



Full wwPDB EM Validation Report ⓘ

Mar 23, 2026 – 01:14 PM UTC

PDB ID : 8BEL / pdb_00008bel
EMDB ID : EMD-16007
Title : Cryo-EM structure of the Arabidopsis thaliana I+III₂ supercomplex (CIII membrane domain)
Authors : Klusch, N.; Kuehlbrandt, W.
Deposited on : 2022-10-21
Resolution : 2.25 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

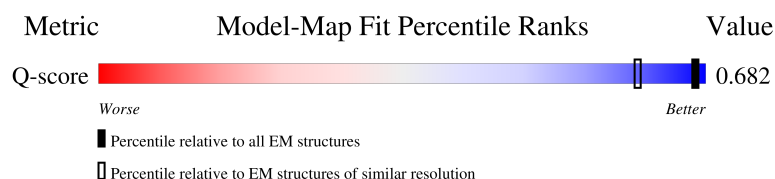
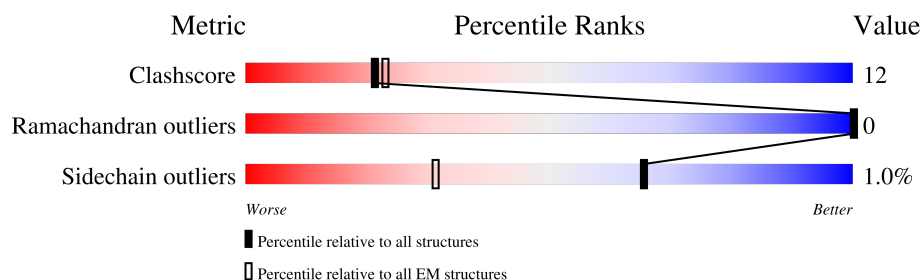
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.25 Å.

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



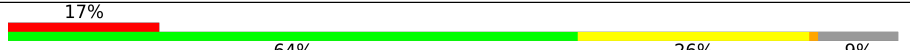
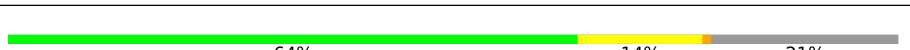
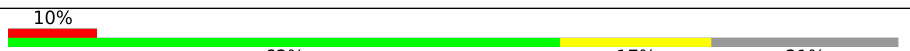
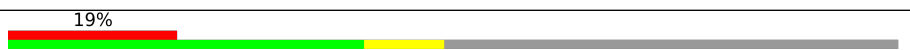
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3458 (1.75 - 2.75)

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 $\leq 5\%$. 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	C	393	
1	M	393	
2	D	272	
2	N	272	

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Mol	Chain	Length	Quality of chain
3	E	307	
3	O	307	
4	G	72	
4	Q	72	
5	H	69	
5	R	69	
6	I	72	
6	S	72	
7	J	57	
7	T	57	

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
14	FES	N	301	-	-	X	-

2 Entry composition [i](#)

There are 18 unique types of molecules in this entry. The entry contains 18929 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 Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	387	Total	C	N	O	S	0	0
			3093	2083	487	508	15		
1	M	387	Total	C	N	O	S	0	0
			3093	2083	487	508	15		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	40	SER	PRO	variant	UNP P42792
M	40	SER	PRO	variant	UNP P42792

- Molecule 2 is a protein called Cytochrome b-c1 complex subunit Rieske-1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	179	Total	C	N	O	S	0	0
			1404	899	244	256	5		
2	N	179	Total	C	N	O	S	0	0
			1404	899	244	256	5		

- Molecule 3 is a protein called Cytochrome c1 2, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	244	Total	C	N	O	S	0	0
			1917	1216	326	364	11		
3	O	244	Total	C	N	O	S	0	0
			1917	1216	326	364	11		

- Molecule 4 is a protein called Cytochrome b-c1 complex subunit 8-1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	69	Total	C	N	O	S	0	0
			581	387	95	98	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	Q	68	Total	C	N	O	S	0	0
			572	382	93	96	1		

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit 6-1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	64	Total	C	N	O	S	0	0
			518	334	87	91	6		
5	R	63	Total	C	N	O	S	0	0
			511	329	86	90	6		

