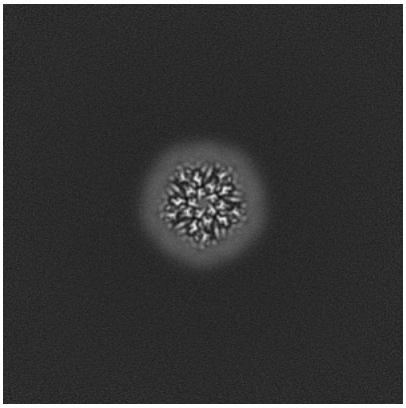
6.3.2 Raw map



X Index: 200



Y Index: 178

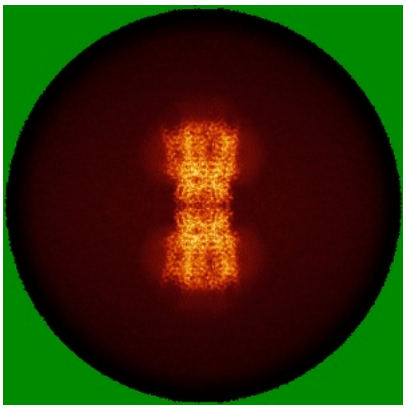


Z Index: 226

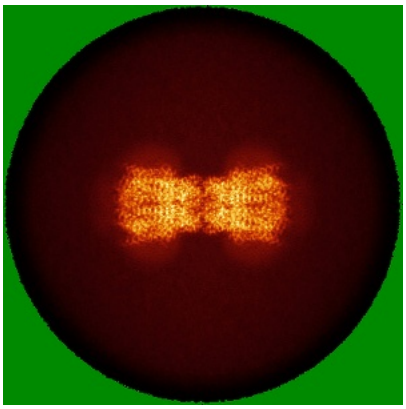
The images above show the largest variance slices of the map in three orthogonal directions.

