Full wwPDB EM Validation Report

Nov 4, 2024 – 02:35 PM JST

PDB ID	:	8HG5
EMDB ID	:	EMD-34735
Title	:	Cryo-EM structure of the prasinophyte-specific light-harvesting complex (Lhcp)from Ostreococcus tauri
Authors	:	Shan, J.; Sheng, X.; Ishii, A.; Watanabe, A.; Song, C.; Murata, K.; Minagawa, J.; Liu, Z.
Deposited on	:	2022-11-13
Resolution	:	2.90 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 (i) symbol.

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

The following versions of software and data (see references (1)) were used in the production of this report:

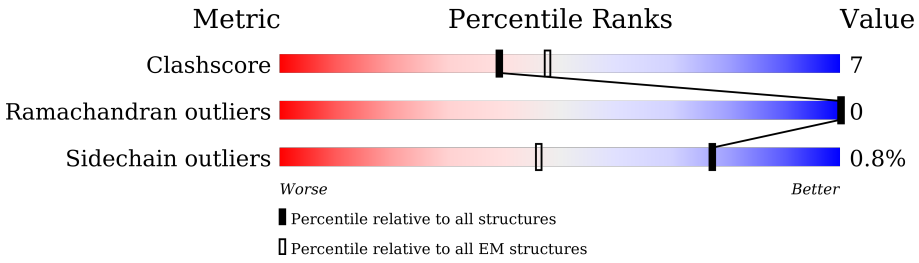
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.90 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	P	233	26% 78% 9% 14%
1	R	233	24% 70% 16% • 14%
2	Q	226	19% 82% 17% •

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CLA	P	301	X	-	-	-
3	CLA	P	302	X	-	-	-
3	CLA	P	303	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CLA	P	309	X	-	-	-
3	CLA	P	310	X	-	-	-
3	CLA	P	311	X	-	-	-
3	CLA	P	312	X	-	-	-
3	CLA	Q	302	X	-	-	-
3	CLA	Q	303	X	-	-	-
3	CLA	Q	304	X	-	-	-
3	CLA	Q	309	X	-	-	-
3	CLA	Q	310	X	-	-	-
3	CLA	Q	311	X	-	-	-
3	CLA	Q	312	X	-	-	-
3	CLA	Q	313	X	-	-	-
3	CLA	R	305	X	-	-	-
3	CLA	R	306	X	-	-	-
3	CLA	R	307	X	-	-	-
3	CLA	R	313	X	-	-	-
3	CLA	R	314	X	-	-	-
3	CLA	R	315	X	-	-	-
3	CLA	R	316	X	-	-	-
4	CHL	P	304	X	-	-	-
4	CHL	P	305	X	-	-	-
4	CHL	P	306	X	-	-	-
4	CHL	P	307	X	-	-	-
4	CHL	P	314	X	-	-	-
4	CHL	Q	305	X	-	-	-
4	CHL	Q	306	X	-	-	-
4	CHL	Q	307	X	-	-	-
4	CHL	Q	314	X	-	-	-
4	CHL	R	302	X	-	-	-
4	CHL	R	308	X	-	-	-
4	CHL	R	309	X	-	-	-
4	CHL	R	310	X	-	-	-
4	CHL	R	311	X	-	-	-
4	CHL	R	318	X	-	-	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 7794 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 Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	P	201	Total	C	N	O	S	0	0
			1507	968	246	287	6		
1	R	201	Total	C	N	O	S	0	0
			1507	968	246	287	6		

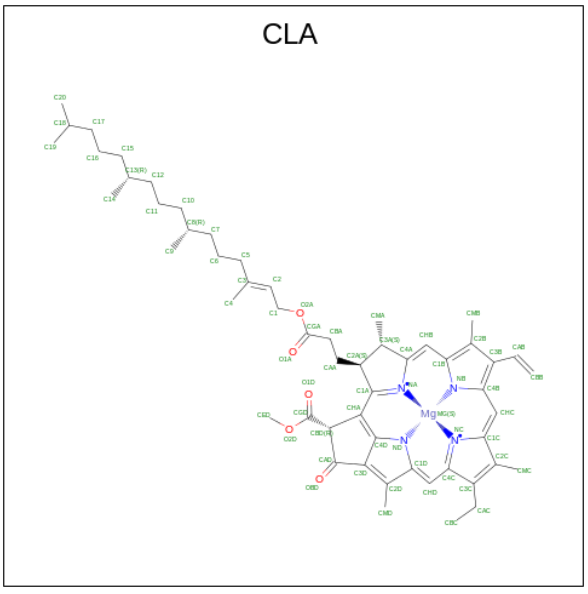
- Molecule 2 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	Q	226	Total	C	N	O	P	S	0	0
			1706	1100	285	313	1	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	28	ACE	-	acetylation	UNP A0A090LYE8

- Molecule 3 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
3	P	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	P	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	P	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
3	P	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
3	P	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
3	P	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
3	P	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
3	P	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
3	Q	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	Q	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
3	Q	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
3	Q	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
3	Q	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
3	Q	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
3	Q	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
3	Q	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
3	R	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	R	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	R	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
3	R	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
3	R	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
3	R	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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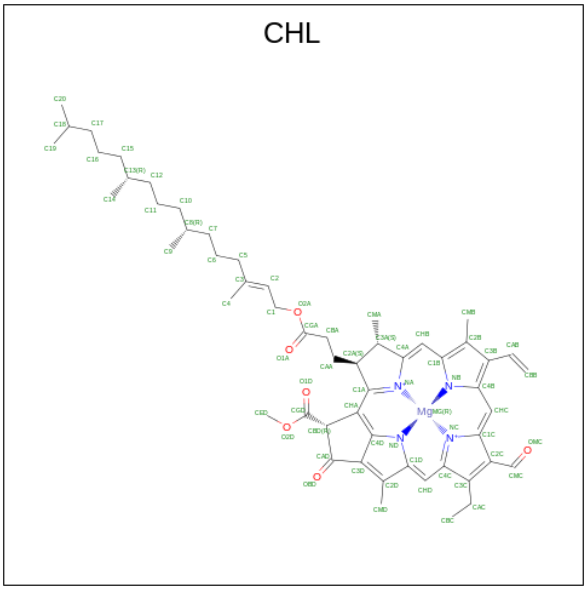
Mol	Chain	Residues	Atoms					AltConf
3	R	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
3	R	1	Total	C	Mg	N	O	0
			48	38	1	4	5	

- Molecule 4 is CHLOROPHYLL B (three-letter code: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
4	P	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
4	P	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
4	P	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
4	P	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
4	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
4	Q	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
4	Q	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
4	Q	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
4	Q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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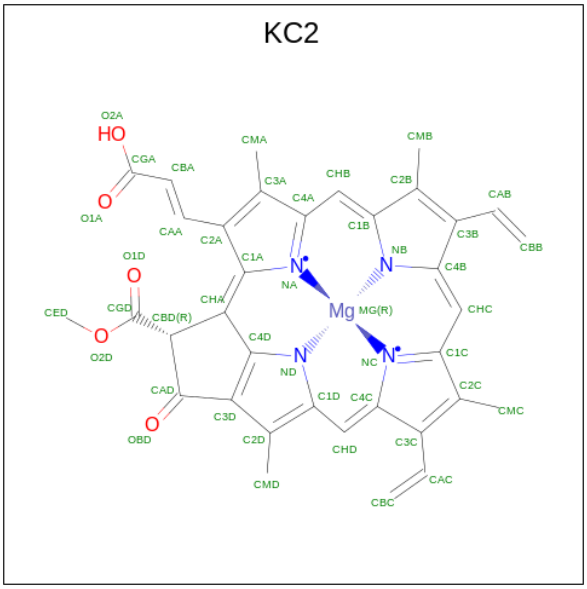
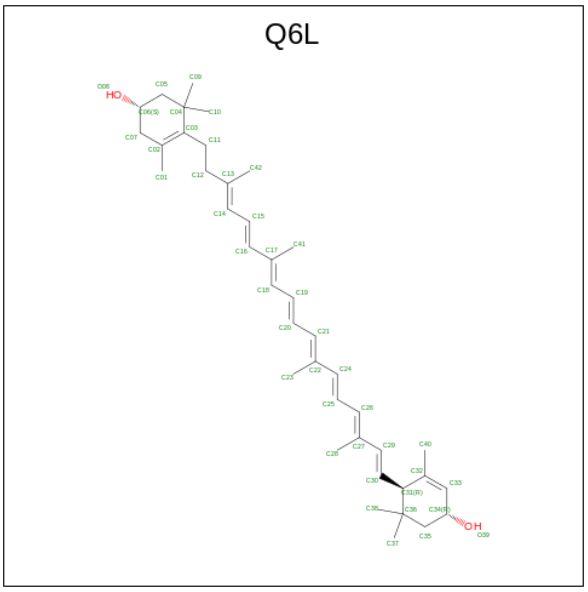
Mol	Chain	Residues	Atoms					AltConf
4	R	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
4	R	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
4	R	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
4	R	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
4	R	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
4	R	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 5 is Chlorophyll c2 (three-letter code: KC2) (formula: $C_{35}H_{28}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
5	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
5	Q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
5	R	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

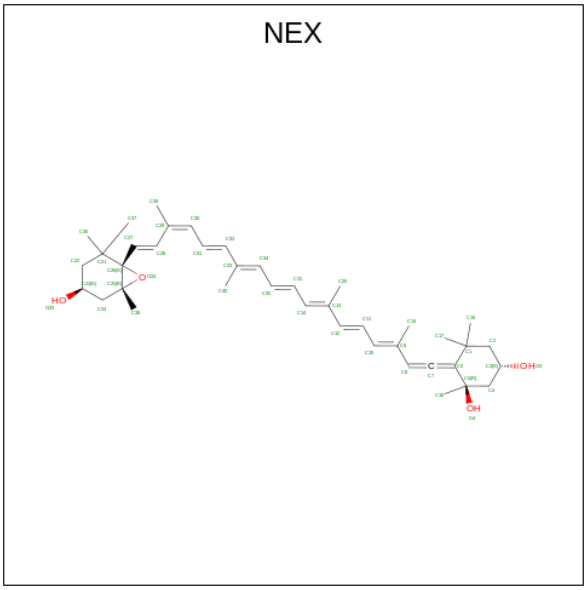
- Molecule 6 is (1 {S})-3,5,5-trimethyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(1 {R},4 {R})-2,6,6-trimethyl-4-oxidanyl-cyclohex-2-en-1-yl] octadeca-3,5,7,9,11,13,15,17-octaenyl]cyclohex-3-en-1-ol (three-letter code: Q6L) (formula: $C_{40}H_{58}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
6	P	1	Total C O 42 40 2	0
6	P	1	Total C O 42 40 2	0
6	P	1	Total C O 42 40 2	0
6	P	1	Total C O 42 40 2	0
6	Q	1	Total C O 42 40 2	0
6	Q	1	Total C O 42 40 2	0
6	Q	1	Total C O 42 40 2	0
6	R	1	Total C O 42 40 2	0
6	R	1	Total C O 42 40 2	0
6	R	1	Total C O 42 40 2	0
6	R	1	Total C O 42 40 2	0
6	R	1	Total C O 42 40 2	0

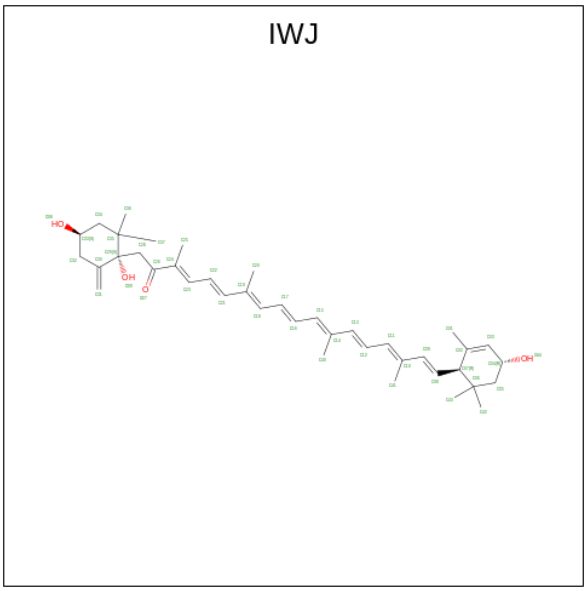
- Molecule 7 is (1R,3R)-6-{(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,

3-DIOL (three-letter code: NEX) (formula: $C_{40}H_{56}O_4$).



Mol	Chain	Residues	Atoms	AltConf
7	P	1	Total C O 44 40 4	0
7	Q	1	Total C O 44 40 4	0
7	R	1	Total C O 44 40 4	0

- Molecule 8 is (3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-1-[(1 {S},4 {S})-2,2-dimethyl-6-methylidene-1,4-bis(oxidanyl)cyclohexyl]-3,7,12,16-tetramethyl-18-[(1 {R},4 {R})-2,6,6-trimethyl-4-oxidanyl-cyclohex-2-en-1-yl]octadeca-3,5,7,9,11,13,15,17-octaen-2-one (three-letter code: IWJ) (formula: $C_{40}H_{56}O_4$).



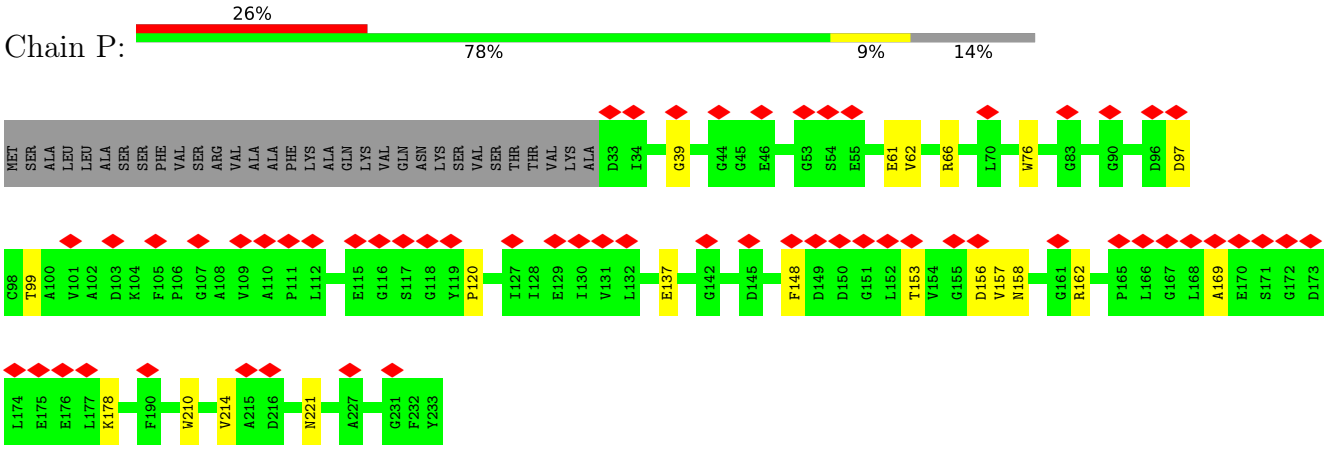
Mol	Chain	Residues	Atoms			AltConf
8	P	1	Total	C	O	0
			44	40	4	
8	P	1	Total	C	O	0
			44	40	4	
8	Q	1	Total	C	O	0
			44	40	4	
8	Q	1	Total	C	O	0
			44	40	4	
8	R	1	Total	C	O	0
			44	40	4	
8	R	1	Total	C	O	0
			44	40	4	

3 Residue-property plots (i)

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

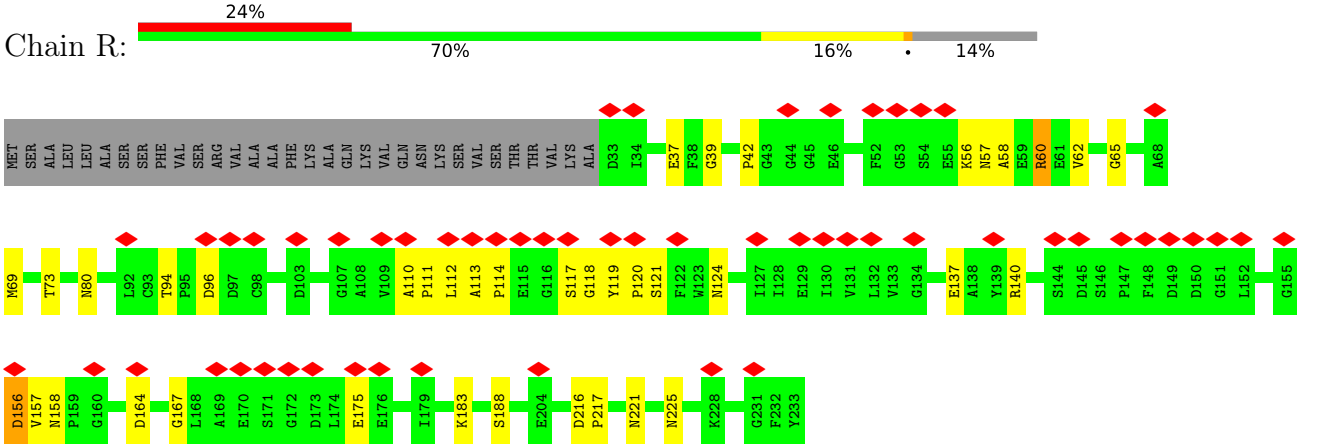
• Molecule 1: Chlorophyll a-b binding protein, chloroplastic

Chain P:



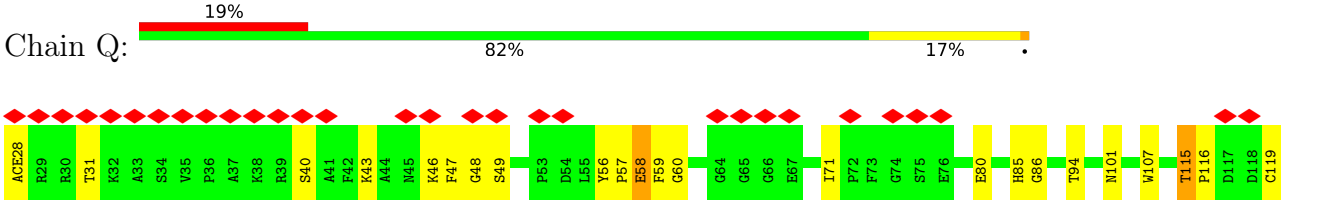
• Molecule 1: Chlorophyll a-b binding protein, chloroplastic

Chain R:



• Molecule 2: Chlorophyll a-b binding protein, chloroplastic

Chain Q:




T120
A121
V122
A123
D124
K125
A131
A134
P135
A136
G137
S138
G139
Y140
E171
D176
V177
T178
E190
A191
G192
D193
L194
E195
K203
H204
S205
M209
A235
D236
N245
Y253

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	80573	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.113	Depositor
Minimum map value	-0.070	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0274	Depositor
Map size (Å)	399.36, 399.36, 399.36	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: KC2, CHL, CLA, TPO, IWJ, NEX, Q6L, ACE

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	P	0.50	1/1553 (0.1%)	0.73	1/2122 (0.0%)
1	R	0.49	0/1553	0.78	6/2122 (0.3%)
2	Q	0.58	2/1746 (0.1%)	0.76	3/2379 (0.1%)
All	All	0.53	3/4852 (0.1%)	0.76	10/6623 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	80	GLU	CD-OE1	-9.19	1.15	1.25
2	Q	115	THR	C-N	5.34	1.44	1.34
1	P	76	TRP	CB-CG	5.28	1.59	1.50

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	R	216	ASP	CB-CG-OD1	8.57	126.02	118.30
1	R	111	PRO	CA-N-CD	-8.16	100.07	111.50
2	Q	236	ASP	CB-CG-OD1	7.88	125.39	118.30
2	Q	28	ACE	O-C-N	-7.25	111.10	122.70
1	R	175	GLU	CG-CD-OE2	6.45	131.19	118.30
2	Q	193	ASP	CB-CG-OD1	6.24	123.92	118.30
1	P	97	ASP	CB-CG-OD1	6.18	123.86	118.30
1	R	110	ALA	C-N-CD	5.84	140.68	128.40
1	R	175	GLU	OE1-CD-OE2	-5.71	116.45	123.30
1	R	156	ASP	CB-CG-OD1	5.43	123.19	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	P	1507	0	1429	19	0
1	R	1507	0	1429	40	0
2	Q	1706	0	1649	32	0
3	P	467	0	454	5	0
3	Q	403	0	338	9	0
3	R	467	0	454	8	0
4	P	233	0	163	1	0
4	Q	185	0	130	1	0
4	R	284	0	200	9	0
5	P	45	0	0	1	0
5	Q	45	0	0	0	0
5	R	45	0	0	2	0
6	P	168	0	0	1	0
6	Q	126	0	0	1	0
6	R	210	0	0	2	0
7	P	44	0	56	1	0
7	Q	44	0	56	0	0
7	R	44	0	56	0	0
8	P	88	0	0	2	0
8	Q	88	0	0	1	0
8	R	88	0	0	1	0
All	All	7794	0	6414	98	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (98) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:209:MET:CE	3:Q:302:CLA:HAB	1.81	1.10
2:Q:209:MET:HE1	3:Q:302:CLA:HAB	1.35	1.03
1:P:66:ARG:HH22	1:P:158:ASN:HB3	1.23	1.01
1:R:114:PRO:HB2	1:R:117:SER:HB3	1.56	0.87
2:Q:209:MET:HE2	3:Q:302:CLA:HAB	1.62	0.80
1:R:114:PRO:HG3	4:R:308:CHL:C3B	2.12	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:121:ALA:O	2:Q:125:LYS:NZ	2.11	0.78
1:R:114:PRO:HG2	1:R:119:TYR:HD1	1.51	0.76
1:R:94:THR:OG1	1:R:96:ASP:OD1	2.03	0.76
1:P:66:ARG:NH2	1:P:158:ASN:HB3	2.01	0.74
1:R:65:GLY:O	1:R:69:MET:HG3	1.89	0.72
1:R:80:ASN:ND2	8:R:322:IWJ:O44	2.26	0.68
1:P:66:ARG:HH22	1:P:158:ASN:CB	2.07	0.64
1:R:137:GLU:OE1	5:R:312:KC2:NB	2.30	0.64
1:R:62:VAL:HG11	1:R:157:VAL:HG11	1.81	0.63
2:Q:177:VAL:HG23	2:Q:178:THR:HG23	1.79	0.63
1:R:113:ALA:HB1	1:R:118:GLY:HA2	1.81	0.62
8:P:320:IWJ:O27	8:P:320:IWJ:O39	2.17	0.62
1:R:69:MET:HG2	1:R:188:SER:OG	2.01	0.61
1:R:56:LYS:HB3	1:R:60:ARG:NH1	2.16	0.60
2:Q:209:MET:HE1	3:Q:302:CLA:CAB	2.23	0.60
1:R:39:GLY:HA3	3:R:305:CLA:HMD1	1.83	0.59
1:R:114:PRO:HD2	1:R:119:TYR:H	1.69	0.58
1:R:164:ASP:OD1	1:R:167:GLY:N	2.36	0.58
1:P:39:GLY:HA3	3:P:301:CLA:HMD1	1.87	0.56
1:R:112:LEU:HD21	4:R:308:CHL:CHD	2.36	0.56
1:P:158:ASN:HB2	3:P:309:CLA:CGD	2.36	0.56
2:Q:58:GLU:OE1	2:Q:203:LYS:NZ	2.34	0.56
2:Q:60:GLY:HA3	3:Q:302:CLA:HMD1	1.87	0.55
2:Q:85:HIS:HB3	2:Q:209:MET:CE	2.37	0.55
2:Q:40:SER:HB3	2:Q:43:LYS:HB2	1.88	0.55
2:Q:57:PRO:HG2	2:Q:58:GLU:OE2	2.06	0.55
2:Q:49:SER:HB3	2:Q:193:ASP:HB3	1.90	0.54
2:Q:57:PRO:HD2	2:Q:203:LYS:HZ1	1.73	0.53
1:R:37:GLU:OE1	1:R:183:LYS:NZ	2.42	0.53
1:R:42:PRO:HA	3:R:305:CLA:HED3	1.90	0.53
1:R:114:PRO:CD	1:R:119:TYR:H	2.22	0.53
2:Q:101:ASN:ND2	8:Q:319:IWJ:O44	2.41	0.53
1:P:61:GLU:OE1	3:P:301:CLA:C4A	2.56	0.52
1:P:137:GLU:OE1	5:P:308:KC2:C4A	2.55	0.52
2:Q:123:ALA:HB1	2:Q:134:ALA:H	1.75	0.52
1:R:62:VAL:CG1	1:R:157:VAL:HG11	2.40	0.52
1:R:120:PRO:HG3	4:R:308:CHL:C4C	2.39	0.52
1:R:69:MET:CG	1:R:188:SER:OG	2.58	0.52
2:Q:85:HIS:HB3	2:Q:209:MET:HE3	1.92	0.51
2:Q:245:ASN:ND2	3:Q:312:CLA:OBD	2.42	0.51
2:Q:46:LYS:HD2	2:Q:191:ALA:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:66:ARG:NH1	1:P:157:VAL:HG12	2.25	0.51
3:P:301:CLA:HMC2	6:P:316:Q6L:C15	2.40	0.50
1:R:156:ASP:OD1	1:R:158:ASN:N	2.41	0.50
1:R:114:PRO:HG2	1:R:119:TYR:CD1	2.40	0.50
8:P:318:IWJ:O39	8:P:318:IWJ:O27	2.29	0.50
1:R:114:PRO:HG3	4:R:308:CHL:C2B	2.41	0.50
1:P:153:THR:O	1:P:156:ASP:HB3	2.11	0.50
2:Q:71:ILE:HG22	3:Q:302:CLA:HBA2	1.93	0.49
3:R:305:CLA:HMC2	6:R:320:Q6L:C15	2.42	0.49
1:P:210:TRP:CZ3	1:P:214:VAL:HG21	2.48	0.49
1:R:140:ARG:HG3	4:R:311:CHL:C1D	2.43	0.49
1:R:69:MET:HG2	1:R:188:SER:CB	2.43	0.48
2:Q:48:GLY:N	2:Q:192:GLY:HA2	2.28	0.48
1:R:140:ARG:HG3	4:R:311:CHL:CHD	2.44	0.48
1:R:58:ALA:HA	3:R:305:CLA:HMA1	1.95	0.47
1:R:121:SER:H	1:R:124:ASN:HB2	1.80	0.47
1:P:148:PHE:HB3	1:P:162:ARG:NH1	2.30	0.46
1:R:73:THR:HG23	3:R:307:CLA:HMC3	1.97	0.46
7:P:317:NEX:H193	7:P:317:NEX:H162	1.96	0.46
1:R:56:LYS:NZ	5:R:312:KC2:O2A	2.47	0.46
2:Q:56:TYR:HE1	2:Q:59:PHE:O	1.98	0.46
2:Q:47:PHE:CE2	2:Q:191:ALA:HB3	2.52	0.45
1:P:66:ARG:HH12	1:P:157:VAL:HG12	1.81	0.45
2:Q:49:SER:HB3	2:Q:193:ASP:CB	2.47	0.45
1:R:57:ASN:OD1	3:R:306:CLA:HED3	2.17	0.45
1:P:62:VAL:CG1	1:P:157:VAL:HG11	2.47	0.44
1:P:153:THR:HG23	1:P:156:ASP:CB	2.47	0.44
2:Q:119:CYS:O	2:Q:122:VAL:HG12	2.17	0.44
1:R:120:PRO:HG3	4:R:308:CHL:C3C	2.47	0.44
2:Q:48:GLY:CA	2:Q:192:GLY:HA2	2.47	0.44
1:P:158:ASN:H	4:P:307:CHL:HMD1	1.82	0.43
1:P:99:THR:HG22	1:P:120:PRO:HG2	2.01	0.43
2:Q:86:GLY:HA3	2:Q:205:SER:HB3	2.00	0.43
1:P:210:TRP:CH2	1:P:214:VAL:HG11	2.54	0.42
2:Q:131:ALA:HB1	4:Q:305:CHL:HMA3	2.01	0.42
2:Q:134:ALA:HA	2:Q:140:TYR:HA	2.01	0.42
1:R:58:ALA:O	1:R:62:VAL:HG23	2.19	0.42
1:P:169:ALA:HB2	3:P:309:CLA:HAA2	2.01	0.42
1:R:225:ASN:ND2	3:R:316:CLA:OBD	2.51	0.42
1:R:120:PRO:HG3	4:R:308:CHL:C1C	2.50	0.42
2:Q:85:HIS:CB	2:Q:209:MET:HE1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:217:PRO:O	1:R:221:ASN:ND2	2.53	0.41
2:Q:107:TRP:O	6:Q:318:Q6L:O08	2.38	0.41
3:R:313:CLA:HMC2	6:R:319:Q6L:C25	2.51	0.41
1:R:114:PRO:HG3	4:R:308:CHL:CAB	2.51	0.41
2:Q:115:THR:CG2	2:Q:116:PRO:HD2	2.51	0.41
1:R:65:GLY:O	1:R:69:MET:CG	2.65	0.41
1:R:96:ASP:OD1	1:R:96:ASP:N	2.54	0.41
1:P:221:ASN:OD1	1:P:221:ASN:N	2.53	0.41
3:Q:312:CLA:H2	3:Q:313:CLA:HMD1	2.03	0.40
2:Q:94:THR:OG1	3:Q:304:CLA:HMC3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	P	199/233 (85%)	191 (96%)	8 (4%)	0	100	100
1	R	199/233 (85%)	185 (93%)	14 (7%)	0	100	100
2	Q	223/226 (99%)	212 (95%)	11 (5%)	0	100	100
All	All	621/692 (90%)	588 (95%)	33 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	P	153/179 (86%)	152 (99%)	1 (1%)	81 94
1	R	153/179 (86%)	152 (99%)	1 (1%)	81 94
2	Q	167/167 (100%)	165 (99%)	2 (1%)	67 89
All	All	473/525 (90%)	469 (99%)	4 (1%)	77 93

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	178	LYS
2	Q	58	GLU
2	Q	190	GLU
1	R	60	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	P	158	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	TPO	Q	31	2	8,10,11	1.69	1 (12%)	10,14,16	1.11	1 (10%)

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	TPO	Q	31	2	-	2/9/11/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	31	TPO	P-O1P	3.45	1.61	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Q	31	TPO	P-OG1-CB	-2.28	116.33	123.21

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	Q	31	TPO	O-C-CA-CB
2	Q	31	TPO	CB-OG1-P-O1P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

63 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	$\#\|Z\|>2$
3	CLA	P	303	-	50,58,73	1.70	5 (10%)	58,95,113	1.55	9 (15%)
6	Q6L	Q	318	-	42,43,43	1.87	7 (16%)	47,60,60	1.71	10 (21%)
7	NEX	P	317	-	38,46,46	1.26	6 (15%)	50,70,70	2.62	17 (34%)
3	CLA	Q	313	-	48,56,73	1.70	7 (14%)	55,92,113	1.62	10 (18%)
4	CHL	R	310	-	52,60,74	1.63	8 (15%)	56,97,114	1.73	11 (19%)
3	CLA	Q	311	-	46,54,73	1.72	8 (17%)	53,90,113	1.66	9 (16%)
7	NEX	Q	315	-	38,46,46	1.33	7 (18%)	50,70,70	2.53	18 (36%)
3	CLA	Q	302	2	65,73,73	1.45	10 (15%)	76,113,113	1.67	9 (11%)
4	CHL	Q	307	-	44,52,74	1.73	6 (13%)	46,87,114	1.61	8 (17%)
4	CHL	P	314	1	45,53,74	1.78	6 (13%)	46,88,114	1.50	8 (17%)
3	CLA	P	302	-	65,73,73	1.50	8 (12%)	76,113,113	1.45	12 (15%)
3	CLA	Q	312	2	53,61,73	1.59	6 (11%)	61,98,113	1.50	9 (14%)
3	CLA	R	313	1	64,72,73	1.54	7 (10%)	74,111,113	1.51	11 (14%)
6	Q6L	P	315	-	42,43,43	1.92	8 (19%)	47,60,60	1.38	5 (10%)
5	KC2	R	312	1	48,53,53	2.61	14 (29%)	54,89,89	2.49	21 (38%)
6	Q6L	R	301	-	42,43,43	1.89	7 (16%)	47,60,60	1.73	6 (12%)
6	Q6L	R	319	-	42,43,43	1.90	7 (16%)	47,60,60	1.47	4 (8%)
5	KC2	P	308	1	48,53,53	2.62	16 (33%)	54,89,89	2.65	21 (38%)
6	Q6L	Q	317	-	42,43,43	1.81	6 (14%)	47,60,60	1.58	6 (12%)
8	IWJ	Q	301	-	43,45,45	1.21	4 (9%)	43,65,65	1.27	6 (13%)
3	CLA	P	311	-	60,68,73	1.51	6 (10%)	70,107,113	1.56	14 (20%)
4	CHL	P	304	1	46,54,74	1.78	6 (13%)	49,90,114	1.95	16 (32%)
8	IWJ	P	320	-	43,45,45	1.20	6 (13%)	43,65,65	1.36	5 (11%)
4	CHL	R	309	-	50,58,74	1.73	6 (12%)	52,94,114	1.57	10 (19%)
3	CLA	R	307	-	50,58,73	1.71	7 (14%)	58,95,113	1.50	7 (12%)
6	Q6L	R	304	-	42,43,43	1.90	7 (16%)	47,60,60	1.45	3 (6%)
3	CLA	R	317	-	48,56,73	1.68	7 (14%)	55,92,113	1.60	9 (16%)
3	CLA	Q	304	-	50,58,73	1.78	7 (14%)	58,95,113	1.78	11 (18%)
8	IWJ	Q	319	-	43,45,45	1.12	4 (9%)	43,65,65	1.29	7 (16%)
8	IWJ	P	318	-	43,45,45	1.16	4 (9%)	43,65,65	1.11	1 (2%)
3	CLA	Q	310	2	42,50,73	1.92	7 (16%)	48,85,113	1.41	7 (14%)
4	CHL	R	318	1	45,53,74	1.80	6 (13%)	46,88,114	1.54	8 (17%)
3	CLA	R	316	1	55,63,73	1.62	5 (9%)	64,101,113	1.74	11 (17%)
3	CLA	Q	303	-	44,52,73	1.76	8 (18%)	49,87,113	1.47	7 (14%)
6	Q6L	R	323	-	42,43,43	1.89	6 (14%)	47,60,60	1.73	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	CHL	P	307	-	44,52,74	1.76	7 (15%)	46,87,114	1.88	10 (21%)
3	CLA	P	301	1	65,73,73	1.43	7 (10%)	76,113,113	1.52	13 (17%)
3	CLA	R	305	1	65,73,73	1.52	7 (10%)	76,113,113	1.50	12 (15%)
4	CHL	P	305	-	46,54,74	1.77	6 (13%)	49,90,114	1.93	11 (22%)
3	CLA	R	315	-	60,68,73	1.59	7 (11%)	70,107,113	1.49	12 (17%)
6	Q6L	P	321	-	42,43,43	1.89	8 (19%)	47,60,60	1.54	6 (12%)
3	CLA	P	310	1	60,68,73	1.58	6 (10%)	70,107,113	1.46	11 (15%)
3	CLA	R	314	1	60,68,73	1.59	6 (10%)	70,107,113	1.58	13 (18%)
5	KC2	Q	308	2	48,53,53	2.58	14 (29%)	54,89,89	2.51	18 (33%)
4	CHL	P	306	-	52,60,74	1.61	8 (15%)	56,97,114	1.70	12 (21%)
8	IWJ	R	303	-	43,45,45	1.18	5 (11%)	43,65,65	1.25	3 (6%)
4	CHL	Q	314	2	45,53,74	1.81	5 (11%)	46,88,114	1.57	11 (23%)
3	CLA	R	306	-	65,73,73	1.45	8 (12%)	76,113,113	1.30	6 (7%)
4	CHL	R	308	1	46,54,74	1.72	5 (10%)	49,90,114	1.50	8 (16%)
4	CHL	Q	306	2	50,58,74	1.71	7 (14%)	52,94,114	1.96	12 (23%)
6	Q6L	R	320	-	42,43,43	1.88	7 (16%)	47,60,60	1.40	5 (10%)
8	IWJ	R	322	-	43,45,45	1.16	4 (9%)	43,65,65	1.00	2 (4%)
3	CLA	Q	309	2	55,63,73	1.55	7 (12%)	64,101,113	1.41	10 (15%)
3	CLA	P	312	1	55,63,73	1.65	5 (9%)	64,101,113	1.57	10 (15%)
6	Q6L	Q	316	-	42,43,43	1.82	6 (14%)	47,60,60	1.61	6 (12%)
6	Q6L	P	319	-	42,43,43	1.87	7 (16%)	47,60,60	1.60	7 (14%)
3	CLA	P	309	1	64,72,73	1.45	5 (7%)	74,111,113	1.64	14 (18%)
7	NEX	R	321	-	38,46,46	1.30	7 (18%)	50,70,70	2.71	17 (34%)
3	CLA	P	313	-	48,56,73	1.74	6 (12%)	55,92,113	1.42	9 (16%)
4	CHL	R	311	-	44,52,74	1.86	8 (18%)	46,87,114	1.59	10 (21%)
4	CHL	R	302	-	47,55,74	1.73	6 (12%)	50,91,114	1.71	13 (26%)
4	CHL	Q	305	2	46,54,74	1.63	4 (8%)	49,90,114	1.65	10 (20%)
6	Q6L	P	316	-	42,43,43	1.91	8 (19%)	47,60,60	1.44	6 (12%)

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
3	CLA	P	303	-	1/1/12/20	11/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	Q6L	Q	318	-	-	5/29/67/67	0/2/2/2
7	NEX	P	317	-	-	2/27/83/83	0/3/3/3
3	CLA	Q	313	-	1/1/11/20	5/17/95/115	-
4	CHL	R	310	-	3/3/17/26	6/23/121/137	-
3	CLA	Q	311	-	1/1/11/20	7/15/93/115	-
7	NEX	Q	315	-	-	3/27/83/83	0/3/3/3
3	CLA	Q	302	2	1/1/15/20	9/37/115/115	-
4	CHL	Q	307	-	3/3/15/26	3/13/111/137	-
4	CHL	P	314	1	3/3/15/26	6/13/112/137	-
3	CLA	P	302	-	1/1/15/20	15/37/115/115	-
3	CLA	Q	312	2	1/1/12/20	12/23/101/115	-
3	CLA	R	313	1	1/1/14/20	17/36/114/115	-
6	Q6L	P	315	-	-	6/29/67/67	0/2/2/2
5	KC2	R	312	1	-	8/15/71/71	-
6	Q6L	R	301	-	-	11/29/67/67	0/2/2/2
6	Q6L	R	319	-	-	10/29/67/67	0/2/2/2
5	KC2	P	308	1	-	9/15/71/71	-
6	Q6L	Q	317	-	-	6/29/67/67	0/2/2/2
8	IWJ	Q	301	-	-	3/33/76/76	0/2/2/2
3	CLA	P	311	-	1/1/14/20	10/31/109/115	-
4	CHL	P	304	1	3/3/16/26	6/15/113/137	-
8	IWJ	P	320	-	-	2/33/76/76	0/2/2/2
4	CHL	R	309	-	3/3/16/26	7/20/118/137	-
3	CLA	R	307	-	1/1/12/20	2/19/97/115	-
6	Q6L	R	304	-	-	5/29/67/67	0/2/2/2
3	CLA	R	317	-	-	6/17/95/115	-
3	CLA	Q	304	-	1/1/12/20	9/19/97/115	-
8	IWJ	Q	319	-	-	12/33/76/76	0/2/2/2
8	IWJ	P	318	-	-	2/33/76/76	0/2/2/2
3	CLA	Q	310	2	1/1/10/20	3/10/88/115	-
4	CHL	R	318	1	3/3/15/26	4/13/112/137	-
3	CLA	R	316	1	1/1/13/20	9/25/103/115	-
3	CLA	Q	303	-	1/1/10/20	0/11/90/115	-
6	Q6L	R	323	-	-	9/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CHL	P	307	-	3/3/15/26	3/13/111/137	-
3	CLA	P	301	1	1/1/15/20	9/37/115/115	-
3	CLA	R	305	1	1/1/15/20	9/37/115/115	-
4	CHL	P	305	-	3/3/16/26	4/15/113/137	-
3	CLA	R	315	-	1/1/14/20	10/31/109/115	-
6	Q6L	P	321	-	-	7/29/67/67	0/2/2/2
3	CLA	P	310	1	1/1/14/20	10/31/109/115	-
3	CLA	R	314	1	1/1/14/20	13/31/109/115	-
5	KC2	Q	308	2	-	6/15/71/71	-
4	CHL	P	306	-	3/3/17/26	7/23/121/137	-
8	IWJ	R	303	-	-	4/33/76/76	0/2/2/2
4	CHL	Q	314	2	3/3/15/26	3/13/112/137	-
3	CLA	R	306	-	1/1/15/20	11/37/115/115	-
4	CHL	R	308	1	3/3/16/26	3/15/113/137	-
4	CHL	Q	306	2	3/3/16/26	4/20/118/137	-
6	Q6L	R	320	-	-	0/29/67/67	0/2/2/2
8	IWJ	R	322	-	-	7/33/76/76	1/2/2/2
3	CLA	Q	309	2	1/1/13/20	8/25/103/115	-
3	CLA	P	312	1	1/1/13/20	12/25/103/115	-
6	Q6L	Q	316	-	-	6/29/67/67	0/2/2/2
6	Q6L	P	319	-	-	6/29/67/67	0/2/2/2
3	CLA	P	309	1	1/1/14/20	15/36/114/115	-
7	NEX	R	321	-	-	3/27/83/83	0/3/3/3
3	CLA	P	313	-	-	4/17/95/115	-
4	CHL	R	311	-	3/3/15/26	3/13/111/137	-
4	CHL	R	302	-	3/3/16/26	5/17/115/137	-
4	CHL	Q	305	2	3/3/16/26	6/15/113/137	-
6	Q6L	P	316	-	-	2/29/67/67	0/2/2/2