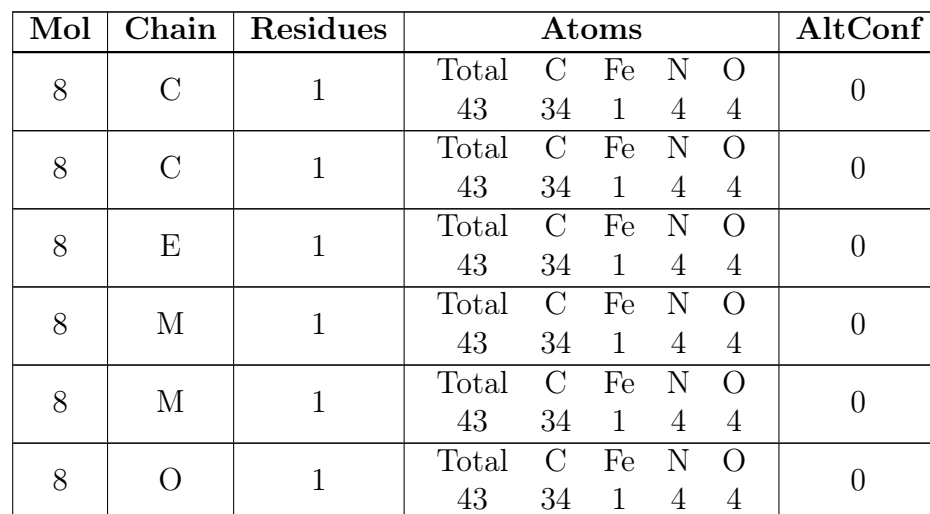
- Molecule 6 is a protein called Cytochrome b-c1 complex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	57	Total	C	N	O	S	0	0
			476	310	85	80	1		
6	S	57	Total	C	N	O	S	0	0
			476	310	85	80	1		

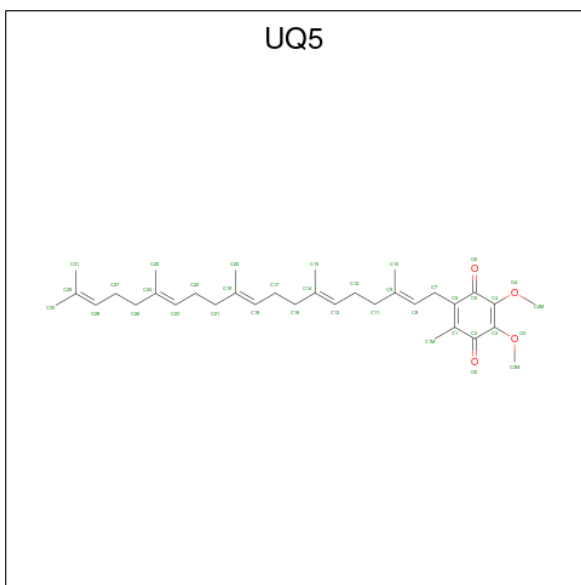
- Molecule 7 is a protein called Cytochrome b-c1 complex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	J	28	Total	C	N	O	0	0
			203	137	33	33		
7	T	28	Total	C	N	O	0	0
			205	139	34	32		

- Molecule 8 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄) (labeled as "Ligand of Interest" by depositor).

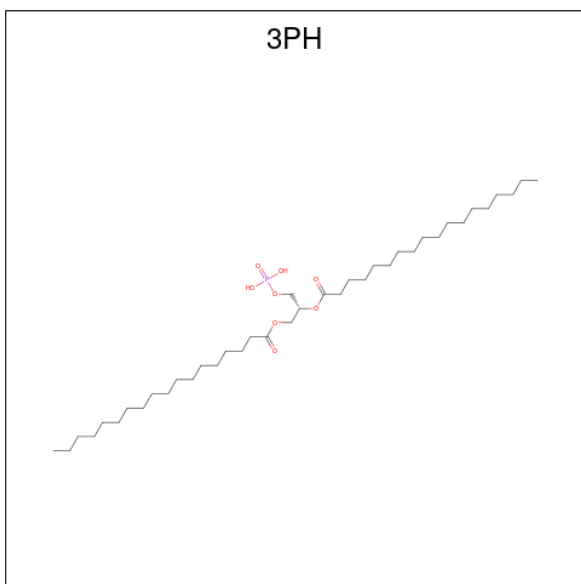


- Molecule 9 is 2,3-DIMETHOXY-5-METHYL-6-(3,11,15,19-TETRAMETHYL-EICOSA-2,6,10,14,18-PENTAENYL)-[1,4]BENZOQUINONE (CCD ID: UQ5) (formula: C₃₄H₅₀O₄) (labeled as "Ligand of Interest" by depositor).