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

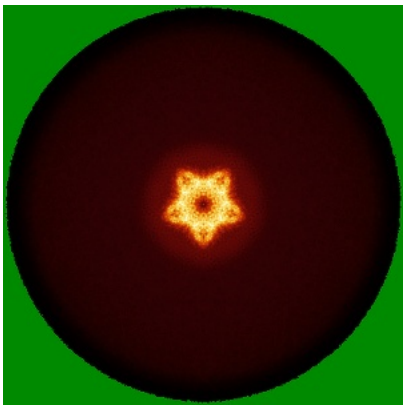
6.4.1 Primary map



X

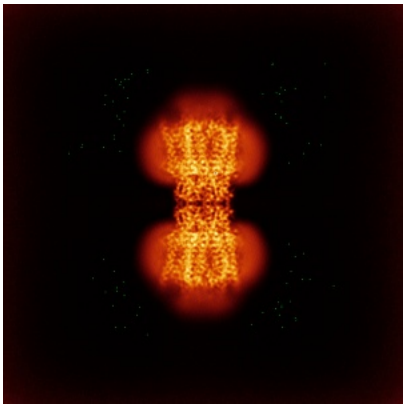


Y

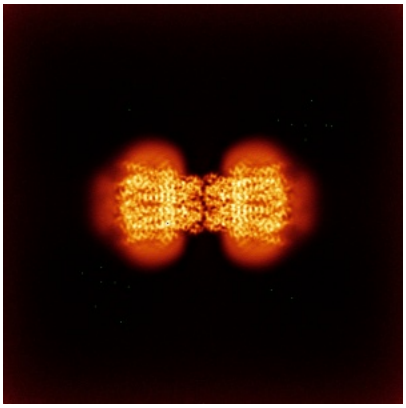


Z

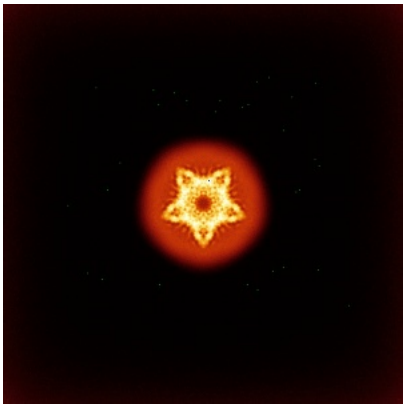
6.4.2 Raw map



X



Y

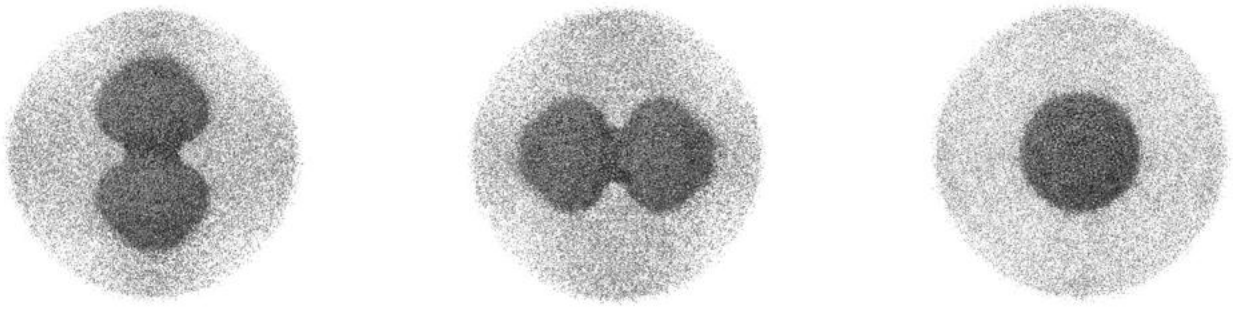


Z

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)

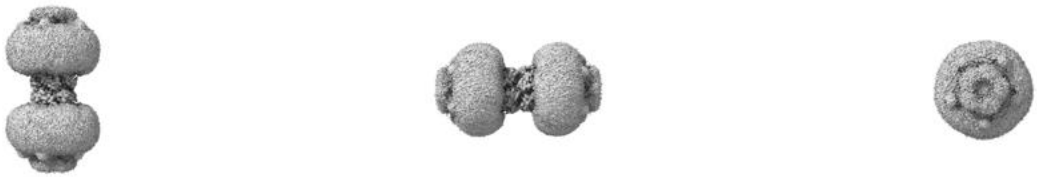
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.21. 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.