All (431) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	P	321	Q6L	C29-C30	8.62	1.52	1.32
6	P	316	Q6L	C29-C30	8.51	1.52	1.32
6	R	304	Q6L	C29-C30	8.49	1.52	1.32
6	R	301	Q6L	C29-C30	8.47	1.52	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	R	319	Q6L	C29-C30	8.45	1.52	1.32
6	P	319	Q6L	C29-C30	8.43	1.52	1.32
6	P	315	Q6L	C29-C30	8.43	1.52	1.32
6	R	323	Q6L	C29-C30	8.43	1.52	1.32
6	R	320	Q6L	C29-C30	8.41	1.52	1.32
5	Q	308	KC2	C2A-C3A	8.28	1.54	1.37
6	Q	316	Q6L	C29-C30	8.27	1.51	1.32
5	R	312	KC2	C2A-C3A	8.24	1.54	1.37
3	Q	310	CLA	C4B-NB	8.23	1.42	1.35
6	Q	318	Q6L	C29-C30	8.23	1.51	1.32
6	Q	317	Q6L	C29-C30	8.06	1.51	1.32
4	P	314	CHL	C4B-NB	7.97	1.42	1.35
3	R	315	CLA	C4B-NB	7.92	1.42	1.35
3	R	313	CLA	C4B-NB	7.90	1.42	1.35
5	P	308	KC2	C2A-C3A	7.83	1.53	1.37
4	R	311	CHL	C4B-NB	7.68	1.42	1.35
4	R	318	CHL	C4B-NB	7.67	1.42	1.35
3	R	316	CLA	C4B-NB	7.65	1.42	1.35
5	P	308	KC2	C1D-ND	7.62	1.42	1.35
4	R	309	CHL	C4B-NB	7.61	1.42	1.35
4	P	305	CHL	C4B-NB	7.59	1.42	1.35
5	R	312	KC2	C3D-C4D	7.51	1.47	1.40
3	P	312	CLA	C4B-NB	7.46	1.41	1.35
3	R	307	CLA	C4B-NB	7.46	1.41	1.35
4	Q	314	CHL	C4B-NB	7.44	1.41	1.35
5	P	308	KC2	C3D-C4D	7.37	1.47	1.40
3	P	313	CLA	C4B-NB	7.34	1.41	1.35
5	Q	308	KC2	C3D-C4D	7.32	1.47	1.40
4	P	304	CHL	C4B-NB	7.32	1.41	1.35
3	Q	313	CLA	C4B-NB	7.31	1.41	1.35
4	Q	307	CHL	C4B-NB	7.31	1.41	1.35
3	R	314	CLA	C4B-NB	7.30	1.41	1.35
3	P	310	CLA	C4B-NB	7.29	1.41	1.35
4	P	307	CHL	C4B-NB	7.26	1.41	1.35
4	R	302	CHL	C4B-NB	7.24	1.41	1.35
3	P	303	CLA	C4B-NB	7.24	1.41	1.35
3	P	311	CLA	C4B-NB	7.11	1.41	1.35
3	P	309	CLA	C4B-NB	7.10	1.41	1.35
3	P	302	CLA	C4B-NB	7.06	1.41	1.35
3	Q	311	CLA	C4B-NB	7.01	1.41	1.35
3	R	317	CLA	C4B-NB	6.97	1.41	1.35
3	Q	303	CLA	C4B-NB	6.94	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	R	308	CHL	C4B-NB	6.93	1.41	1.35
3	Q	304	CLA	C4B-NB	6.85	1.41	1.35
4	Q	306	CHL	C4B-NB	6.83	1.41	1.35
3	R	305	CLA	C4B-NB	6.82	1.41	1.35
4	P	306	CHL	C4B-NB	6.82	1.41	1.35
4	R	310	CHL	C4B-NB	6.69	1.41	1.35
5	Q	308	KC2	C1D-ND	6.66	1.41	1.35
3	Q	312	CLA	C4B-NB	6.64	1.41	1.35
5	R	312	KC2	C1D-ND	6.54	1.41	1.35
3	Q	309	CLA	C4B-NB	6.48	1.41	1.35
3	R	306	CLA	C4B-NB	6.42	1.40	1.35
5	Q	308	KC2	CBA-CAA	6.32	1.52	1.33
4	Q	305	CHL	C4B-NB	6.27	1.40	1.35
3	P	301	CLA	C4B-NB	6.21	1.40	1.35
5	P	308	KC2	CBA-CAA	6.00	1.51	1.33
5	R	312	KC2	CBA-CAA	5.99	1.51	1.33
6	R	301	Q6L	C12-C11	-5.62	1.34	1.52
3	Q	302	CLA	C4B-NB	5.58	1.40	1.35
6	R	323	Q6L	C12-C11	-5.55	1.34	1.52
6	P	315	Q6L	C12-C11	-5.54	1.34	1.52
6	Q	316	Q6L	C12-C11	-5.46	1.34	1.52
6	R	319	Q6L	C12-C11	-5.38	1.34	1.52
6	P	321	Q6L	C12-C11	-5.37	1.34	1.52
6	Q	318	Q6L	C12-C11	-5.37	1.34	1.52
6	Q	317	Q6L	C12-C11	-5.33	1.35	1.52
6	R	304	Q6L	C12-C11	-5.30	1.35	1.52
6	R	320	Q6L	C12-C11	-5.27	1.35	1.52
6	P	316	Q6L	C12-C11	-5.23	1.35	1.52
6	P	319	Q6L	C12-C11	-5.21	1.35	1.52
3	Q	304	CLA	C4D-ND	-4.91	1.31	1.37
4	Q	306	CHL	CMD-C2D	-4.39	1.41	1.50
5	R	312	KC2	C4A-C3A	4.30	1.52	1.44
4	Q	314	CHL	C1D-ND	4.27	1.43	1.37
5	P	308	KC2	C4A-C3A	4.08	1.52	1.44
3	R	313	CLA	C1D-ND	4.03	1.42	1.37
3	P	310	CLA	C1D-ND	4.03	1.42	1.37
3	R	314	CLA	C1D-ND	3.86	1.42	1.37
4	P	304	CHL	CHC-C1C	3.77	1.44	1.35
3	R	305	CLA	C1D-ND	3.76	1.42	1.37
7	R	321	NEX	C7-C8	-3.76	1.25	1.32
3	P	302	CLA	C1D-ND	3.75	1.42	1.37
3	P	303	CLA	C1D-ND	3.75	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	313	CLA	C1D-ND	3.74	1.42	1.37
8	Q	301	IWJ	C09-C10	3.70	1.53	1.45
5	Q	308	KC2	C4A-C3A	3.70	1.51	1.44
4	R	311	CHL	C1D-ND	3.69	1.42	1.37
4	P	307	CHL	C1D-ND	3.67	1.42	1.37
3	R	316	CLA	C1D-ND	3.64	1.42	1.37
4	R	309	CHL	C1D-ND	3.63	1.42	1.37
4	R	302	CHL	C1D-ND	3.63	1.42	1.37
3	R	317	CLA	C1D-ND	3.62	1.42	1.37
3	Q	309	CLA	C1D-ND	3.61	1.42	1.37
4	R	318	CHL	C1D-ND	3.59	1.42	1.37
3	P	311	CLA	C1D-ND	3.59	1.42	1.37
4	R	311	CHL	CMD-C2D	-3.58	1.43	1.50
4	Q	305	CHL	C1D-ND	3.57	1.42	1.37
3	Q	303	CLA	C1D-ND	3.57	1.42	1.37
3	P	301	CLA	C1D-ND	3.57	1.42	1.37
3	Q	304	CLA	C1D-ND	3.56	1.42	1.37
3	Q	313	CLA	C1D-ND	3.56	1.42	1.37
3	R	315	CLA	C1D-ND	3.56	1.42	1.37
3	P	312	CLA	C4D-ND	-3.55	1.32	1.37
4	R	309	CHL	C4D-ND	-3.55	1.32	1.37
3	P	312	CLA	C1D-ND	3.55	1.42	1.37
3	Q	310	CLA	C1D-ND	3.55	1.42	1.37
3	Q	302	CLA	C1D-ND	3.54	1.42	1.37
3	R	306	CLA	C4D-ND	-3.49	1.32	1.37
3	Q	311	CLA	C1D-ND	3.46	1.42	1.37
4	Q	307	CHL	C1D-ND	3.45	1.42	1.37
4	P	304	CHL	C1D-ND	3.43	1.42	1.37
4	P	305	CHL	C4D-ND	-3.43	1.33	1.37
3	R	307	CLA	C1D-ND	3.40	1.42	1.37
4	P	304	CHL	C4D-ND	-3.40	1.33	1.37
8	R	303	IWJ	C09-C10	3.39	1.53	1.45
3	Q	302	CLA	C4D-ND	-3.38	1.33	1.37
8	R	322	IWJ	C09-C10	3.38	1.53	1.45
3	P	309	CLA	C1D-ND	3.36	1.41	1.37
3	R	317	CLA	CHC-C1C	3.35	1.43	1.35
3	R	305	CLA	C4D-ND	-3.35	1.33	1.37
3	P	301	CLA	C4D-ND	-3.34	1.33	1.37
4	R	310	CHL	C1D-ND	3.34	1.41	1.37
7	Q	315	NEX	C7-C8	-3.33	1.26	1.32
3	R	306	CLA	C1D-ND	3.33	1.41	1.37
4	R	302	CHL	C4D-ND	-3.29	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	R	311	CHL	CHC-C1C	3.27	1.43	1.35
4	R	308	CHL	C4D-ND	-3.25	1.33	1.37
4	P	306	CHL	C1D-ND	3.24	1.41	1.37
4	Q	314	CHL	C4D-ND	-3.24	1.33	1.37
8	P	320	IWJ	C09-C10	3.23	1.52	1.45
8	Q	319	IWJ	C09-C10	3.21	1.52	1.45
3	Q	312	CLA	C1D-ND	3.21	1.41	1.37
3	P	311	CLA	C4D-ND	-3.20	1.33	1.37
3	Q	312	CLA	C4D-ND	-3.20	1.33	1.37
8	P	318	IWJ	C09-C10	3.19	1.52	1.45
3	P	301	CLA	CHC-C1C	3.19	1.43	1.35
3	P	303	CLA	CHC-C1C	3.19	1.43	1.35
3	R	315	CLA	CHC-C1C	3.19	1.43	1.35
4	R	308	CHL	C1D-ND	3.17	1.41	1.37
3	P	312	CLA	CHC-C1C	3.14	1.43	1.35
3	P	313	CLA	C4D-ND	-3.14	1.33	1.37
3	R	317	CLA	C4D-ND	-3.11	1.33	1.37
3	R	307	CLA	CHC-C1C	3.11	1.42	1.35
5	P	308	KC2	C4B-NB	3.11	1.41	1.37
4	R	318	CHL	CHC-C1C	3.10	1.42	1.35
3	P	310	CLA	CHC-C1C	3.09	1.42	1.35
3	P	302	CLA	CHC-C1C	3.08	1.42	1.35
4	Q	307	CHL	C4D-ND	-3.08	1.33	1.37
4	P	307	CHL	C4D-ND	-3.07	1.33	1.37
4	P	305	CHL	C1D-ND	3.07	1.41	1.37
4	Q	306	CHL	CHC-C1C	3.07	1.42	1.35
3	Q	311	CLA	C4D-ND	-3.06	1.33	1.37
3	Q	310	CLA	CHC-C1C	3.06	1.42	1.35
3	Q	313	CLA	C4D-ND	-3.05	1.33	1.37
5	R	312	KC2	C4D-ND	-3.04	1.32	1.35
3	P	309	CLA	CHC-C1C	3.04	1.42	1.35
3	R	314	CLA	C4D-ND	-3.03	1.33	1.37
4	P	307	CHL	CHC-C1C	3.03	1.42	1.35
5	Q	308	KC2	C2A-C1A	3.02	1.53	1.44
3	P	313	CLA	CHC-C1C	3.01	1.42	1.35
3	R	314	CLA	CHC-C1C	3.00	1.42	1.35
3	P	302	CLA	C4D-ND	-3.00	1.33	1.37
3	Q	304	CLA	CMB-C2B	-3.00	1.45	1.51
6	P	315	Q6L	C34-C33	2.99	1.54	1.50
4	P	314	CHL	CHC-C1C	2.99	1.42	1.35
3	R	305	CLA	CMA-C3A	-2.99	1.46	1.53
3	Q	302	CLA	CHC-C1C	2.98	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	R	322	IWJ	C04-C03	2.98	1.54	1.50
3	Q	303	CLA	CMD-C2D	-2.98	1.44	1.50
4	P	314	CHL	C4D-ND	-2.98	1.33	1.37
6	R	323	Q6L	C34-C33	2.98	1.54	1.50
6	Q	318	Q6L	C34-C33	2.98	1.54	1.50
3	R	313	CLA	CHC-C1C	2.98	1.42	1.35
3	Q	309	CLA	C4D-ND	-2.97	1.33	1.37
3	P	310	CLA	C4D-ND	-2.97	1.33	1.37
4	P	305	CHL	CHC-C1C	2.97	1.42	1.35
3	P	303	CLA	C4D-ND	-2.97	1.33	1.37
8	Q	319	IWJ	C04-C03	2.96	1.54	1.50
8	P	318	IWJ	C29-C35	-2.96	1.51	1.56
4	Q	307	CHL	CHC-C1C	2.96	1.42	1.35
3	Q	304	CLA	CHC-C1C	2.96	1.42	1.35
3	Q	309	CLA	CHC-C1C	2.95	1.42	1.35
3	R	316	CLA	CHC-C1C	2.94	1.42	1.35
3	Q	313	CLA	CHC-C1C	2.94	1.42	1.35
5	P	308	KC2	C4D-ND	-2.94	1.32	1.35
8	P	320	IWJ	C04-C03	2.93	1.54	1.50
3	Q	312	CLA	CHC-C1C	2.92	1.42	1.35
5	R	312	KC2	C4B-NB	2.90	1.41	1.37
8	R	303	IWJ	C04-C03	2.90	1.54	1.50
4	R	310	CHL	CMD-C2D	-2.90	1.44	1.50
8	Q	301	IWJ	C04-C03	2.90	1.54	1.50
6	R	301	Q6L	C12-C13	-2.90	1.45	1.51
4	R	318	CHL	C4D-ND	-2.89	1.33	1.37
3	Q	311	CLA	CHC-C1C	2.89	1.42	1.35
4	R	309	CHL	CHC-C1C	2.89	1.42	1.35
4	P	306	CHL	C4D-ND	-2.88	1.33	1.37
6	P	315	Q6L	C12-C13	-2.88	1.45	1.51
3	Q	310	CLA	C4D-ND	-2.88	1.33	1.37
3	R	307	CLA	C4D-ND	-2.88	1.33	1.37
6	P	316	Q6L	C02-C03	2.85	1.38	1.34
3	P	311	CLA	CHC-C1C	2.85	1.42	1.35
6	R	320	Q6L	C34-C33	2.85	1.54	1.50
3	Q	303	CLA	C4D-ND	-2.84	1.33	1.37
3	P	309	CLA	C4D-ND	-2.84	1.33	1.37
5	Q	308	KC2	C4B-NB	2.82	1.41	1.37
3	R	316	CLA	C4D-ND	-2.81	1.33	1.37
3	Q	312	CLA	CMD-C2D	-2.81	1.44	1.50
7	P	317	NEX	C7-C8	-2.81	1.27	1.32
4	Q	314	CHL	CHC-C1C	2.81	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	P	318	IWJ	C04-C03	2.80	1.54	1.50
4	Q	306	CHL	C4D-ND	-2.80	1.33	1.37
7	P	317	NEX	C12-C13	2.80	1.52	1.45
6	R	323	Q6L	C12-C13	-2.78	1.45	1.51
3	R	305	CLA	CHC-C1C	2.78	1.42	1.35
5	R	312	KC2	CMD-C2D	-2.76	1.45	1.51
4	Q	305	CHL	CHC-C1C	2.76	1.42	1.35
4	R	311	CHL	CMB-C2B	-2.76	1.45	1.51
3	Q	303	CLA	CHC-C1C	2.76	1.42	1.35
5	R	312	KC2	C2A-C1A	2.76	1.53	1.44
4	Q	306	CHL	C1D-ND	2.75	1.41	1.37
6	R	304	Q6L	C34-C33	2.75	1.54	1.50
5	Q	308	KC2	CMD-C2D	-2.75	1.45	1.51
6	R	319	Q6L	C02-C03	2.74	1.38	1.34
3	R	306	CLA	CHC-C1C	2.73	1.42	1.35
4	R	310	CHL	CHC-C1C	2.72	1.41	1.35
3	P	302	CLA	C3B-C2B	-2.71	1.36	1.40
3	R	306	CLA	CMD-C2D	-2.71	1.45	1.50
8	Q	301	IWJ	C03-C02	2.71	1.36	1.33
4	Q	305	CHL	C4D-ND	-2.70	1.34	1.37
6	P	316	Q6L	C34-C33	2.70	1.54	1.50
6	Q	316	Q6L	C12-C13	-2.70	1.45	1.51
5	Q	308	KC2	C4D-ND	-2.69	1.32	1.35
6	Q	318	Q6L	C33-C32	2.69	1.36	1.33
5	P	308	KC2	CMD-C2D	-2.68	1.46	1.51
6	R	320	Q6L	C12-C13	-2.67	1.45	1.51
3	R	316	CLA	CMB-C2B	-2.66	1.46	1.51
3	Q	303	CLA	CMB-C2B	-2.65	1.46	1.51
3	R	307	CLA	CMB-C2B	-2.65	1.46	1.51
8	P	320	IWJ	O39-C29	-2.64	1.39	1.43
6	R	319	Q6L	C12-C13	-2.62	1.45	1.51
6	P	319	Q6L	C02-C03	2.62	1.37	1.34
6	P	319	Q6L	C33-C32	2.61	1.36	1.33
7	Q	315	NEX	C12-C13	2.61	1.51	1.45
4	R	302	CHL	CHC-C1C	2.61	1.41	1.35
8	R	322	IWJ	C03-C02	2.60	1.36	1.33
4	R	308	CHL	CHC-C1C	2.60	1.41	1.35
6	P	316	Q6L	C12-C13	-2.60	1.45	1.51
4	Q	307	CHL	CMB-C2B	-2.59	1.46	1.51
3	R	313	CLA	C4D-ND	-2.58	1.34	1.37
4	R	310	CHL	C4D-ND	-2.58	1.34	1.37
7	Q	315	NEX	C22-C21	-2.58	1.50	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	305	CLA	C3B-C2B	-2.57	1.36	1.40
6	R	301	Q6L	C34-C33	2.57	1.53	1.50
4	Q	306	CHL	CMB-C2B	-2.57	1.46	1.51
5	R	312	KC2	CMC-C2C	-2.56	1.45	1.50
3	R	315	CLA	CMB-C2B	-2.56	1.46	1.51
3	P	313	CLA	CMB-C2B	-2.56	1.46	1.51
8	P	320	IWJ	C03-C02	2.55	1.36	1.33
3	R	306	CLA	CMB-C2B	-2.55	1.46	1.51
3	R	317	CLA	CMC-C2C	-2.55	1.45	1.50
3	Q	310	CLA	CMB-C2B	-2.55	1.46	1.51
6	R	304	Q6L	C12-C13	-2.54	1.46	1.51
5	P	308	KC2	C2A-C1A	2.54	1.52	1.44
8	R	303	IWJ	C03-C02	2.54	1.36	1.33
6	Q	317	Q6L	C02-C03	2.53	1.37	1.34
6	Q	317	Q6L	C12-C13	-2.52	1.46	1.51
6	R	319	Q6L	C34-C33	2.52	1.53	1.50
3	Q	302	CLA	C3B-C2B	-2.52	1.36	1.40
6	P	321	Q6L	C12-C13	-2.51	1.46	1.51
3	Q	302	CLA	CAA-C2A	-2.51	1.49	1.54
4	R	311	CHL	C4D-ND	-2.51	1.34	1.37
4	P	307	CHL	CMB-C2B	-2.50	1.46	1.51
4	P	314	CHL	C1D-ND	2.49	1.40	1.37
5	Q	308	KC2	CHD-C4C	2.49	1.41	1.35
5	Q	308	KC2	C1B-C2B	2.49	1.50	1.45
6	R	304	Q6L	C02-C03	2.49	1.37	1.34
6	R	301	Q6L	C33-C32	2.49	1.36	1.33
3	P	302	CLA	C3B-CAB	-2.48	1.42	1.47
3	R	314	CLA	CMB-C2B	-2.48	1.46	1.51
3	Q	311	CLA	CMB-C2B	-2.47	1.46	1.51
6	Q	316	Q6L	C34-C33	2.47	1.53	1.50
8	Q	319	IWJ	C03-C02	2.47	1.36	1.33
4	P	306	CHL	CMB-C2B	-2.46	1.46	1.51
6	Q	318	Q6L	C12-C13	-2.46	1.46	1.51
3	P	302	CLA	CMB-C2B	-2.46	1.46	1.51
5	Q	308	KC2	O2A-CGA	2.46	1.36	1.30
5	Q	308	KC2	CMC-C2C	-2.45	1.45	1.50
6	Q	318	Q6L	C02-C03	2.44	1.37	1.34
3	P	301	CLA	CMB-C2B	-2.43	1.46	1.51
3	R	315	CLA	C4D-ND	-2.43	1.34	1.37
3	P	309	CLA	CMB-C2B	-2.43	1.46	1.51
6	P	319	Q6L	C34-C33	2.42	1.53	1.50
5	P	308	KC2	CMC-C2C	-2.42	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	R	304	Q6L	C33-C32	2.41	1.36	1.33
6	R	320	Q6L	C02-C03	2.41	1.37	1.34
3	P	310	CLA	CMB-C2B	-2.41	1.46	1.51
5	P	308	KC2	CMB-C2B	-2.40	1.45	1.50
7	Q	315	NEX	C38-C25	2.39	1.55	1.51
5	P	308	KC2	O2A-CGA	2.38	1.36	1.30
4	P	306	CHL	CMD-C2D	-2.37	1.45	1.50
6	P	319	Q6L	C01-C02	2.37	1.54	1.50
7	R	321	NEX	C28-C29	2.37	1.51	1.45
6	P	316	Q6L	C33-C32	2.37	1.36	1.33
5	R	312	KC2	MG-NB	-2.37	2.01	2.05
3	Q	313	CLA	CMB-C2B	-2.37	1.46	1.51
3	P	303	CLA	CMB-C2B	-2.36	1.46	1.51
4	R	318	CHL	CMD-C2D	-2.36	1.45	1.50
6	R	319	Q6L	C01-C02	2.36	1.54	1.50
6	P	315	Q6L	C02-C03	2.35	1.37	1.34
6	R	323	Q6L	C01-C02	2.34	1.54	1.50
8	Q	319	IWJ	C29-C35	-2.34	1.52	1.56
6	P	321	Q6L	C01-C02	2.33	1.54	1.50
6	R	304	Q6L	C01-C02	2.33	1.54	1.50
3	R	307	CLA	C3B-C2B	-2.33	1.37	1.40
6	P	315	Q6L	C01-C02	2.33	1.54	1.50
3	R	306	CLA	C3B-C2B	-2.33	1.37	1.40
5	R	312	KC2	O2A-CGA	2.33	1.36	1.30
5	R	312	KC2	CMB-C2B	-2.33	1.45	1.50
7	R	321	NEX	C32-C33	2.32	1.50	1.45
3	P	312	CLA	CMB-C2B	-2.32	1.46	1.51
6	P	321	Q6L	C34-C33	2.31	1.53	1.50
7	R	321	NEX	C12-C13	2.31	1.50	1.45
8	R	303	IWJ	C29-C35	-2.30	1.52	1.56
4	Q	307	CHL	CMD-C2D	-2.30	1.45	1.50
3	P	311	CLA	CMB-C2B	-2.30	1.46	1.51
7	P	317	NEX	C28-C29	2.30	1.50	1.45
5	P	308	KC2	CHD-C4C	2.30	1.40	1.35
4	R	311	CHL	CMC-C2C	2.30	1.50	1.45
6	P	319	Q6L	C12-C13	-2.29	1.46	1.51
6	Q	316	Q6L	C02-C03	2.29	1.37	1.34
3	Q	302	CLA	C4B-CHC	-2.29	1.34	1.41
4	Q	306	CHL	MG-ND	-2.29	2.01	2.05
4	R	302	CHL	CMB-C2B	-2.28	1.46	1.51
3	Q	311	CLA	CMD-C2D	-2.27	1.46	1.50
8	R	322	IWJ	C29-C35	-2.27	1.52	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	314	CLA	C3B-C2B	-2.27	1.37	1.40
3	R	313	CLA	CMB-C2B	-2.26	1.46	1.51
7	P	317	NEX	C32-C33	2.26	1.50	1.45
6	P	316	Q6L	C01-C02	2.25	1.54	1.50
3	Q	302	CLA	CMB-C2B	-2.25	1.47	1.51
4	R	310	CHL	CMB-C2B	-2.25	1.47	1.51
3	P	301	CLA	C3B-C2B	-2.24	1.37	1.40
3	Q	309	CLA	CMB-C2B	-2.24	1.47	1.51
7	Q	315	NEX	C32-C33	2.24	1.50	1.45
4	P	314	CHL	CMB-C2B	-2.24	1.47	1.51
6	P	321	Q6L	C33-C32	2.23	1.35	1.33
8	P	320	IWJ	C29-C35	-2.23	1.53	1.56
3	Q	311	CLA	C3B-C2B	-2.23	1.37	1.40
6	Q	317	Q6L	C34-C33	2.23	1.53	1.50
8	P	318	IWJ	C26-C24	-2.22	1.45	1.49
3	Q	309	CLA	C3B-C2B	-2.21	1.37	1.40
7	P	317	NEX	C35-C15	-2.20	1.30	1.36
4	P	306	CHL	CHC-C1C	2.19	1.40	1.35
3	Q	311	CLA	C4B-CHC	-2.18	1.34	1.41
6	P	315	Q6L	C33-C32	2.18	1.35	1.33
3	R	307	CLA	CMD-C2D	-2.18	1.46	1.50
4	Q	314	CHL	CMB-C2B	-2.18	1.47	1.51
3	R	317	CLA	CMB-C2B	-2.18	1.47	1.51
6	R	323	Q6L	C33-C32	2.18	1.35	1.33
4	P	305	CHL	CMD-C2D	-2.18	1.46	1.50
6	P	321	Q6L	C02-C03	2.17	1.37	1.34
4	P	305	CHL	CMB-C2B	-2.17	1.47	1.51
6	R	320	Q6L	C33-C32	2.16	1.35	1.33
6	R	319	Q6L	C33-C32	2.16	1.35	1.33
6	Q	318	Q6L	C01-C02	2.16	1.54	1.50
3	Q	310	CLA	CMD-C2D	-2.16	1.46	1.50
6	Q	317	Q6L	C01-C02	2.16	1.54	1.50
3	Q	302	CLA	CMA-C3A	-2.15	1.48	1.53
4	P	304	CHL	MG-ND	-2.15	2.01	2.05
3	Q	313	CLA	CMD-C2D	-2.15	1.46	1.50
4	P	314	CHL	CMD-C2D	-2.15	1.46	1.50
4	R	308	CHL	MG-ND	-2.15	2.01	2.05
8	Q	301	IWJ	O39-C29	-2.14	1.39	1.43
3	Q	304	CLA	MG-ND	-2.13	2.01	2.05
6	P	321	Q6L	C29-C27	2.13	1.50	1.45
3	Q	309	CLA	C3B-CAB	-2.12	1.43	1.47
4	P	306	CHL	C4B-CHC	-2.12	1.35	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	P	316	Q6L	C29-C27	2.12	1.50	1.45
4	R	318	CHL	CMB-C2B	-2.11	1.47	1.51
7	R	321	NEX	C35-C15	-2.11	1.30	1.36
3	R	315	CLA	CMD-C2D	-2.11	1.46	1.50
6	P	315	Q6L	C11-C03	-2.11	1.48	1.51
7	Q	315	NEX	C35-C15	-2.11	1.30	1.36
6	Q	316	Q6L	C01-C02	2.10	1.54	1.50
7	R	321	NEX	C22-C21	-2.10	1.51	1.54
5	P	308	KC2	CHB-C1B	2.10	1.42	1.38
8	R	303	IWJ	O39-C29	-2.10	1.39	1.43
7	P	317	NEX	C22-C21	-2.09	1.51	1.54
4	R	310	CHL	MG-ND	-2.09	2.01	2.05
3	Q	303	CLA	C4B-CHC	-2.09	1.35	1.41
6	R	320	Q6L	C01-C02	2.09	1.54	1.50
6	R	301	Q6L	C02-C03	2.09	1.37	1.34
7	Q	315	NEX	C1-C6	-2.08	1.51	1.54
4	P	306	CHL	CMC-C2C	2.08	1.49	1.45
3	Q	304	CLA	C3B-C2B	-2.08	1.37	1.40
3	Q	313	CLA	CMC-C2C	-2.08	1.46	1.50
4	P	307	CHL	CMC-C2C	2.08	1.49	1.45
3	Q	310	CLA	C3B-C2B	-2.07	1.37	1.40
4	R	311	CHL	C2C-C3C	2.07	1.41	1.36
5	R	312	KC2	C1B-C2B	2.07	1.49	1.45
5	P	308	KC2	C1B-C2B	2.06	1.49	1.45
4	P	307	CHL	CMD-C2D	-2.06	1.46	1.50
4	R	310	CHL	CMC-C2C	2.06	1.49	1.45
7	R	321	NEX	O24-C25	-2.06	1.43	1.46
3	R	306	CLA	CMC-C2C	-2.06	1.46	1.50
3	R	313	CLA	CAA-C2A	-2.06	1.50	1.54
4	R	309	CHL	CMB-C2B	-2.05	1.47	1.51
3	P	301	CLA	CMD-C2D	-2.05	1.46	1.50
3	Q	302	CLA	CMD-C2D	-2.04	1.46	1.50
3	Q	312	CLA	C3B-CAB	-2.03	1.43	1.47
4	R	309	CHL	OBD-CAD	-2.03	1.19	1.22
5	Q	308	KC2	CMB-C2B	-2.03	1.46	1.50
3	P	313	CLA	C3B-C2B	-2.03	1.37	1.40
3	R	317	CLA	C4B-CHC	-2.03	1.35	1.41
8	P	320	IWJ	C26-C24	-2.03	1.45	1.49
5	P	308	KC2	MG-NB	-2.03	2.01	2.05
3	R	315	CLA	C3B-C2B	-2.03	1.37	1.40
3	Q	303	CLA	C3B-C2B	-2.03	1.37	1.40
3	P	302	CLA	CMD-C2D	-2.02	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	310	CLA	C3B-C2B	-2.02	1.37	1.40
6	R	301	Q6L	C01-C02	2.02	1.54	1.50
4	P	304	CHL	CMD-C2D	-2.02	1.46	1.50
3	R	313	CLA	MG-NA	2.01	2.11	2.06
3	R	305	CLA	CMB-C2B	-2.00	1.47	1.51
4	R	302	CHL	CMA-C3A	-2.00	1.48	1.53
3	P	311	CLA	C3D-C4D	2.00	1.48	1.44