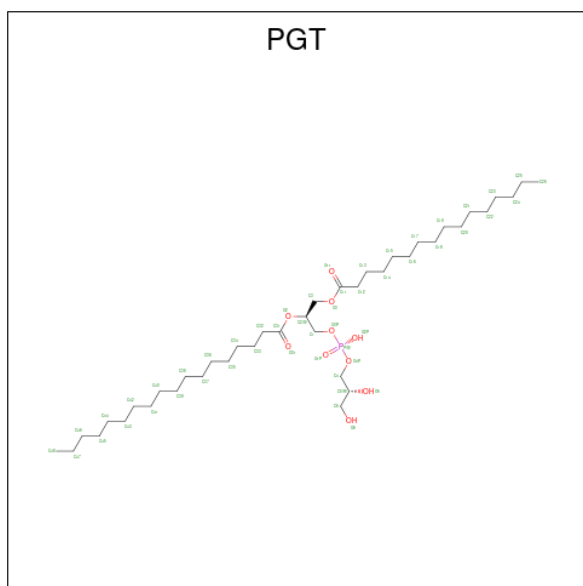
Mol	Chain	Residues	Atoms			AltConf
9	C	1	Total	C	O	0
			38	34	4	
9	C	1	Total	C	O	0
			38	34	4	
9	M	1	Total	C	O	0
			38	34	4	

- Molecule 10 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula: $C_{39}H_{77}O_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
10	C	1	Total	C	O	P	0
			33	24	8	1	
10	G	1	Total	C	O	P	0
			33	24	8	1	
10	I	1	Total	C	O	P	0
			32	23	8	1	
10	M	1	Total	C	O	P	0
			44	35	8	1	
10	T	1	Total	C	O	P	0
			41	32	8	1	
10	T	1	Total	C	O	P	0
			48	39	8	1	

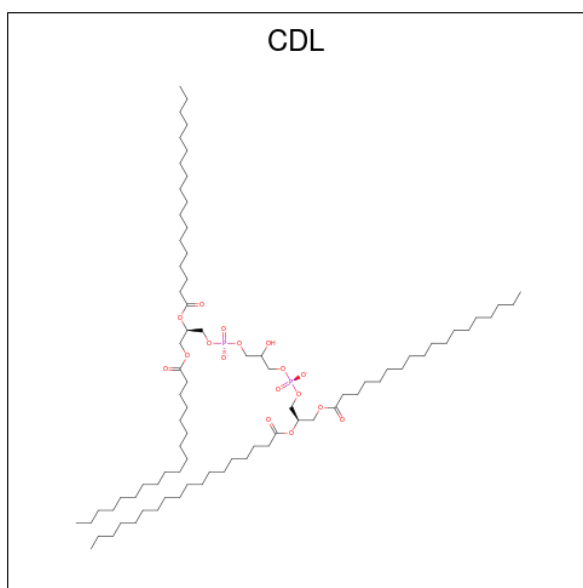
- Molecule 11 is (1S)-2-{{[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (CCD ID: PGT) (formula: C₄₀H₇₉O₁₀P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
11	C	1	Total	C	O	P	0
			41	30	10	1	
11	C	1	Total	C	O	P	0
			51	40	10	1	
11	G	1	Total	C	O	P	0
			51	40	10	1	
11	M	1	Total	C	O	P	0
			37	26	10	1	