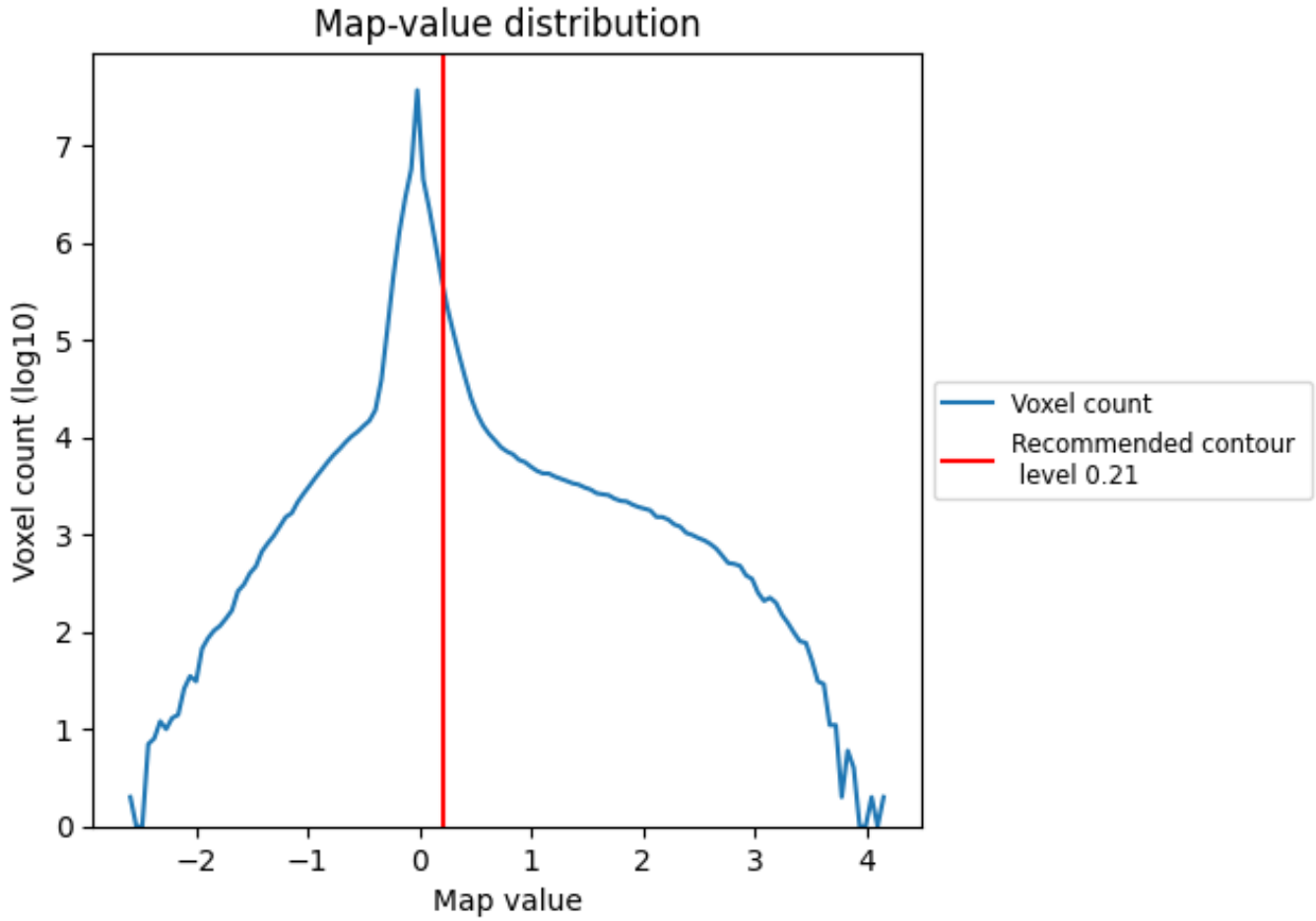
6.6 Mask visualisation (i)