All (610) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	R	321	NEX	O24-C25-C24	13.41	123.46	113.38
7	Q	315	NEX	O24-C25-C24	10.78	121.48	113.38
7	P	317	NEX	O24-C25-C24	10.32	121.14	113.38
5	P	308	KC2	C1A-NA-C4A	8.78	110.65	106.71
5	P	308	KC2	CMA-C3A-C2A	-8.68	107.06	128.30
5	R	312	KC2	C1A-NA-C4A	8.43	110.50	106.71
3	Q	302	CLA	C4A-NA-C1A	8.05	110.32	106.71
5	P	308	KC2	CMA-C3A-C4A	-7.40	113.77	125.04
5	Q	308	KC2	CMA-C3A-C4A	-7.30	113.92	125.04
6	R	323	Q6L	C11-C12-C13	7.18	133.09	112.69
5	Q	308	KC2	C1A-NA-C4A	7.11	109.90	106.71
6	R	301	Q6L	C11-C12-C13	7.10	132.87	112.69
7	P	317	NEX	C16-C1-C6	7.05	116.78	110.47
5	Q	308	KC2	C2A-C3A-C4A	-6.78	101.45	106.49
6	Q	316	Q6L	C11-C12-C13	6.65	131.59	112.69
6	P	321	Q6L	C11-C12-C13	6.59	131.41	112.69
4	P	305	CHL	C4A-NA-C1A	6.56	109.65	106.71
4	P	307	CHL	CMB-C2B-C1B	-6.43	118.58	128.46
3	R	316	CLA	C4A-NA-C1A	6.37	109.57	106.71
5	R	312	KC2	CMA-C3A-C2A	-6.28	112.93	128.30
3	Q	311	CLA	C4A-NA-C1A	6.27	109.52	106.71
6	R	319	Q6L	C11-C12-C13	6.24	130.41	112.69
6	P	319	Q6L	C11-C12-C13	6.13	130.11	112.69
6	Q	318	Q6L	C11-C12-C13	5.90	129.45	112.69
4	Q	306	CHL	CMB-C2B-C1B	-5.86	119.46	128.46
6	R	304	Q6L	C11-C12-C13	5.80	129.18	112.69
4	P	304	CHL	C4A-NA-C1A	5.57	109.21	106.71
6	Q	317	Q6L	C11-C12-C13	5.56	128.48	112.69
3	Q	304	CLA	CMB-C2B-C1B	-5.54	119.94	128.46
3	R	316	CLA	C4-C3-C5	5.49	124.50	115.27
5	R	312	KC2	CMA-C3A-C4A	-5.45	116.74	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	P	315	Q6L	C11-C12-C13	5.44	128.15	112.69
4	R	311	CHL	CMB-C2B-C1B	-5.36	120.22	128.46
3	R	315	CLA	C4A-NA-C1A	5.36	109.12	106.71
3	Q	312	CLA	C4A-NA-C1A	5.29	109.08	106.71
3	Q	313	CLA	C4A-NA-C1A	5.27	109.08	106.71
4	Q	306	CHL	C4A-NA-C1A	5.21	109.05	106.71
4	R	310	CHL	C4-C3-C5	5.19	121.91	115.98
4	Q	305	CHL	CMB-C2B-C1B	-5.05	120.70	128.46
3	P	312	CLA	C4A-NA-C1A	5.05	108.97	106.71
7	Q	315	NEX	C26-C27-C28	-5.04	115.33	125.99
4	Q	307	CHL	CMB-C2B-C1B	-5.03	120.73	128.46
3	P	309	CLA	C4A-NA-C1A	5.02	108.96	106.71
5	R	312	KC2	C1A-C2A-C3A	-4.97	103.17	107.11
6	P	316	Q6L	C40-C32-C33	-4.96	112.95	123.56
3	R	313	CLA	CMB-C2B-C1B	-4.96	120.85	128.46
3	P	301	CLA	C4A-NA-C1A	4.94	108.93	106.71
3	P	311	CLA	C4A-NA-C1A	4.92	108.92	106.71
5	Q	308	KC2	CMA-C3A-C2A	-4.90	116.31	128.30
4	P	305	CHL	CMB-C2B-C1B	-4.88	120.96	128.46
5	R	312	KC2	CMD-C2D-C1D	-4.85	121.01	128.46
7	R	321	NEX	C26-C27-C28	-4.82	115.81	125.99
3	R	317	CLA	C4A-NA-C1A	4.80	108.87	106.71
5	Q	308	KC2	CHB-C4A-C3A	-4.80	117.48	124.98
6	P	319	Q6L	C40-C32-C33	-4.66	113.58	123.56
5	R	312	KC2	CMD-C2D-C3D	4.66	133.40	124.68
6	R	304	Q6L	C40-C32-C33	-4.65	113.61	123.56
3	R	305	CLA	C4A-NA-C1A	4.65	108.80	106.71
3	Q	304	CLA	CHD-C1D-ND	-4.65	120.18	124.45
7	Q	315	NEX	C28-C29-C30	4.63	126.04	118.94
4	P	306	CHL	C1C-C2C-C3C	-4.62	103.45	107.11
3	R	317	CLA	CMB-C2B-C1B	-4.62	121.37	128.46
4	R	309	CHL	CMB-C2B-C1B	-4.60	121.40	128.46
3	R	316	CLA	CMB-C2B-C1B	-4.59	121.41	128.46
7	P	317	NEX	C28-C29-C30	4.55	125.92	118.94
3	Q	304	CLA	C4D-C3D-CAD	-4.54	102.75	108.10
7	P	317	NEX	C26-C27-C28	-4.53	116.42	125.99
3	Q	302	CLA	O2A-CGA-O1A	-4.49	112.25	123.59
3	R	307	CLA	CMB-C2B-C1B	-4.48	121.58	128.46
4	P	305	CHL	CED-O2D-CGD	4.47	126.05	115.94
8	R	303	IWJ	C01-C02-C03	-4.46	114.03	123.56
3	P	303	CLA	CMB-C2B-C1B	-4.44	121.64	128.46
4	P	304	CHL	CMB-C2B-C1B	-4.44	121.64	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	P	307	CHL	CMB-C2B-C3B	4.39	132.90	124.68
4	Q	306	CHL	CHB-C4A-NA	4.39	130.58	124.51
3	Q	313	CLA	CMB-C2B-C1B	-4.39	121.72	128.46
3	P	302	CLA	C4A-NA-C1A	4.38	108.67	106.71
6	Q	318	Q6L	C05-C06-C07	4.38	116.30	110.30
4	Q	307	CHL	C4A-NA-C1A	4.37	108.67	106.71
3	P	301	CLA	C4-C3-C5	4.35	122.59	115.27
7	Q	315	NEX	C19-C9-C10	4.34	129.01	122.92
6	P	321	Q6L	C40-C32-C33	-4.34	114.28	123.56
4	P	304	CHL	CMB-C2B-C3B	4.32	132.76	124.68
6	P	316	Q6L	C11-C12-C13	4.26	124.81	112.69
8	Q	301	IWJ	C01-C02-C03	-4.26	114.44	123.56
7	R	321	NEX	C28-C29-C30	4.26	125.47	118.94
8	P	320	IWJ	C01-C02-C03	-4.25	114.47	123.56
3	Q	304	CLA	CMB-C2B-C3B	4.23	132.59	124.68
7	R	321	NEX	C19-C9-C10	4.22	128.83	122.92
6	R	301	Q6L	C40-C32-C33	-4.21	114.54	123.56
3	R	307	CLA	C4A-NA-C1A	4.21	108.60	106.71
3	R	314	CLA	C4A-NA-C1A	4.21	108.60	106.71
5	P	308	KC2	C1A-C2A-C3A	-4.21	103.77	107.11
6	R	320	Q6L	C11-C12-C13	4.21	124.64	112.69
3	Q	302	CLA	CHB-C4A-NA	4.20	130.32	124.51
5	Q	308	KC2	CBA-CAA-C2A	-4.17	109.36	125.27
7	Q	315	NEX	C16-C1-C6	4.14	114.18	110.47
3	R	313	CLA	CMB-C2B-C3B	4.14	132.42	124.68
4	Q	306	CHL	CMB-C2B-C3B	4.13	132.41	124.68
4	Q	305	CHL	CMB-C2B-C3B	4.13	132.41	124.68
4	R	318	CHL	CMB-C2B-C1B	-4.08	122.19	128.46
3	R	315	CLA	O2D-CGD-O1D	-4.08	115.86	123.84
6	R	320	Q6L	C40-C32-C33	-4.07	114.85	123.56
4	Q	306	CHL	C2D-C1D-ND	-4.07	107.11	110.10
3	P	303	CLA	CMB-C2B-C3B	4.05	132.26	124.68
8	Q	319	IWJ	C01-C02-C03	-4.05	114.89	123.56
7	P	317	NEX	O24-C25-C38	4.03	119.89	115.06
4	P	305	CHL	C1B-CHB-C4A	-4.03	122.13	130.12
3	R	314	CLA	O2D-CGD-O1D	-4.03	115.96	123.84
4	P	314	CHL	CMB-C2B-C1B	-4.00	122.31	128.46
8	R	322	IWJ	C01-C02-C03	-4.00	115.00	123.56
3	P	311	CLA	CMB-C2B-C1B	-4.00	122.32	128.46
7	P	317	NEX	C38-C25-C26	-4.00	115.56	122.26
3	R	306	CLA	C4A-NA-C1A	3.98	108.50	106.71
4	P	304	CHL	C1B-CHB-C4A	-3.96	122.28	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	Q	305	CHL	CHB-C4A-NA	3.95	129.97	124.51
6	R	319	Q6L	C40-C32-C33	-3.94	115.13	123.56
3	Q	302	CLA	C1B-CHB-C4A	-3.94	122.32	130.12
3	Q	310	CLA	O2D-CGD-O1D	-3.89	116.23	123.84
3	R	317	CLA	CMB-C2B-C3B	3.89	131.95	124.68
4	P	314	CHL	C4A-NA-C1A	3.86	108.44	106.71
3	Q	311	CLA	CHB-C4A-NA	3.85	129.83	124.51
8	P	318	IWJ	C01-C02-C03	-3.82	115.38	123.56
6	Q	317	Q6L	C40-C32-C33	-3.80	115.42	123.56
6	R	323	Q6L	C40-C32-C33	-3.80	115.44	123.56
3	P	312	CLA	CMB-C2B-C1B	-3.78	122.65	128.46
4	Q	314	CHL	CMB-C2B-C1B	-3.78	122.65	128.46
3	Q	303	CLA	CMB-C2B-C1B	-3.76	122.68	128.46
4	R	302	CHL	CMB-C2B-C1B	-3.76	122.69	128.46
3	R	307	CLA	CMB-C2B-C3B	3.75	131.69	124.68
4	P	306	CHL	C2C-C3C-C4C	3.75	109.16	106.49
4	P	306	CHL	C4A-NA-C1A	3.73	108.38	106.71
3	P	310	CLA	CMB-C2B-C1B	-3.73	122.74	128.46
7	P	317	NEX	C39-C29-C30	-3.72	117.71	122.92
3	R	305	CLA	C1B-CHB-C4A	-3.71	122.77	130.12
6	Q	316	Q6L	C40-C32-C33	-3.70	115.65	123.56
3	P	301	CLA	C1B-CHB-C4A	-3.70	122.80	130.12
3	P	309	CLA	O2D-CGD-O1D	-3.69	116.62	123.84
4	R	318	CHL	O2D-CGD-O1D	-3.68	116.64	123.84
6	Q	318	Q6L	C40-C32-C33	-3.68	115.69	123.56
7	R	321	NEX	C39-C29-C30	-3.68	117.78	122.92
3	P	309	CLA	CMB-C2B-C1B	-3.67	122.82	128.46
4	R	310	CHL	CHB-C4A-NA	3.66	129.57	124.51
3	P	309	CLA	O2D-CGD-CBD	3.66	117.77	111.27
5	Q	308	KC2	CMD-C2D-C1D	-3.65	122.86	128.46
3	P	302	CLA	O2D-CGD-O1D	-3.61	116.78	123.84
3	R	306	CLA	C1B-CHB-C4A	-3.61	122.97	130.12
3	R	305	CLA	C1D-ND-C4D	-3.61	103.77	106.33
4	P	306	CHL	CMB-C2B-C1B	-3.59	122.94	128.46
4	R	318	CHL	C1B-CHB-C4A	-3.59	123.01	130.12
6	R	323	Q6L	C35-C34-C33	3.59	115.82	111.74
4	R	308	CHL	C1B-CHB-C4A	-3.56	123.06	130.12
3	P	310	CLA	C4A-NA-C1A	3.56	108.31	106.71
4	R	302	CHL	C2C-C3C-C4C	3.55	109.02	106.49
3	Q	313	CLA	CMB-C2B-C3B	3.55	131.33	124.68
4	R	310	CHL	CMB-C2B-C1B	-3.55	123.00	128.46
4	R	309	CHL	C4A-NA-C1A	3.55	108.30	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	P	306	CHL	CHB-C4A-NA	3.54	129.40	124.51
3	R	315	CLA	CMB-C2B-C1B	-3.52	123.05	128.46
3	P	311	CLA	CMB-C2B-C3B	3.52	131.26	124.68
3	R	307	CLA	CHD-C1D-ND	-3.51	121.22	124.45
4	R	302	CHL	C4A-NA-C1A	3.49	108.28	106.71
3	P	312	CLA	O2A-C1-C2	3.49	117.81	108.64
3	P	309	CLA	CHB-C4A-NA	3.49	129.33	124.51
4	R	318	CHL	C4A-NA-C1A	3.48	108.27	106.71
5	P	308	KC2	CBA-CAA-C2A	-3.47	112.03	125.27
3	P	310	CLA	CMB-C2B-C3B	3.47	131.17	124.68
3	P	312	CLA	CHD-C1D-ND	-3.46	121.27	124.45
3	R	316	CLA	CMB-C2B-C3B	3.45	131.14	124.68
3	P	301	CLA	CMB-C2B-C1B	-3.45	123.17	128.46
3	Q	312	CLA	C4-C3-C5	3.44	121.06	115.27
3	P	309	CLA	CHD-C1D-ND	-3.43	121.30	124.45
4	R	310	CHL	C2D-C1D-ND	-3.43	107.58	110.10
4	R	308	CHL	CMB-C2B-C1B	-3.42	123.20	128.46
4	R	309	CHL	CMB-C2B-C3B	3.42	131.08	124.68
4	R	310	CHL	C1B-CHB-C4A	-3.41	123.37	130.12
6	P	315	Q6L	C40-C32-C33	-3.41	116.27	123.56
3	P	312	CLA	CMB-C2B-C3B	3.40	131.04	124.68
3	P	302	CLA	C1B-CHB-C4A	-3.39	123.41	130.12
4	R	311	CHL	C1C-C2C-C3C	-3.37	104.44	107.11
4	Q	305	CHL	O2D-CGD-O1D	-3.36	117.26	123.84
3	P	309	CLA	C4-C3-C5	3.36	120.93	115.27
4	P	306	CHL	C1B-CHB-C4A	-3.36	123.47	130.12
3	P	311	CLA	C4-C3-C2	-3.35	115.08	123.68
6	P	315	Q6L	C05-C06-C07	3.35	114.89	110.30
3	Q	310	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
3	R	306	CLA	CMB-C2B-C1B	-3.34	123.34	128.46
3	Q	303	CLA	C2D-C1D-ND	-3.33	107.65	110.10
3	P	303	CLA	C4A-NA-C1A	3.32	108.20	106.71
3	P	303	CLA	CHD-C1D-ND	-3.32	121.40	124.45
3	R	314	CLA	CMB-C2B-C1B	-3.31	123.37	128.46
3	P	309	CLA	C1B-CHB-C4A	-3.31	123.56	130.12
5	P	308	KC2	O2D-CGD-O1D	-3.31	117.37	123.84
4	R	302	CHL	CHB-C4A-NA	3.30	129.08	124.51
4	P	307	CHL	CHB-C4A-NA	3.29	129.07	124.51
4	P	307	CHL	C2C-C3C-C4C	3.29	108.84	106.49
4	Q	307	CHL	CMB-C2B-C3B	3.29	130.84	124.68
3	Q	313	CLA	C1-O2A-CGA	3.28	125.06	116.44
3	Q	311	CLA	CMB-C2B-C1B	-3.28	123.42	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	Q	302	CLA	CMB-C2B-C3B	3.28	130.82	124.68
3	P	313	CLA	C4A-NA-C1A	3.28	108.18	106.71
5	Q	308	KC2	CMD-C2D-C3D	3.28	130.81	124.68
3	Q	309	CLA	C1B-CHB-C4A	-3.27	123.63	130.12
3	R	313	CLA	C1B-CHB-C4A	-3.27	123.64	130.12
3	P	309	CLA	CMB-C2B-C3B	3.27	130.80	124.68
6	P	319	Q6L	C20-C21-C22	3.27	131.98	127.31
4	R	302	CHL	C1B-CHB-C4A	-3.27	123.64	130.12
4	P	305	CHL	CMB-C2B-C3B	3.26	130.78	124.68
5	R	312	KC2	CBA-CAA-C2A	-3.26	112.83	125.27
4	Q	314	CHL	C4A-NA-C1A	3.26	108.17	106.71
6	R	301	Q6L	C42-C13-C12	3.26	120.75	115.27
3	P	310	CLA	O2D-CGD-O1D	-3.25	117.48	123.84
5	P	308	KC2	CHB-C1B-NB	3.25	127.44	124.45
4	Q	314	CHL	O2D-CGD-O1D	-3.25	117.49	123.84
3	Q	309	CLA	O2D-CGD-O1D	-3.20	117.58	123.84
4	P	314	CHL	C1B-CHB-C4A	-3.20	123.78	130.12
4	R	309	CHL	O2D-CGD-O1D	-3.19	117.60	123.84
3	P	301	CLA	CHB-C4A-NA	3.19	128.92	124.51
7	Q	315	NEX	C11-C10-C9	-3.18	122.77	127.31
3	Q	303	CLA	C4A-NA-C1A	3.18	108.14	106.71
4	R	302	CHL	C1C-C2C-C3C	-3.18	104.59	107.11
5	Q	308	KC2	O2D-CGD-O1D	-3.17	117.63	123.84
6	R	301	Q6L	C12-C13-C14	-3.17	112.38	121.98
3	P	301	CLA	CMB-C2B-C3B	3.17	130.60	124.68
3	Q	304	CLA	C1B-CHB-C4A	-3.16	123.85	130.12
3	R	305	CLA	CBA-CAA-C2A	3.16	123.19	113.86
3	P	313	CLA	CMB-C2B-C1B	-3.16	123.61	128.46
3	P	310	CLA	C1B-CHB-C4A	-3.16	123.86	130.12
7	Q	315	NEX	C39-C29-C30	-3.16	118.50	122.92
3	Q	304	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
4	Q	307	CHL	C1B-CHB-C4A	-3.15	123.88	130.12
4	Q	307	CHL	CHB-C4A-NA	3.15	128.86	124.51
4	P	307	CHL	C1C-C2C-C3C	-3.14	104.62	107.11
3	Q	309	CLA	CMB-C2B-C3B	3.13	130.53	124.68
4	R	308	CHL	C1C-C2C-C3C	-3.12	104.64	107.11
3	Q	313	CLA	O2A-CGA-O1A	-3.12	115.72	123.59
3	R	313	CLA	O2D-CGD-CBD	3.12	116.81	111.27
4	R	311	CHL	CMB-C2B-C3B	3.12	130.51	124.68
4	P	307	CHL	C1B-CHB-C4A	-3.11	123.95	130.12
3	P	303	CLA	CHB-C4A-NA	3.11	128.81	124.51
4	Q	305	CHL	C1B-CHB-C4A	-3.10	123.97	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	P	307	CHL	CBA-CAA-C2A	3.10	120.57	114.02
3	R	314	CLA	CMB-C2B-C3B	3.10	130.48	124.68
4	Q	314	CHL	C1B-CHB-C4A	-3.10	123.98	130.12
6	Q	317	Q6L	C06-C07-C02	3.09	118.02	111.85
3	Q	311	CLA	CMB-C2B-C3B	3.09	130.46	124.68
4	R	308	CHL	CMB-C2B-C3B	3.09	130.45	124.68
3	P	303	CLA	C1B-CHB-C4A	-3.08	124.01	130.12
5	R	312	KC2	O2D-CGD-O1D	-3.08	117.81	123.84
3	R	314	CLA	C1B-CHB-C4A	-3.08	124.01	130.12
5	P	308	KC2	CHB-C4A-NA	3.08	129.06	124.20
3	P	302	CLA	CHB-C4A-NA	3.08	128.77	124.51
3	R	305	CLA	CHB-C4A-NA	3.08	128.76	124.51
6	Q	317	Q6L	C05-C06-C07	3.07	114.51	110.30
3	Q	302	CLA	CMB-C2B-C1B	-3.05	123.77	128.46
3	Q	303	CLA	CMB-C2B-C3B	3.05	130.39	124.68
3	P	313	CLA	C1B-CHB-C4A	-3.05	124.07	130.12
3	P	312	CLA	C1B-CHB-C4A	-3.05	124.08	130.12
3	R	314	CLA	CHB-C4A-NA	3.05	128.73	124.51
3	P	313	CLA	CHD-C1D-ND	-3.04	121.66	124.45
3	R	317	CLA	CHD-C1D-ND	-3.03	121.67	124.45
6	Q	317	Q6L	C23-C22-C21	3.03	127.16	122.92
6	Q	316	Q6L	C42-C13-C12	3.03	120.36	115.27
7	Q	315	NEX	C12-C13-C14	-3.03	114.30	118.94
3	Q	309	CLA	C4A-NA-C1A	3.03	108.07	106.71
3	R	306	CLA	CHB-C4A-NA	3.02	128.69	124.51
3	Q	312	CLA	C1B-CHB-C4A	-3.02	124.13	130.12
5	Q	308	KC2	CBD-CHA-C1A	3.02	134.52	128.88
6	R	323	Q6L	C42-C13-C12	3.01	120.34	115.27
4	R	308	CHL	CHB-C4A-NA	3.01	128.68	124.51
6	R	301	Q6L	C05-C06-C07	3.01	114.42	110.30
7	Q	315	NEX	O24-C25-C38	3.01	118.66	115.06
7	P	317	NEX	C11-C10-C9	-3.00	123.03	127.31
3	Q	309	CLA	CMB-C2B-C1B	-2.99	123.87	128.46
3	P	311	CLA	O2A-CGA-O1A	-2.98	116.07	123.59
4	P	314	CHL	CHB-C4A-NA	2.98	128.63	124.51
3	R	314	CLA	O2D-CGD-CBD	2.97	116.55	111.27
3	R	316	CLA	CBA-CAA-C2A	2.97	122.64	113.86
4	R	318	CHL	CMB-C2B-C3B	2.97	130.24	124.68
3	R	306	CLA	CMB-C2B-C3B	2.96	130.22	124.68
4	R	310	CHL	C1C-C2C-C3C	-2.96	104.76	107.11
5	Q	308	KC2	CHB-C4A-NA	2.96	128.87	124.20
6	R	320	Q6L	C35-C34-C33	2.96	115.11	111.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	R	321	NEX	C16-C1-C6	2.96	113.12	110.47
3	Q	311	CLA	C1B-CHB-C4A	-2.96	124.26	130.12
3	R	316	CLA	C5-C3-C2	-2.95	115.14	121.12
3	Q	310	CLA	C1B-CHB-C4A	-2.95	124.27	130.12
3	P	310	CLA	O2A-CGA-O1A	-2.95	116.16	123.59
3	Q	309	CLA	CHB-C4A-NA	2.94	128.58	124.51
7	P	317	NEX	C40-C33-C32	2.94	122.72	118.08
3	Q	303	CLA	C1B-CHB-C4A	-2.94	124.29	130.12
3	P	302	CLA	CMB-C2B-C3B	2.94	130.17	124.68
4	P	304	CHL	CMA-C3A-C4A	2.93	119.64	111.77
3	R	317	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
3	P	302	CLA	CMB-C2B-C1B	-2.92	123.98	128.46
3	Q	310	CLA	CMB-C2B-C3B	2.92	130.13	124.68
4	R	309	CHL	C1C-C2C-C3C	-2.92	104.80	107.11
4	R	302	CHL	O2D-CGD-O1D	-2.91	118.14	123.84
6	R	323	Q6L	C12-C13-C14	-2.91	113.16	121.98
3	R	317	CLA	C1B-CHB-C4A	-2.91	124.35	130.12
3	P	310	CLA	CHD-C1D-ND	-2.91	121.78	124.45
3	Q	303	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
7	P	317	NEX	C20-C13-C12	2.89	122.63	118.08
7	Q	315	NEX	C15-C35-C34	-2.88	117.56	123.47
3	P	301	CLA	CMC-C2C-C1C	2.88	129.43	125.04
3	Q	313	CLA	C1B-CHB-C4A	-2.88	124.42	130.12
7	R	321	NEX	C38-C25-C26	-2.87	117.45	122.26
3	Q	312	CLA	CMB-C2B-C3B	2.87	130.05	124.68
6	P	316	Q6L	C10-C04-C03	2.87	113.81	109.71
6	P	319	Q6L	C23-C22-C21	2.87	126.94	122.92
3	Q	311	CLA	CHD-C1D-ND	-2.86	121.82	124.45
4	R	310	CHL	CAC-C3C-C4C	2.86	128.52	124.81
3	R	313	CLA	CHD-C1D-ND	-2.86	121.83	124.45
3	Q	309	CLA	CBA-CAA-C2A	2.86	122.30	113.86
3	P	302	CLA	C4-C3-C5	2.85	120.06	115.27
3	P	311	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
4	R	318	CHL	CHB-C4A-NA	2.83	128.43	124.51
3	Q	309	CLA	C1-C2-C3	-2.83	121.14	126.04
4	P	307	CHL	C3C-C4C-NC	-2.83	107.40	110.57
3	R	316	CLA	CHB-C4A-NA	2.83	128.42	124.51
4	Q	307	CHL	OMC-CMC-C2C	-2.82	119.30	125.69
4	Q	306	CHL	C1B-CHB-C4A	-2.82	124.53	130.12
5	P	308	KC2	CHC-C4B-NB	2.82	127.05	124.45
3	R	313	CLA	O2A-CGA-O1A	-2.82	116.47	123.59
4	R	308	CHL	C4A-NA-C1A	2.81	107.97	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	R	310	CHL	CMB-C2B-C3B	2.81	129.94	124.68
3	P	310	CLA	CHB-C4A-NA	2.81	128.40	124.51
7	R	321	NEX	C11-C10-C9	-2.81	123.30	127.31
3	Q	309	CLA	O2D-CGD-CBD	2.80	116.25	111.27
4	P	314	CHL	CMB-C2B-C3B	2.79	129.91	124.68
4	P	306	CHL	C4-C3-C5	2.79	119.17	115.98
3	Q	309	CLA	CHD-C1D-ND	-2.78	121.89	124.45
5	P	308	KC2	CAA-C2A-C1A	-2.78	111.96	124.75
5	Q	308	KC2	O2A-CGA-O1A	-2.78	116.89	122.67
4	R	302	CHL	C3C-C4C-NC	-2.78	107.45	110.57
3	P	302	CLA	O2D-CGD-CBD	2.77	116.20	111.27
4	Q	314	CHL	CMB-C2B-C3B	2.77	129.87	124.68
3	R	305	CLA	CAA-CBA-CGA	2.76	121.32	113.25
7	R	321	NEX	C40-C33-C32	2.76	122.42	118.08
6	P	321	Q6L	C19-C18-C17	-2.75	123.38	127.31
3	R	305	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
5	P	308	KC2	CMD-C2D-C3D	2.75	129.81	124.68
4	R	310	CHL	C4A-NA-C1A	2.74	107.94	106.71
4	Q	307	CHL	O2D-CGD-O1D	-2.74	118.48	123.84
3	Q	304	CLA	CBA-CAA-C2A	2.74	121.94	113.86
7	P	317	NEX	C12-C13-C14	-2.73	114.76	118.94
3	Q	312	CLA	CHB-C4A-NA	2.73	128.28	124.51
3	P	302	CLA	CHD-C1D-ND	-2.73	121.95	124.45
3	R	306	CLA	CHD-C1D-ND	-2.73	121.95	124.45
3	R	315	CLA	O2A-CGA-O1A	-2.73	116.71	123.59
3	R	307	CLA	CHB-C4A-NA	2.72	128.27	124.51
4	P	304	CHL	O2D-CGD-O1D	-2.71	118.55	123.84
4	P	314	CHL	O2D-CGD-O1D	-2.71	118.55	123.84
3	R	307	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
4	P	304	CHL	CHB-C4A-NA	2.70	128.25	124.51
3	R	315	CLA	O2D-CGD-CBD	2.70	116.06	111.27
4	Q	306	CHL	C1C-C2C-C3C	-2.70	104.97	107.11
3	R	313	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
3	R	315	CLA	CMB-C2B-C3B	2.69	129.71	124.68
3	R	305	CLA	CMC-C2C-C1C	2.69	129.13	125.04
3	R	305	CLA	CMB-C2B-C3B	2.69	129.70	124.68
4	Q	306	CHL	C2C-C3C-C4C	2.68	108.40	106.49
4	P	306	CHL	O2D-CGD-O1D	-2.68	118.60	123.84
3	R	307	CLA	C1B-CHB-C4A	-2.67	124.82	130.12
4	R	311	CHL	C1B-CHB-C4A	-2.67	124.82	130.12
5	Q	308	KC2	C3A-C4A-NA	2.67	113.49	110.57
4	Q	305	CHL	O2D-CGD-CBD	2.67	116.00	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	R	309	CHL	O2A-CGA-O1A	-2.66	116.87	123.59
4	Q	314	CHL	CHB-C4A-NA	2.66	128.19	124.51
3	R	314	CLA	CHD-C1D-ND	-2.66	122.01	124.45
5	R	312	KC2	O1A-CGA-CBA	2.66	129.29	120.99
3	Q	310	CLA	C4A-NA-C1A	2.66	107.90	106.71
5	P	308	KC2	CMD-C2D-C1D	-2.65	124.39	128.46
6	P	316	Q6L	C01-C02-C07	-2.65	109.45	114.36
3	P	311	CLA	C4-C3-C5	2.65	119.72	115.27
8	Q	319	IWJ	O27-C26-C28	-2.64	116.29	121.66
4	P	305	CHL	C1C-C2C-C3C	-2.64	105.02	107.11
5	R	312	KC2	C4C-C3C-C2C	-2.64	105.02	107.11
5	R	312	KC2	CAA-C2A-C1A	-2.64	112.62	124.75
3	R	317	CLA	CHB-C4A-NA	2.64	128.16	124.51
4	R	302	CHL	CMB-C2B-C3B	2.63	129.61	124.68
3	P	313	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
3	P	313	CLA	CAA-C2A-C3A	-2.63	105.57	112.78
3	P	312	CLA	CHB-C4A-NA	2.63	128.15	124.51
4	P	307	CHL	O2D-CGD-O1D	-2.63	118.70	123.84
3	R	316	CLA	C1B-CHB-C4A	-2.61	124.95	130.12
3	Q	312	CLA	CMB-C2B-C1B	-2.61	124.46	128.46
3	Q	313	CLA	CHB-C4A-NA	2.60	128.11	124.51
3	Q	312	CLA	CBA-CAA-C2A	2.60	121.54	113.86
7	R	321	NEX	C20-C13-C12	2.59	122.17	118.08
3	Q	313	CLA	CHD-C1D-ND	-2.59	122.07	124.45
5	R	312	KC2	C2A-C3A-C4A	-2.59	104.56	106.49
3	P	313	CLA	CMB-C2B-C3B	2.59	129.52	124.68
3	P	311	CLA	CHB-C4A-NA	2.59	128.09	124.51
4	P	305	CHL	CHB-C4A-NA	2.59	128.09	124.51
3	R	313	CLA	C1D-ND-C4D	-2.58	104.50	106.33
3	R	315	CLA	CHB-C4A-NA	2.58	128.08	124.51
5	R	312	KC2	CAA-CBA-CGA	-2.58	114.01	127.26
3	Q	304	CLA	CGD-CBD-CAD	-2.58	102.39	110.73
5	P	308	KC2	CHB-C4A-C3A	-2.57	120.96	124.98
4	P	314	CHL	C1C-C2C-C3C	-2.57	105.08	107.11
6	R	323	Q6L	C10-C04-C03	-2.56	106.05	109.71
3	R	316	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
8	P	320	IWJ	C25-C24-C26	2.56	120.32	116.02
5	P	308	KC2	CAA-CBA-CGA	-2.56	114.11	127.26
3	R	305	CLA	CMB-C2B-C1B	-2.55	124.54	128.46
5	R	312	KC2	C3C-C2C-C1C	2.55	108.38	106.49
3	R	314	CLA	O2A-CGA-O1A	-2.55	117.17	123.59
8	P	320	IWJ	C21-C19-C18	-2.54	115.04	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	R	316	CLA	CHD-C1D-ND	-2.54	122.12	124.45
3	P	311	CLA	C1B-CHB-C4A	-2.54	125.09	130.12
3	P	311	CLA	CHD-C1D-ND	-2.53	122.12	124.45
7	R	321	NEX	C12-C13-C14	-2.53	115.05	118.94
4	R	309	CHL	C1B-CHB-C4A	-2.53	125.11	130.12
4	P	304	CHL	CBA-CAA-C2A	2.53	121.32	113.86
3	Q	313	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
4	P	306	CHL	C3C-C4C-NC	-2.51	107.75	110.57
3	P	312	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
7	Q	315	NEX	C15-C14-C13	-2.51	123.73	127.31
7	R	321	NEX	C15-C35-C34	-2.51	118.33	123.47
4	R	302	CHL	CAC-C3C-C4C	2.51	128.06	124.81
4	R	311	CHL	C2C-C3C-C4C	2.51	108.28	106.49
3	P	309	CLA	CAA-C2A-C3A	2.50	119.62	112.78
3	R	305	CLA	O2A-CGA-O1A	-2.50	117.28	123.59
5	P	308	KC2	C2B-C1B-NB	-2.50	108.27	110.10
6	R	320	Q6L	C19-C20-C21	-2.49	118.38	123.47
6	Q	318	Q6L	C01-C02-C07	-2.49	109.75	114.36
4	Q	306	CHL	C3C-C4C-NC	-2.48	107.80	110.57
3	P	302	CLA	C11-C12-C13	2.47	123.91	115.92
3	R	314	CLA	C1-O2A-CGA	2.47	122.92	116.44
3	P	303	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
3	P	309	CLA	CBA-CAA-C2A	2.46	121.13	113.86
4	R	311	CHL	C2D-C1D-ND	-2.46	108.29	110.10
7	P	317	NEX	C15-C35-C34	-2.46	118.44	123.47
4	P	304	CHL	C2A-C1A-CHA	2.46	128.16	123.86
5	R	312	KC2	CHC-C4B-NB	2.46	126.71	124.45
7	P	317	NEX	C32-C33-C34	-2.46	115.17	118.94
5	P	308	KC2	O2A-CGA-O1A	-2.45	117.58	122.67
4	P	306	CHL	CMB-C2B-C3B	2.45	129.26	124.68
7	P	317	NEX	C31-C30-C29	-2.45	123.81	127.31
4	P	314	CHL	CHD-C1D-ND	-2.45	122.20	124.45
3	Q	312	CLA	O2D-CGD-O1D	-2.44	119.06	123.84
3	P	301	CLA	C5-C3-C2	-2.43	116.20	121.12
6	R	304	Q6L	C19-C18-C17	-2.43	123.84	127.31
8	P	320	IWJ	C23-C22-C21	-2.42	115.67	123.22
4	Q	314	CHL	O2D-CGD-CBD	2.42	115.57	111.27
3	P	311	CLA	CAC-C3C-C4C	2.40	127.93	124.81
3	R	314	CLA	C1-C2-C3	-2.39	121.91	126.04
4	Q	305	CHL	C4A-NA-C1A	2.39	107.78	106.71
6	P	319	Q6L	C06-C07-C02	2.38	116.60	111.85
4	R	318	CHL	C1C-C2C-C3C	-2.38	105.23	107.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	P	319	Q6L	C19-C20-C21	-2.38	118.61	123.47
6	P	316	Q6L	C19-C20-C21	-2.37	118.62	123.47
3	P	312	CLA	O2D-CGD-CBD	2.37	115.48	111.27
4	Q	306	CHL	CHA-C4D-ND	2.37	137.45	132.50
6	Q	316	Q6L	C12-C13-C14	-2.36	114.83	121.98
3	P	302	CLA	C14-C13-C15	2.36	119.83	111.29
4	P	304	CHL	O2D-CGD-CBD	2.35	115.45	111.27
8	Q	319	IWJ	C25-C24-C26	2.35	119.98	116.02
3	R	315	CLA	C5-C3-C2	2.35	125.88	121.12
3	P	313	CLA	CBA-CAA-C2A	2.35	120.80	113.86
8	Q	319	IWJ	C16-C17-C18	-2.35	118.67	123.47
6	Q	317	Q6L	C10-C04-C03	2.35	113.06	109.71
6	Q	316	Q6L	C36-C31-C32	2.34	115.62	111.42
7	R	321	NEX	C38-C25-C24	-2.34	111.64	114.28
7	Q	315	NEX	C20-C13-C12	2.34	121.77	118.08
6	R	320	Q6L	C24-C22-C21	-2.34	115.35	118.94
7	Q	315	NEX	C38-C25-C26	-2.34	118.35	122.26
7	Q	315	NEX	C32-C33-C34	-2.33	115.36	118.94
3	P	310	CLA	C11-C10-C8	2.32	123.43	115.92
3	P	309	CLA	C11-C12-C13	-2.32	108.41	115.92
3	Q	312	CLA	CAC-C3C-C4C	2.32	127.82	124.81
3	R	313	CLA	CAA-C2A-C1A	-2.32	104.37	111.97
5	P	308	KC2	CAC-C3C-C2C	-2.32	120.97	128.60
5	R	312	KC2	CAC-C3C-C2C	-2.32	120.98	128.60
3	R	317	CLA	O2A-CGA-O1A	-2.30	117.78	123.59
4	R	311	CHL	CHB-C4A-NA	2.30	127.70	124.51
7	Q	315	NEX	C31-C30-C29	-2.30	124.03	127.31
5	R	312	KC2	CBD-CHA-C1A	2.29	133.15	128.88
7	Q	315	NEX	C24-C23-C22	-2.28	106.36	110.77
4	R	302	CHL	C2A-C1A-CHA	2.28	127.85	123.86
4	R	302	CHL	CHA-C1A-NA	-2.27	121.19	126.40
4	P	305	CHL	C2C-C3C-C4C	2.27	108.11	106.49
6	P	316	Q6L	C24-C22-C21	-2.27	115.46	118.94
5	Q	308	KC2	CAA-CBA-CGA	-2.27	115.62	127.26
3	R	315	CLA	CHD-C1D-ND	-2.26	122.38	124.45
5	R	312	KC2	O2A-CGA-O1A	-2.26	117.98	122.67
4	R	310	CHL	O2D-CGD-O1D	-2.26	119.42	123.84
3	P	303	CLA	CBA-CAA-C2A	2.26	120.52	113.86
6	Q	318	Q6L	C06-C07-C02	2.25	116.35	111.85
3	Q	304	CLA	O2D-CGD-CBD	2.25	115.28	111.27
8	Q	301	IWJ	C12-C11-C10	2.25	130.53	127.31
7	P	317	NEX	C35-C15-C14	-2.25	118.86	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	P	313	CLA	CHB-C4A-NA	2.25	127.62	124.51
4	P	305	CHL	CMA-C3A-C4A	2.25	117.81	111.77
7	R	321	NEX	O24-C25-C38	2.25	117.75	115.06
3	R	314	CLA	CMA-C3A-C4A	2.24	117.80	111.77
4	Q	306	CHL	C3D-C2D-C1D	2.24	108.88	105.83
7	R	321	NEX	C31-C30-C29	-2.24	124.12	127.31
8	R	303	IWJ	C21-C19-C18	-2.23	115.51	118.94
4	P	304	CHL	CED-O2D-CGD	2.23	120.99	115.94
4	P	304	CHL	C1D-CHD-C4C	-2.23	121.25	126.06
4	R	310	CHL	O2A-CGA-O1A	-2.23	117.97	123.59
3	P	311	CLA	CBA-CAA-C2A	2.23	120.44	113.86
3	P	301	CLA	CAC-C3C-C4C	2.22	127.69	124.81
4	P	304	CHL	C3B-C4B-NB	-2.22	106.34	109.21
8	Q	301	IWJ	C36-C35-C34	-2.21	105.14	108.98
3	P	301	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
3	Q	310	CLA	O1D-CGD-CBD	2.21	129.00	124.48
3	P	302	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
3	Q	313	CLA	O2A-CGA-CBA	2.21	118.83	111.91
4	R	309	CHL	CHB-C4A-NA	2.20	127.56	124.51
8	Q	301	IWJ	C21-C19-C18	-2.20	115.56	118.94
3	P	301	CLA	C6-C5-C3	2.20	119.23	113.45
3	Q	302	CLA	O2A-CGA-CBA	2.20	118.81	111.91
3	Q	304	CLA	CHA-C1A-NA	-2.20	121.37	126.40
4	Q	314	CHL	C1C-C2C-C3C	-2.19	105.37	107.11
5	Q	308	KC2	CAC-C3C-C2C	-2.19	121.40	128.60
3	P	303	CLA	C1-C2-C3	-2.19	123.22	126.75
3	Q	303	CLA	CHB-C4A-NA	2.18	127.53	124.51
5	P	308	KC2	O1A-CGA-CBA	2.18	127.81	120.99
4	R	308	CHL	O2A-CGA-O1A	-2.17	117.89	123.30
3	Q	310	CLA	CHD-C1D-ND	-2.17	122.46	124.45
3	Q	311	CLA	O2D-CGD-O1D	-2.17	119.60	123.84
5	P	308	KC2	C3C-C2C-C1C	2.16	108.09	106.49
5	P	308	KC2	C4C-C3C-C2C	-2.16	105.40	107.11
4	P	306	CHL	CAA-C2A-C3A	2.16	118.68	112.78
3	R	314	CLA	CHA-C1A-NA	-2.15	121.47	126.40
6	R	319	Q6L	C01-C02-C07	-2.15	110.38	114.36
3	Q	302	CLA	C1D-ND-C4D	-2.14	104.81	106.33
6	Q	318	Q6L	C35-C34-C33	2.14	114.18	111.74
4	R	302	CHL	O2D-CGD-CBD	2.14	115.07	111.27
3	P	309	CLA	C1-C2-C3	-2.14	122.34	126.04
3	R	316	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
8	R	303	IWJ	C36-C35-C34	-2.14	105.27	108.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	R	308	CHL	C2A-C1A-CHA	2.13	127.59	123.86
7	R	321	NEX	C35-C15-C14	-2.13	119.11	123.47
3	P	311	CLA	CMC-C2C-C1C	2.13	128.28	125.04
4	R	311	CHL	CHA-C4D-ND	2.11	136.92	132.50
4	Q	307	CHL	O2D-CGD-CBD	2.11	115.02	111.27
8	Q	319	IWJ	C21-C19-C18	-2.11	115.70	118.94
6	P	321	Q6L	C01-C02-C03	2.11	127.27	124.49
3	Q	311	CLA	C2A-C1A-CHA	2.11	127.55	123.86
8	R	322	IWJ	C36-C35-C34	-2.11	105.32	108.98
6	Q	318	Q6L	C25-C26-C27	-2.11	124.30	127.31
4	R	311	CHL	O2D-CGD-O1D	-2.10	119.73	123.84
4	Q	314	CHL	CMA-C3A-C4A	2.10	117.42	111.77
3	R	305	CLA	C2C-C1C-NC	2.10	111.94	109.97
5	Q	308	KC2	O1A-CGA-CBA	2.10	127.55	120.99
4	P	304	CHL	C3A-C2A-C1A	2.10	104.48	101.34
5	P	308	KC2	CBD-CHA-C1A	2.09	132.79	128.88
4	P	306	CHL	C2D-C1D-ND	-2.09	108.56	110.10
4	Q	305	CHL	O2A-CGA-O1A	-2.09	118.08	123.30
3	R	315	CLA	C1B-CHB-C4A	-2.09	125.98	130.12
3	Q	304	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
3	P	309	CLA	C6-C5-C3	2.09	118.93	113.45
8	Q	319	IWJ	C05-C04-C03	2.09	114.11	111.74
6	R	319	Q6L	C12-C13-C14	-2.08	115.67	121.98
6	Q	318	Q6L	C42-C13-C12	2.08	118.77	115.27
4	Q	305	CHL	CAC-C3C-C4C	2.08	127.51	124.81
3	R	313	CLA	CAA-C2A-C3A	2.08	118.48	112.78
6	P	321	Q6L	C05-C06-C07	2.08	113.15	110.30
4	P	305	CHL	C3C-C4C-NC	-2.08	108.24	110.57
3	P	301	CLA	CHD-C1D-ND	-2.08	122.55	124.45
6	Q	318	Q6L	C38-C36-C35	-2.08	105.50	109.44
3	R	315	CLA	CBA-CAA-C2A	2.07	119.98	113.86
3	R	313	CLA	CMC-C2C-C1C	2.07	128.20	125.04
5	Q	308	KC2	CHB-C1B-NB	2.07	126.36	124.45
3	R	315	CLA	CAC-C3C-C4C	2.07	127.50	124.81
5	Q	308	KC2	CHC-C4B-NB	2.07	126.36	124.45
3	P	312	CLA	CBA-CAA-C2A	2.07	119.97	113.86
5	R	312	KC2	O1D-CGD-CBD	2.07	128.72	124.48
6	P	315	Q6L	C19-C20-C21	-2.07	119.24	123.47
5	R	312	KC2	CHB-C4A-NA	2.07	127.46	124.20
3	Q	311	CLA	CMC-C2C-C1C	2.07	128.18	125.04
7	R	321	NEX	C15-C14-C13	-2.06	124.37	127.31
4	Q	314	CHL	CHA-C1A-NA	-2.06	121.68	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	P	310	CLA	CHA-C1A-NA	-2.06	121.68	126.40
8	P	320	IWJ	C36-C35-C34	-2.06	105.41	108.98
6	Q	318	Q6L	C16-C17-C18	-2.06	115.79	118.94
6	P	315	Q6L	C01-C02-C07	-2.05	110.56	114.36
7	P	317	NEX	C36-C21-C22	-2.05	105.42	108.98
8	Q	301	IWJ	C25-C24-C26	2.05	119.47	116.02
8	Q	319	IWJ	C36-C35-C34	-2.05	105.43	108.98
4	R	309	CHL	CHA-C4D-ND	2.04	136.77	132.50
6	P	321	Q6L	C19-C20-C21	-2.04	119.30	123.47
3	P	301	CLA	C1D-ND-C4D	-2.03	104.89	106.33
8	Q	301	IWJ	C33-C32-C30	2.03	115.51	112.04
4	P	305	CHL	O1A-CGA-CBA	2.03	129.60	123.08
6	R	301	Q6L	C19-C20-C21	-2.03	119.32	123.47
4	Q	305	CHL	C1C-C2C-C3C	-2.03	105.51	107.11
5	R	312	KC2	CAC-C3C-C4C	2.02	133.89	124.47
6	R	323	Q6L	C19-C20-C21	-2.02	119.33	123.47
6	Q	316	Q6L	C16-C17-C18	-2.02	115.84	118.94
6	P	319	Q6L	C01-C02-C07	-2.02	110.61	114.36
4	P	304	CHL	CHA-C1A-NA	-2.02	121.77	126.40
7	P	317	NEX	C19-C9-C10	2.02	125.75	122.92
7	Q	315	NEX	C35-C15-C14	-2.01	119.35	123.47
4	Q	306	CHL	C2A-C3A-C4A	2.01	105.12	101.87
3	P	311	CLA	C5-C3-C2	2.01	125.19	121.12
4	R	311	CHL	C4A-NA-C1A	2.01	107.61	106.71
4	R	318	CHL	O1D-CGD-CBD	2.01	128.60	124.48
4	P	304	CHL	O1A-CGA-CBA	2.01	129.54	123.08
3	P	310	CLA	C1-C2-C3	-2.01	122.57	126.04
3	R	317	CLA	CAC-C3C-C4C	2.01	127.42	124.81
4	P	307	CHL	O2D-CGD-CBD	2.01	114.83	111.27
4	Q	314	CHL	C1D-CHD-C4C	-2.01	121.73	126.06
4	R	309	CHL	O2D-CGD-CBD	2.00	114.83	111.27
3	Q	302	CLA	CHD-C1D-ND	-2.00	122.61	124.45
7	Q	315	NEX	C40-C33-C32	2.00	121.23	118.08

All (67) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	P	301	CLA	ND
3	P	302	CLA	ND
3	P	303	CLA	ND
3	P	309	CLA	ND
3	P	310	CLA	ND

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Mol	Chain	Res	Type	Atom
3	P	311	CLA	ND
3	P	312	CLA	ND
3	Q	302	CLA	ND
3	Q	303	CLA	ND
3	Q	304	CLA	ND
3	Q	309	CLA	ND
3	Q	310	CLA	ND
3	Q	311	CLA	ND
3	Q	312	CLA	ND
3	Q	313	CLA	ND
3	R	305	CLA	ND
3	R	306	CLA	ND
3	R	307	CLA	ND
3	R	313	CLA	ND
3	R	314	CLA	ND
3	R	315	CLA	ND
3	R	316	CLA	ND
4	P	304	CHL	NC
4	P	304	CHL	NA
4	P	304	CHL	ND
4	P	305	CHL	NC
4	P	305	CHL	NA
4	P	305	CHL	ND
4	P	306	CHL	NC
4	P	306	CHL	NA
4	P	306	CHL	ND
4	P	307	CHL	NC
4	P	307	CHL	NA
4	P	307	CHL	ND
4	P	314	CHL	NC
4	P	314	CHL	NA
4	P	314	CHL	ND
4	Q	305	CHL	NC
4	Q	305	CHL	NA
4	Q	305	CHL	ND
4	Q	306	CHL	NC
4	Q	306	CHL	NA
4	Q	306	CHL	ND
4	Q	307	CHL	NC
4	Q	307	CHL	NA
4	Q	307	CHL	ND
4	Q	314	CHL	NC

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Mol	Chain	Res	Type	Atom
4	Q	314	CHL	NA
4	Q	314	CHL	ND
4	R	302	CHL	NC
4	R	302	CHL	NA
4	R	302	CHL	ND
4	R	308	CHL	NC
4	R	308	CHL	NA
4	R	308	CHL	ND
4	R	309	CHL	NC
4	R	309	CHL	NA
4	R	309	CHL	ND
4	R	310	CHL	NC
4	R	310	CHL	NA
4	R	310	CHL	ND
4	R	311	CHL	NC
4	R	311	CHL	NA
4	R	311	CHL	ND
4	R	318	CHL	NC
4	R	318	CHL	NA
4	R	318	CHL	ND

All (420) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	P	301	CLA	C3A-C2A-CAA-CBA
3	P	301	CLA	C2-C3-C5-C6
3	P	301	CLA	C4-C3-C5-C6
3	P	302	CLA	CHA-CBD-CGD-O1D
3	P	302	CLA	CHA-CBD-CGD-O2D
3	P	302	CLA	CAD-CBD-CGD-O1D
3	P	302	CLA	CAD-CBD-CGD-O2D
3	P	303	CLA	C1A-C2A-CAA-CBA
3	P	303	CLA	C3A-C2A-CAA-CBA
3	P	303	CLA	CBD-CGD-O2D-CED
3	P	309	CLA	C3A-C2A-CAA-CBA
3	P	310	CLA	CHA-CBD-CGD-O1D
3	P	310	CLA	CHA-CBD-CGD-O2D
3	P	312	CLA	CHA-CBD-CGD-O1D
3	P	312	CLA	CHA-CBD-CGD-O2D
3	Q	304	CLA	C1A-C2A-CAA-CBA
3	Q	309	CLA	C1A-C2A-CAA-CBA
3	Q	310	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
3	Q	310	CLA	CHA-CBD-CGD-O1D
3	Q	311	CLA	CBA-CGA-O2A-C1
3	Q	312	CLA	CHA-CBD-CGD-O1D
3	Q	312	CLA	CHA-CBD-CGD-O2D
3	R	305	CLA	C1A-C2A-CAA-CBA
3	R	313	CLA	C1A-C2A-CAA-CBA
3	R	313	CLA	C3A-C2A-CAA-CBA
3	R	314	CLA	C3A-C2A-CAA-CBA
3	R	315	CLA	CHA-CBD-CGD-O1D
3	R	315	CLA	CHA-CBD-CGD-O2D
3	R	315	CLA	CAD-CBD-CGD-O1D
3	R	316	CLA	C1A-C2A-CAA-CBA
3	R	316	CLA	C3A-C2A-CAA-CBA
3	R	316	CLA	C4-C3-C5-C6
3	R	317	CLA	O1A-CGA-O2A-C1
4	P	304	CHL	C1A-C2A-CAA-CBA
4	P	304	CHL	C3A-C2A-CAA-CBA
4	P	304	CHL	C1C-C2C-CMC-OMC
4	P	304	CHL	C3C-C2C-CMC-OMC
4	P	304	CHL	CBD-CGD-O2D-CED
4	P	314	CHL	C1A-C2A-CAA-CBA
4	P	314	CHL	CHA-CBD-CGD-O1D
4	P	314	CHL	CHA-CBD-CGD-O2D
4	R	302	CHL	CBA-CGA-O2A-C1
4	R	308	CHL	CHA-CBD-CGD-O1D
4	R	308	CHL	CHA-CBD-CGD-O2D
4	R	309	CHL	CBD-CGD-O2D-CED
4	R	310	CHL	C2-C3-C5-C6
4	R	310	CHL	C4-C3-C5-C6
4	R	311	CHL	CBD-CGD-O2D-CED
4	R	318	CHL	CBD-CGD-O2D-CED
5	P	308	KC2	C1A-C2A-CAA-CBA
5	P	308	KC2	C2A-CAA-CBA-CGA
5	Q	308	KC2	C1A-C2A-CAA-CBA
5	Q	308	KC2	C3A-C2A-CAA-CBA
5	Q	308	KC2	C2A-CAA-CBA-CGA
5	R	312	KC2	C1A-C2A-CAA-CBA
5	R	312	KC2	C2A-CAA-CBA-CGA
6	P	315	Q6L	C28-C27-C29-C30
6	P	315	Q6L	C26-C27-C29-C30
6	P	315	Q6L	C15-C16-C17-C18
6	P	315	Q6L	C15-C16-C17-C41

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Mol	Chain	Res	Type	Atoms
6	P	319	Q6L	C11-C12-C13-C14
6	P	319	Q6L	C11-C12-C13-C42
6	Q	316	Q6L	C02-C03-C11-C12
6	Q	316	Q6L	C11-C12-C13-C14
6	Q	316	Q6L	C11-C12-C13-C42
6	Q	316	Q6L	C28-C27-C29-C30
6	Q	316	Q6L	C26-C27-C29-C30
6	Q	316	Q6L	C27-C29-C30-C31
6	Q	317	Q6L	C28-C27-C29-C30
6	Q	317	Q6L	C26-C27-C29-C30
6	R	301	Q6L	C04-C03-C11-C12
6	R	301	Q6L	C11-C12-C13-C42
6	R	301	Q6L	C21-C22-C24-C25
6	R	301	Q6L	C23-C22-C24-C25
6	R	301	Q6L	C28-C27-C29-C30
6	R	301	Q6L	C26-C27-C29-C30
6	R	301	Q6L	C29-C30-C31-C32
6	R	301	Q6L	C27-C29-C30-C31
6	R	319	Q6L	C11-C12-C13-C14
6	R	319	Q6L	C11-C12-C13-C42
6	R	319	Q6L	C21-C22-C24-C25
6	R	319	Q6L	C23-C22-C24-C25
6	R	319	Q6L	C29-C30-C31-C36
6	R	319	Q6L	C29-C30-C31-C32
6	R	323	Q6L	C11-C12-C13-C42
6	R	323	Q6L	C28-C27-C29-C30
6	R	323	Q6L	C27-C29-C30-C31
7	Q	315	NEX	O24-C26-C27-C28
8	P	318	IWJ	C18-C19-C21-C22
8	P	318	IWJ	C20-C19-C21-C22
8	P	320	IWJ	C26-C28-C29-C30
8	P	320	IWJ	C26-C28-C29-O39
8	Q	301	IWJ	C26-C28-C29-C30
8	Q	301	IWJ	C26-C28-C29-O39
8	Q	319	IWJ	C18-C19-C21-C22
8	Q	319	IWJ	C20-C19-C21-C22
8	Q	319	IWJ	C26-C28-C29-C30
8	Q	319	IWJ	C26-C28-C29-C35
8	Q	319	IWJ	C26-C28-C29-O39
8	R	303	IWJ	C26-C28-C29-C30
8	R	303	IWJ	C26-C28-C29-C35
8	R	303	IWJ	C26-C28-C29-O39

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Mol	Chain	Res	Type	Atoms
8	R	322	IWJ	C18-C19-C21-C22
8	R	322	IWJ	C20-C19-C21-C22
8	R	322	IWJ	C26-C28-C29-C30
8	R	322	IWJ	C26-C28-C29-C35
8	R	322	IWJ	C26-C28-C29-O39
4	P	304	CHL	O1D-CGD-O2D-CED
3	P	311	CLA	CBD-CGD-O2D-CED
3	Q	312	CLA	CBD-CGD-O2D-CED
3	R	306	CLA	CBD-CGD-O2D-CED
3	R	316	CLA	CBD-CGD-O2D-CED
3	Q	313	CLA	O1A-CGA-O2A-C1
3	R	314	CLA	O1A-CGA-O2A-C1
3	Q	311	CLA	O1A-CGA-O2A-C1
3	P	303	CLA	O1D-CGD-O2D-CED
3	R	306	CLA	O1D-CGD-O2D-CED
4	R	309	CHL	O1D-CGD-O2D-CED
3	Q	313	CLA	CBA-CGA-O2A-C1
3	R	317	CLA	CBA-CGA-O2A-C1
3	Q	309	CLA	CBD-CGD-O2D-CED
4	Q	305	CHL	CBD-CGD-O2D-CED
5	P	308	KC2	CBD-CGD-O2D-CED
3	P	302	CLA	O1A-CGA-O2A-C1
3	P	311	CLA	O1A-CGA-O2A-C1
3	Q	302	CLA	O1A-CGA-O2A-C1
3	R	305	CLA	O1A-CGA-O2A-C1
3	R	315	CLA	O1A-CGA-O2A-C1
4	P	306	CHL	O1A-CGA-O2A-C1
4	R	310	CHL	O1A-CGA-O2A-C1
4	R	302	CHL	O1A-CGA-O2A-C1
4	R	311	CHL	O1D-CGD-O2D-CED
4	R	318	CHL	O1D-CGD-O2D-CED
3	P	309	CLA	CBD-CGD-O2D-CED
3	P	311	CLA	O1D-CGD-O2D-CED
3	R	315	CLA	C3-C5-C6-C7
3	P	302	CLA	CBA-CGA-O2A-C1
3	Q	302	CLA	CBA-CGA-O2A-C1
3	R	305	CLA	CBA-CGA-O2A-C1
3	R	314	CLA	CBA-CGA-O2A-C1
3	R	316	CLA	CBA-CGA-O2A-C1
4	P	306	CHL	CBA-CGA-O2A-C1
3	R	316	CLA	C2-C3-C5-C6
6	R	301	Q6L	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
6	R	323	Q6L	C11-C12-C13-C14
3	Q	302	CLA	CBD-CGD-O2D-CED
3	Q	312	CLA	C2A-CAA-CBA-CGA
4	Q	306	CHL	C2A-CAA-CBA-CGA
3	P	311	CLA	CBA-CGA-O2A-C1
3	Q	312	CLA	CBA-CGA-O2A-C1
3	R	315	CLA	CBA-CGA-O2A-C1
4	R	310	CHL	CBA-CGA-O2A-C1
3	Q	312	CLA	O1A-CGA-O2A-C1
6	P	321	Q6L	C13-C14-C15-C16
6	R	323	Q6L	C24-C25-C26-C27
3	Q	304	CLA	CBD-CGD-O2D-CED
3	R	307	CLA	CBD-CGD-O2D-CED
4	P	306	CHL	CBD-CGD-O2D-CED
3	Q	302	CLA	C3-C5-C6-C7
3	Q	312	CLA	O1D-CGD-O2D-CED
3	R	316	CLA	O1A-CGA-O2A-C1
6	Q	318	Q6L	C11-C12-C13-C42
6	Q	318	Q6L	C11-C12-C13-C14
3	R	316	CLA	O1D-CGD-O2D-CED
4	Q	305	CHL	O1D-CGD-O2D-CED
5	R	312	KC2	CAA-CBA-CGA-O1A
3	P	301	CLA	CBA-CGA-O2A-C1
6	P	319	Q6L	C13-C14-C15-C16
3	Q	312	CLA	C2-C3-C5-C6
3	P	310	CLA	C11-C10-C8-C9
3	R	315	CLA	C11-C10-C8-C9
5	P	308	KC2	O1D-CGD-O2D-CED
4	P	314	CHL	CBD-CGD-O2D-CED
6	P	321	Q6L	C28-C27-C29-C30
6	Q	318	Q6L	C28-C27-C29-C30
6	R	304	Q6L	C28-C27-C29-C30
6	R	319	Q6L	C15-C16-C17-C41
6	R	323	Q6L	C23-C22-C24-C25
6	P	319	Q6L	C26-C27-C29-C30
6	P	321	Q6L	C26-C27-C29-C30
6	Q	318	Q6L	C26-C27-C29-C30
6	R	304	Q6L	C26-C27-C29-C30
6	R	323	Q6L	C26-C27-C29-C30
5	R	312	KC2	CAA-CBA-CGA-O2A
3	R	305	CLA	C13-C15-C16-C17
3	Q	309	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
3	P	301	CLA	C10-C11-C12-C13
3	R	306	CLA	C10-C11-C12-C13
3	Q	302	CLA	O1D-CGD-O2D-CED
3	R	306	CLA	C15-C16-C17-C18
3	P	310	CLA	C8-C10-C11-C12
3	P	311	CLA	C8-C10-C11-C12
3	P	309	CLA	O1D-CGD-O2D-CED
3	P	301	CLA	O1A-CGA-O2A-C1
3	R	314	CLA	C5-C6-C7-C8
3	R	313	CLA	C8-C10-C11-C12
3	R	314	CLA	C3-C5-C6-C7
3	P	310	CLA	CBA-CGA-O2A-C1
3	Q	304	CLA	O1D-CGD-O2D-CED
3	R	314	CLA	CBD-CGD-O2D-CED
3	P	309	CLA	C13-C15-C16-C17
6	P	315	Q6L	C11-C12-C13-C42
4	Q	306	CHL	CBA-CGA-O2A-C1
4	R	309	CHL	CBA-CGA-O2A-C1
3	P	310	CLA	O1A-CGA-O2A-C1
4	R	309	CHL	O1A-CGA-O2A-C1
6	P	319	Q6L	C28-C27-C29-C30
6	R	319	Q6L	C28-C27-C29-C30
6	R	319	Q6L	C26-C27-C29-C30
6	R	323	Q6L	C21-C22-C24-C25
3	R	307	CLA	O1D-CGD-O2D-CED
3	Q	309	CLA	C6-C7-C8-C10
4	P	306	CHL	O1D-CGD-O2D-CED
3	Q	304	CLA	C3A-C2A-CAA-CBA
3	Q	309	CLA	C3A-C2A-CAA-CBA
3	Q	311	CLA	C3A-C2A-CAA-CBA
3	R	305	CLA	C3A-C2A-CAA-CBA
4	P	305	CHL	C3A-C2A-CAA-CBA
4	P	314	CHL	C3A-C2A-CAA-CBA
4	Q	305	CHL	C3A-C2A-CAA-CBA
4	R	302	CHL	C3A-C2A-CAA-CBA
3	Q	309	CLA	C6-C7-C8-C9
3	Q	304	CLA	CBA-CGA-O2A-C1
6	Q	317	Q6L	C11-C12-C13-C14
3	R	306	CLA	C3-C5-C6-C7
3	P	302	CLA	C2-C1-O2A-CGA
3	Q	313	CLA	C2-C1-O2A-CGA
4	P	306	CHL	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
3	P	311	CLA	C5-C6-C7-C8
3	P	313	CLA	CBA-CGA-O2A-C1
3	P	313	CLA	O2A-C1-C2-C3
3	Q	312	CLA	C4-C3-C5-C6
6	Q	317	Q6L	C11-C12-C13-C42
3	Q	302	CLA	C6-C7-C8-C10
3	R	306	CLA	C11-C12-C13-C15
6	P	321	Q6L	C11-C12-C13-C14
3	P	312	CLA	CBA-CGA-O2A-C1
3	R	313	CLA	CBA-CGA-O2A-C1
3	R	315	CLA	C2A-CAA-CBA-CGA
3	Q	302	CLA	C10-C11-C12-C13
3	R	306	CLA	C8-C10-C11-C12
4	Q	306	CHL	O1A-CGA-O2A-C1
5	P	308	KC2	C4C-C3C-CAC-CBC
5	Q	308	KC2	C4C-C3C-CAC-CBC
3	R	314	CLA	O1D-CGD-O2D-CED
6	P	321	Q6L	C11-C12-C13-C42
6	P	315	Q6L	C11-C12-C13-C14
6	R	304	Q6L	C11-C12-C13-C14
3	Q	302	CLA	C6-C7-C8-C9
3	P	312	CLA	C2A-CAA-CBA-CGA
3	R	313	CLA	C2A-CAA-CBA-CGA
4	P	314	CHL	O1D-CGD-O2D-CED
3	Q	304	CLA	O1A-CGA-O2A-C1
3	R	313	CLA	O1A-CGA-O2A-C1
3	P	301	CLA	C1A-C2A-CAA-CBA
3	P	309	CLA	C1A-C2A-CAA-CBA
3	Q	311	CLA	C1A-C2A-CAA-CBA
3	R	306	CLA	C1A-C2A-CAA-CBA
3	R	314	CLA	C1A-C2A-CAA-CBA
4	P	305	CHL	C1A-C2A-CAA-CBA
4	P	307	CHL	C1A-C2A-CAA-CBA
4	Q	305	CHL	C1A-C2A-CAA-CBA
4	R	302	CHL	C1A-C2A-CAA-CBA
3	P	312	CLA	O1A-CGA-O2A-C1
3	P	313	CLA	O1A-CGA-O2A-C1
3	R	305	CLA	CBD-CGD-O2D-CED
3	R	317	CLA	O2A-C1-C2-C3
6	R	304	Q6L	C11-C12-C13-C42
3	P	311	CLA	C11-C12-C13-C14
3	P	309	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
3	P	309	CLA	C15-C16-C17-C18
3	P	310	CLA	C11-C10-C8-C7
3	R	305	CLA	C11-C12-C13-C15
3	P	312	CLA	C3-C5-C6-C7
3	P	309	CLA	O1A-CGA-O2A-C1
3	R	305	CLA	C11-C12-C13-C14
3	R	306	CLA	C11-C12-C13-C14
3	P	303	CLA	CBA-CGA-O2A-C1
3	P	311	CLA	C2A-CAA-CBA-CGA
8	Q	301	IWJ	O27-C26-C28-C29
8	Q	319	IWJ	O27-C26-C28-C29
8	R	322	IWJ	O27-C26-C28-C29
3	P	311	CLA	C11-C12-C13-C15
4	Q	314	CHL	C3C-C2C-CMC-OMC
4	R	302	CHL	C3C-C2C-CMC-OMC
5	P	308	KC2	C3A-C2A-CAA-CBA
3	P	312	CLA	O1D-CGD-O2D-CED
8	Q	319	IWJ	C23-C24-C26-C28
3	R	313	CLA	C12-C13-C15-C16
3	R	314	CLA	C6-C7-C8-C10
3	Q	311	CLA	C2A-CAA-CBA-CGA
3	R	316	CLA	C5-C6-C7-C8
3	P	303	CLA	CAD-CBD-CGD-O2D
3	R	315	CLA	CAD-CBD-CGD-O2D
3	R	317	CLA	CAD-CBD-CGD-O2D
4	P	307	CHL	CAD-CBD-CGD-O2D
4	Q	307	CHL	CAD-CBD-CGD-O2D
5	R	312	KC2	CAD-CBD-CGD-O2D
3	R	315	CLA	C10-C11-C12-C13
8	Q	319	IWJ	C25-C24-C26-O27
3	P	312	CLA	CBD-CGD-O2D-CED
4	Q	306	CHL	O2A-C1-C2-C3
5	R	312	KC2	C4C-C3C-CAC-CBC
3	Q	310	CLA	CHA-CBD-CGD-O2D
3	R	313	CLA	CHA-CBD-CGD-O1D
3	R	313	CLA	CHA-CBD-CGD-O2D
3	R	314	CLA	CHA-CBD-CGD-O1D
3	R	314	CLA	CHA-CBD-CGD-O2D
3	P	303	CLA	O1A-CGA-O2A-C1
6	R	301	Q6L	C02-C03-C11-C12
8	Q	319	IWJ	C23-C24-C26-O27
3	R	305	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
3	Q	304	CLA	C2A-CAA-CBA-CGA
8	Q	319	IWJ	C08-C09-C10-C41
6	R	319	Q6L	C15-C16-C17-C18
6	P	319	Q6L	C04-C03-C11-C12
6	Q	317	Q6L	C04-C03-C11-C12
4	R	310	CHL	C2-C1-O2A-CGA
3	P	310	CLA	CAA-CBA-CGA-O2A
4	R	308	CHL	CAD-CBD-CGD-O1D
3	P	309	CLA	C6-C7-C8-C10
3	P	309	CLA	C11-C12-C13-C15
6	P	321	Q6L	C29-C30-C31-C32
4	Q	307	CHL	C1C-C2C-CMC-OMC
3	R	313	CLA	C14-C13-C15-C16
3	R	314	CLA	C6-C7-C8-C9
8	Q	319	IWJ	C08-C09-C10-C11
8	Q	319	IWJ	C25-C24-C26-C28
3	P	309	CLA	C11-C12-C13-C14
3	P	302	CLA	C13-C15-C16-C17
3	Q	313	CLA	O2A-C1-C2-C3
3	P	301	CLA	C8-C10-C11-C12
3	R	306	CLA	C5-C6-C7-C8
6	Q	317	Q6L	C24-C25-C26-C27
6	Q	318	Q6L	C24-C25-C26-C27
3	R	313	CLA	C4-C3-C5-C6
4	R	309	CHL	C2-C1-O2A-CGA
3	P	312	CLA	C3A-C2A-CAA-CBA
3	P	313	CLA	C3A-C2A-CAA-CBA
3	Q	312	CLA	C3A-C2A-CAA-CBA
4	Q	314	CHL	C3A-C2A-CAA-CBA
4	R	309	CHL	O2A-C1-C2-C3
3	P	302	CLA	C11-C12-C13-C14
7	P	317	NEX	C39-C29-C30-C31
7	Q	315	NEX	C39-C29-C30-C31
7	R	321	NEX	C39-C29-C30-C31
3	R	317	CLA	C2A-CAA-CBA-CGA
3	P	312	CLA	C1A-C2A-CAA-CBA
3	Q	312	CLA	C1A-C2A-CAA-CBA
4	R	318	CHL	C1A-C2A-CAA-CBA
3	P	302	CLA	C11-C12-C13-C15
6	R	301	Q6L	C17-C18-C19-C20
5	Q	308	KC2	O1D-CGD-O2D-CED
4	Q	307	CHL	C3C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
3	Q	312	CLA	C5-C6-C7-C8
3	Q	302	CLA	C2A-CAA-CBA-CGA
5	R	312	KC2	C3A-C2A-CAA-CBA
7	P	317	NEX	C28-C29-C30-C31
7	Q	315	NEX	C28-C29-C30-C31
7	R	321	NEX	C28-C29-C30-C31
5	P	308	KC2	CAA-CBA-CGA-O2A
3	R	317	CLA	C2-C1-O2A-CGA
3	P	310	CLA	C6-C7-C8-C9
6	P	316	Q6L	C24-C25-C26-C27
6	P	321	Q6L	C24-C25-C26-C27
4	P	305	CHL	CAA-CBA-CGA-O2A
3	P	302	CLA	C5-C6-C7-C8
3	R	313	CLA	C6-C7-C8-C10
3	P	302	CLA	CAA-CBA-CGA-O2A
5	P	308	KC2	CAA-CBA-CGA-O1A
3	P	302	CLA	C8-C10-C11-C12
3	P	309	CLA	C6-C7-C8-C9
3	P	309	CLA	CAD-CBD-CGD-O2D
3	P	311	CLA	CAD-CBD-CGD-O2D
3	Q	309	CLA	CAD-CBD-CGD-O2D
3	Q	313	CLA	CAD-CBD-CGD-O2D
4	R	309	CHL	CAD-CBD-CGD-O2D
4	R	311	CHL	CAD-CBD-CGD-O2D
4	P	305	CHL	CAA-CBA-CGA-O1A
4	Q	305	CHL	CAA-CBA-CGA-O2A
3	Q	311	CLA	CAA-CBA-CGA-O2A
3	R	313	CLA	CAA-CBA-CGA-O2A
7	R	321	NEX	O24-C26-C27-C28
5	Q	308	KC2	CBD-CGD-O2D-CED
3	P	303	CLA	CAA-CBA-CGA-O2A
3	P	301	CLA	O2A-C1-C2-C3
5	R	312	KC2	C4B-C3B-CAB-CBB
3	P	303	CLA	C2A-CAA-CBA-CGA
4	Q	305	CHL	CAA-CBA-CGA-O1A
3	P	303	CLA	CHA-CBD-CGD-O2D
3	Q	304	CLA	CHA-CBD-CGD-O1D
3	Q	304	CLA	CHA-CBD-CGD-O2D
3	P	312	CLA	CAA-CBA-CGA-O2A
3	R	313	CLA	C15-C16-C17-C18
3	R	313	CLA	C6-C7-C8-C9
8	R	322	IWJ	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
3	P	312	CLA	CAA-CBA-CGA-O1A
4	P	306	CHL	C1A-C2A-CAA-CBA
4	Q	314	CHL	C1A-C2A-CAA-CBA
3	P	309	CLA	C2-C1-O2A-CGA
3	Q	309	CLA	C5-C6-C7-C8
3	P	302	CLA	CAA-CBA-CGA-O1A
3	P	303	CLA	CAA-CBA-CGA-O1A
3	R	313	CLA	C16-C17-C18-C19
3	Q	311	CLA	CAA-CBA-CGA-O1A
3	R	313	CLA	CAA-CBA-CGA-O1A
4	R	310	CHL	C4C-C3C-CAC-CBC
4	P	306	CHL	C2-C3-C5-C6
4	R	318	CHL	CAD-CBD-CGD-O1D
5	P	308	KC2	CAD-CBD-CGD-O1D
3	P	302	CLA	C10-C11-C12-C13
3	R	314	CLA	CAA-CBA-CGA-O2A
3	P	309	CLA	C4-C3-C5-C6
3	R	306	CLA	C12-C13-C15-C16
4	P	307	CHL	C3A-C2A-CAA-CBA
6	R	304	Q6L	C29-C30-C31-C32
6	R	323	Q6L	C29-C30-C31-C32
6	P	316	Q6L	C15-C16-C17-C18
8	R	303	IWJ	O27-C26-C28-C29
3	P	310	CLA	C2A-CAA-CBA-CGA