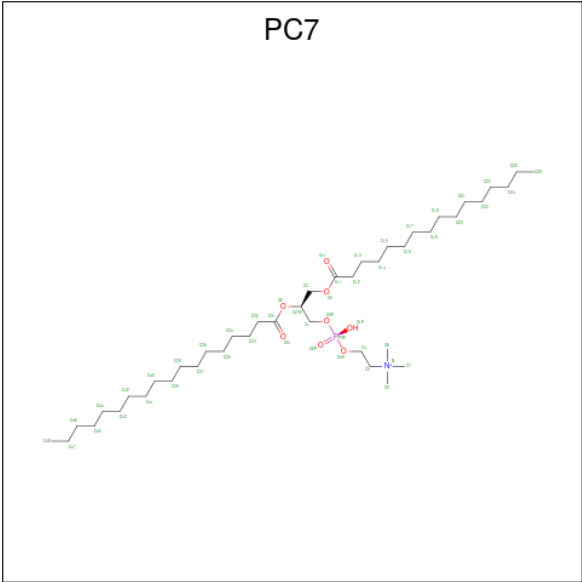
- Molecule 12 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂) (labeled as "Ligand

of Interest" by depositor).



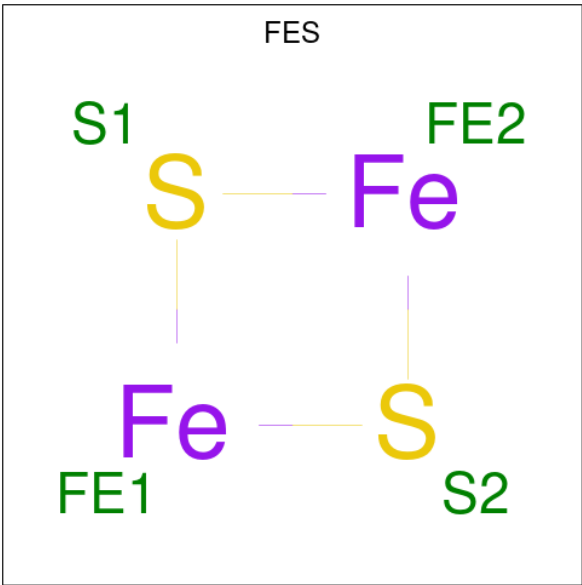
Mol	Chain	Residues	Atoms				AltConf
12	C	1	Total	C	O	P	0
			81	62	17	2	
12	C	1	Total	C	O	P	0
			85	66	17	2	
12	G	1	Total	C	O	P	0
			85	66	17	2	
12	M	1	Total	C	O	P	0
			77	58	17	2	
12	N	1	Total	C	O	P	0
			81	62	17	2	
12	O	1	Total	C	O	P	0
			88	69	17	2	
12	Q	1	Total	C	O	P	0
			70	51	17	2	

- Molecule 13 is (7S)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY) METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSAN-1-AMINIUM 4-OXIDE (CCD ID: PC7) (formula: C₄₂H₈₅NO₈P) (labeled as "Ligand of Interest" by depositor).



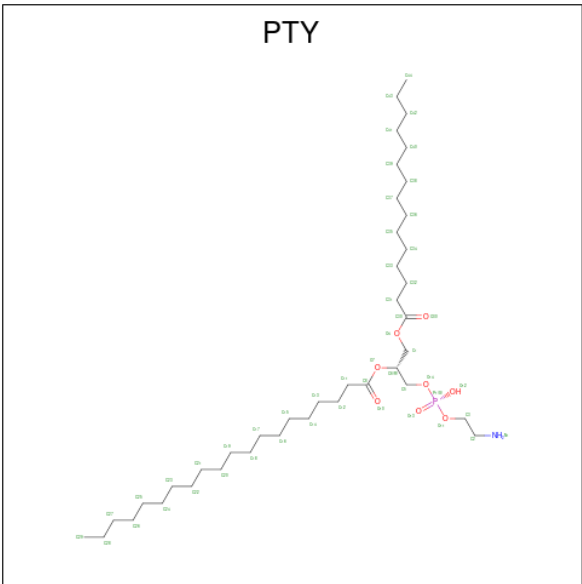
Mol	Chain	Residues	Atoms					AltConf
13	C	1	Total	C	N	O	P	0
			51	41	1	8	1	
13	D	1	Total	C	N	O	P	0
			34	24	1	8	1	
13	G	1	Total	C	N	O	P	0
			52	42	1	8	1	
13	M	1	Total	C	N	O	P	0
			45	35	1	8	1	
13	N	1	Total	C	N	O	P	0
			39	29	1	8	1	

- Molecule 14 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
14	D	1	Total	Fe	S	0
			4	2	2	
14	N	1	Total	Fe	S	0
			4	2	2	

- Molecule 15 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: $C_{40}H_{80}NO_8P$) (labeled as "Ligand of Interest" by depositor).