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

7 Map analysis

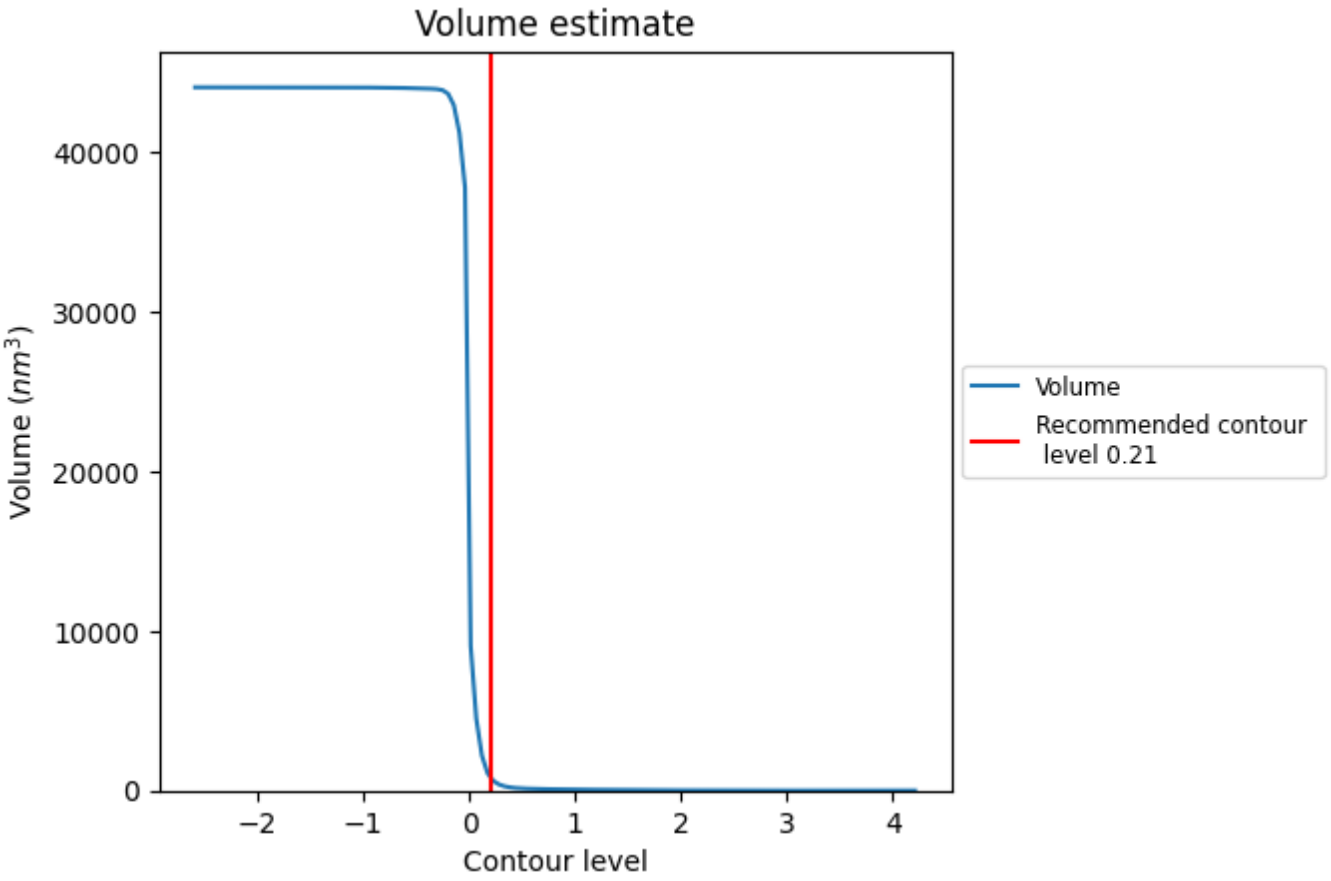
This section contains the results of statistical analysis of the map.

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.