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	R	322	IWJ	C29-C30-C32-C33-C34-C35

26 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	Q	318	Q6L	1	0
7	P	317	NEX	1	0
3	Q	313	CLA	1	0
3	Q	302	CLA	6	0
3	Q	312	CLA	2	0
3	R	313	CLA	1	0
5	R	312	KC2	2	0
6	R	319	Q6L	1	0
5	P	308	KC2	1	0

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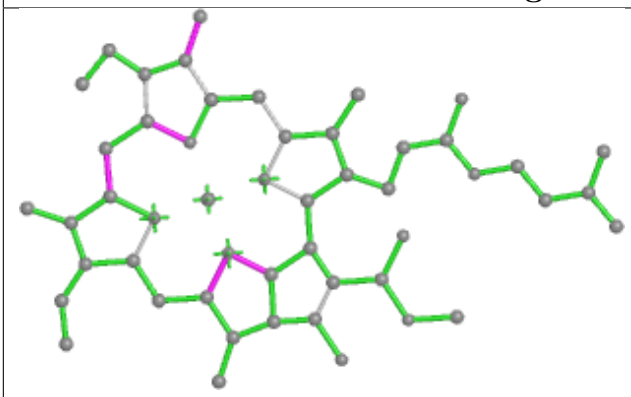
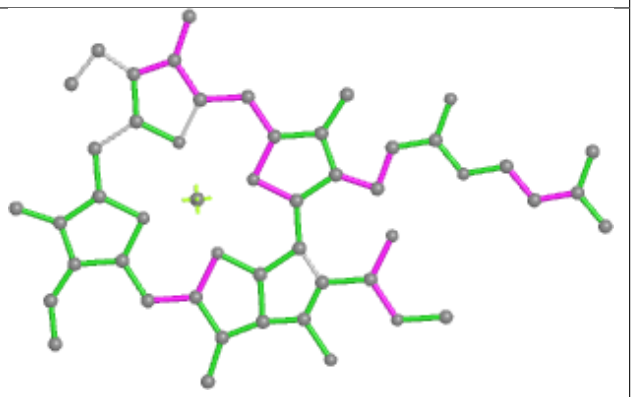
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	P	320	IWJ	1	0
3	R	307	CLA	1	0
3	Q	304	CLA	1	0
8	Q	319	IWJ	1	0
8	P	318	IWJ	1	0
3	R	316	CLA	1	0
4	P	307	CHL	1	0
3	P	301	CLA	3	0
3	R	305	CLA	4	0
3	R	306	CLA	1	0
4	R	308	CHL	7	0
6	R	320	Q6L	1	0
8	R	322	IWJ	1	0
3	P	309	CLA	2	0
4	R	311	CHL	2	0
4	Q	305	CHL	1	0
6	P	316	Q6L	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

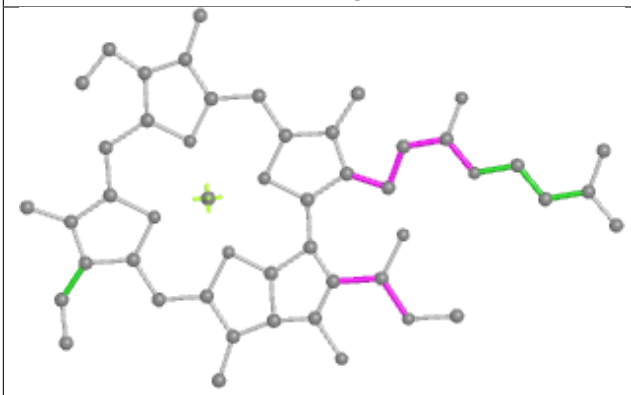
Ligand CLA P 303



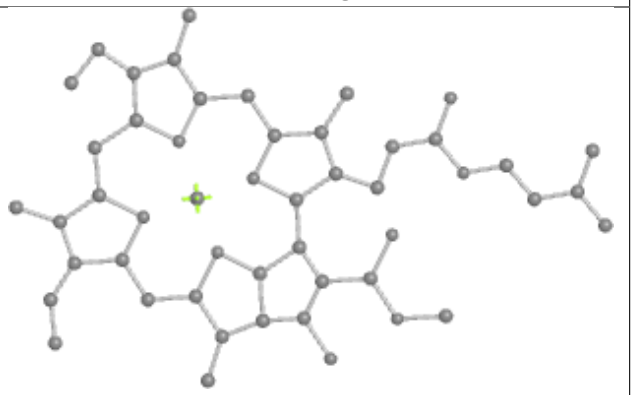
Bond lengths



Bond angles

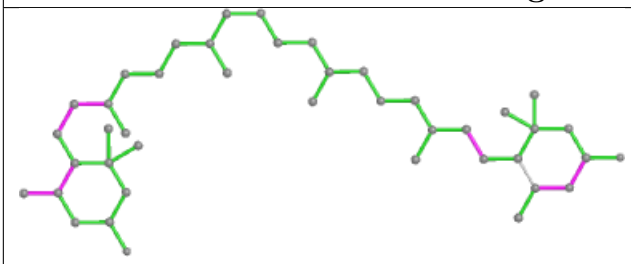


Torsions

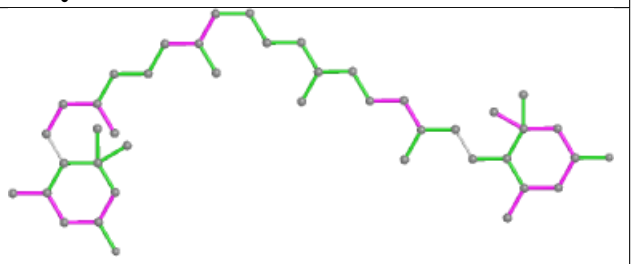


Rings

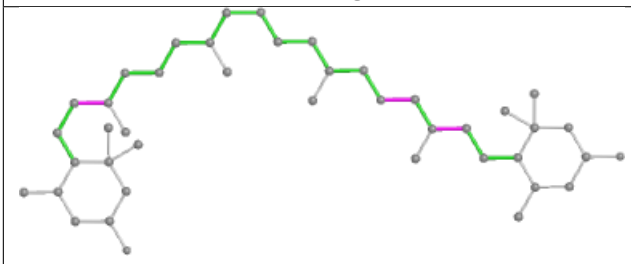
Ligand Q6L Q 318



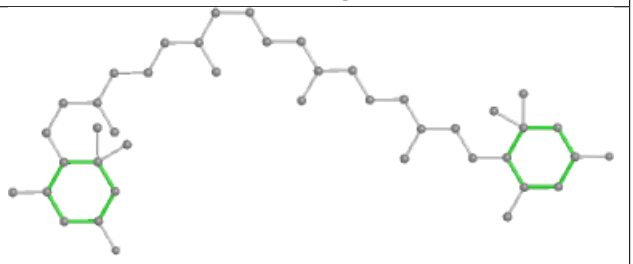
Bond lengths



Bond angles

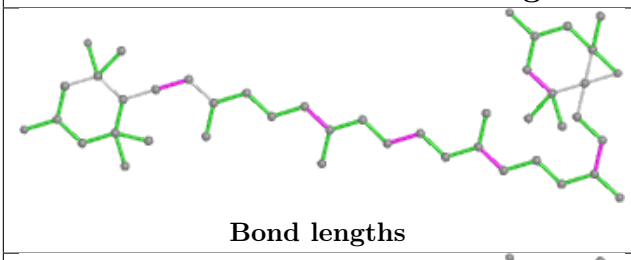


Torsions

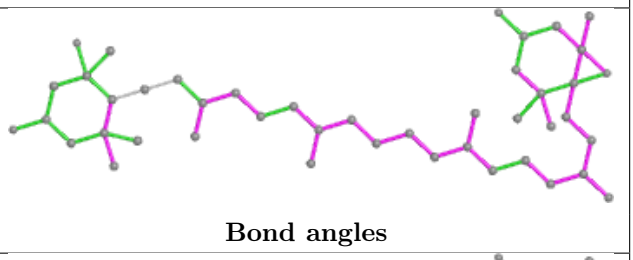


Rings

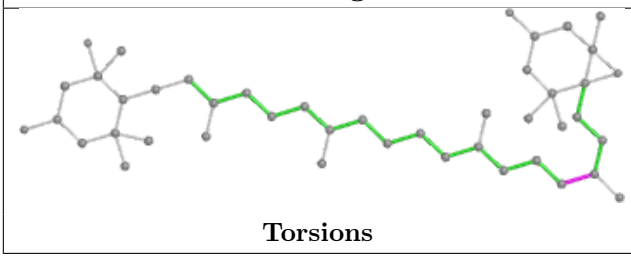
Ligand NEX P 317



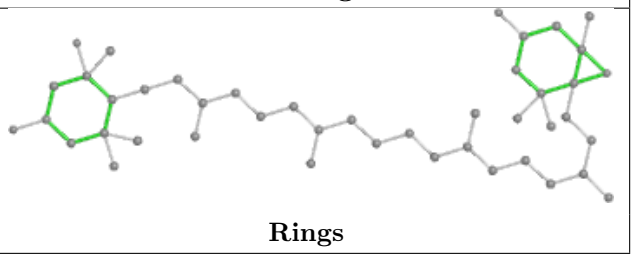
Bond lengths



Bond angles

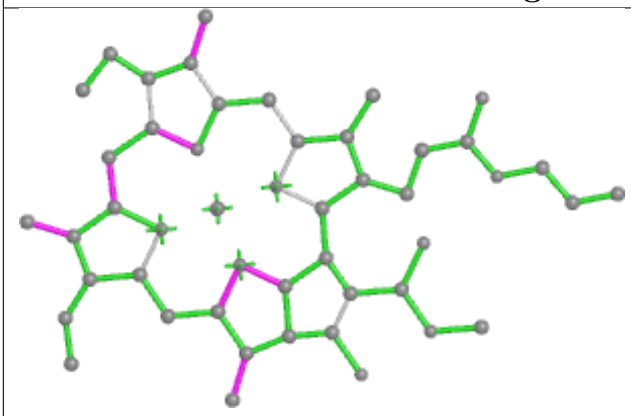


Torsions

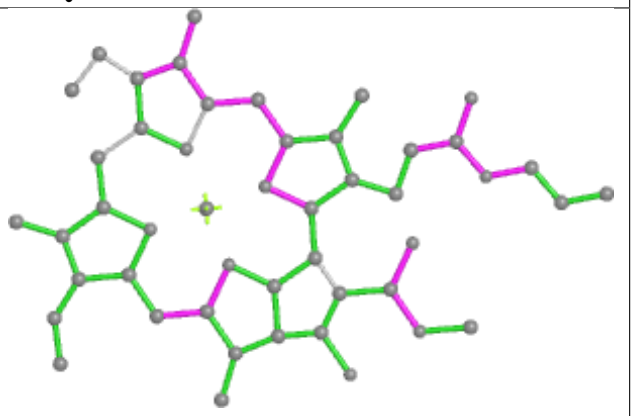


Rings

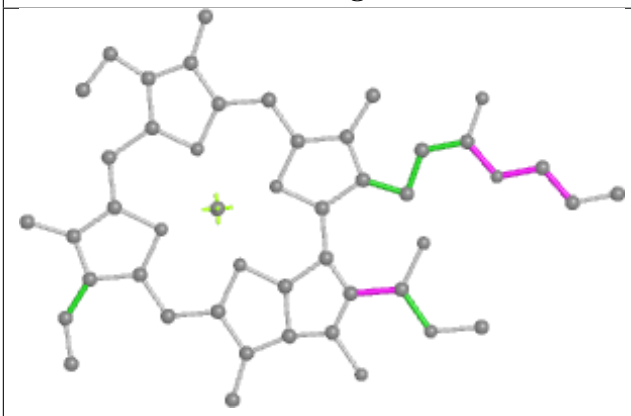
Ligand CLA Q 313



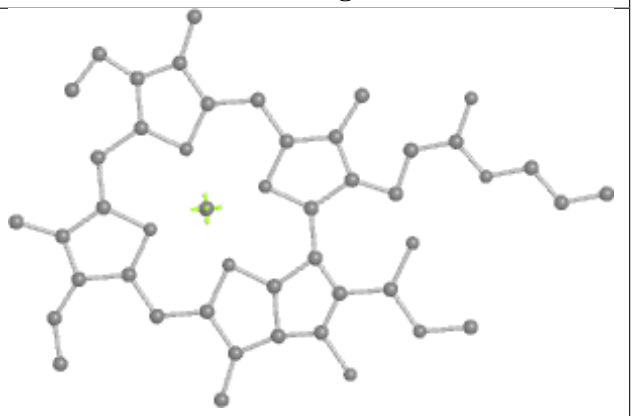
Bond lengths



Bond angles

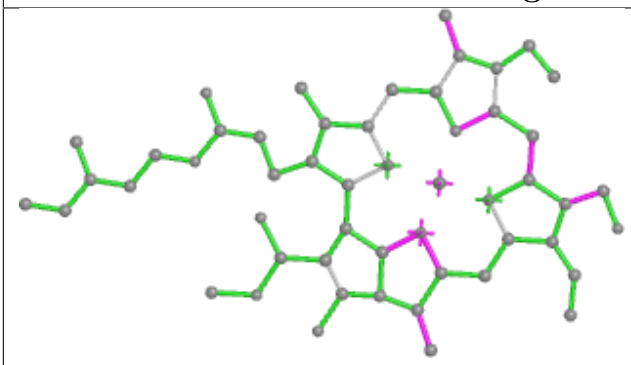


Torsions

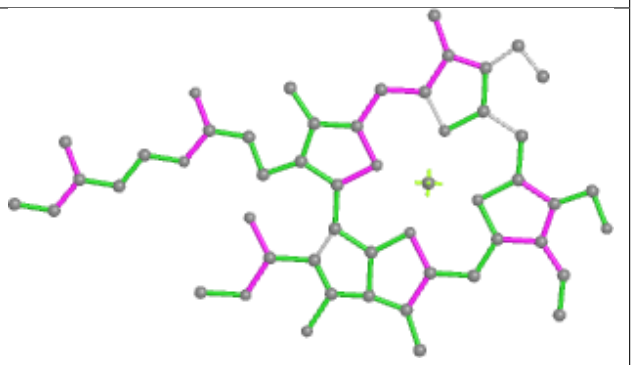


Rings

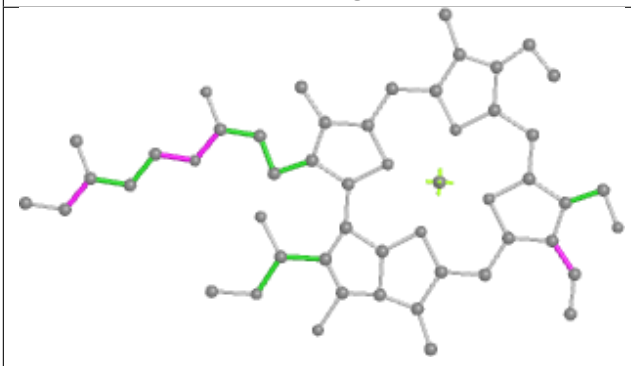
Ligand CHL R 310



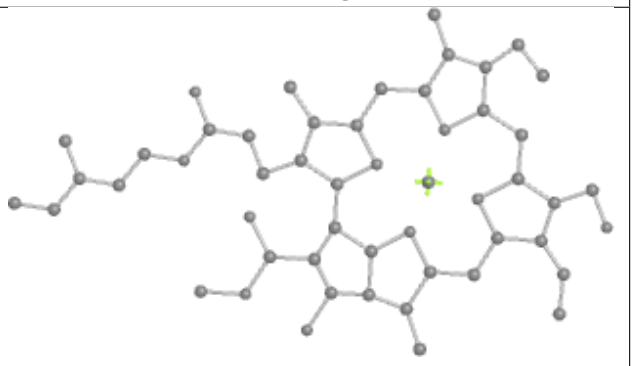
Bond lengths



Bond angles

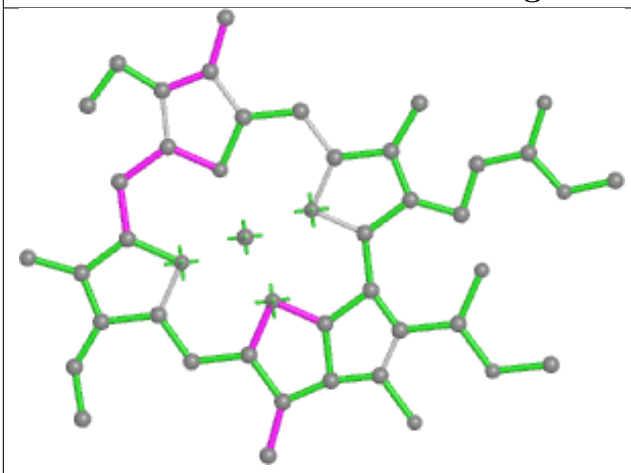


Torsions

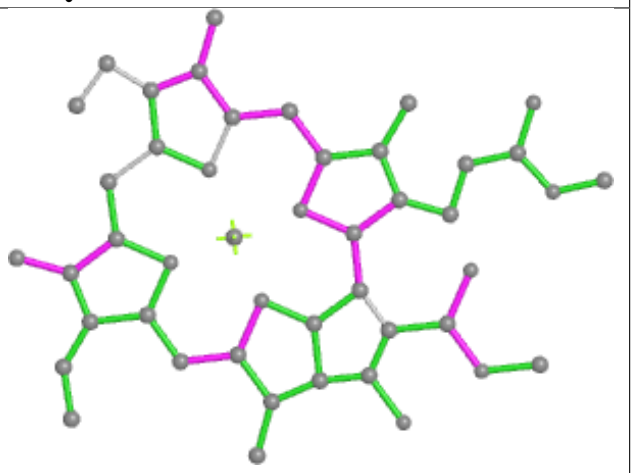


Rings

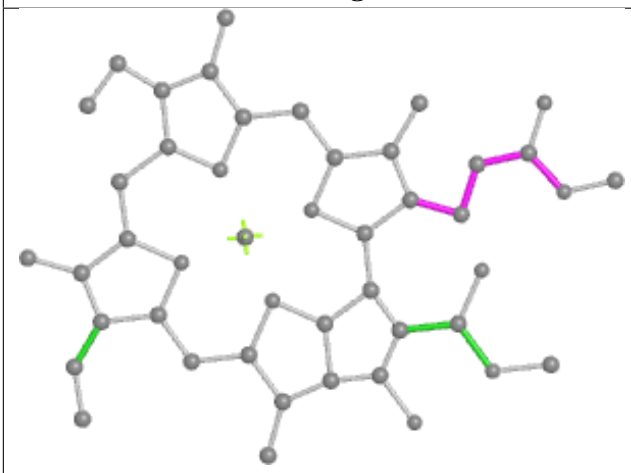
Ligand CLA Q 311



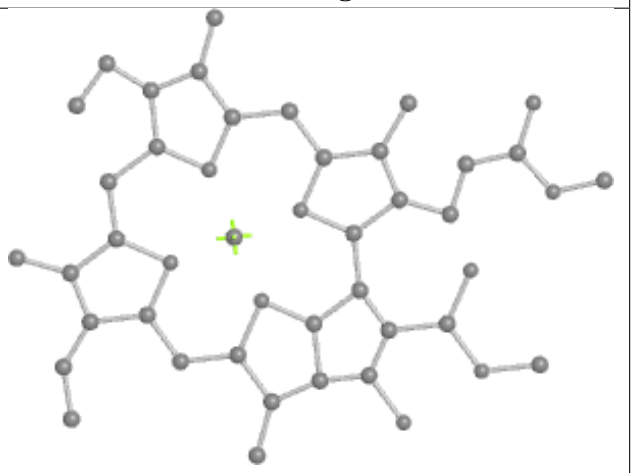
Bond lengths



Bond angles

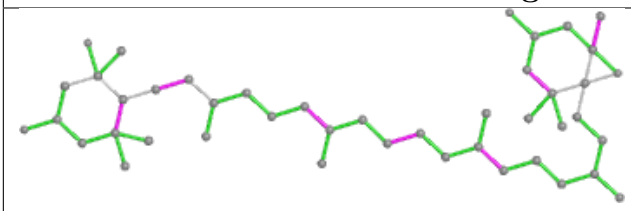


Torsions

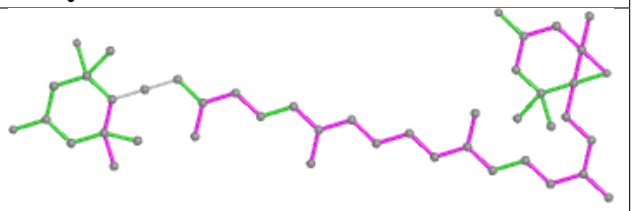


Rings

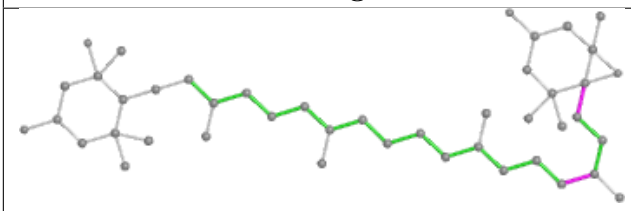
Ligand NEX Q 315



Bond lengths



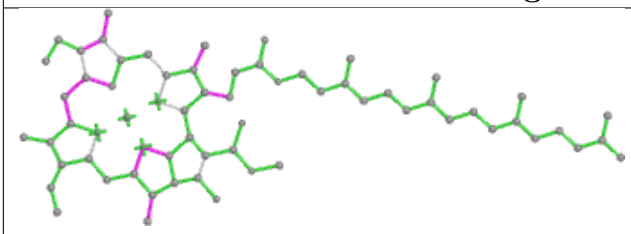
Bond angles



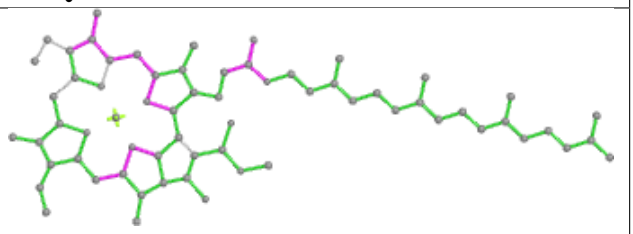
Torsions

Rings

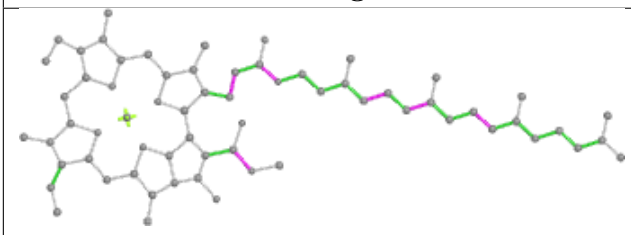
Ligand CLA Q 302



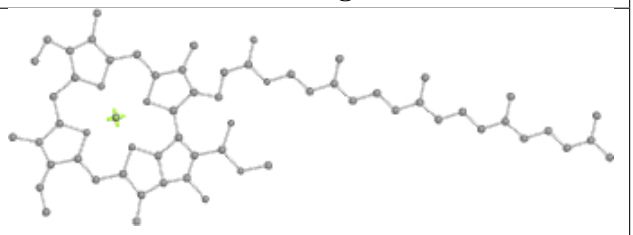
Bond lengths



Bond angles

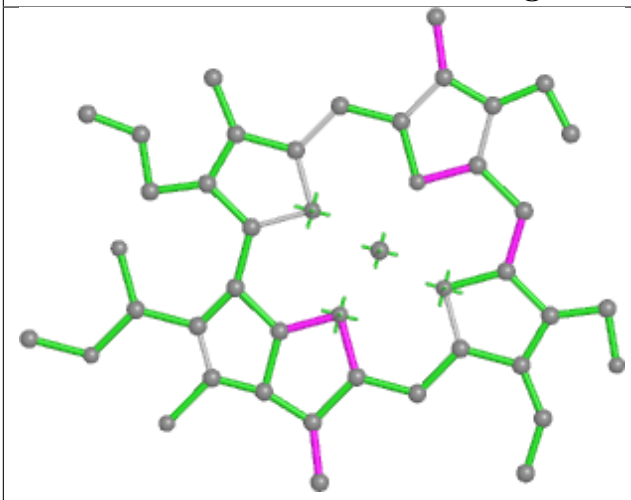


Torsions

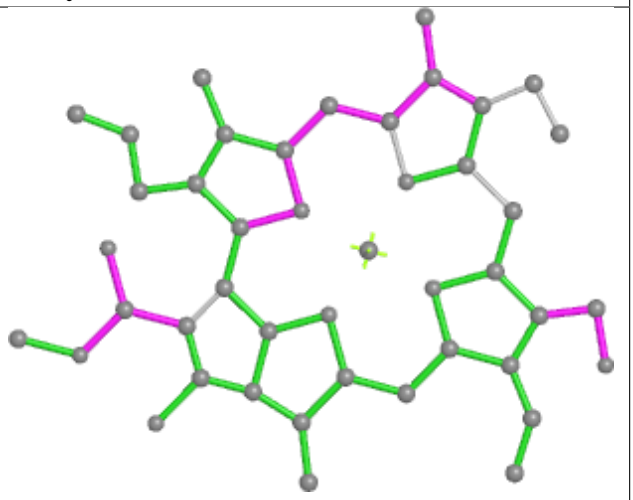


Rings

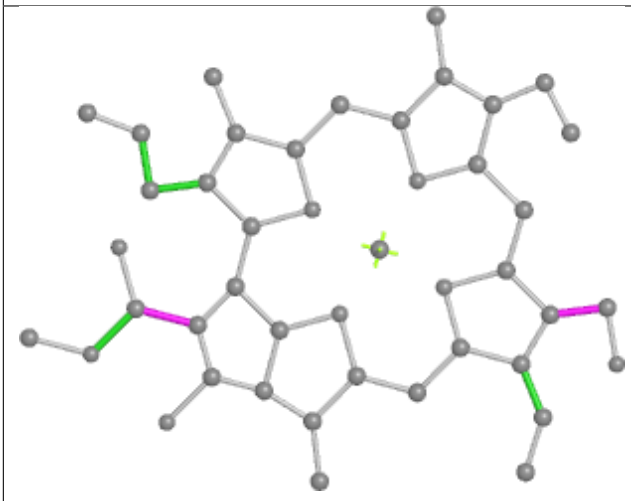
Ligand CHL Q 307



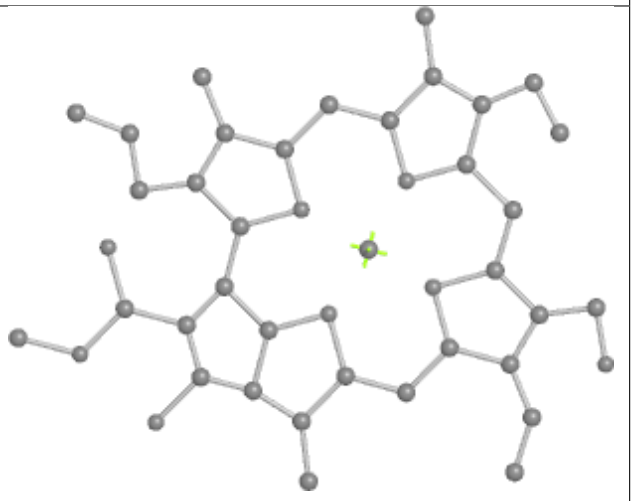
Bond lengths



Bond angles

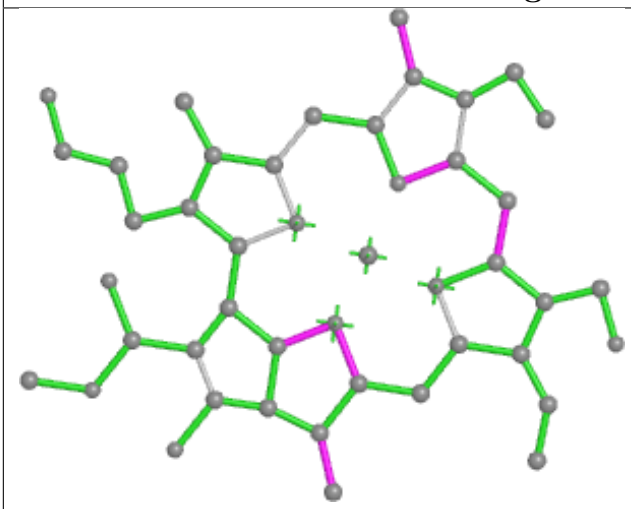


Torsions

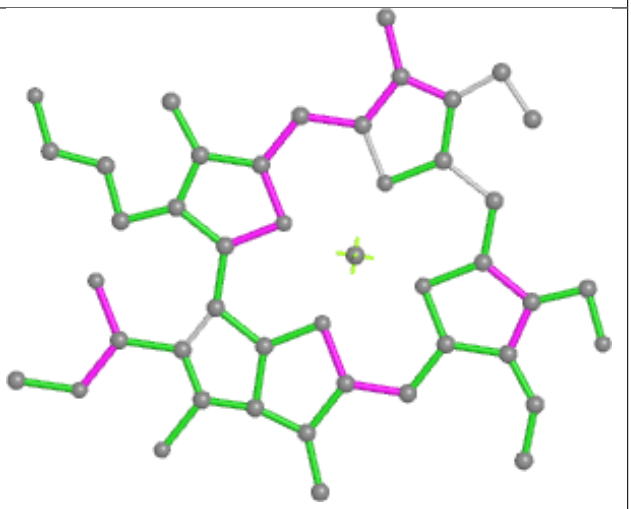


Rings

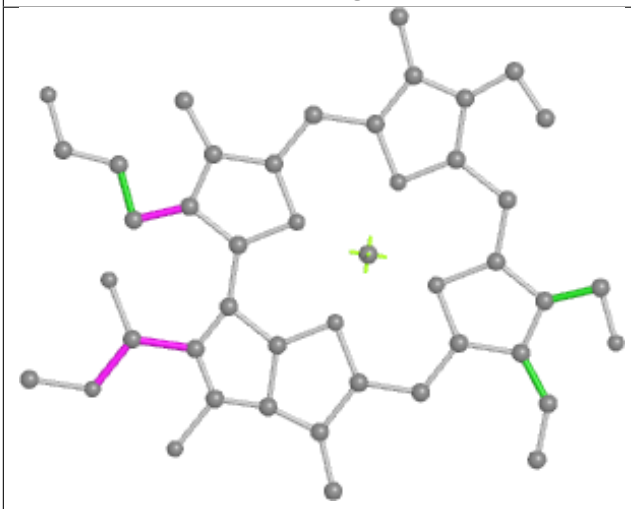
Ligand CHL P 314



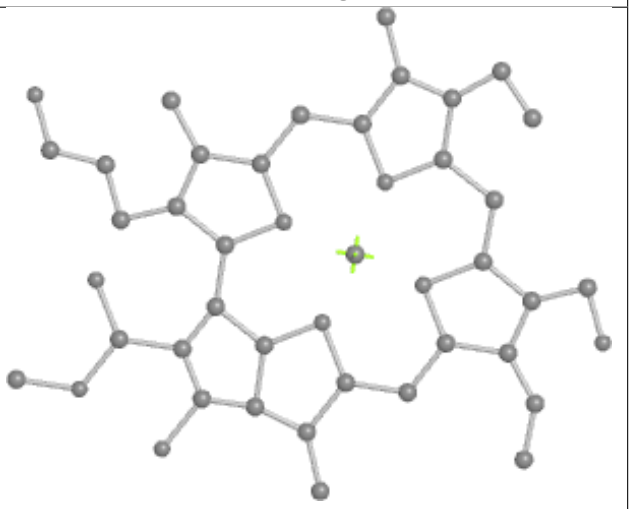
Bond lengths



Bond angles

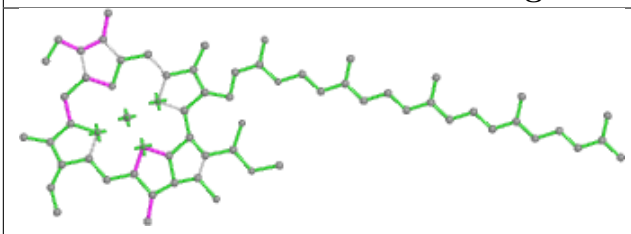


Torsions

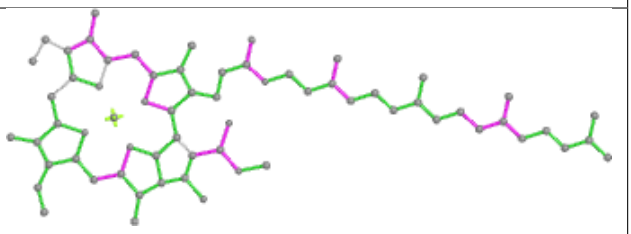


Rings

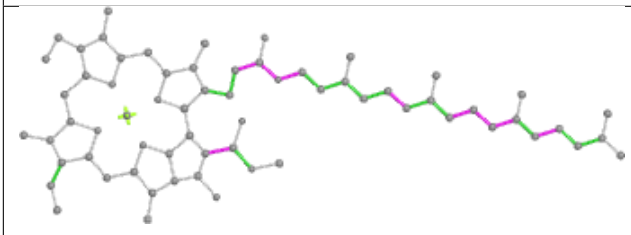
Ligand CLA P 302



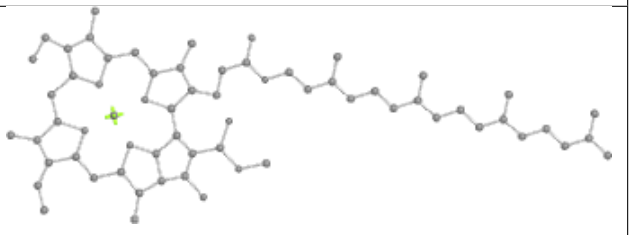
Bond lengths



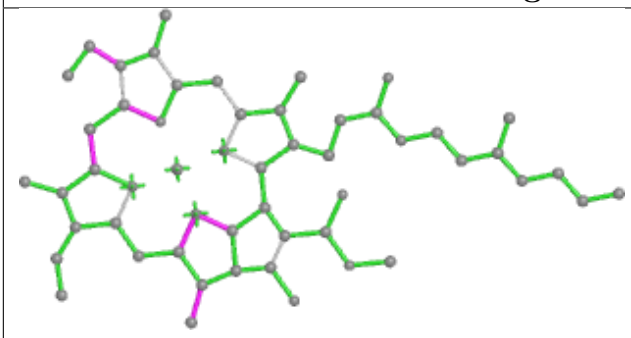
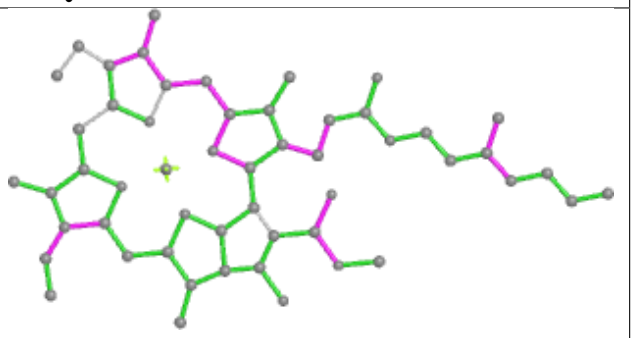
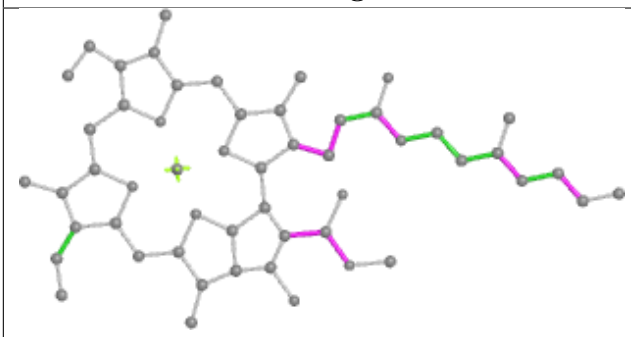
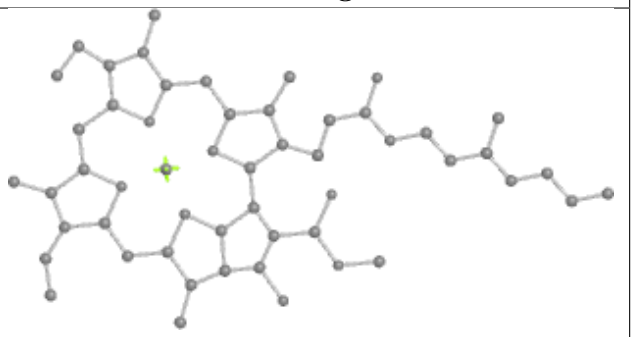
Bond angles