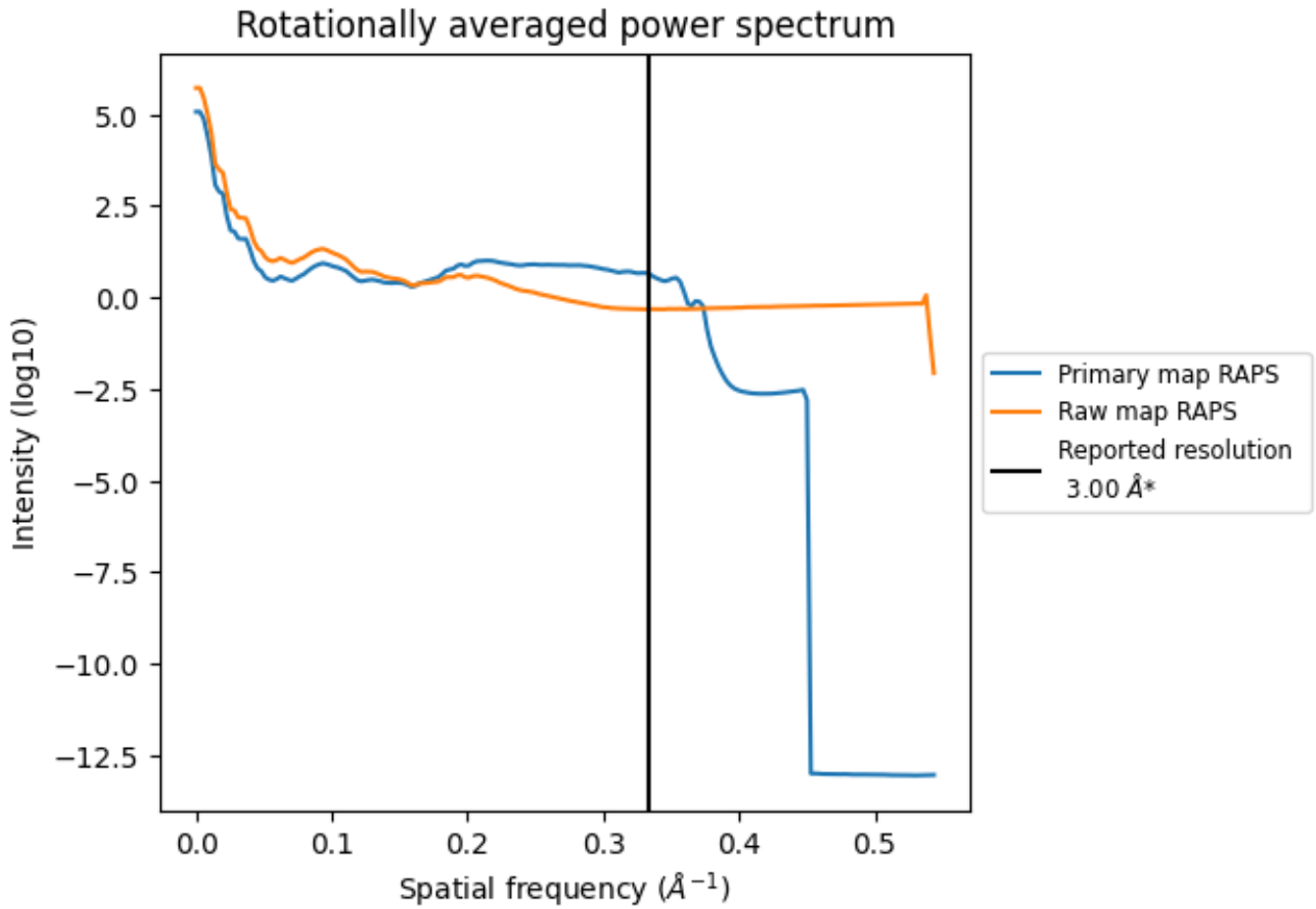
7.2 Volume estimate



The volume at the recommended contour level is 767 nm^3; this corresponds to an approximate mass of 693 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)

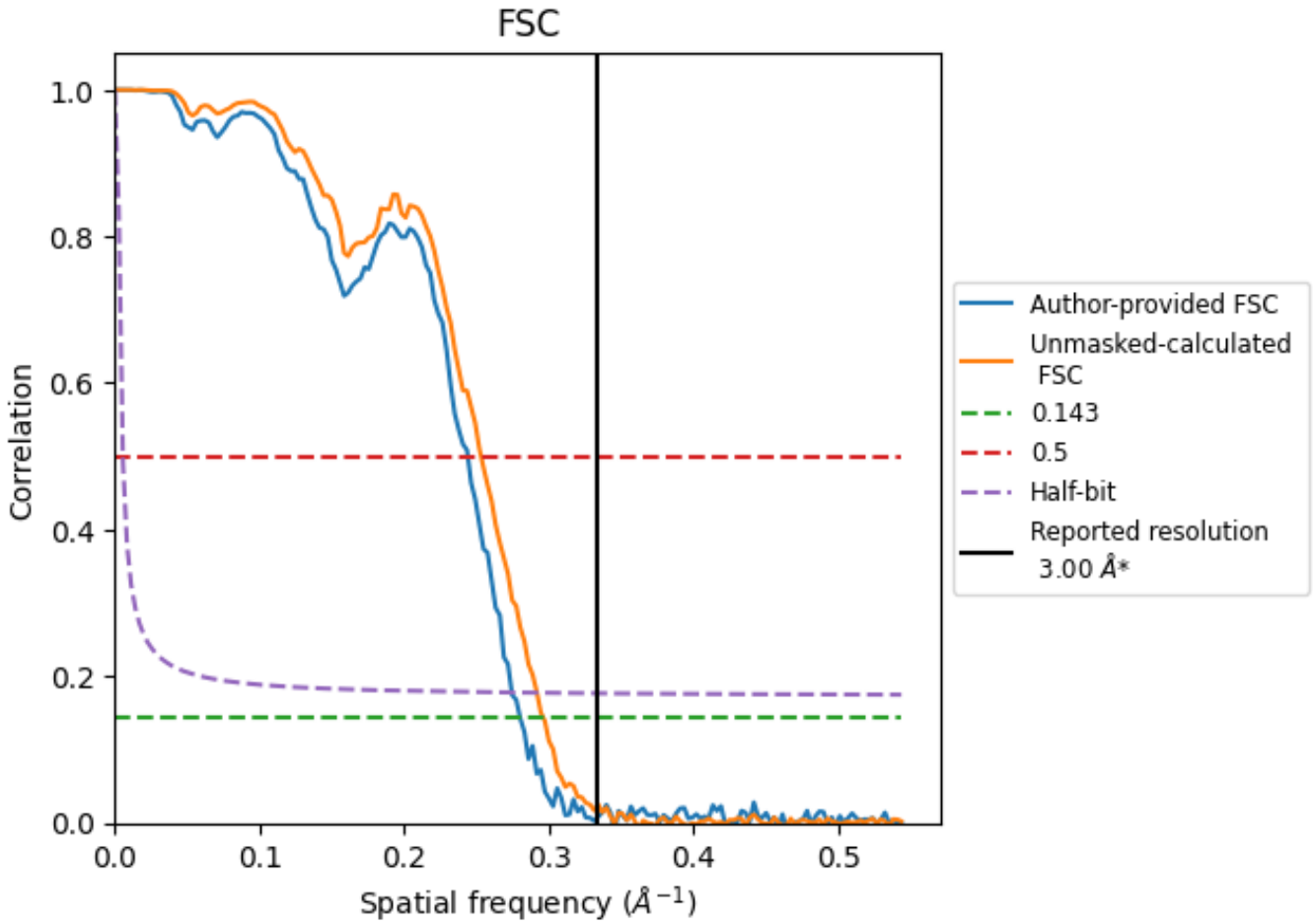


*Reported resolution corresponds to spatial frequency of 0.333 $Å^{-1}$

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 0.333 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.57	4.10	3.65
Unmasked-calculated*	3.38	3.95	3.43

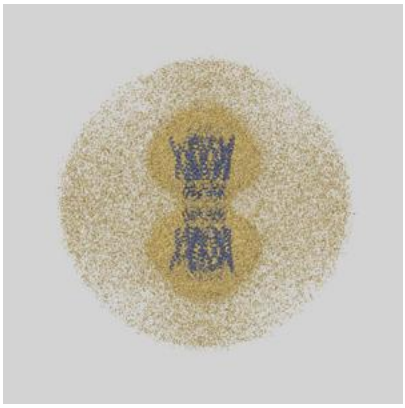
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.57 differs from the reported value 3.0 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.38 differs from the reported value 3.0 by more than 10 %

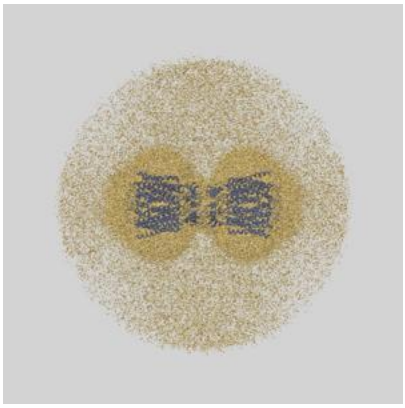
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-34156 and PDB model 8GN7. Per-residue inclusion information can be found in section 3 on page 9.