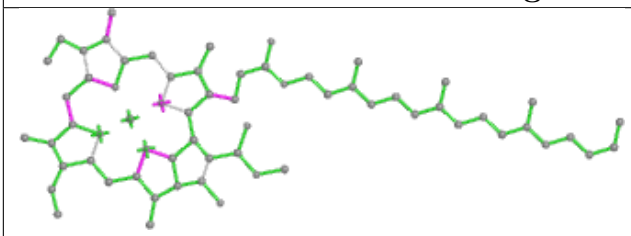
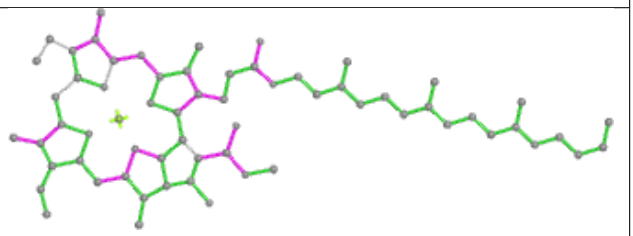
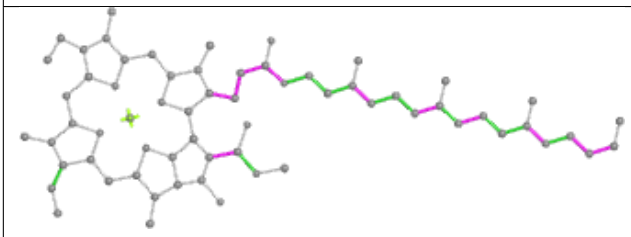
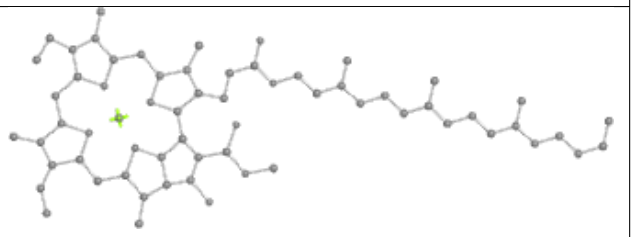


Torsions

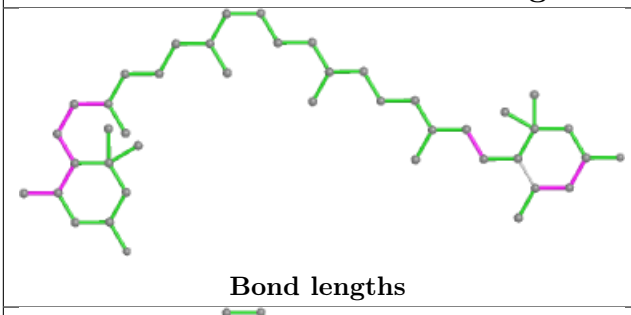


Rings

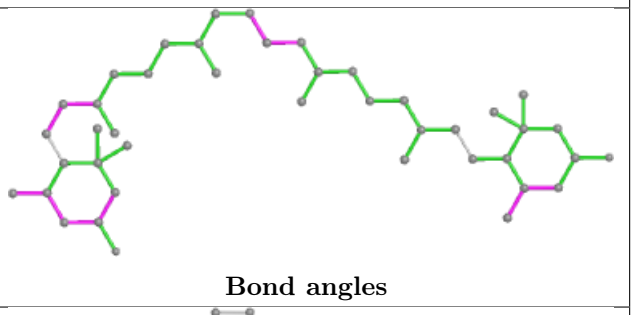
Ligand CLA Q 312	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA R 313	
 Bond lengths	 Bond angles
 Torsions	 Rings

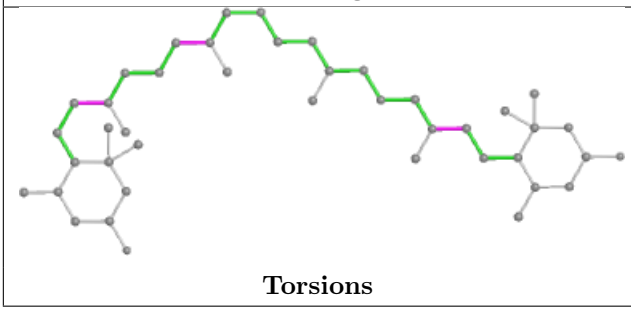
Ligand Q6L P 315



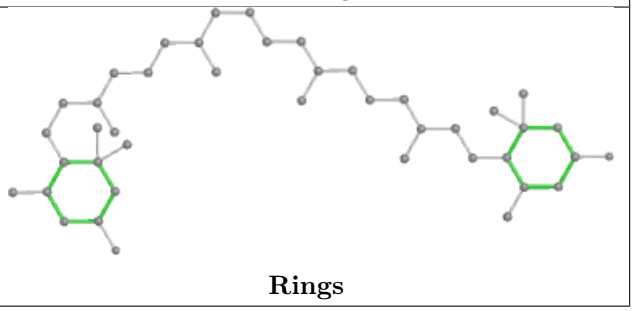
Bond lengths



Bond angles

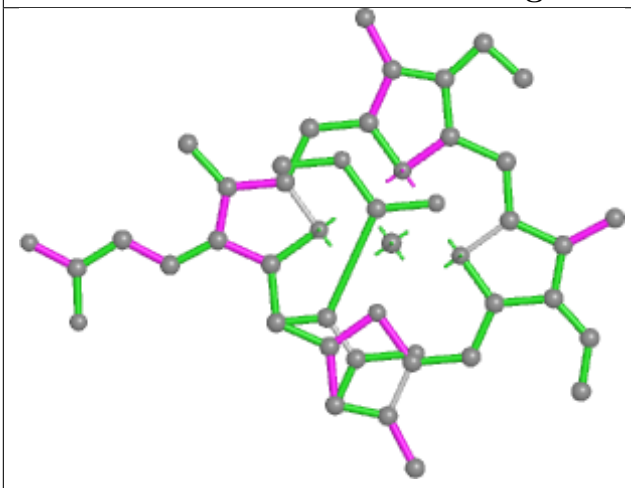


Torsions

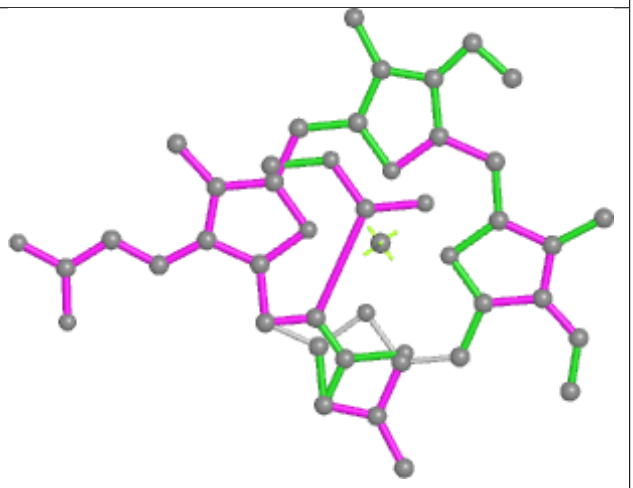


Rings

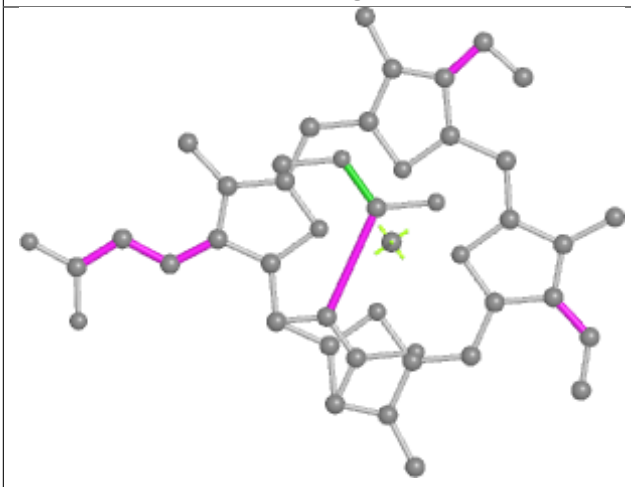
Ligand KC2 R 312



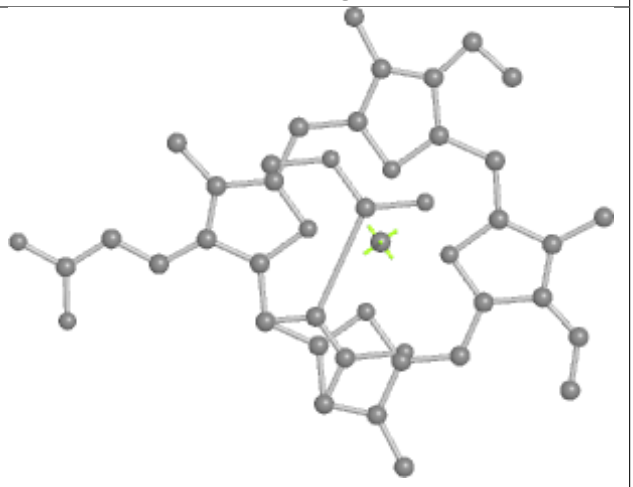
Bond lengths



Bond angles

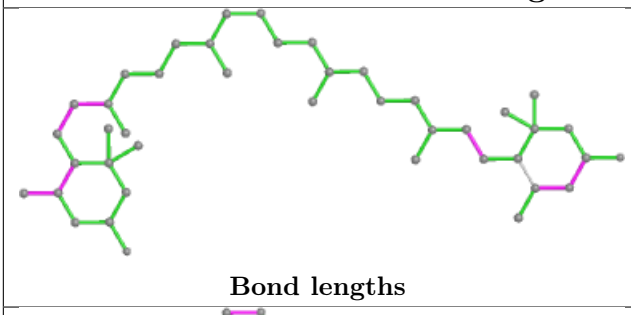


Torsions

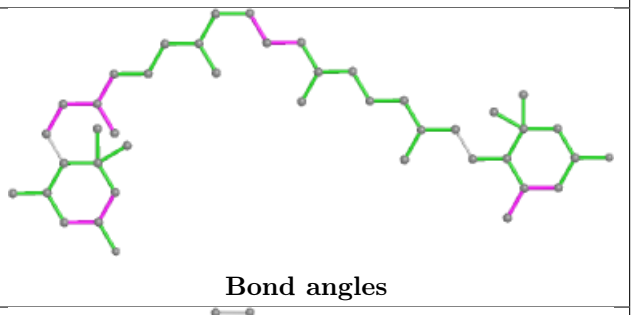


Rings

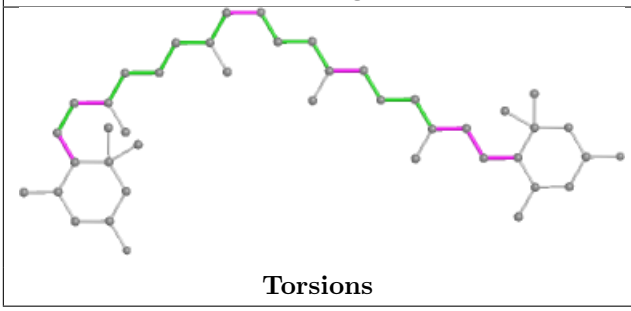
Ligand Q6L R 301



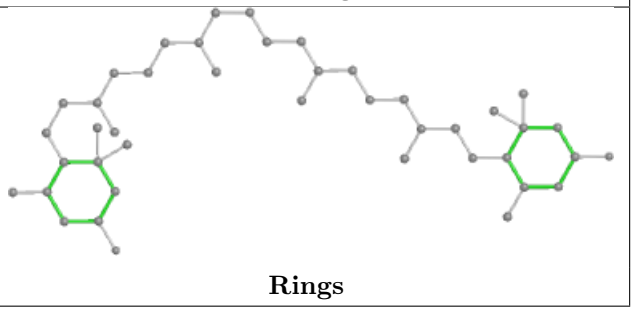
Bond lengths



Bond angles

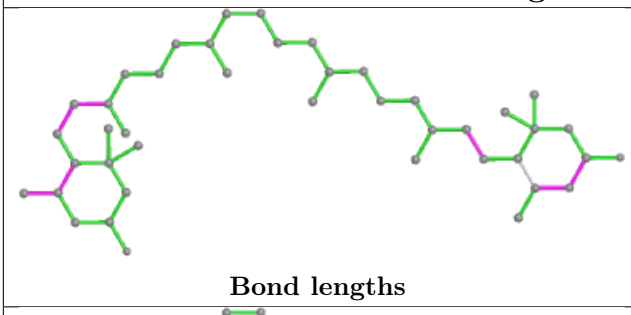


Torsions

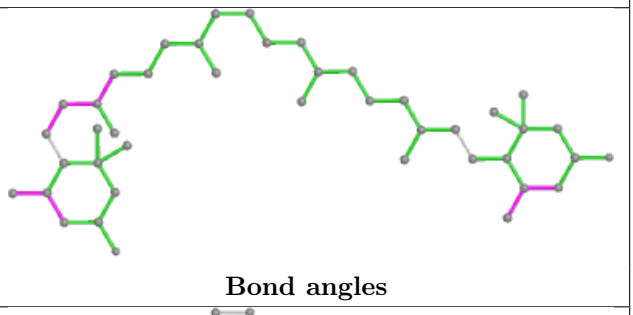


Rings

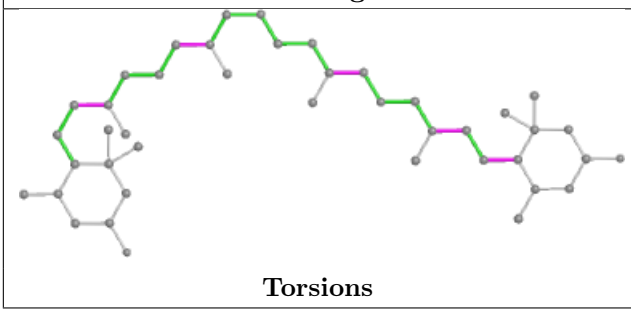
Ligand Q6L R 319



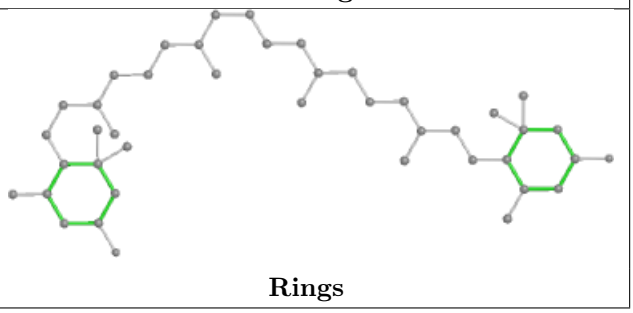
Bond lengths



Bond angles

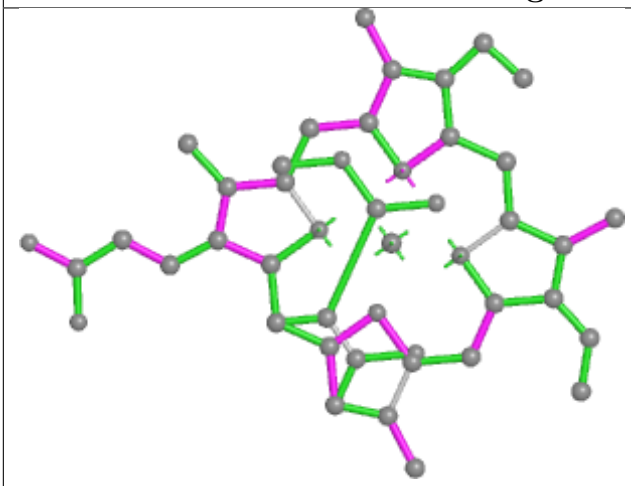


Torsions

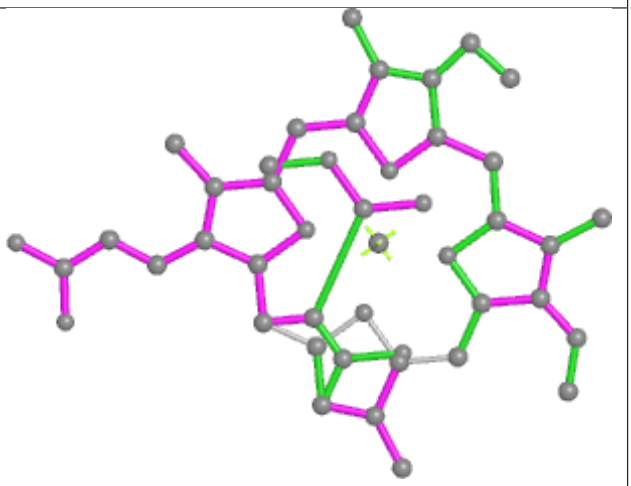


Rings

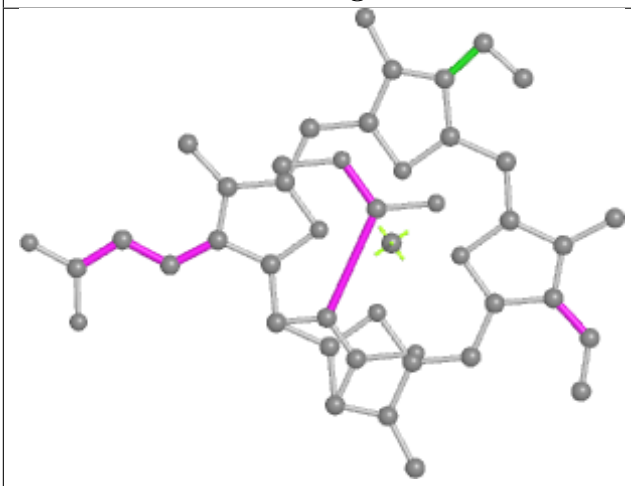
Ligand KC2 P 308



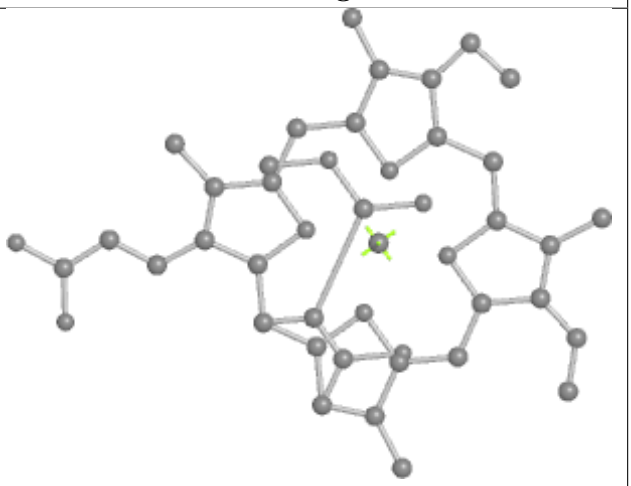
Bond lengths



Bond angles

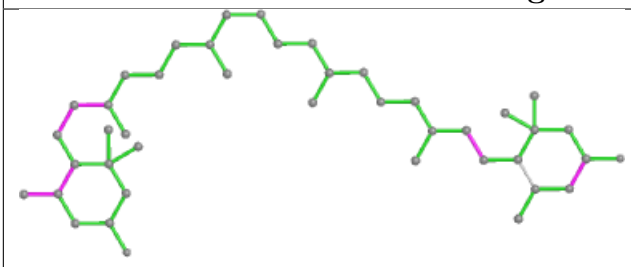


Torsions

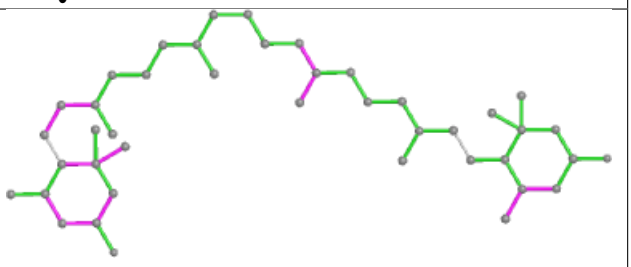


Rings

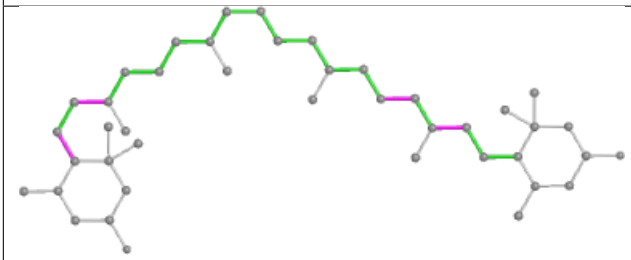
Ligand Q6L Q 317



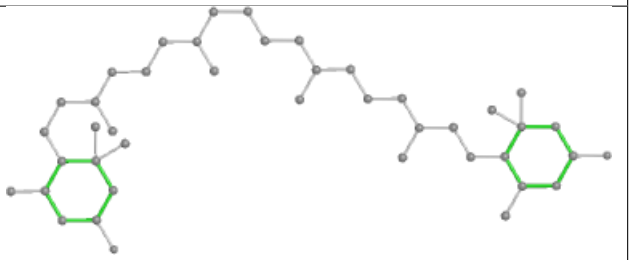
Bond lengths



Bond angles

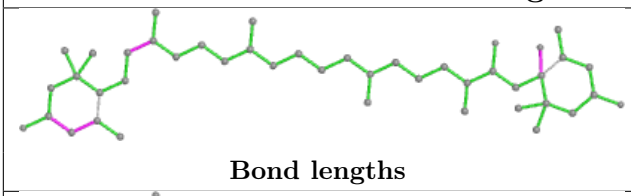


Torsions

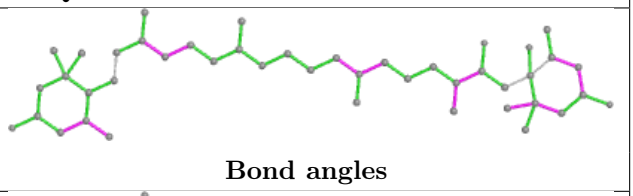


Rings

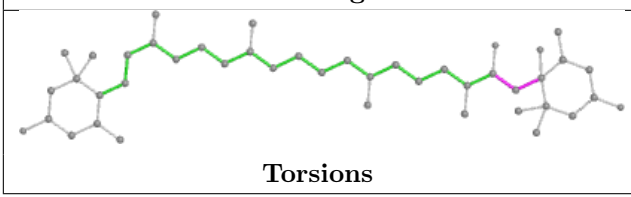
Ligand IWJ Q 301



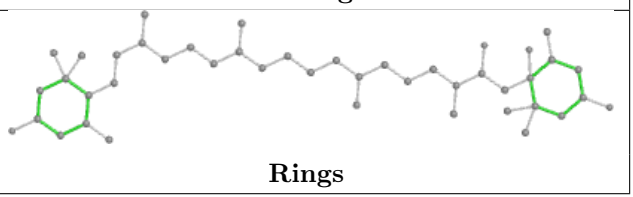
Bond lengths



Bond angles

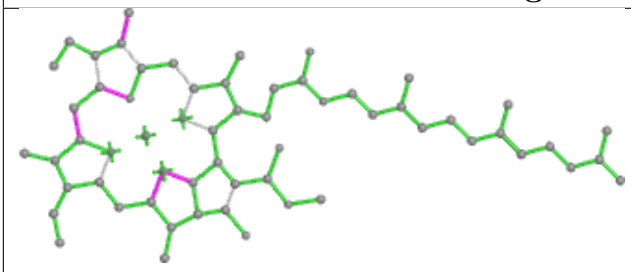


Torsions

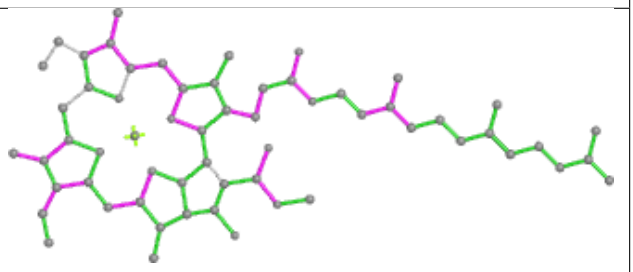


Rings

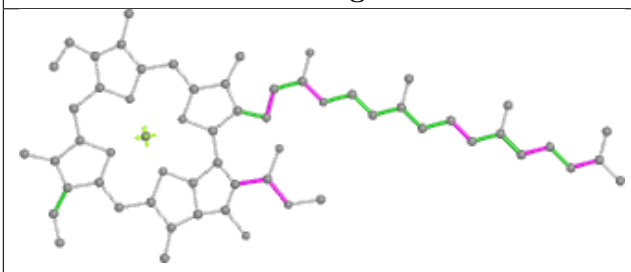
Ligand CLA P 311



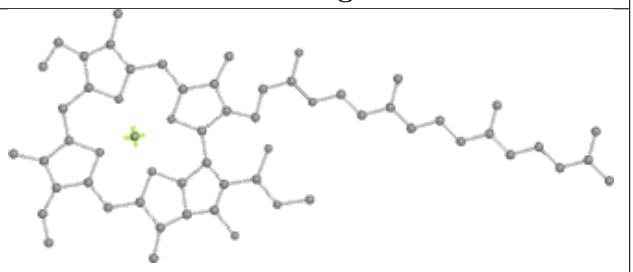
Bond lengths



Bond angles

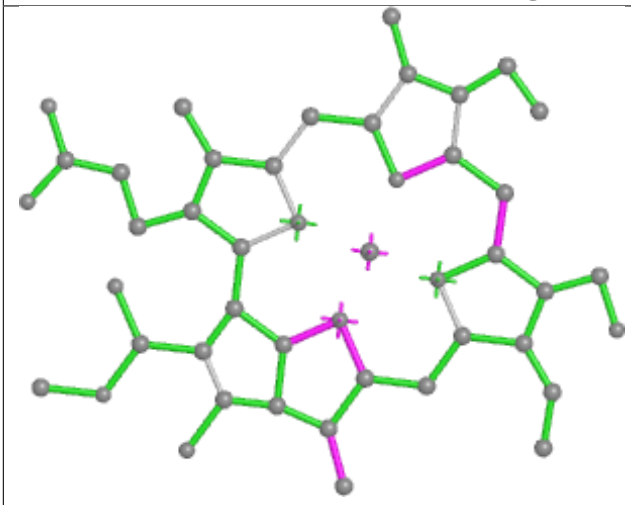


Torsions

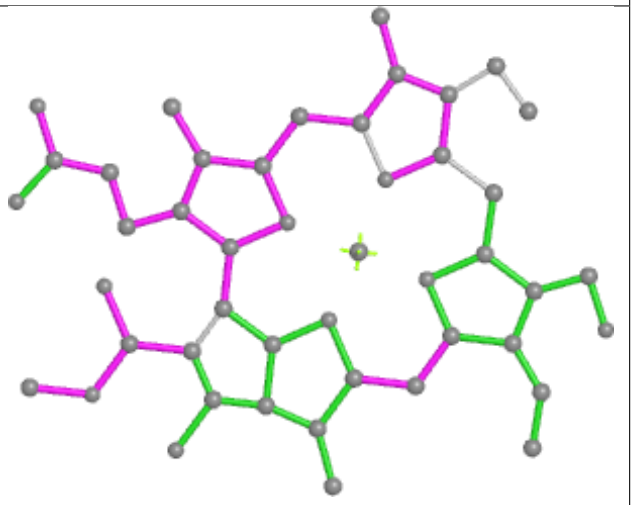


Rings

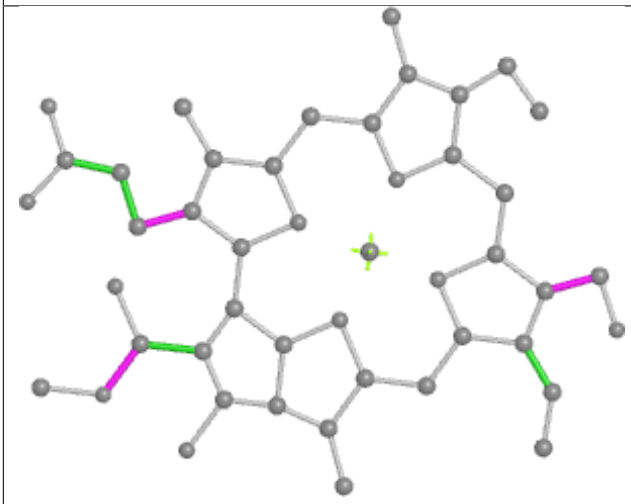
Ligand CHL P 304



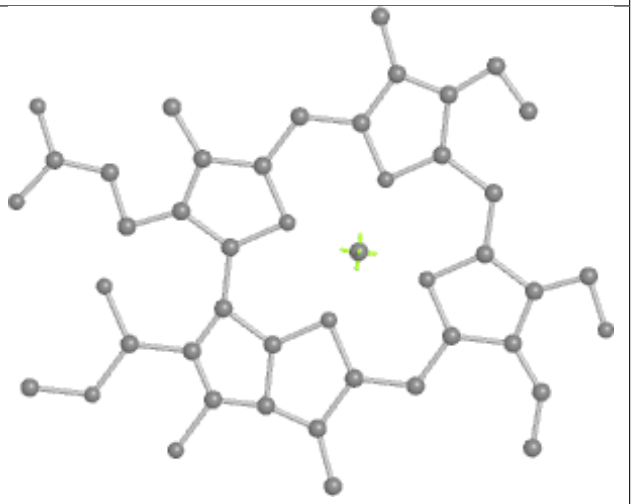
Bond lengths



Bond angles

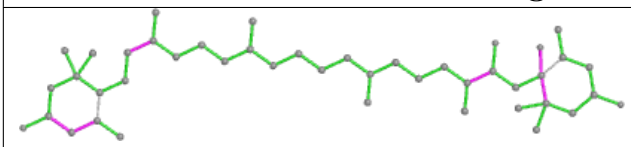


Torsions

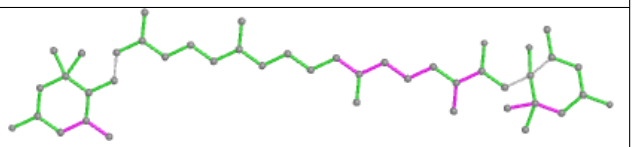


Rings

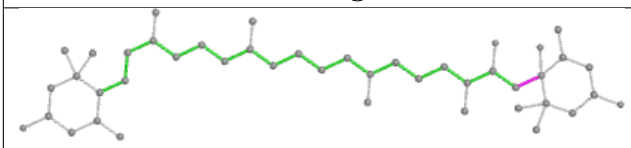
Ligand IWJ P 320



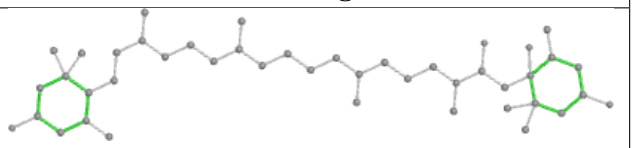
Bond lengths



Bond angles

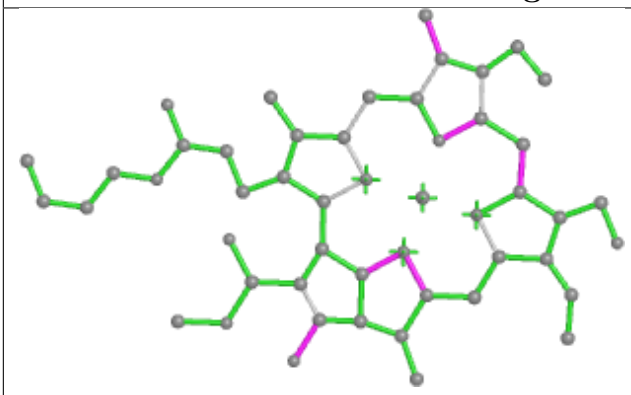


Torsions

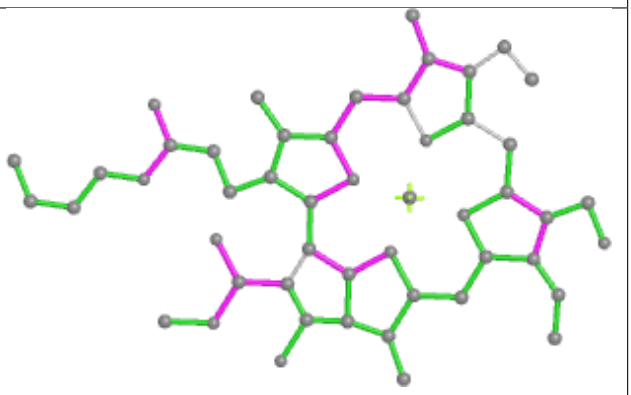


Rings

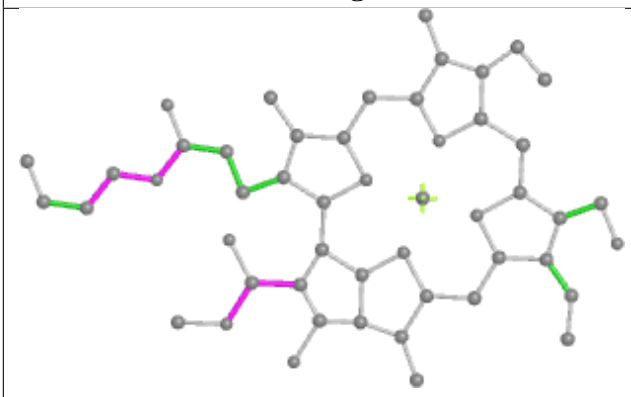
Ligand CHL R 309



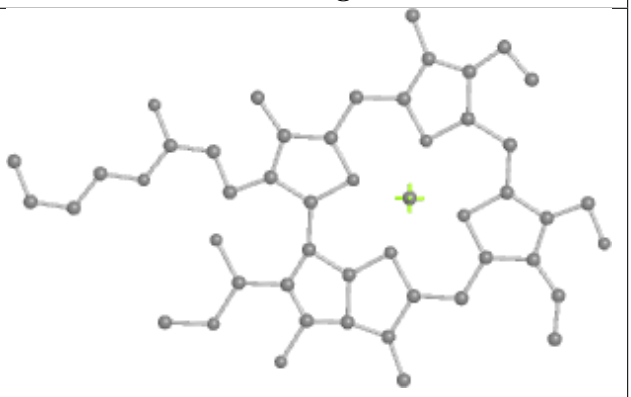
Bond lengths



Bond angles

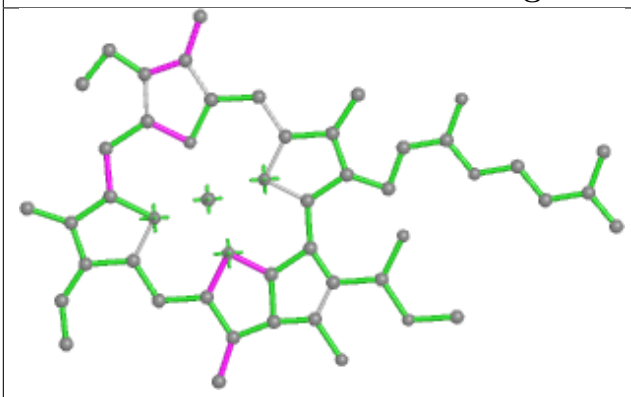


Torsions

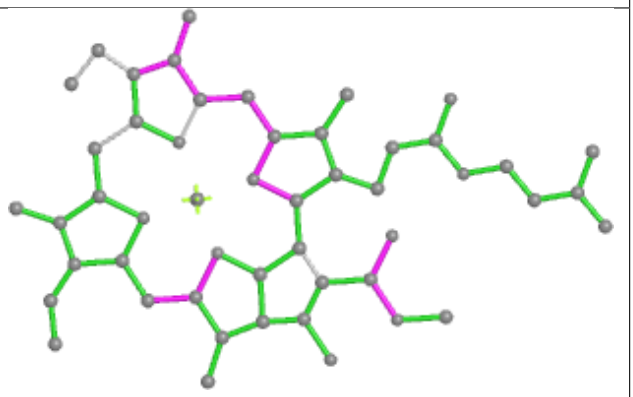


Rings

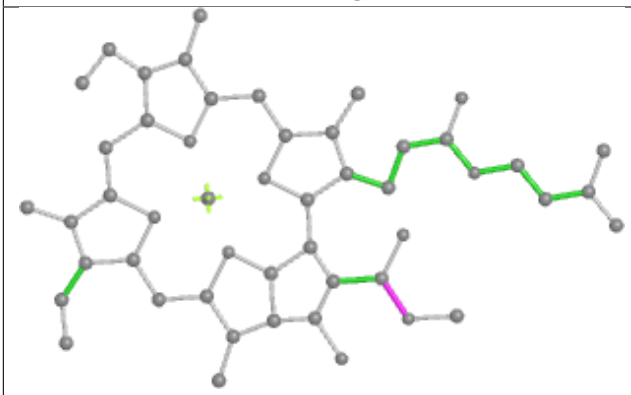
Ligand CLA R 307



Bond lengths



Bond angles



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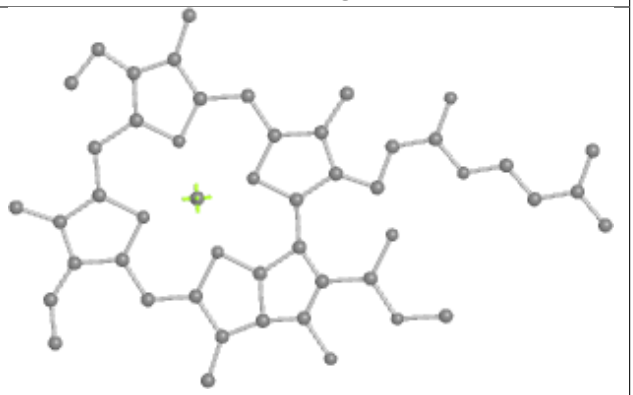
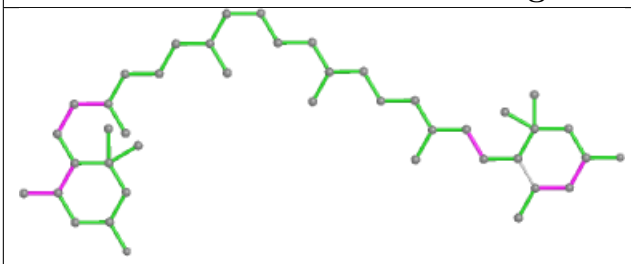
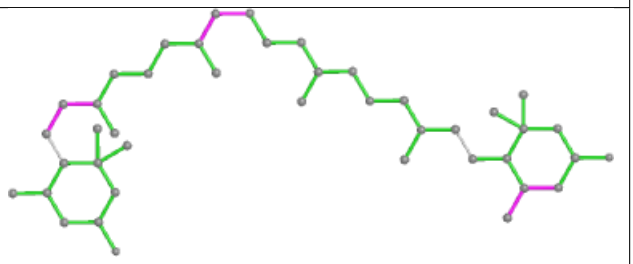


Rings

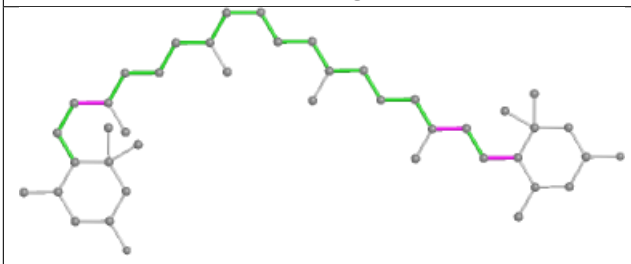
Ligand Q6L R 304



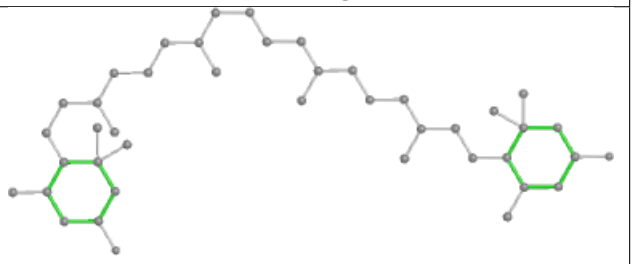
Bond lengths



Bond angles

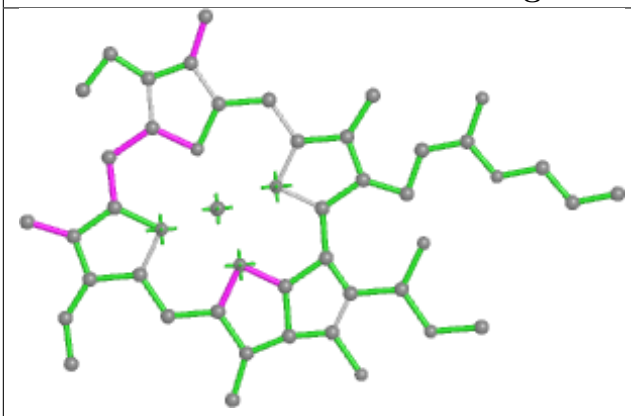


Torsions

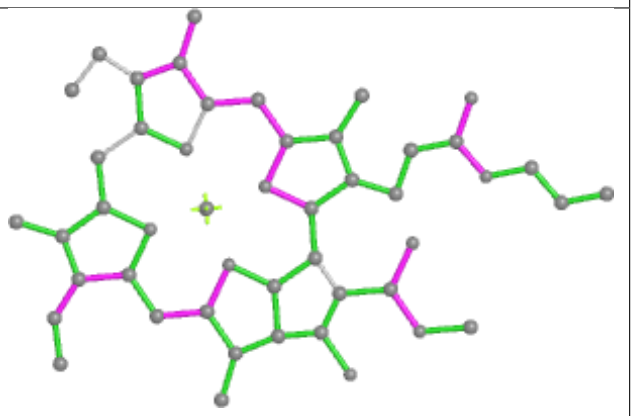


Rings

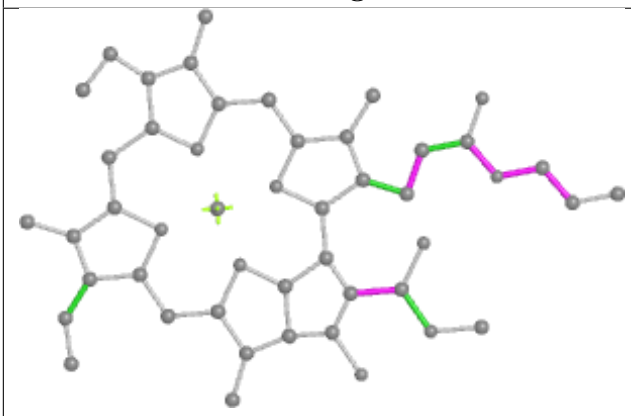
Ligand CLA R 317



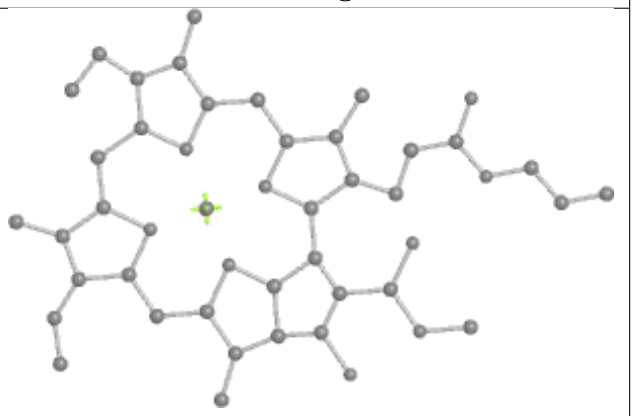
Bond lengths



Bond angles

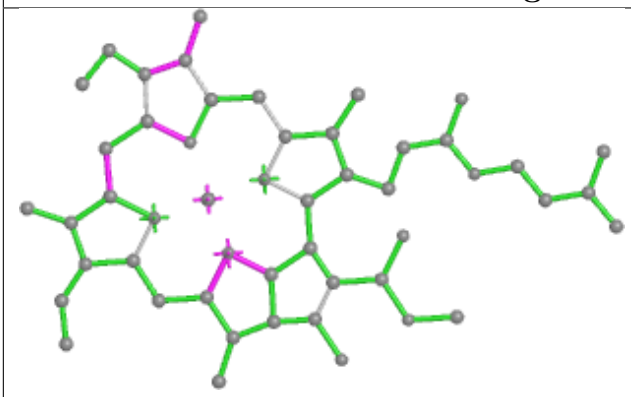


Torsions

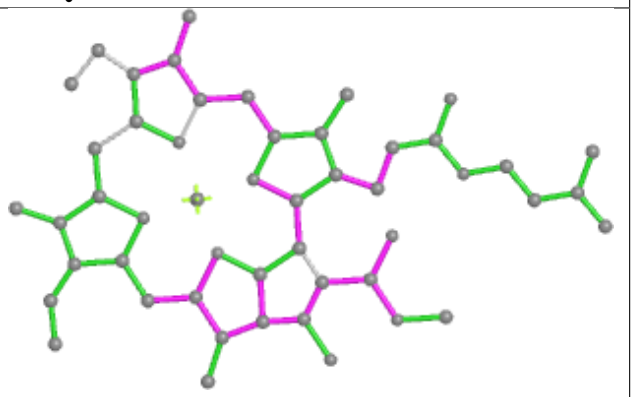


Rings

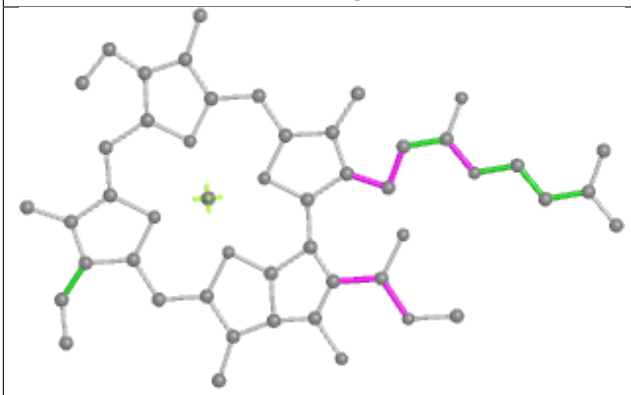
Ligand CLA Q 304



Bond lengths



Bond angles



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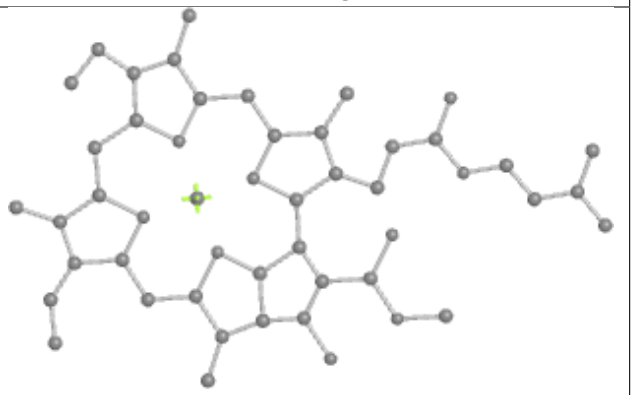
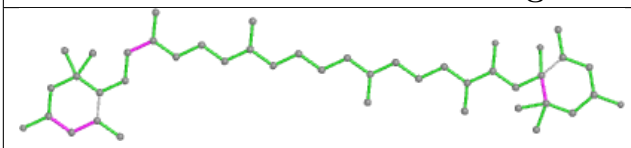
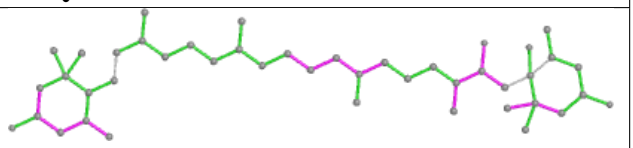