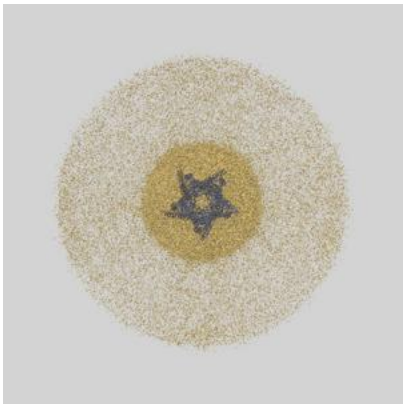
9.1 Map-model overlay



X



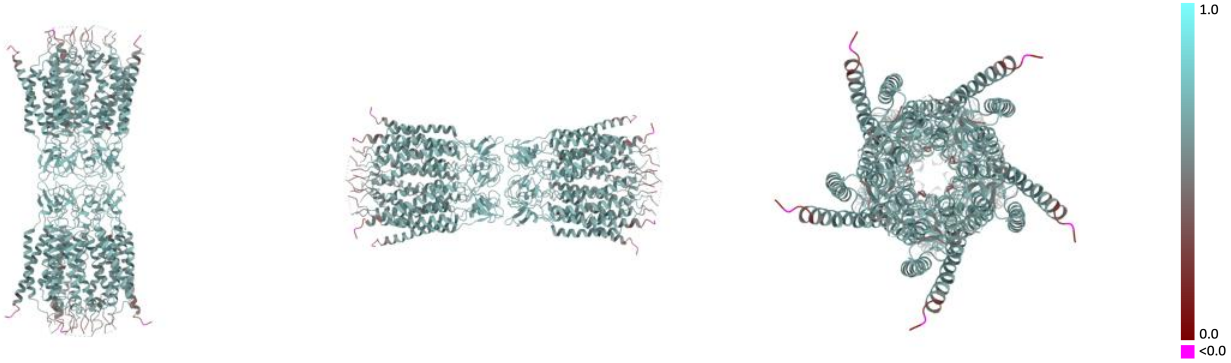
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.21 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.

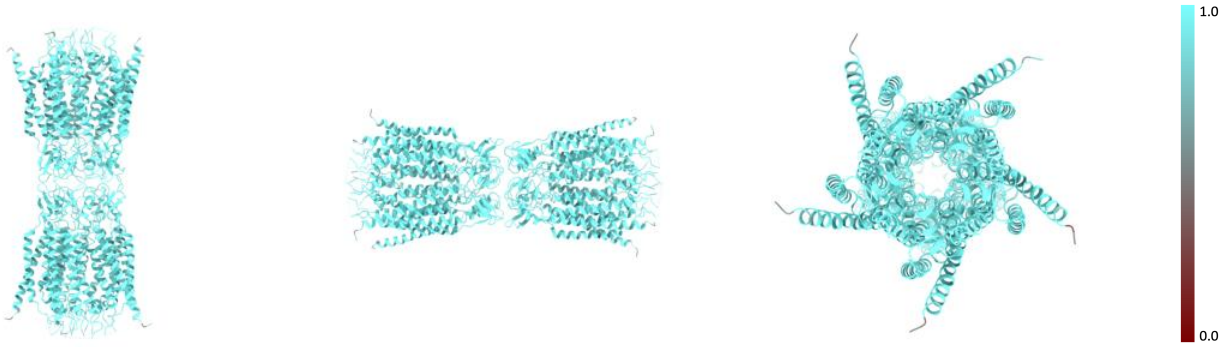
9.2 Q-score mapped to coordinate model (i)



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.