Rings

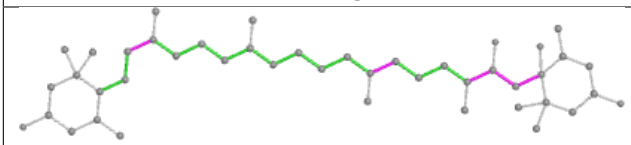
Ligand IWJ Q 319



Bond lengths



Bond angles



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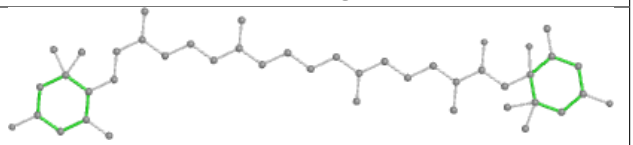
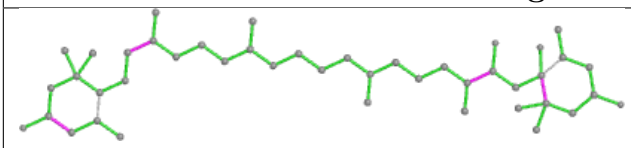
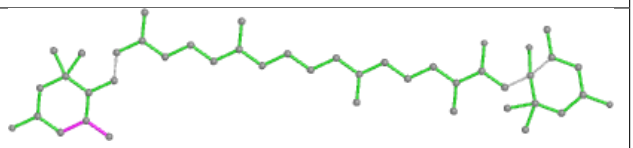


Rings

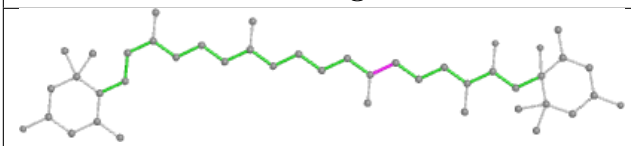
Ligand IWJ P 318



Bond lengths



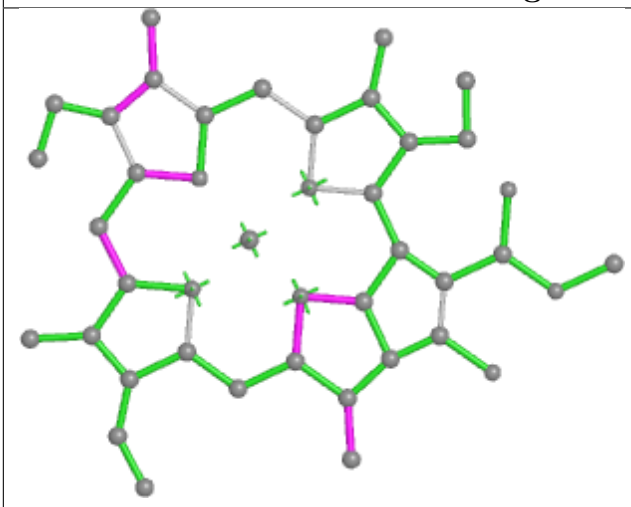
Bond angles



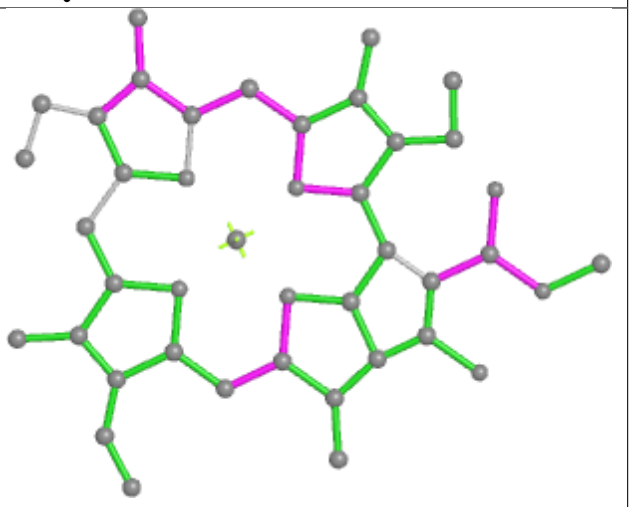
Torsions

Rings

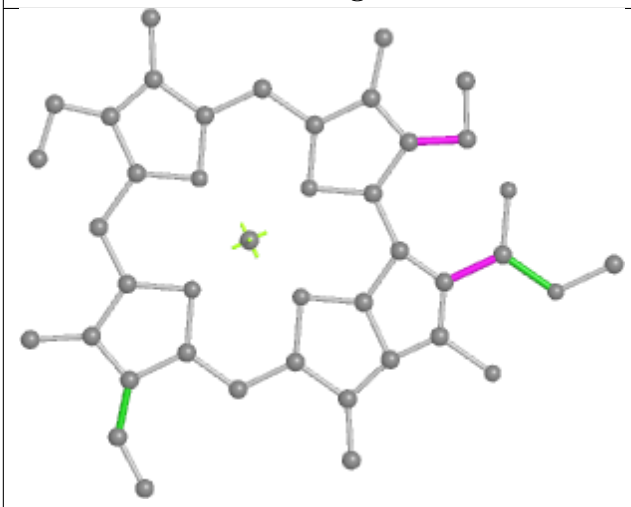
Ligand CLA Q 310



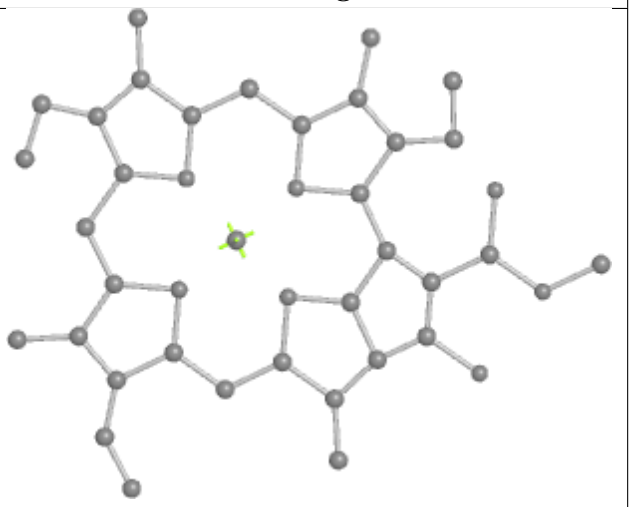
Bond lengths



Bond angles

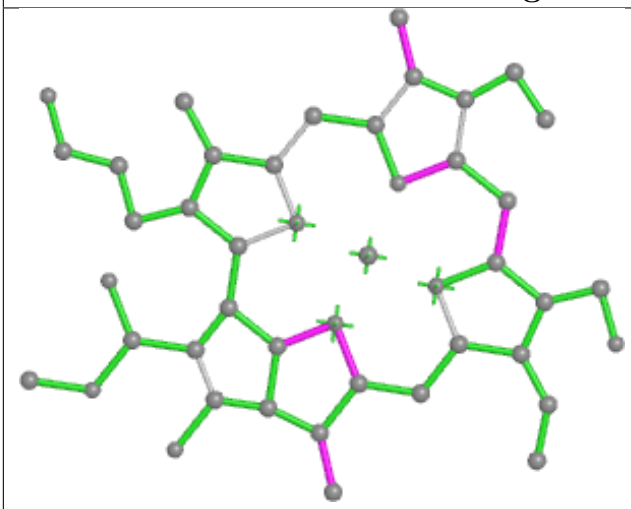


Torsions



Rings

Ligand CHL R 318



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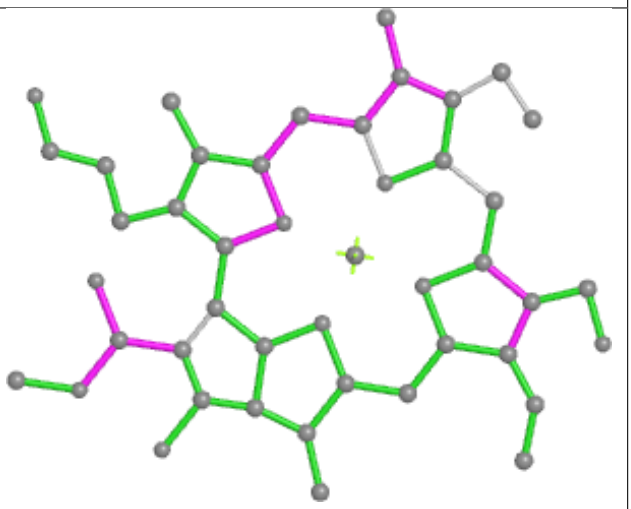
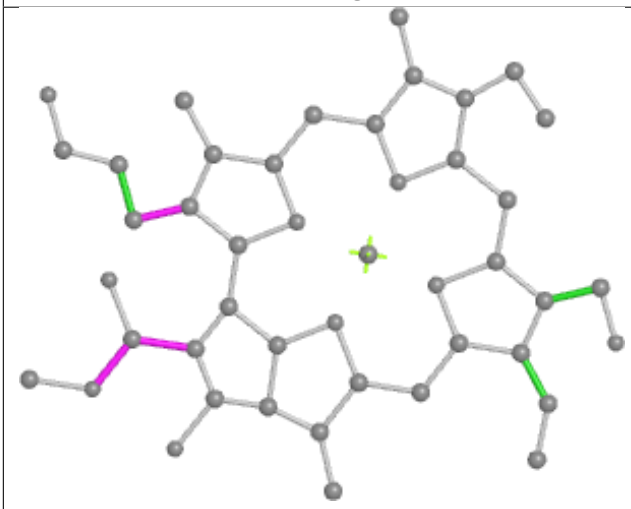
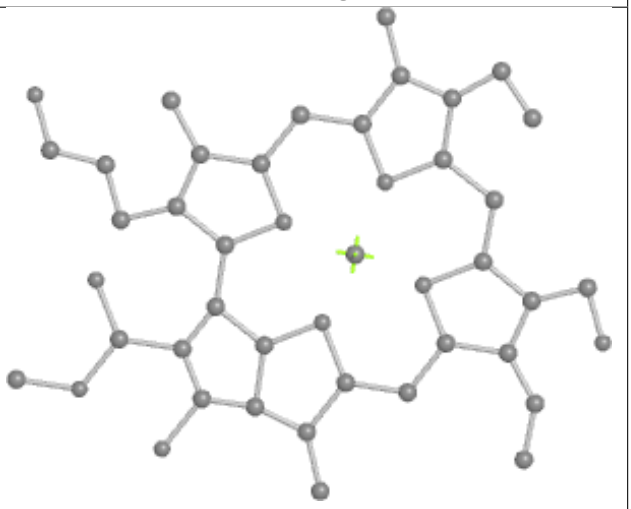


Bond angles

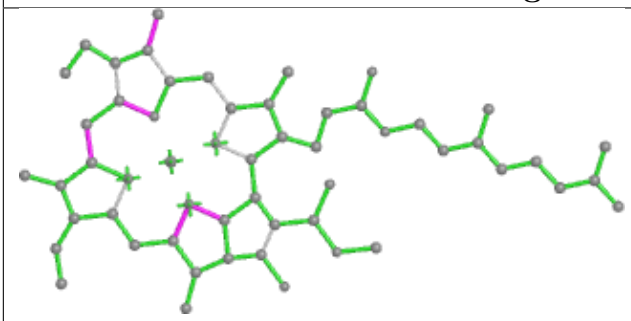


Torsions



Rings

Ligand CLA R 316



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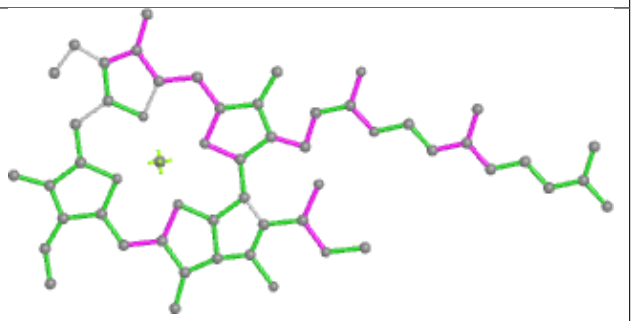
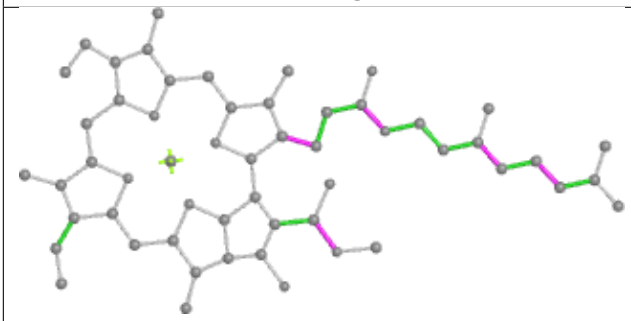
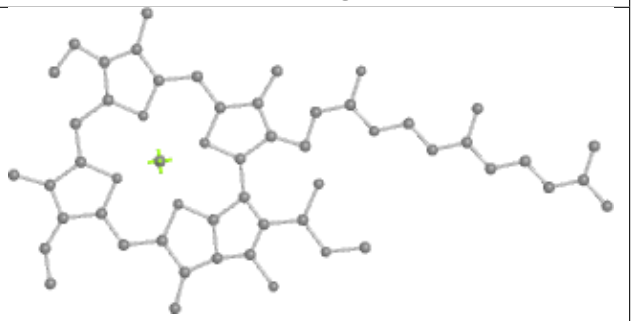


Bond angles

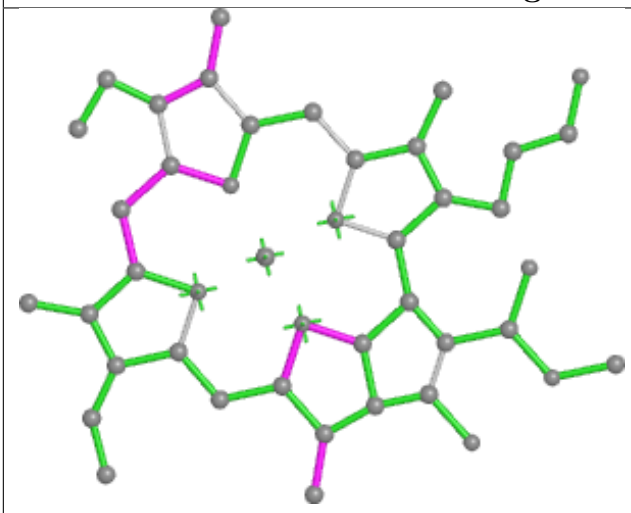


Torsions

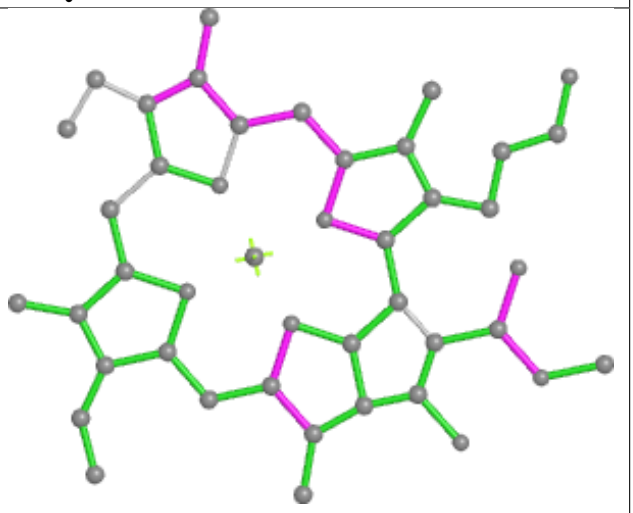


Rings

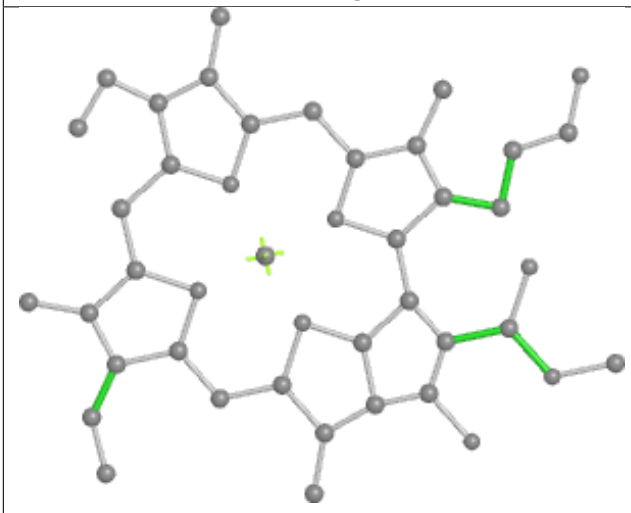
Ligand CLA Q 303



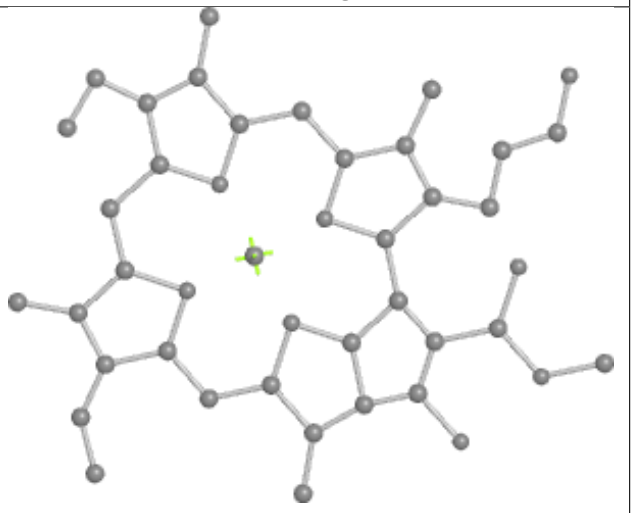
Bond lengths



Bond angles

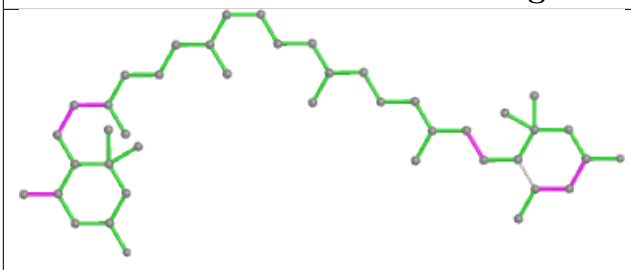


Torsions

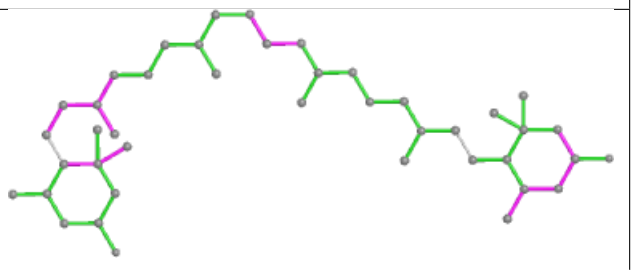


Rings

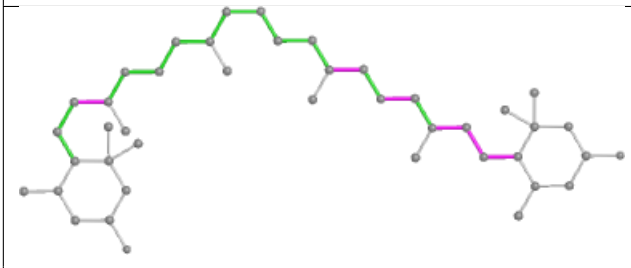
Ligand Q6L R 323



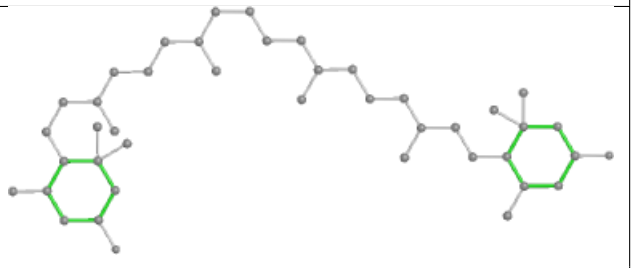
Bond lengths



Bond angles

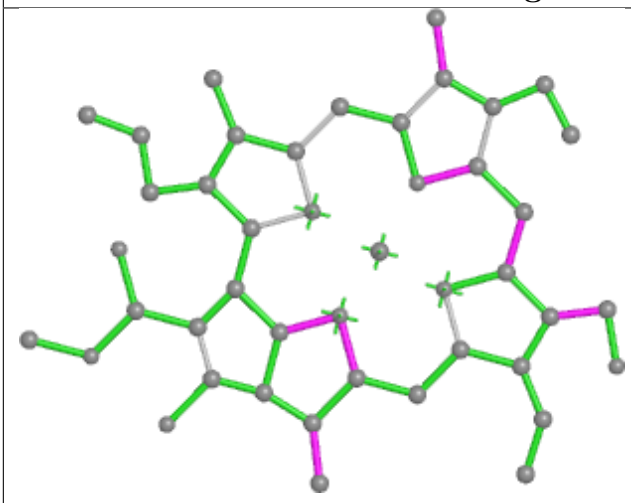


Torsions

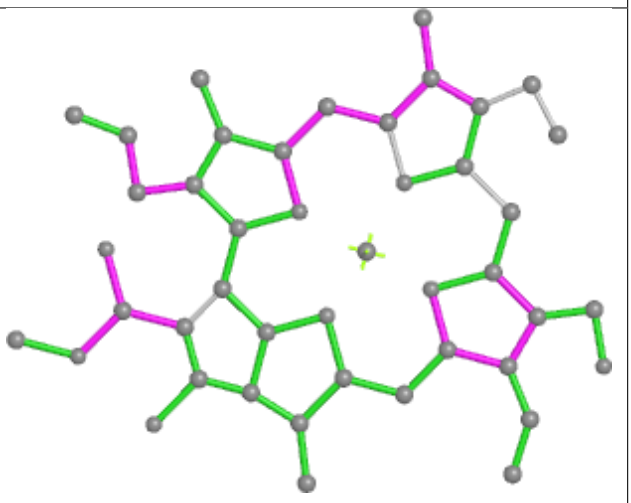


Rings

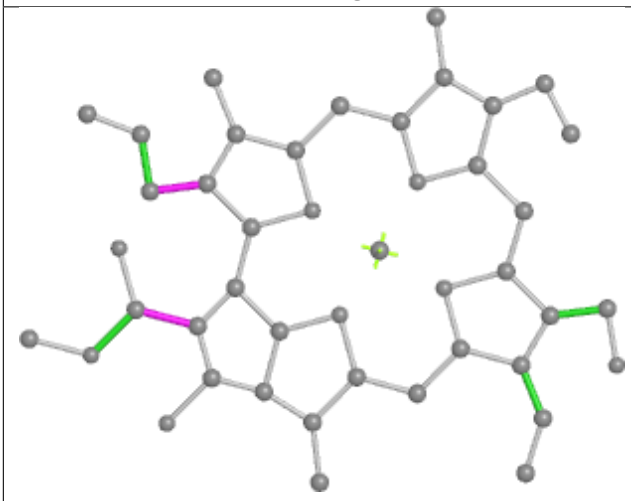
Ligand CHL P 307



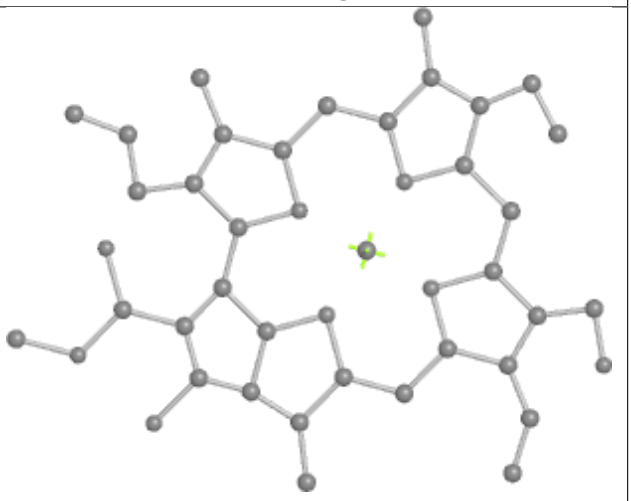
Bond lengths



Bond angles

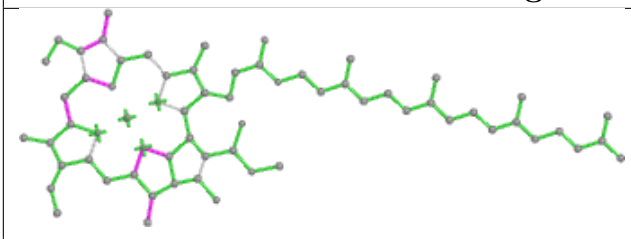


Torsions

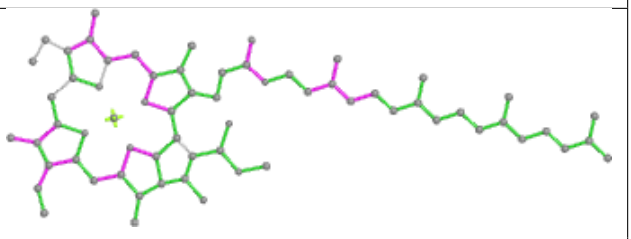


Rings

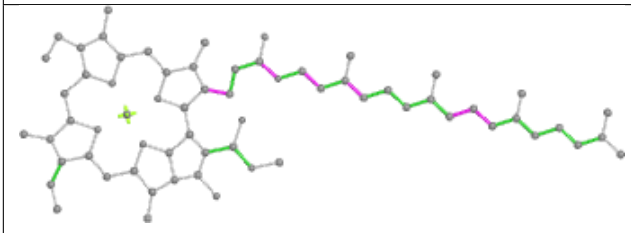
Ligand CLA P 301



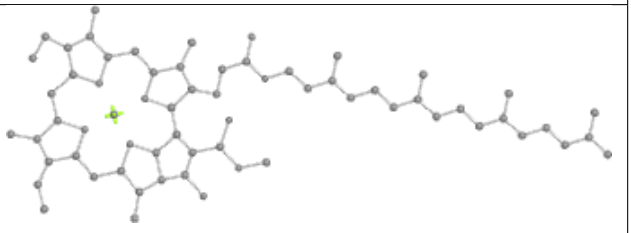
Bond lengths



Bond angles

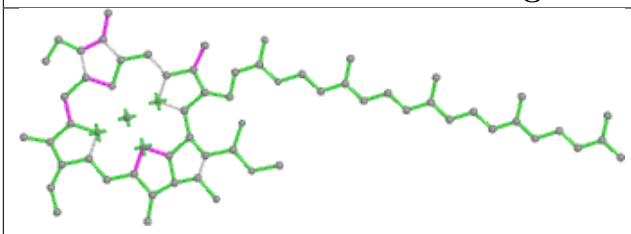


Torsions

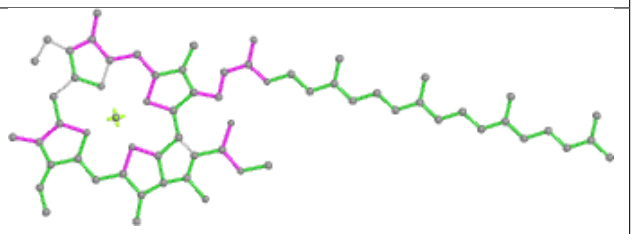


Rings

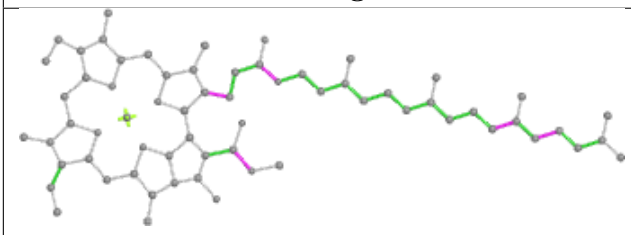
Ligand CLA R 305



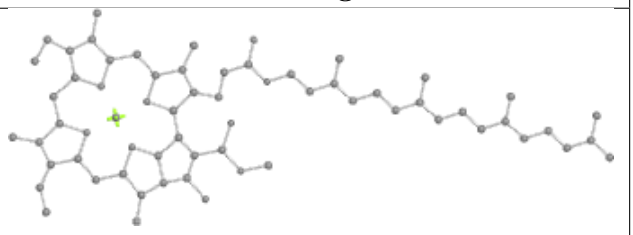
Bond lengths



Bond angles

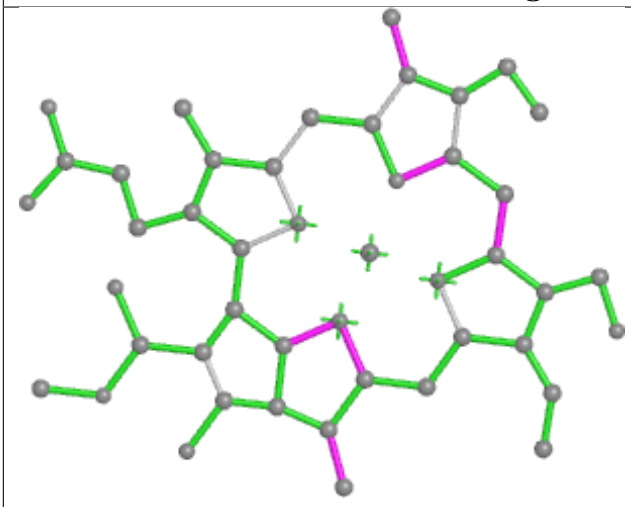


Torsions

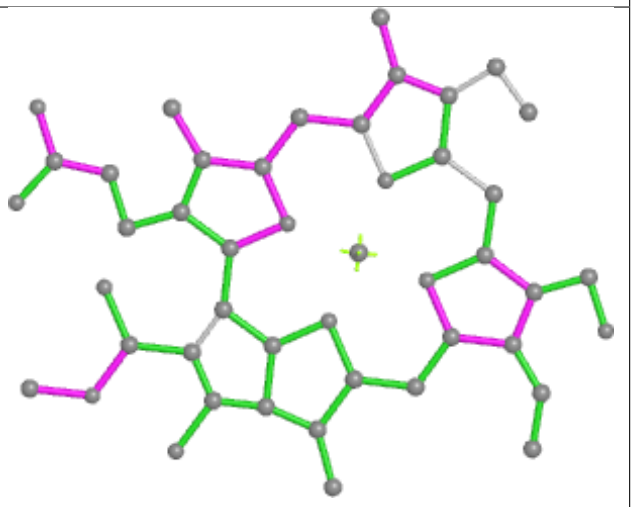


Rings

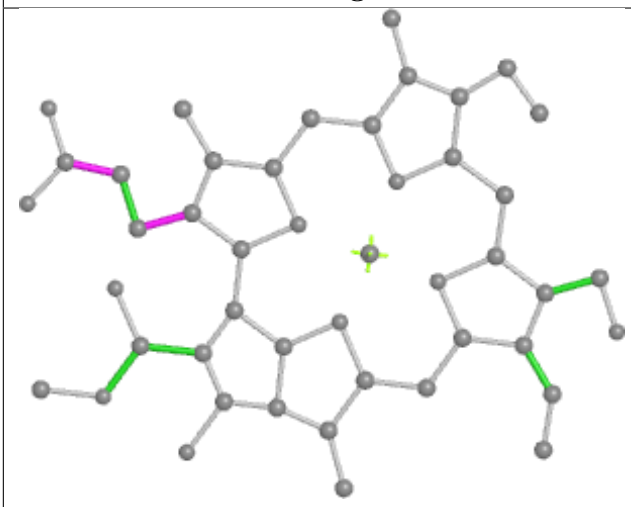
Ligand CHL P 305



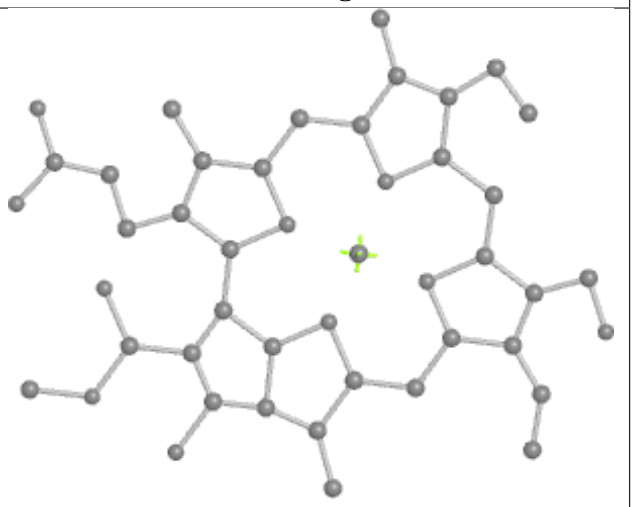
Bond lengths



Bond angles

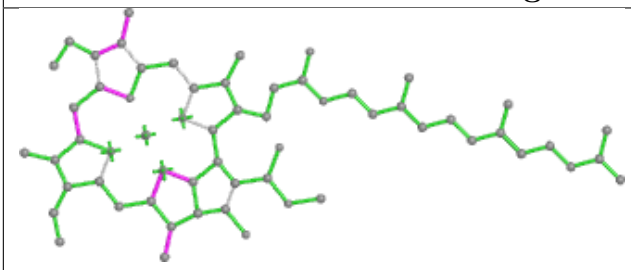


Torsions

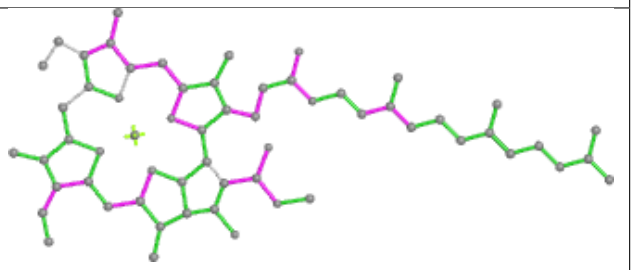


Rings

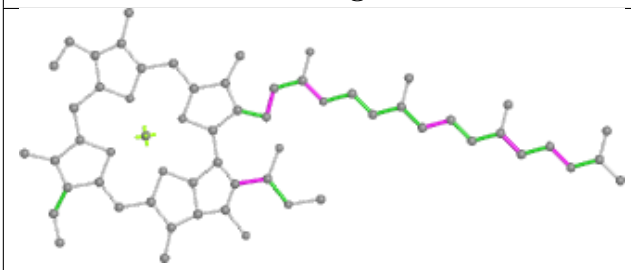
Ligand CLA R 315



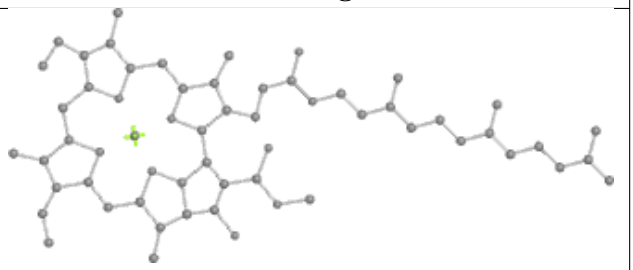
Bond lengths



Bond angles

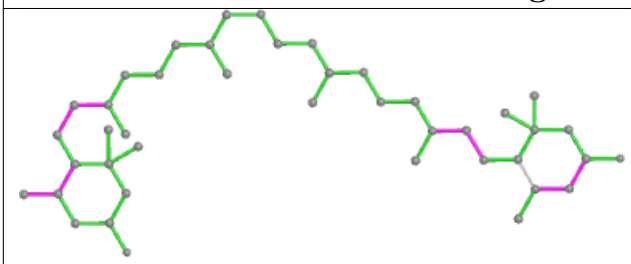


Torsions

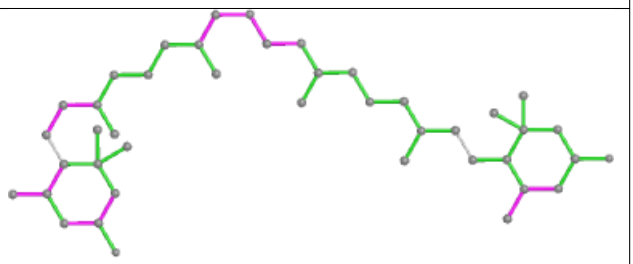


Rings

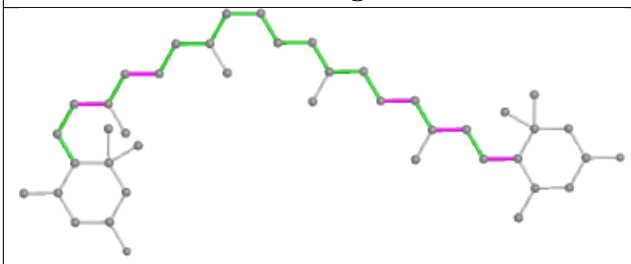
Ligand Q6L P 321



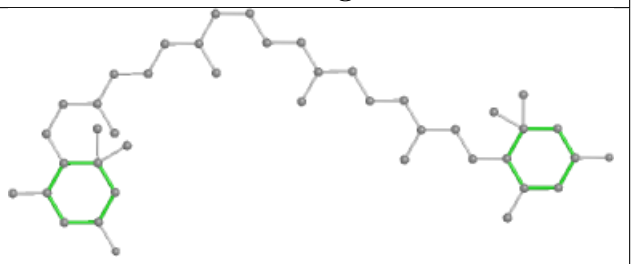
Bond lengths



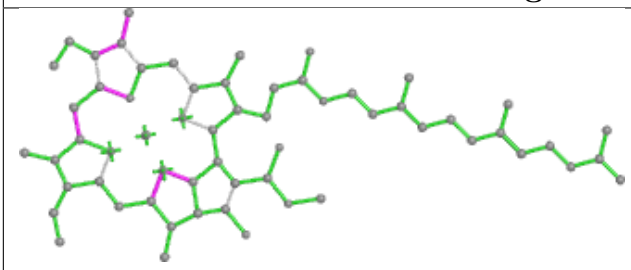
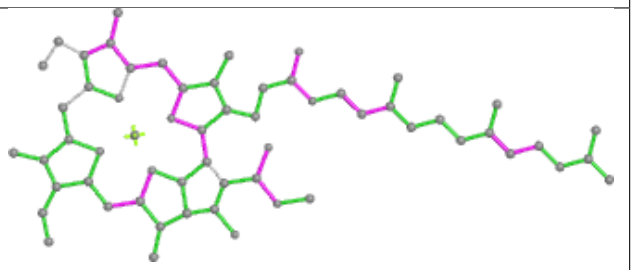
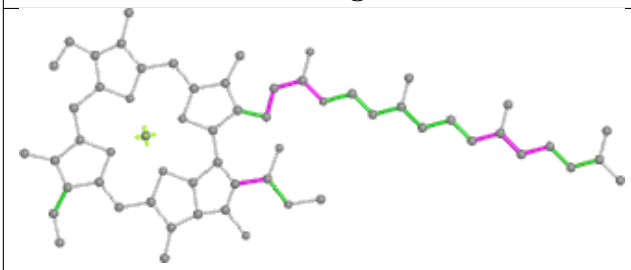
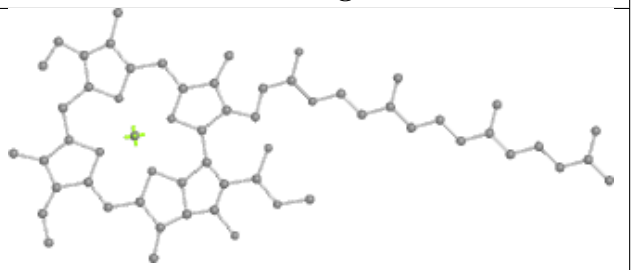
Bond angles

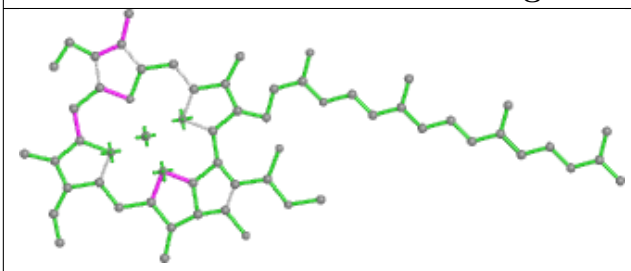
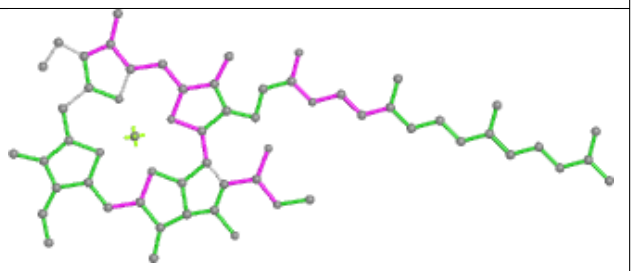
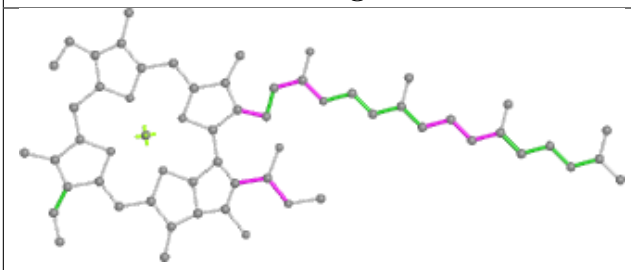
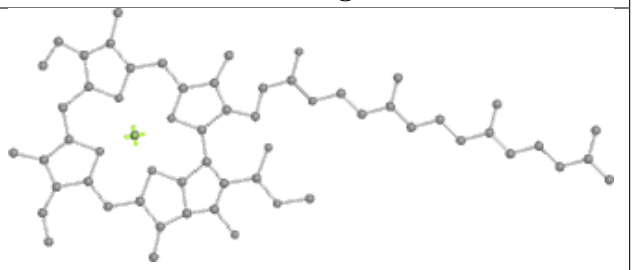


Torsions

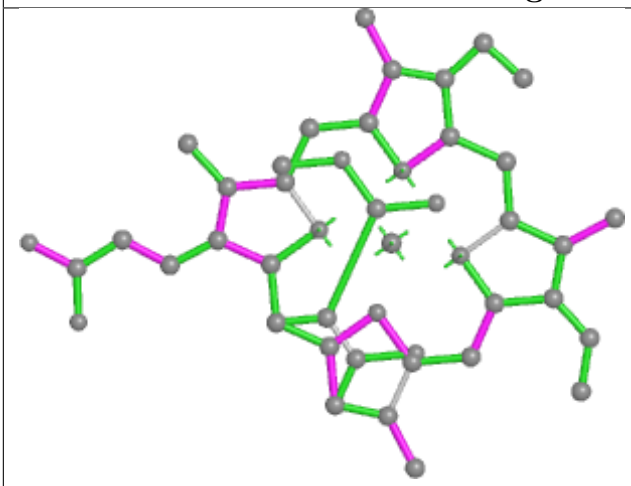


Rings

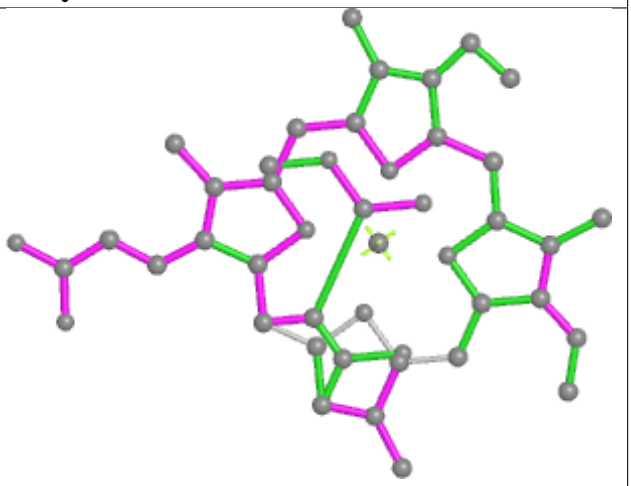
Ligand CLA P 310	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA R 314	
 Bond lengths	 Bond angles
 Torsions	 Rings