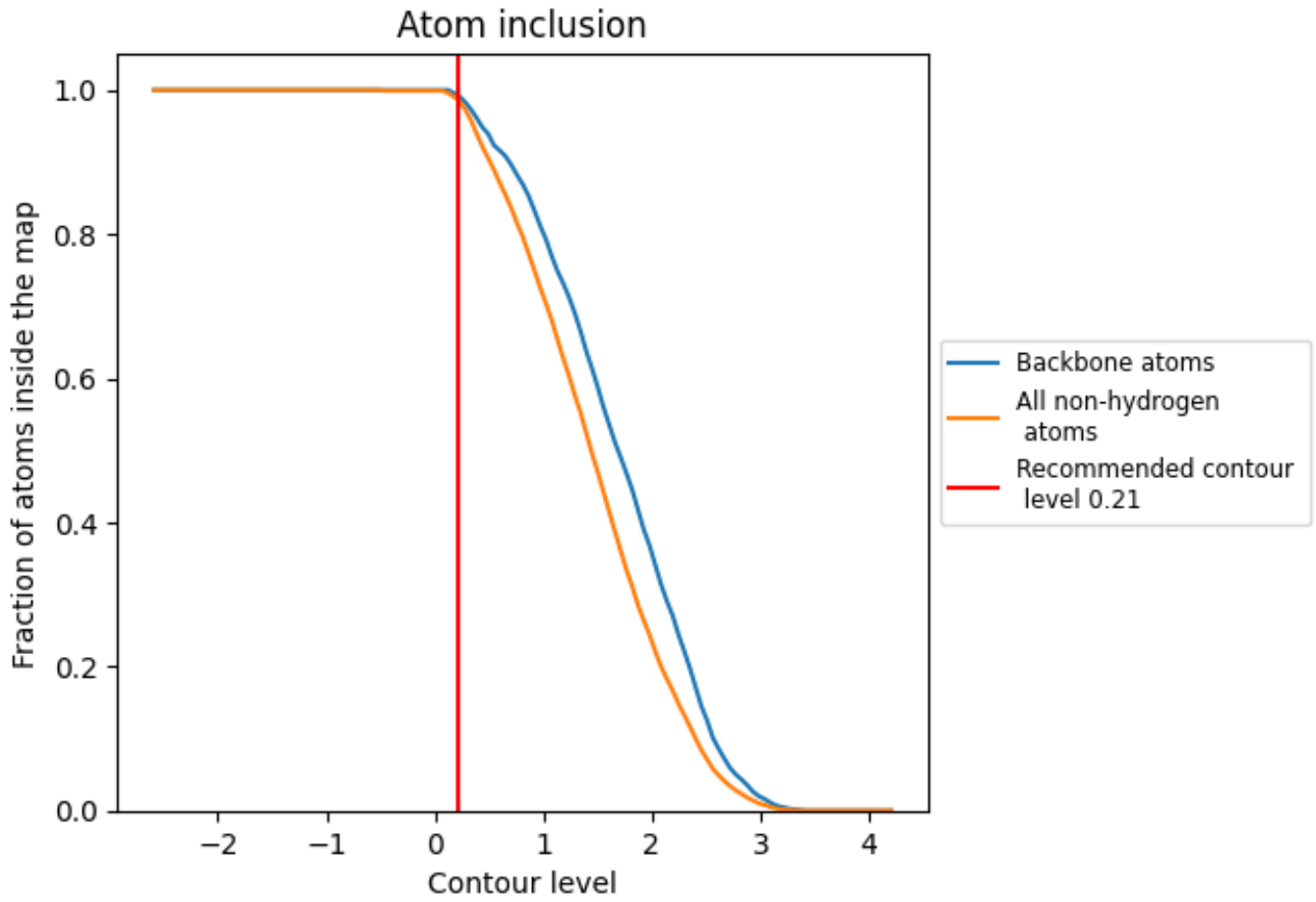
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.21).

9.4 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 99% 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 (0.21) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9870	0.5870
A	0.9850	0.5870
B	0.9870	0.5860
G	0.9870	0.5870
J	0.9880	0.5880
M	0.9850	0.5850
P	0.9870	0.5870
S	0.9880	0.5870
V	0.9890	0.5880
Y	0.9850	0.5870
b	0.9850	0.5870