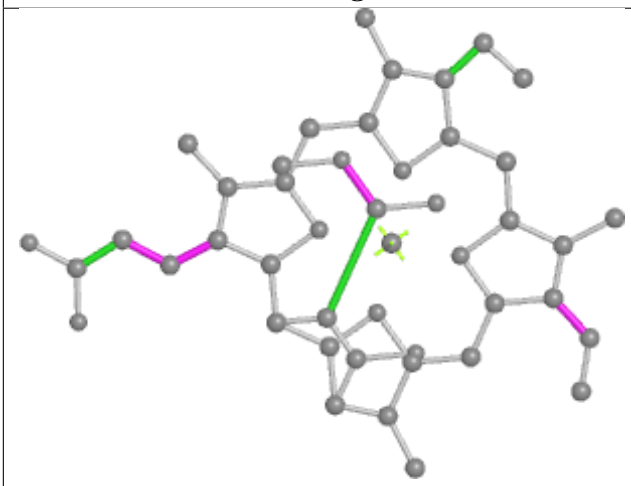
Ligand KC2 Q 308



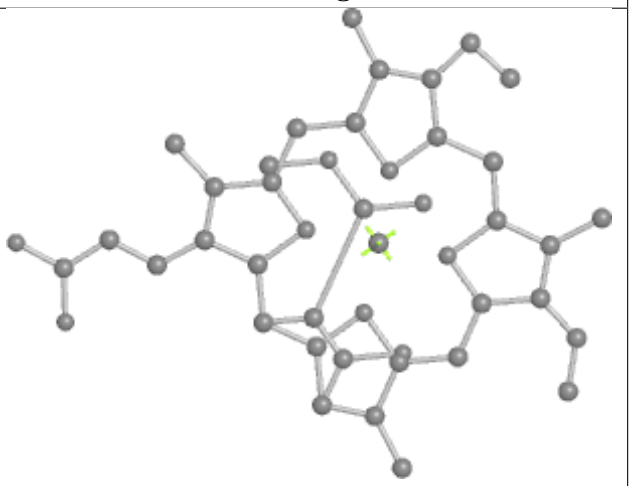
Bond lengths



Bond angles

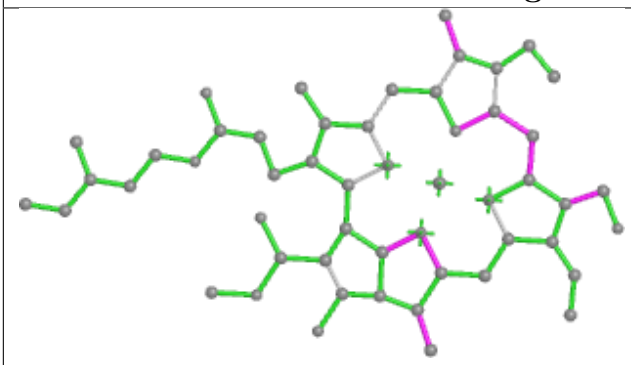


Torsions

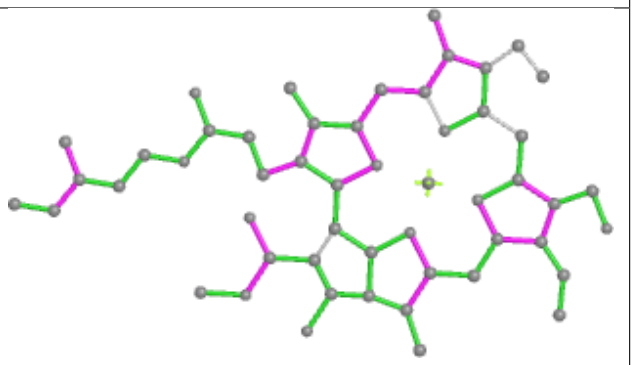


Rings

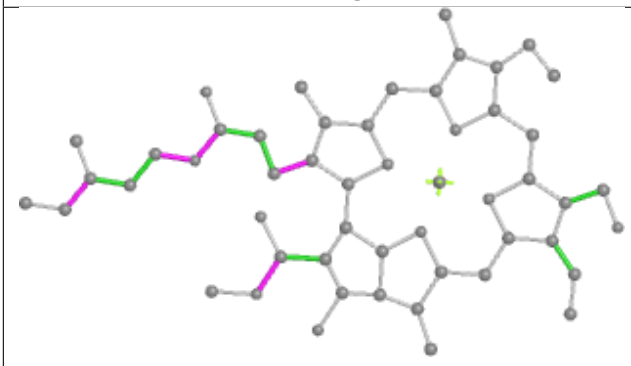
Ligand CHL P 306



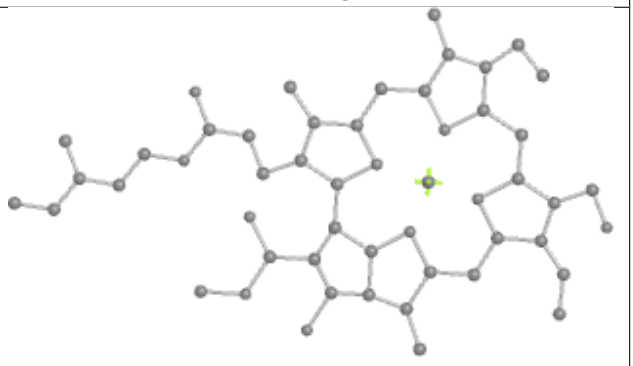
Bond lengths



Bond angles

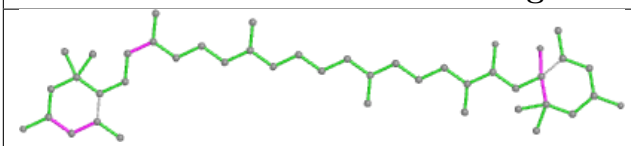


Torsions

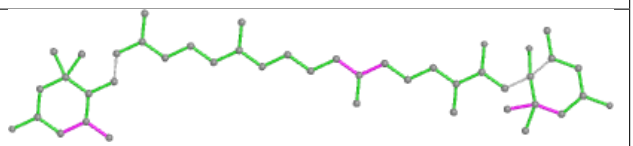


Rings

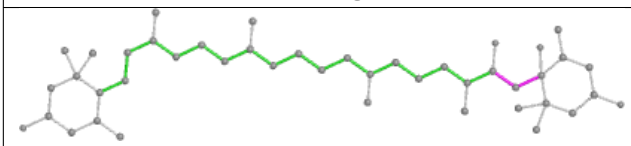
Ligand IWJ R 303



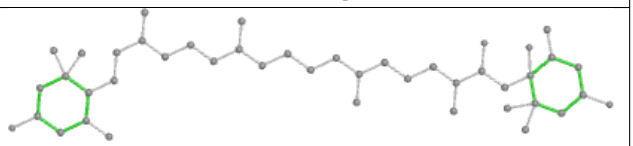
Bond lengths



Bond angles

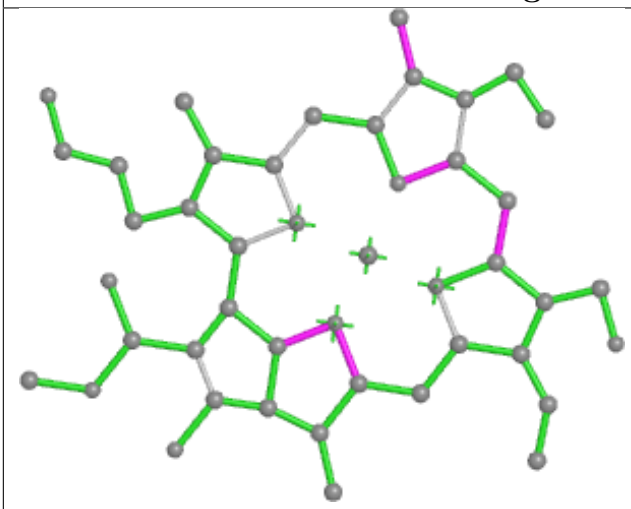


Torsions

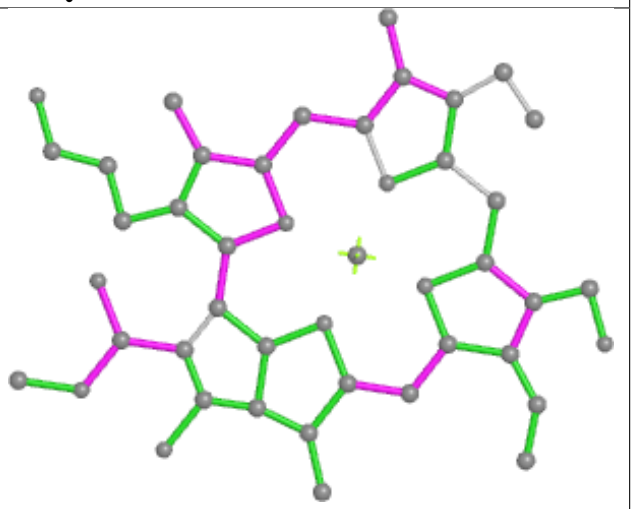


Rings

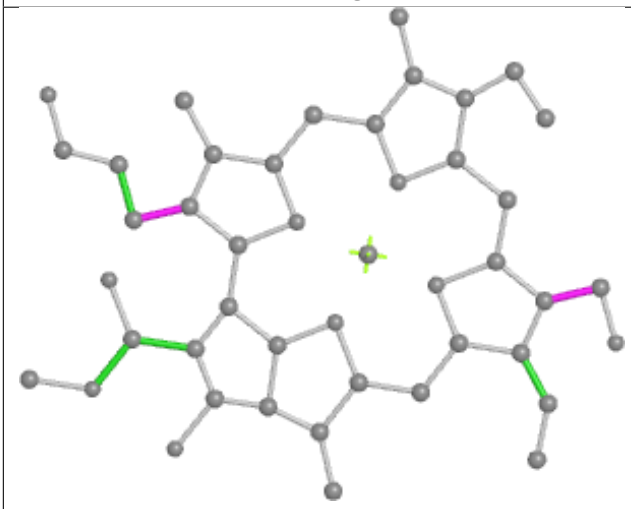
Ligand CHL Q 314



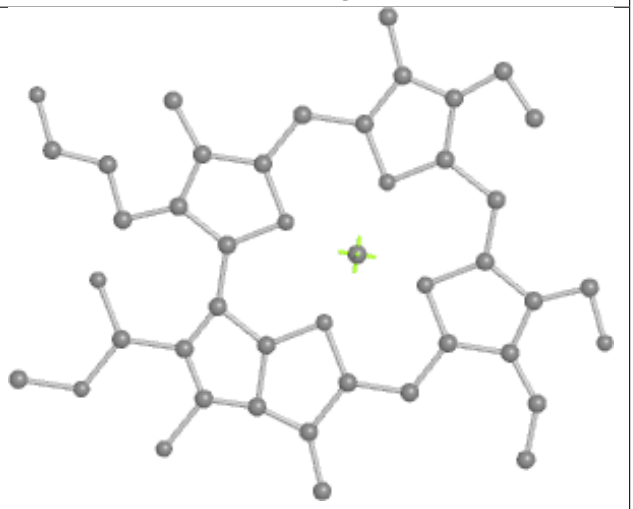
Bond lengths



Bond angles

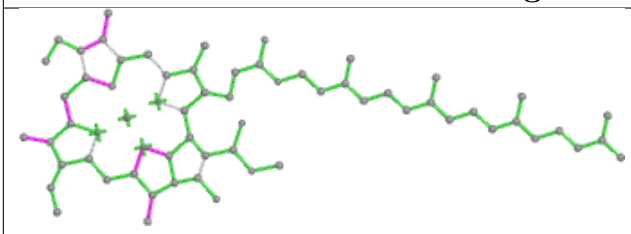


Torsions

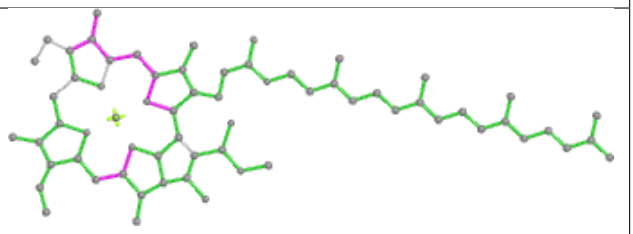


Rings

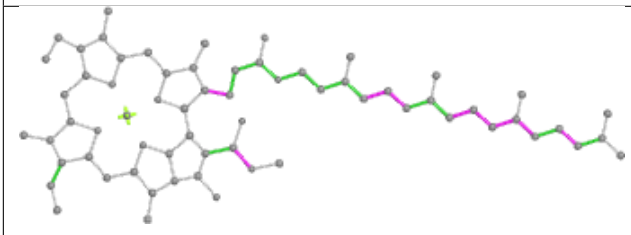
Ligand CLA R 306



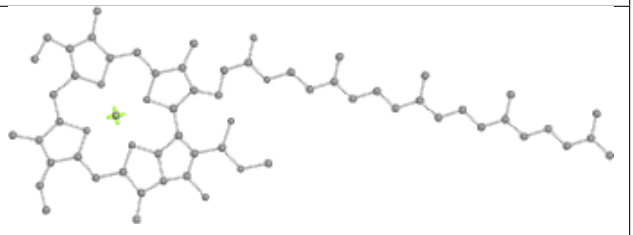
Bond lengths



Bond angles

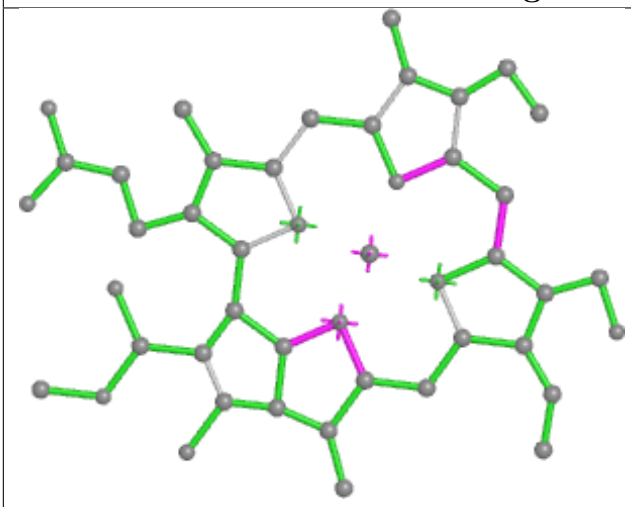


Torsions

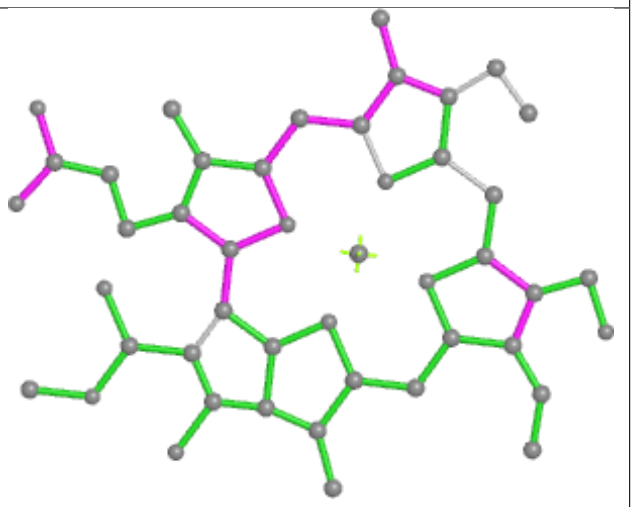


Rings

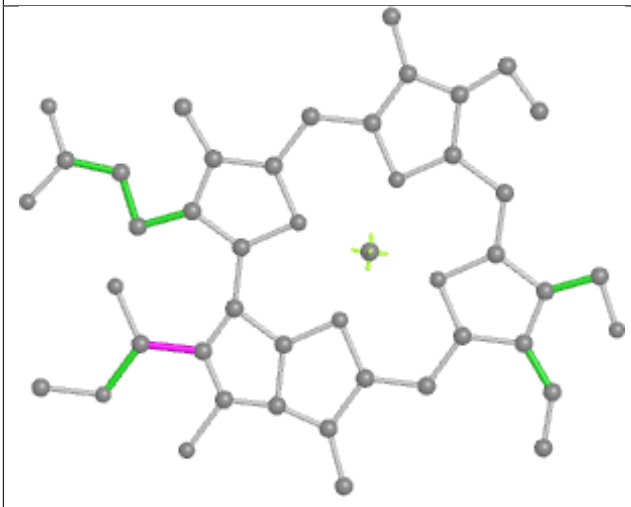
Ligand CHL R 308



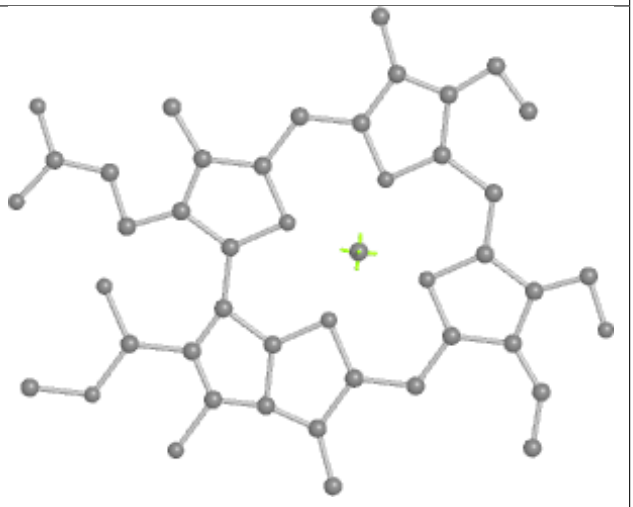
Bond lengths



Bond angles

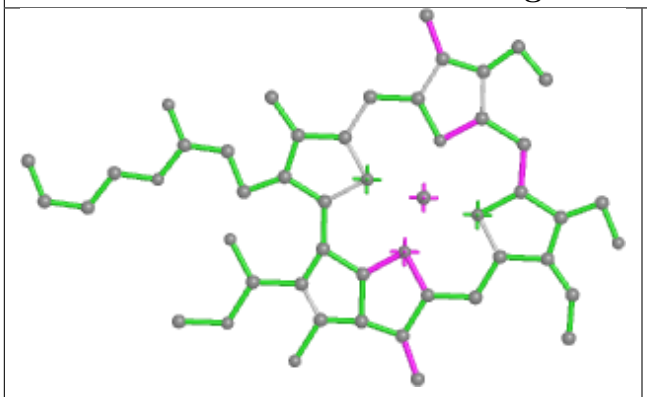


Torsions

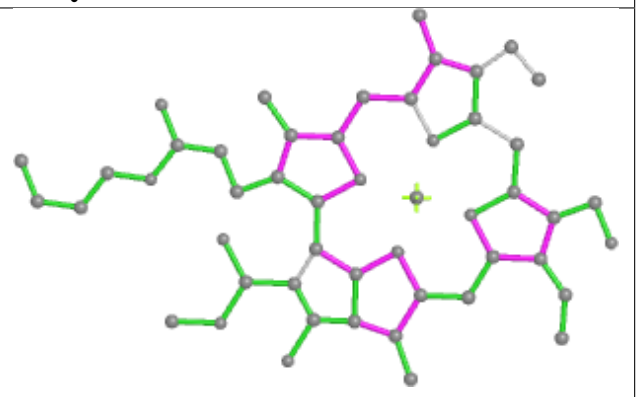


Rings

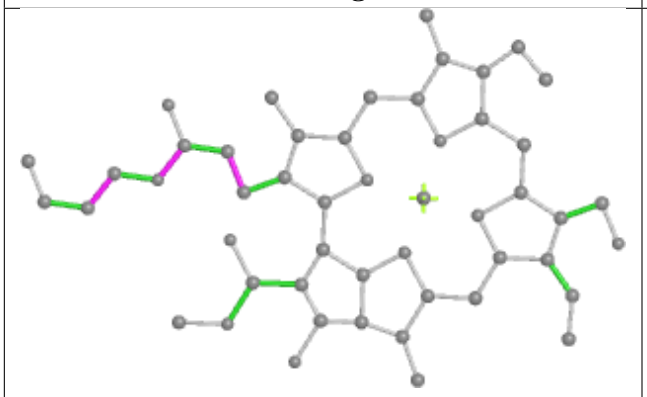
Ligand CHL Q 306



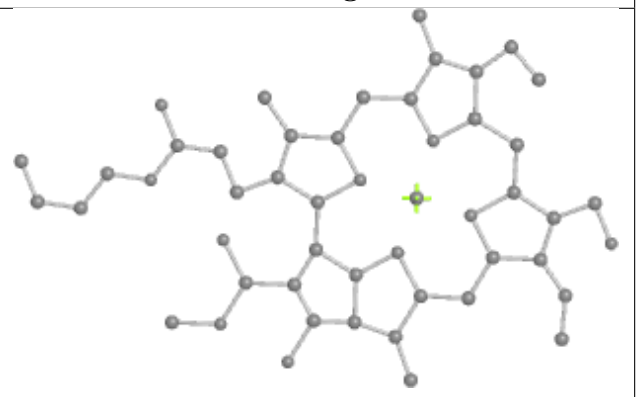
Bond lengths



Bond angles

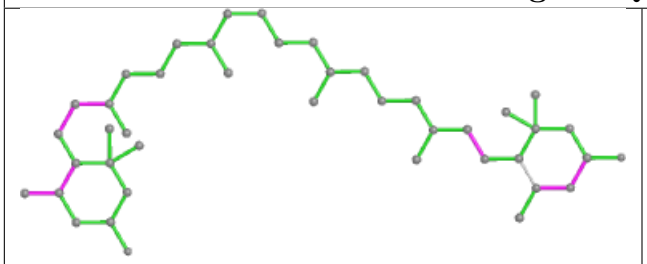


Torsions

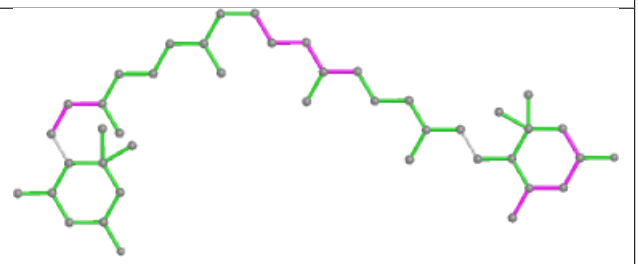


Rings

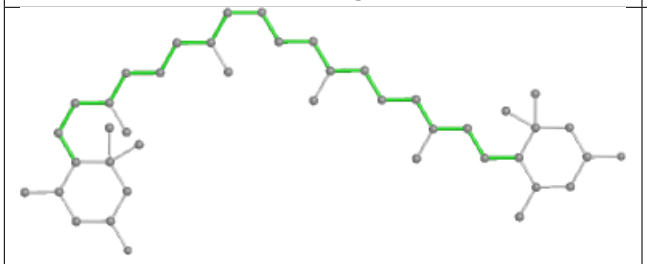
Ligand Q6L R 320



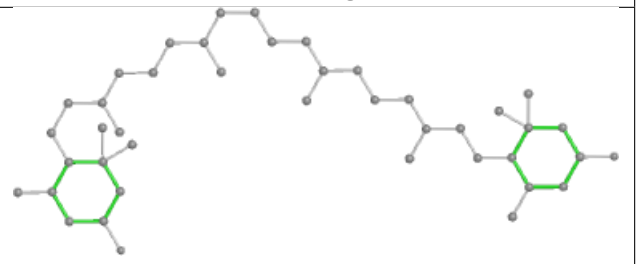
Bond lengths



Bond angles

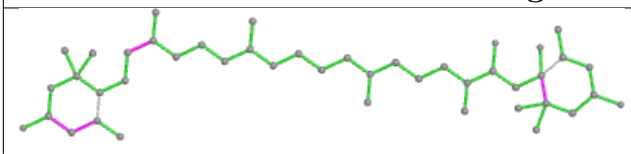


Torsions

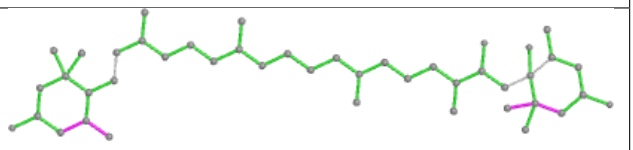


Rings

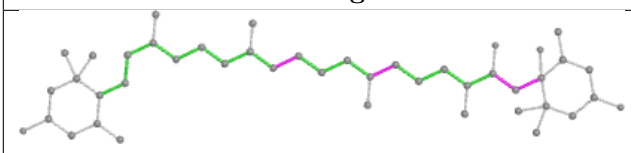
Ligand IWJ R 322



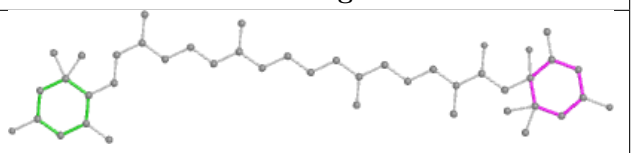
Bond lengths



Bond angles

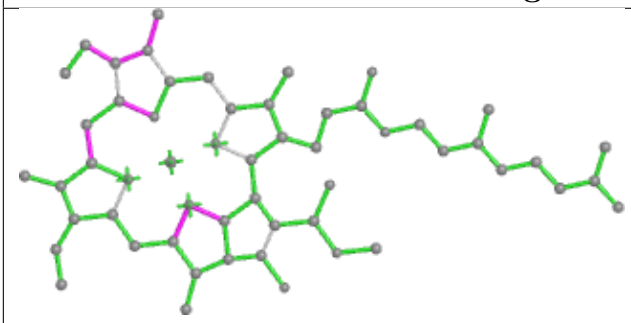


Torsions

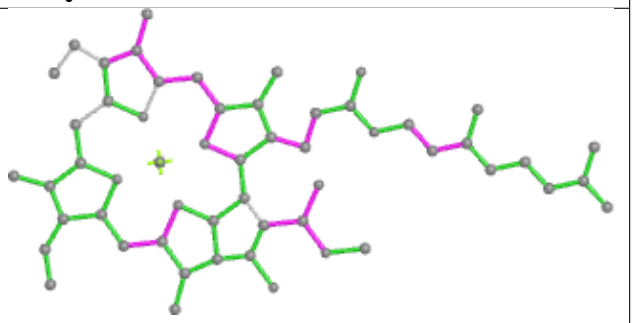


Rings

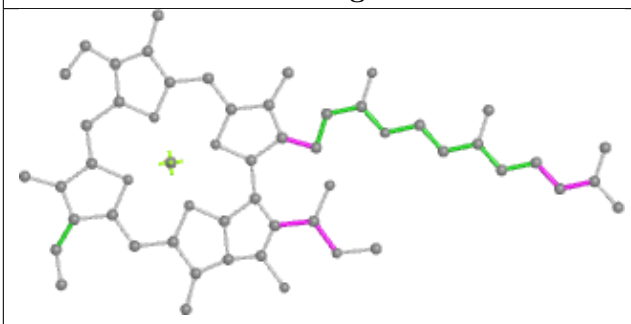
Ligand CLA Q 309



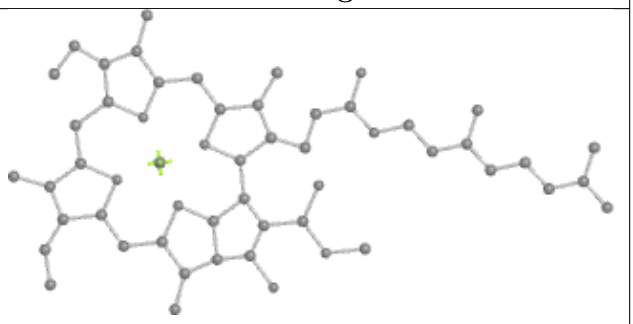
Bond lengths



Bond angles

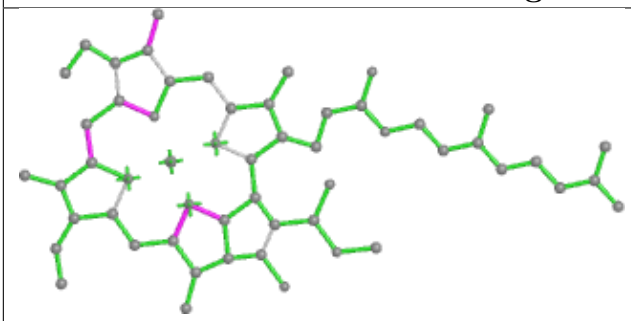


Torsions

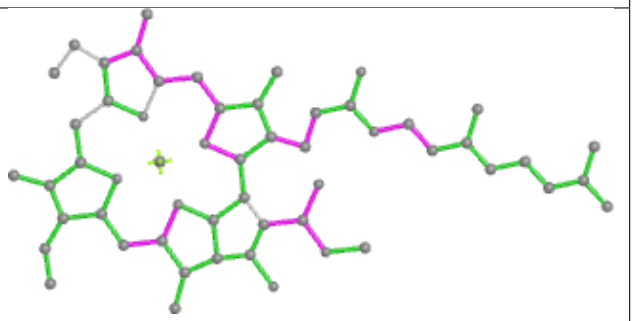


Rings

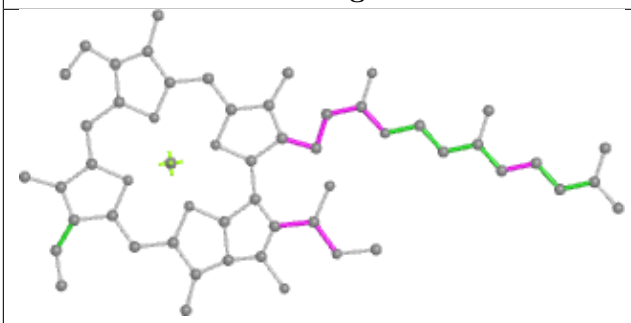
Ligand CLA P 312



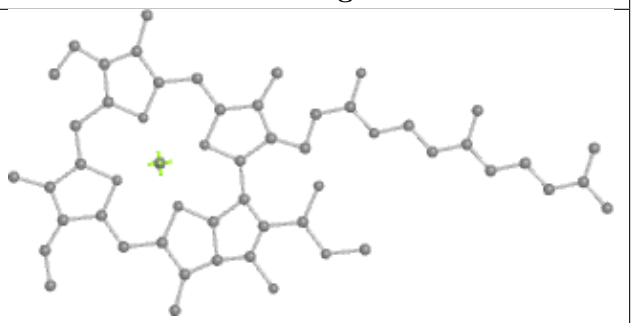
Bond lengths



Bond angles

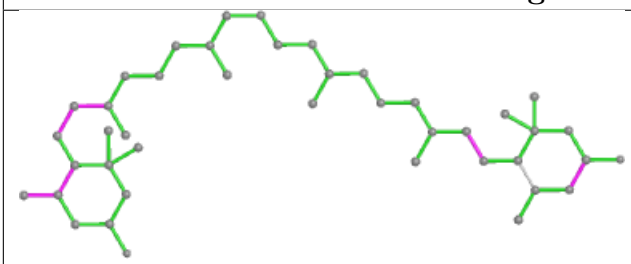


Torsions

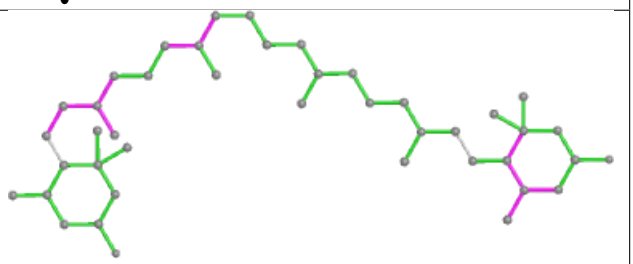


Rings

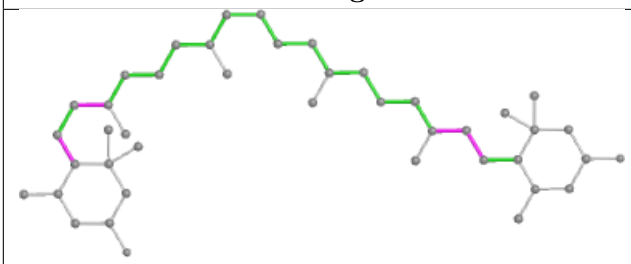
Ligand Q6L Q 316



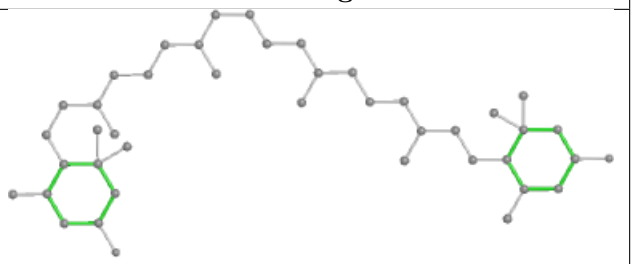
Bond lengths



Bond angles

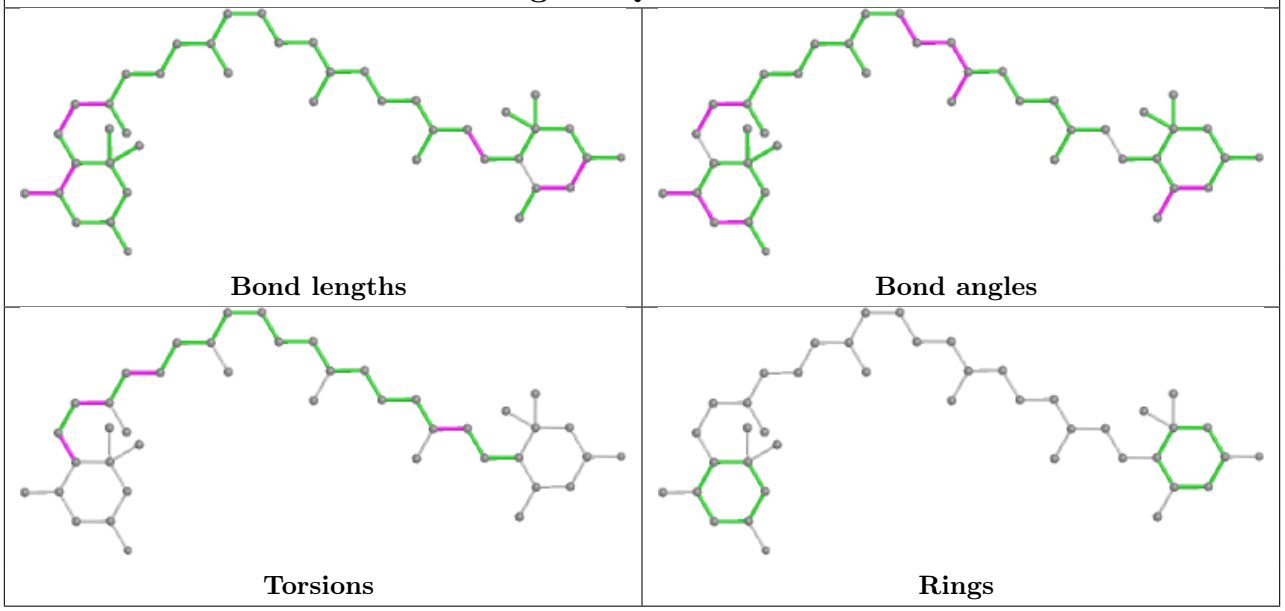


Torsions

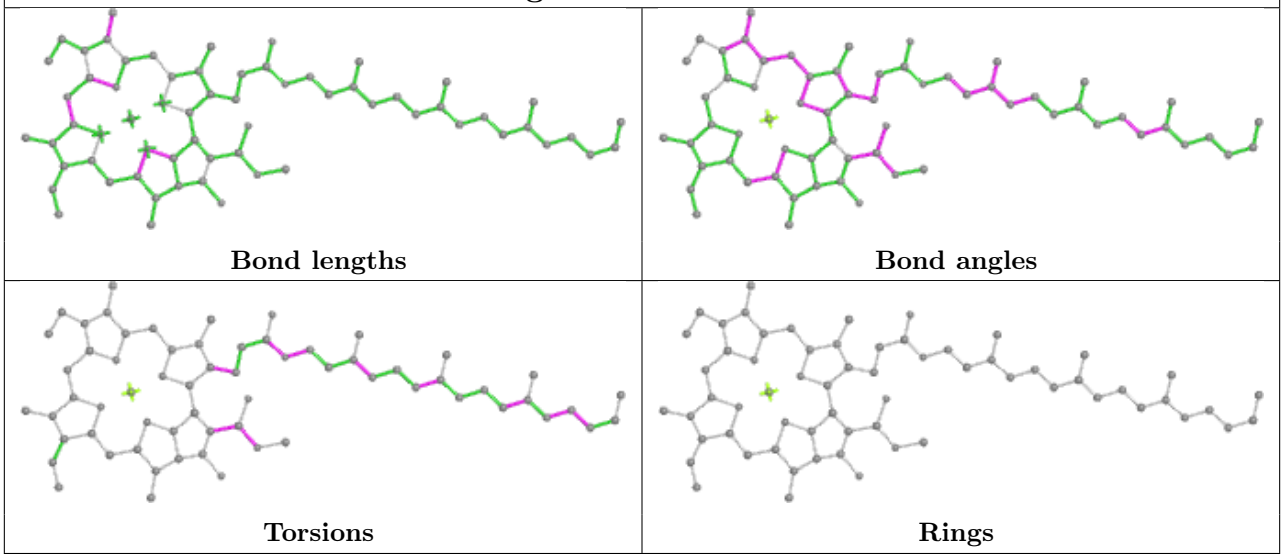


Rings

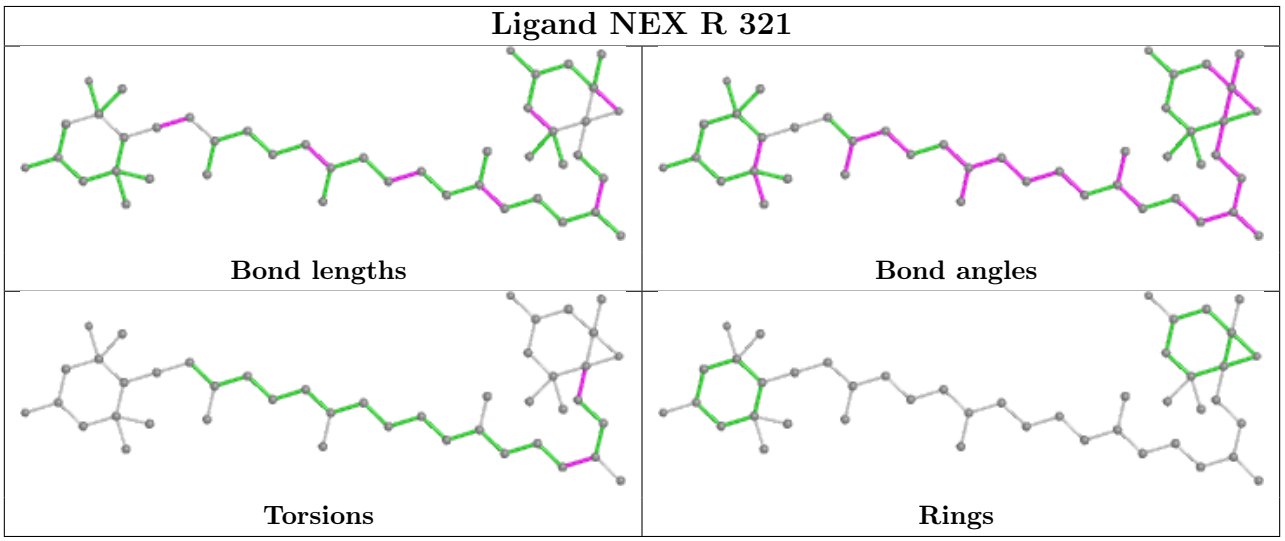
Ligand Q6L P 319



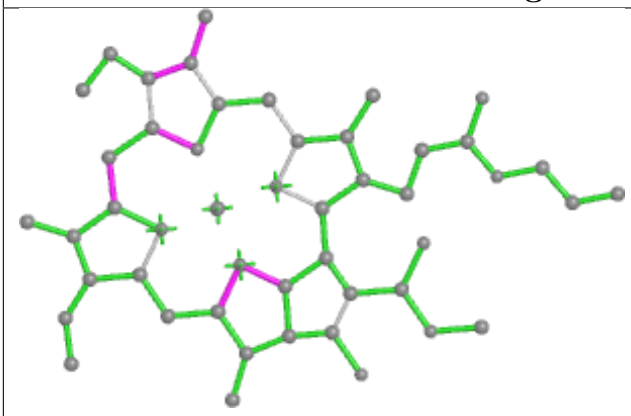
Ligand CLA P 309



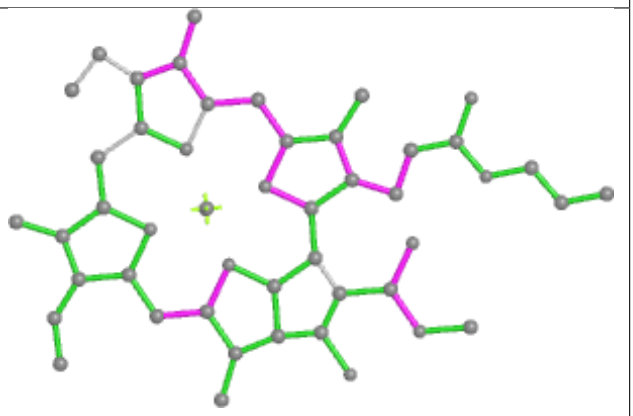
Ligand NEX R 321



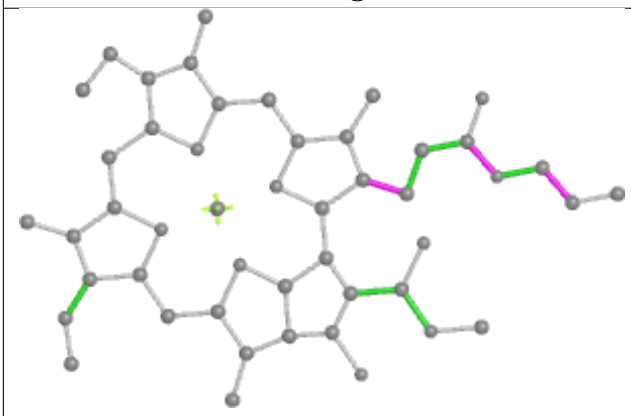
Ligand CLA P 313



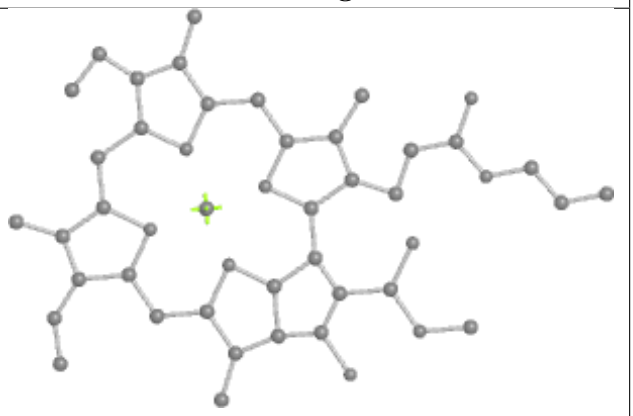
Bond lengths



Bond angles

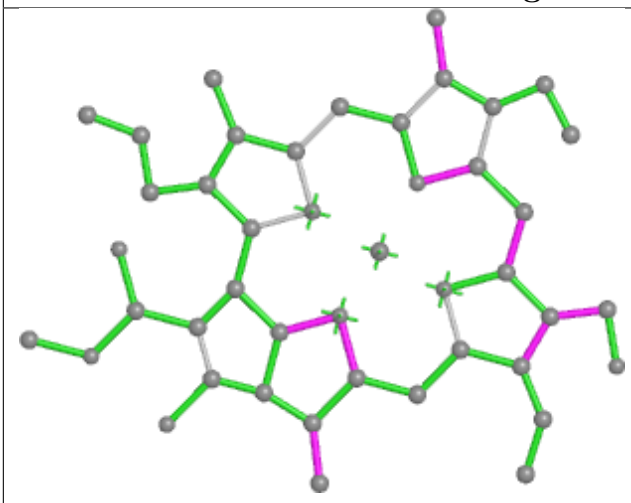


Torsions

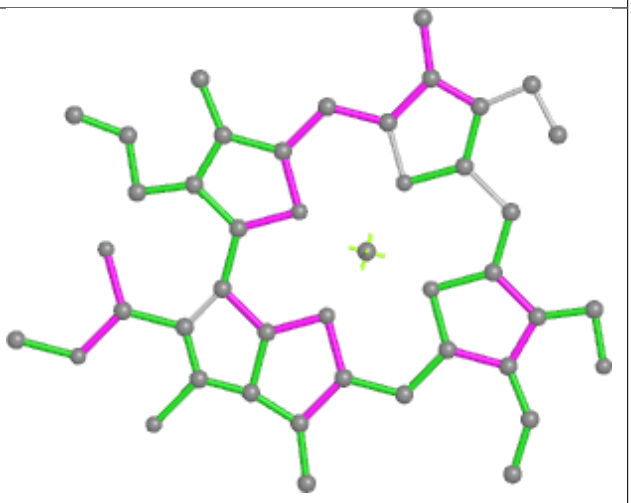


Rings

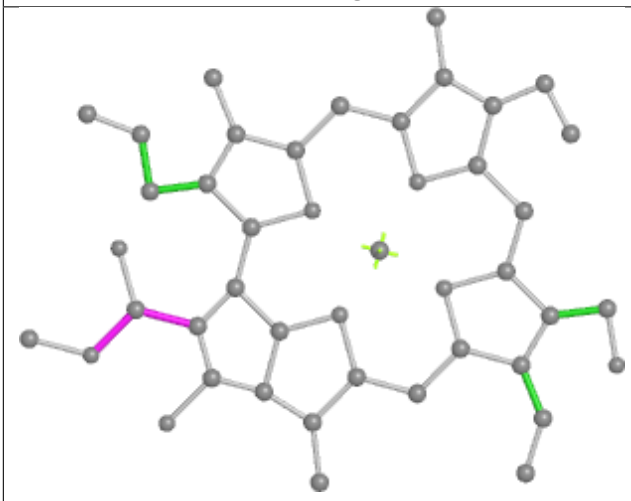
Ligand CHL R 311



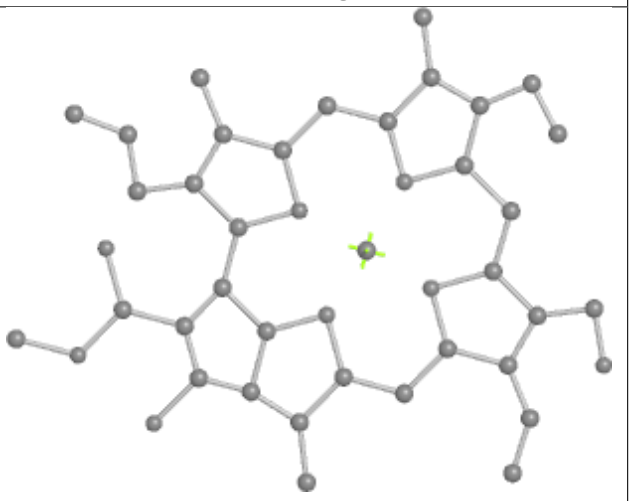
Bond lengths



Bond angles

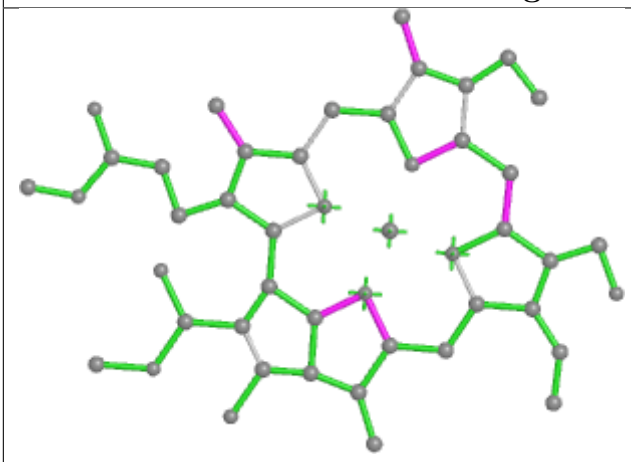


Torsions

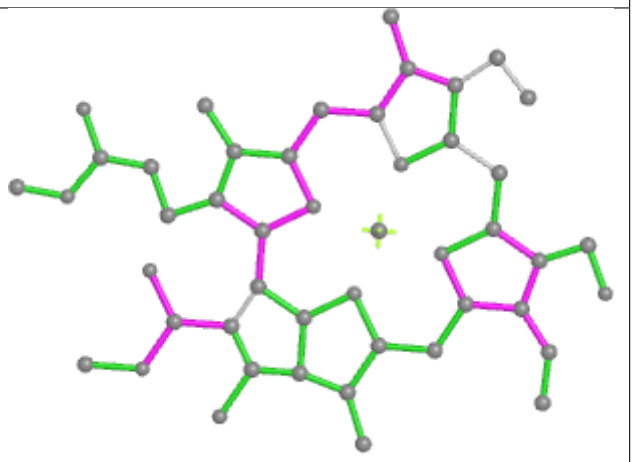


Rings

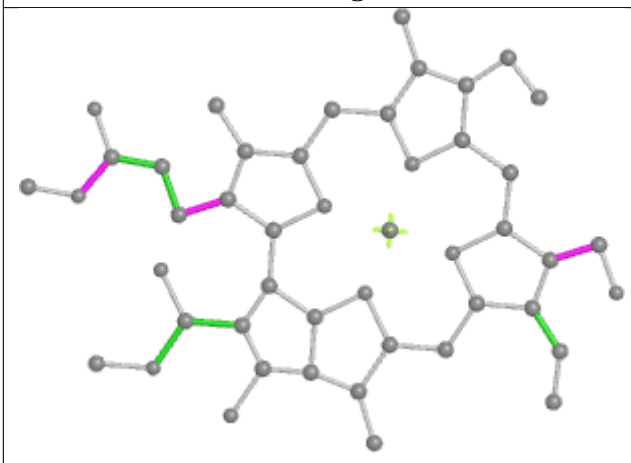
Ligand CHL R 302



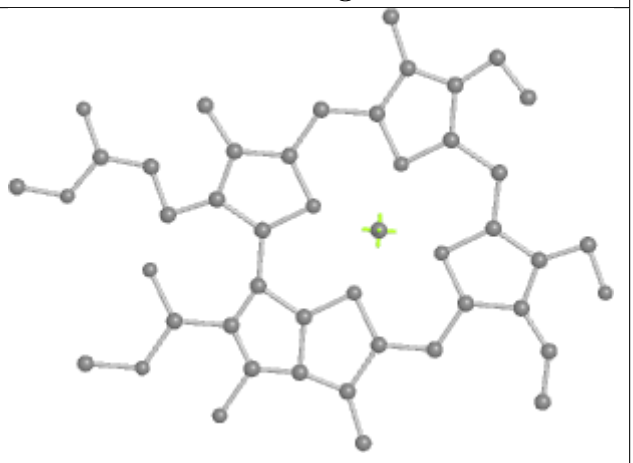
Bond lengths



Bond angles

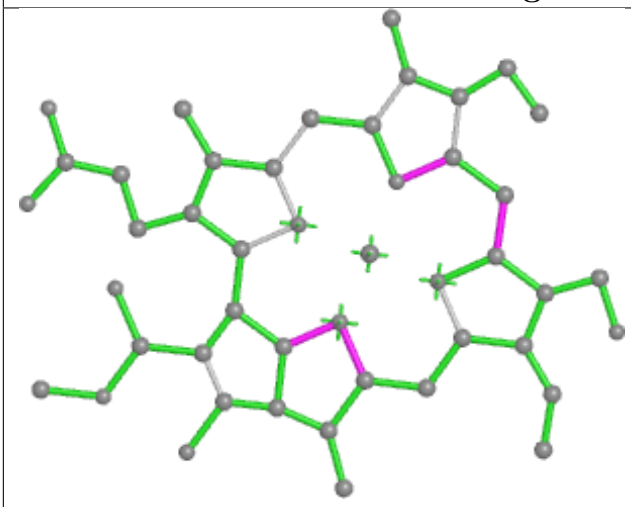


Torsions

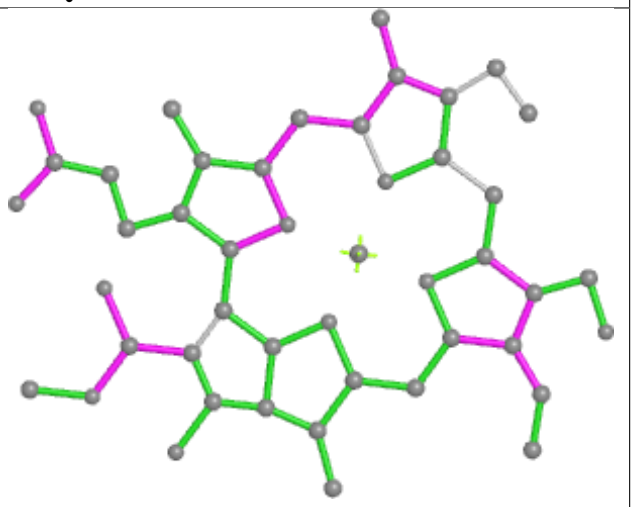


Rings

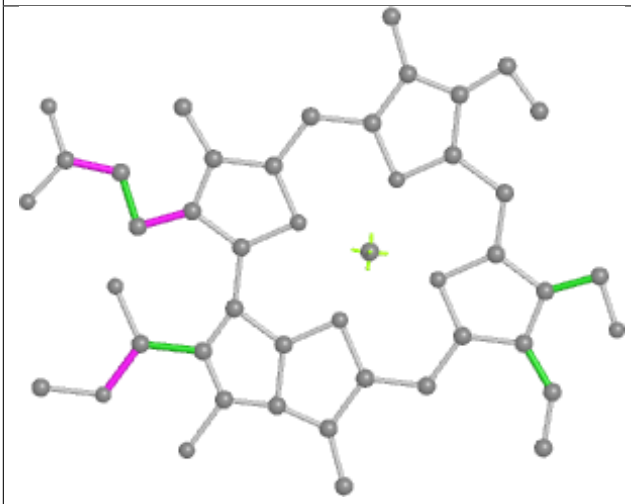
Ligand CHL Q 305



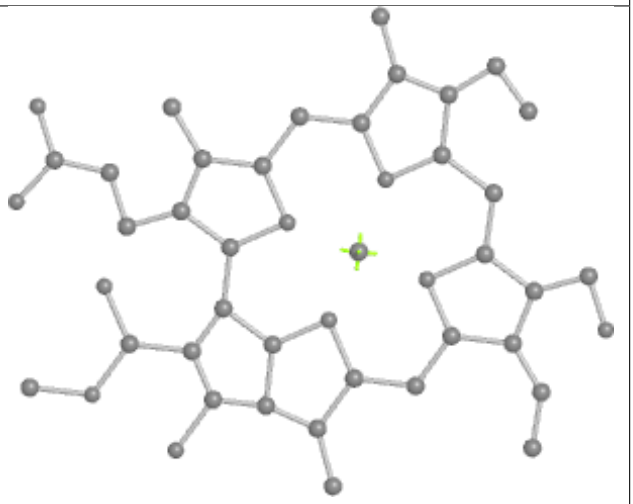
Bond lengths



Bond angles

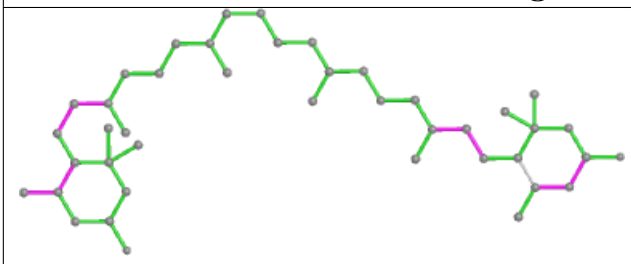


Torsions

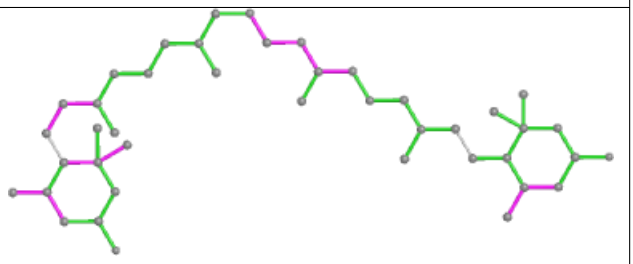


Rings

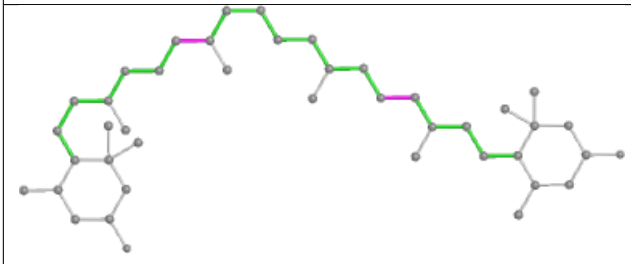
Ligand Q6L P 316



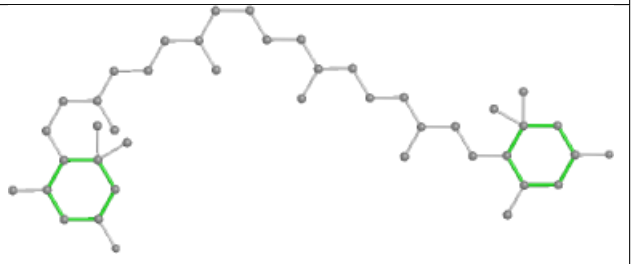
Bond lengths



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.

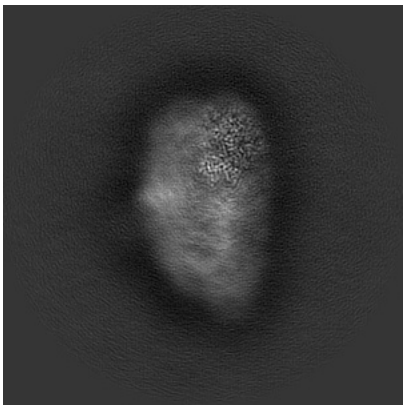
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-34735. These allow visual inspection of the internal detail of the map and identification of artifacts.

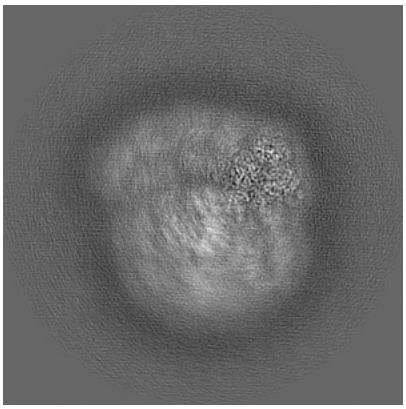
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

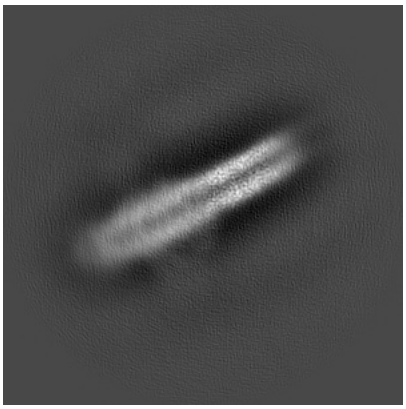
6.1.1 Primary map



X

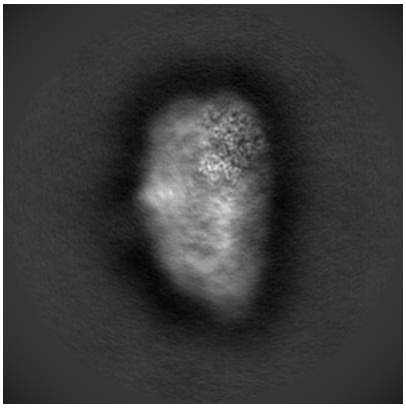


Y

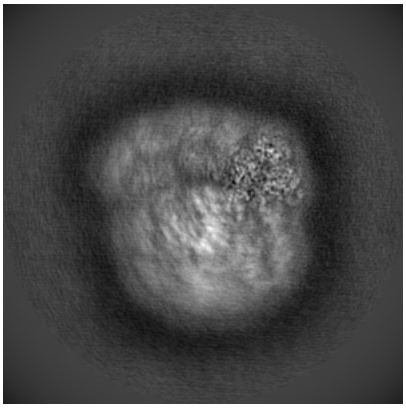


Z

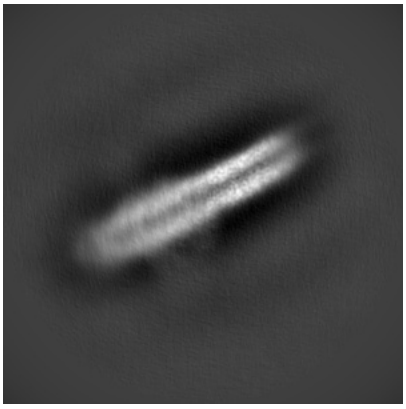
6.1.2 Raw map



X



Y

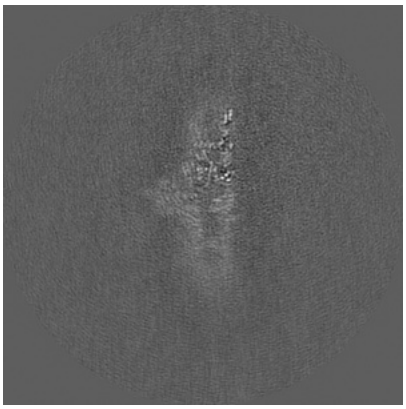


Z

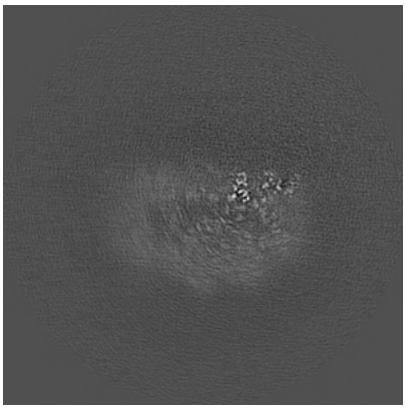
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

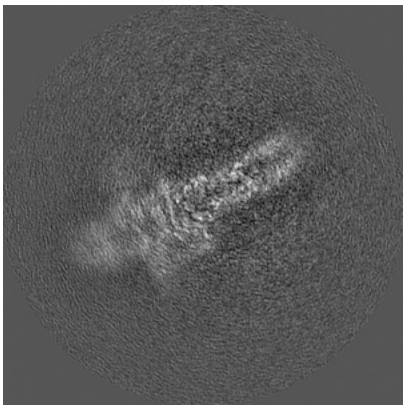
6.2.1 Primary map



X Index: 192

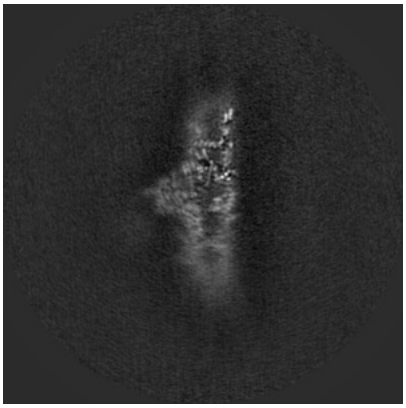


Y Index: 192

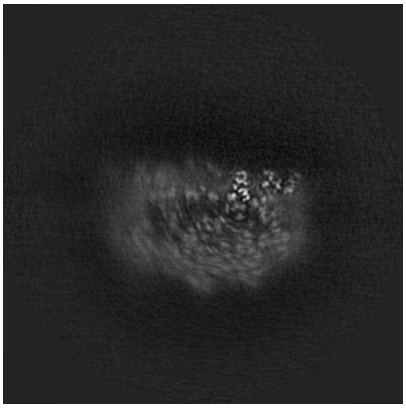


Z Index: 192

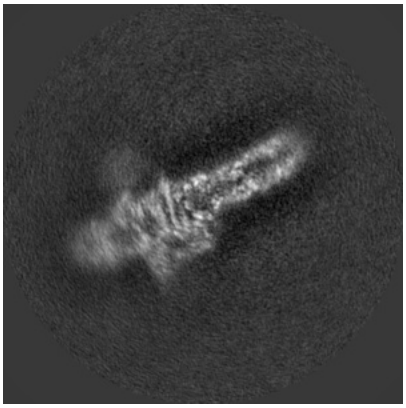
6.2.2 Raw map



X Index: 192



Y Index: 192

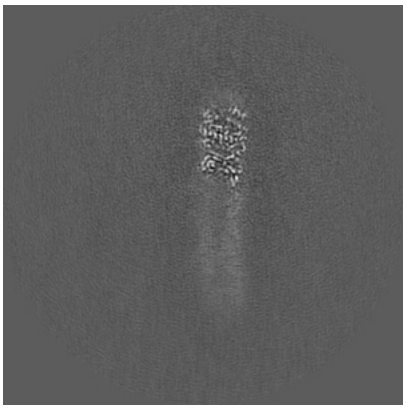


Z Index: 192

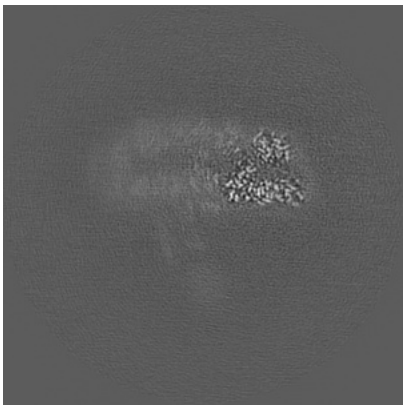
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

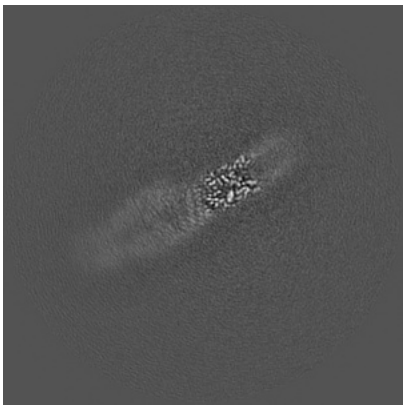
6.3.1 Primary map



X Index: 212

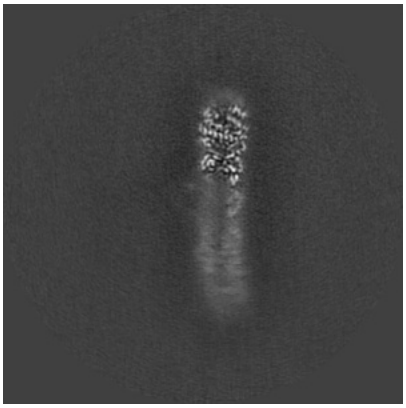


Y Index: 219

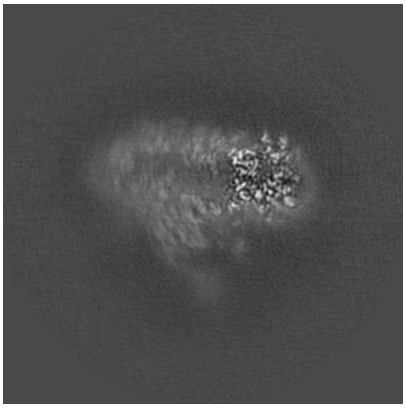


Z Index: 228

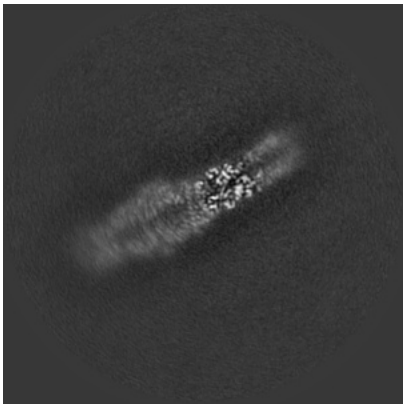
6.3.2 Raw map



X Index: 212



Y Index: 213

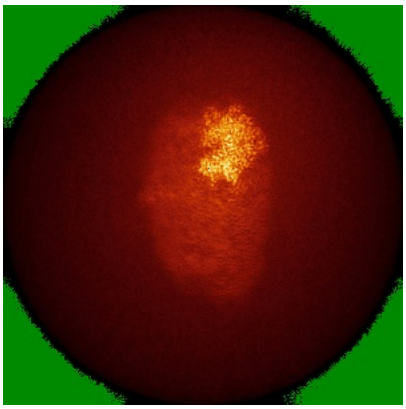


Z Index: 225

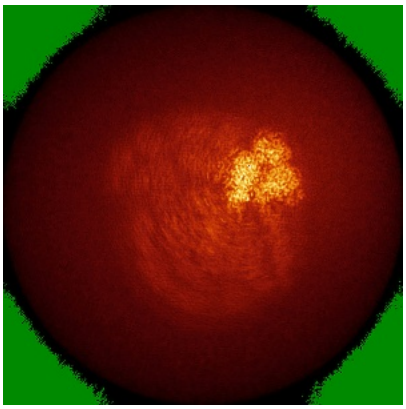
The images above show the largest variance slices of the map in three orthogonal directions.

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

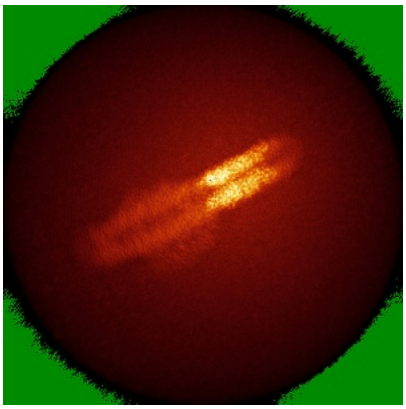
6.4.1 Primary map



X

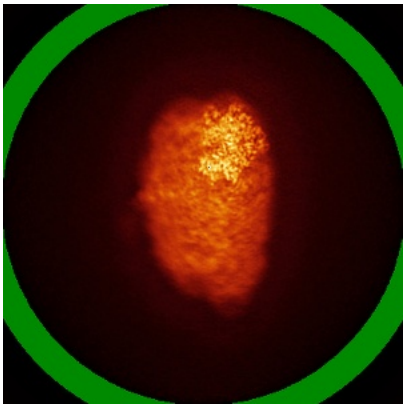


Y

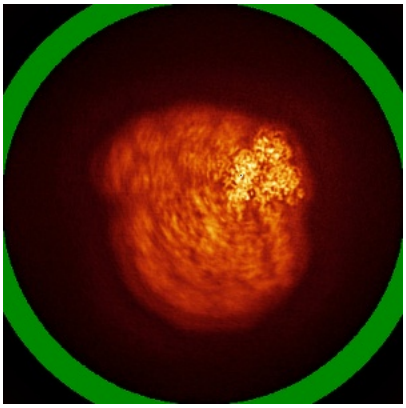


Z

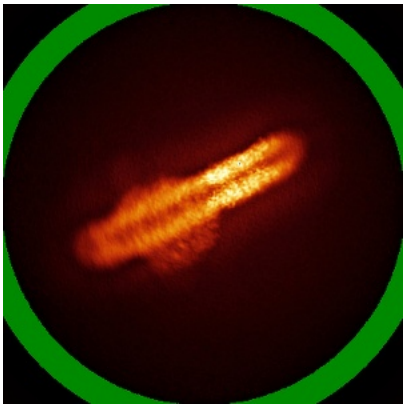
6.4.2 Raw map



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 0.0274. 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.

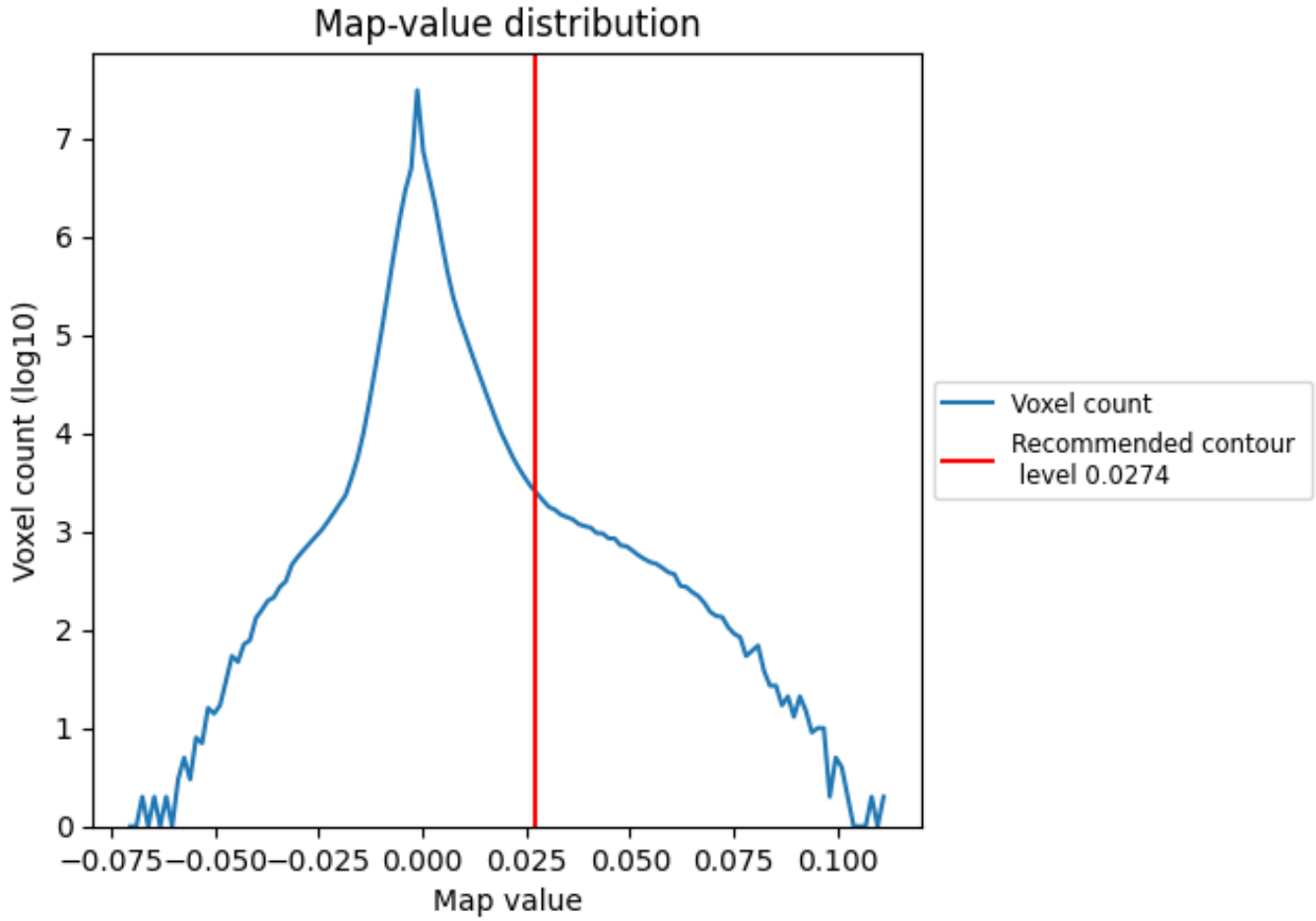
6.6 Mask visualisation (i)

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

7 Map analysis

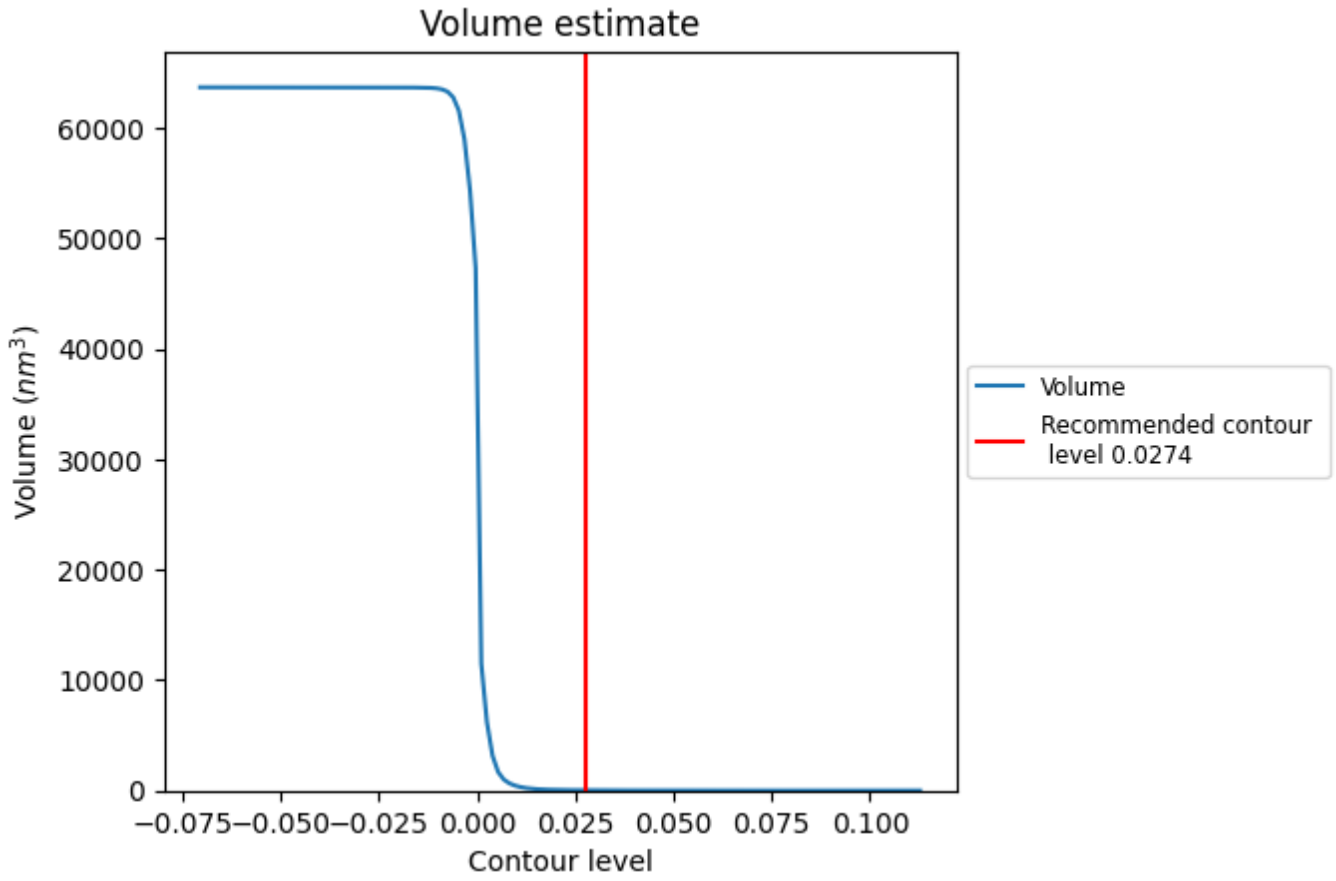
This section contains the results of statistical analysis of the map.

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.

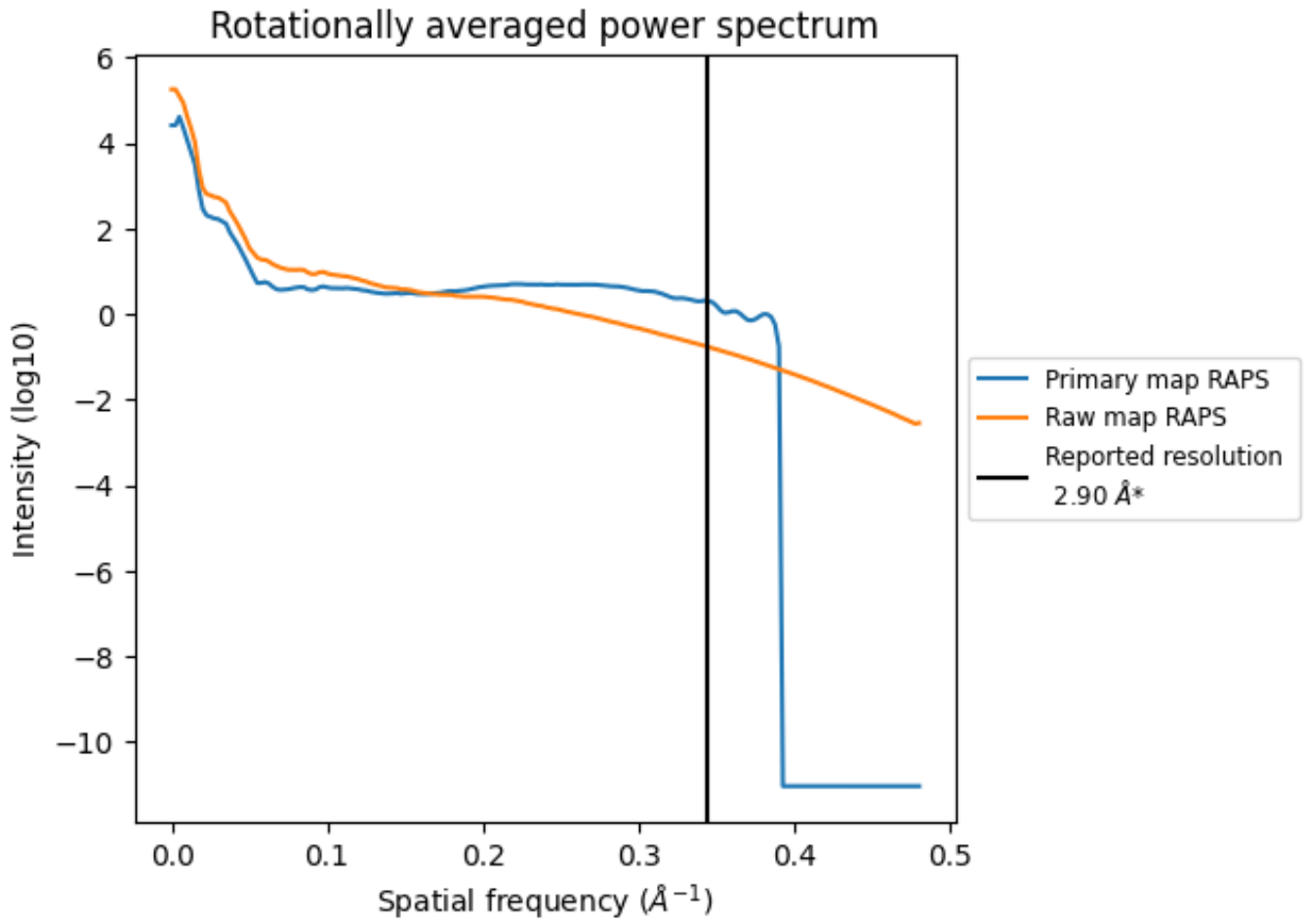
7.2 Volume estimate



The volume at the recommended contour level is 31 nm^3; this corresponds to an approximate mass of 28 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)

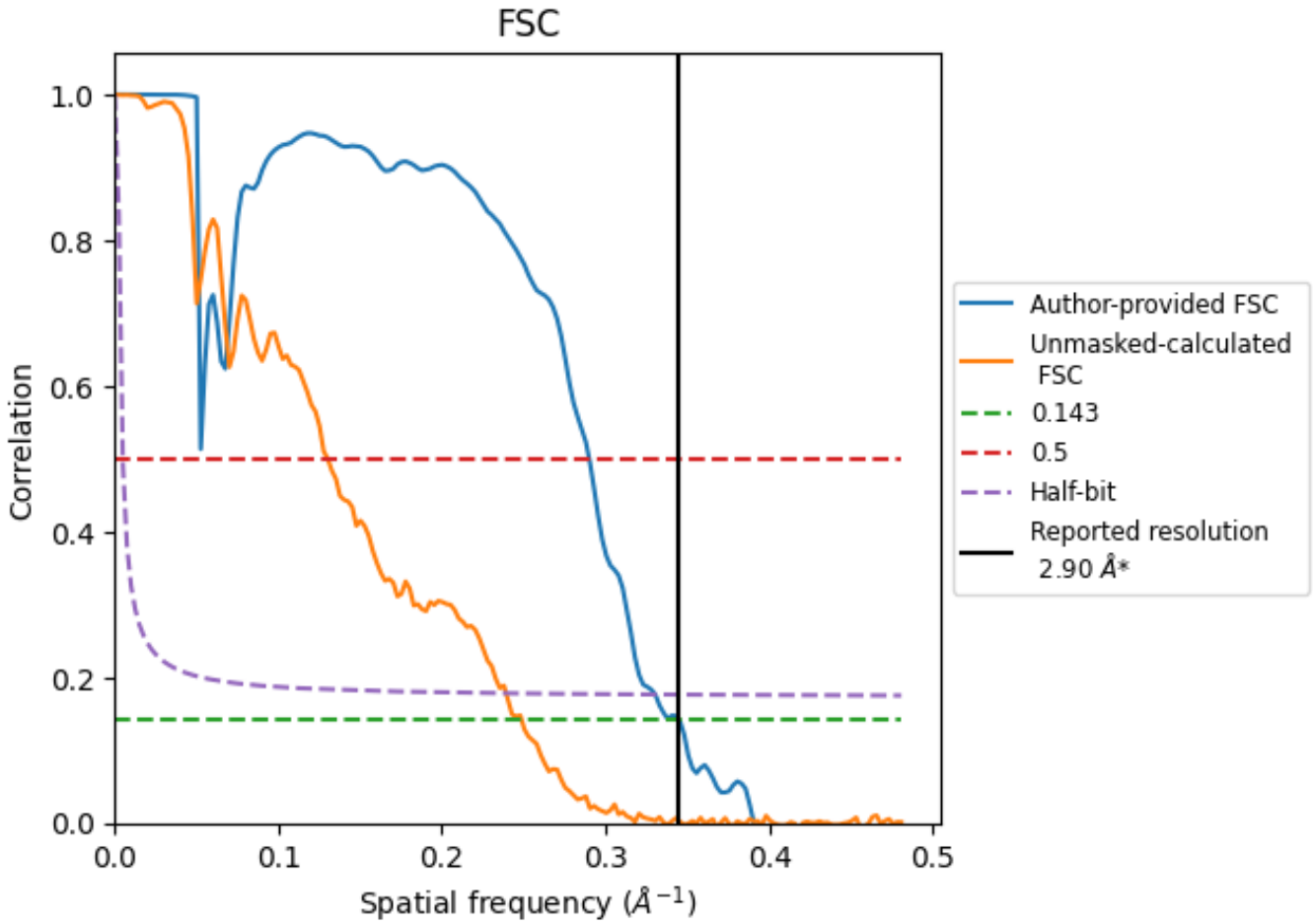


*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

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 0.345 Å^{-1}

8.2 Resolution estimates (i)

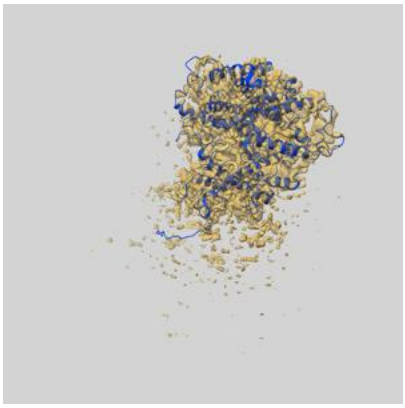
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.96	3.45	3.03
Unmasked-calculated*	4.02	7.69	4.18

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.02 differs from the reported value 2.9 by more than 10 %

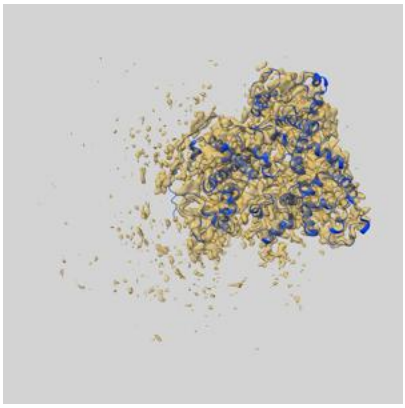
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-34735 and PDB model 8HG5. Per-residue inclusion information can be found in section 3 on page 11.

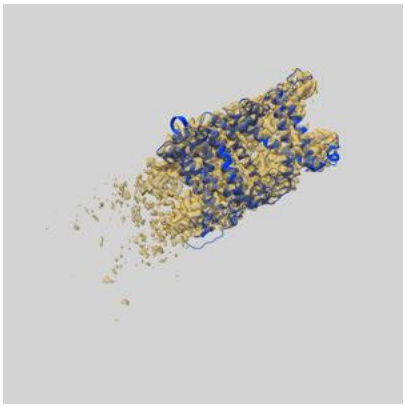
9.1 Map-model overlay



X



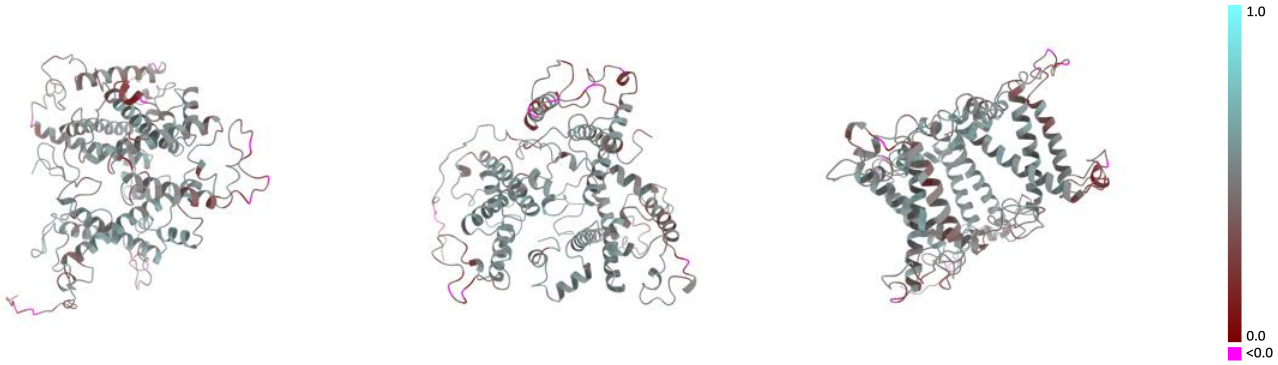
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0274 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.

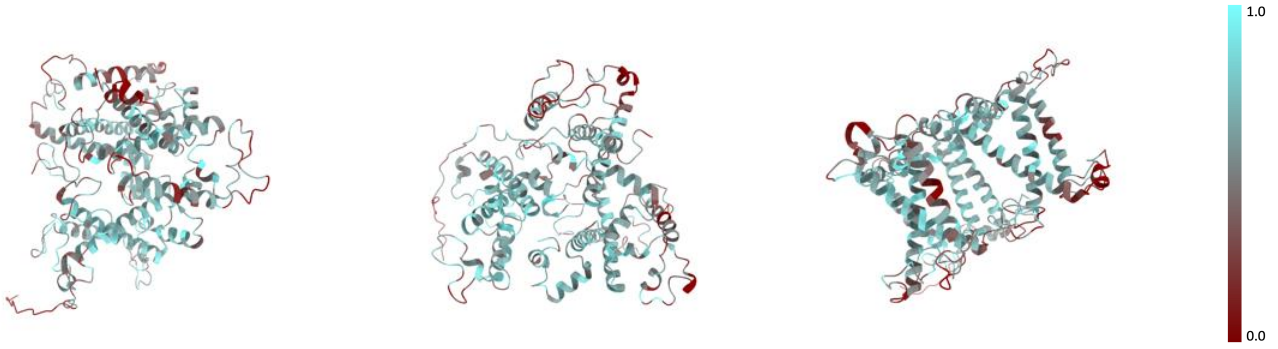
9.2 Q-score mapped to coordinate model (i)



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.

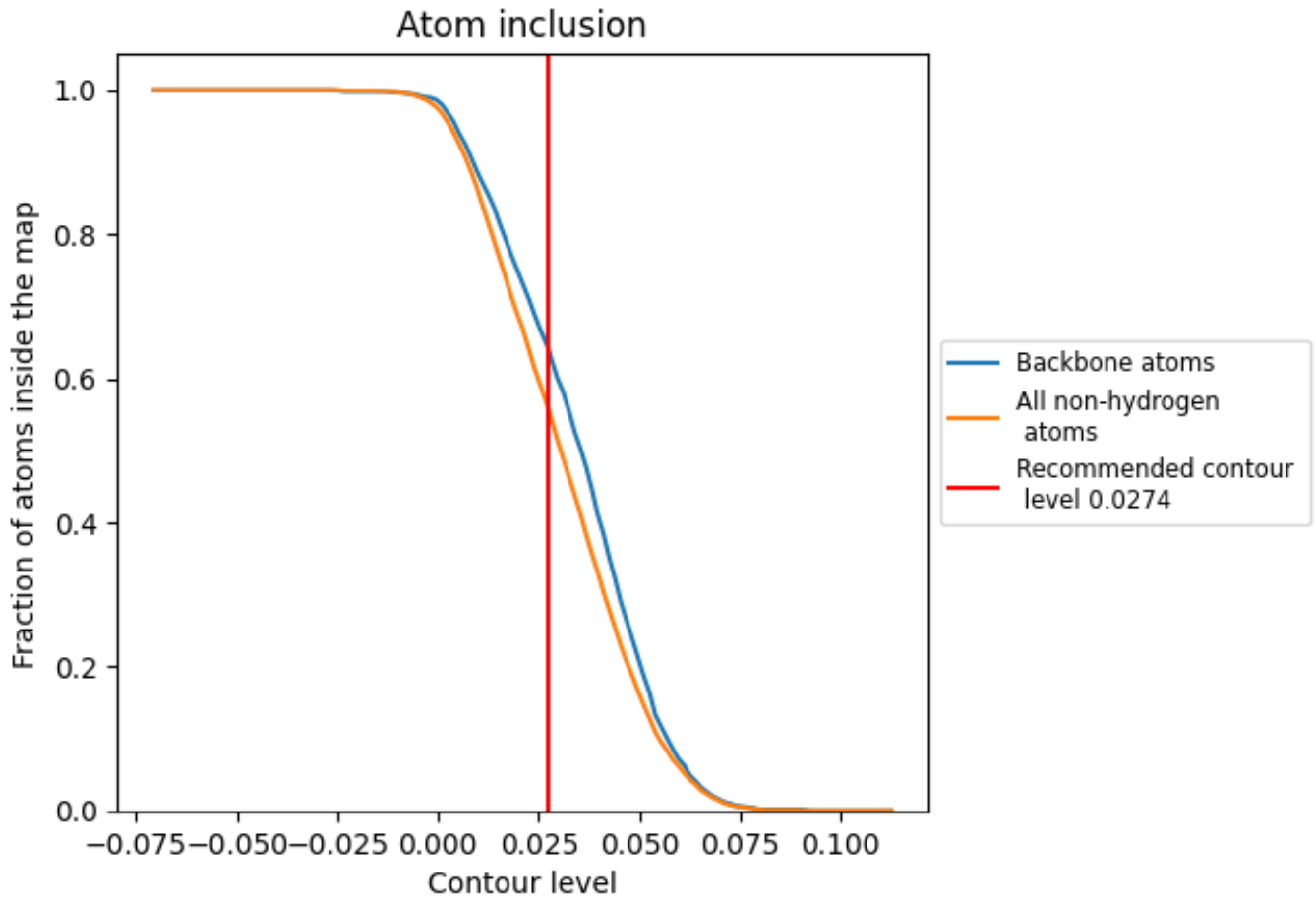
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0274).

9.4 Atom inclusion (i)



At the recommended contour level, 64% of all backbone atoms, 56% 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 (0.0274) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5590	0.4860
P	0.5090	0.4720
Q	0.6270	0.5010
R	0.5400	0.4850