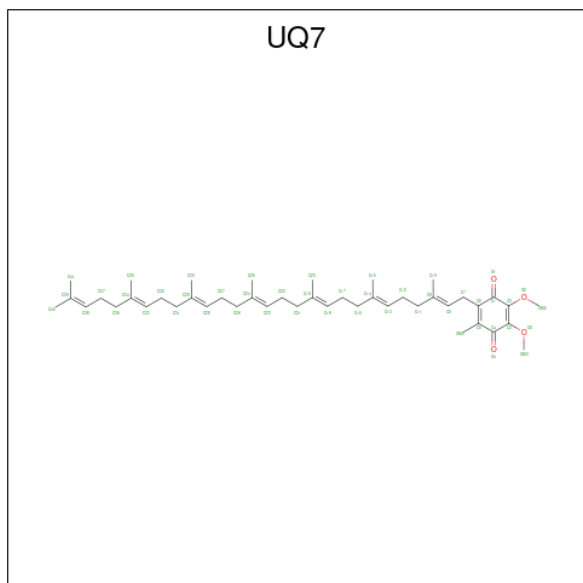
Mol	Chain	Residues	Atoms					AltConf
15	J	1	Total	C	N	O	P	0
			41	31	1	8	1	

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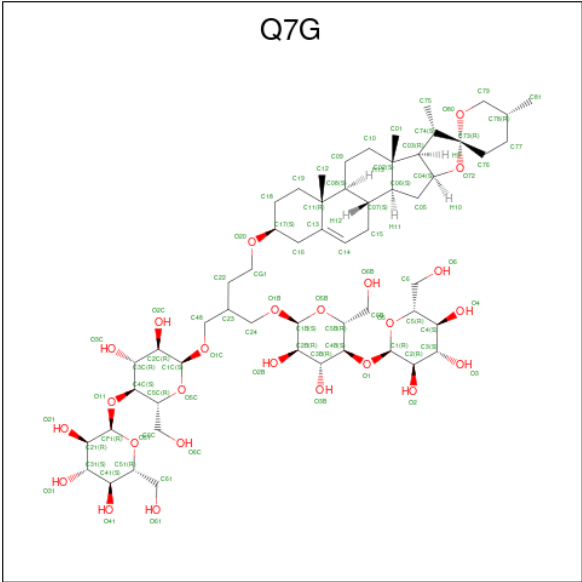
Mol	Chain	Residues	Atoms					AltConf
15	M	1	Total	C	N	O	P	0
			40	30	1	8	1	
15	T	1	Total	C	N	O	P	0
			29	19	1	8	1	

- Molecule 16 is UBIQUINONE-7 (CCD ID: UQ7) (formula: $C_{44}H_{66}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
16	M	1	Total	C	O	0
			48	44	4	

- Molecule 17 is 2-[[[(4-O-alpha-D-glucopyranosyl-alpha-D-glucopyranosyl)oxy]methyl]-4-[[[(3 beta,9beta,14beta,17beta,25R)-spirost-5-en-3-yl]oxy]butyl 4-O-alpha-D-glucopyranosyl-alpha-D-glucopyranoside (CCD ID: Q7G) (formula: $C_{56}H_{92}O_{25}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
17	M	1	Total	C	O	0
			39	34	5	
17	M	1	Total	C	O	0
			39	34	5	

- Molecule 18 is water.

Mol	Chain	Residues	Atoms		AltConf
18	C	179	Total	O	0
			179	179	
18	D	32	Total	O	0
			32	32	
18	E	159	Total	O	0
			159	159	
18	G	30	Total	O	0
			30	30	
18	H	13	Total	O	0
			13	13	
18	I	20	Total	O	0
			20	20	
18	M	138	Total	O	0
			138	138	
18	N	33	Total	O	0
			33	33	
18	O	111	Total	O	0
			111	111	
18	Q	13	Total	O	0
			13	13	

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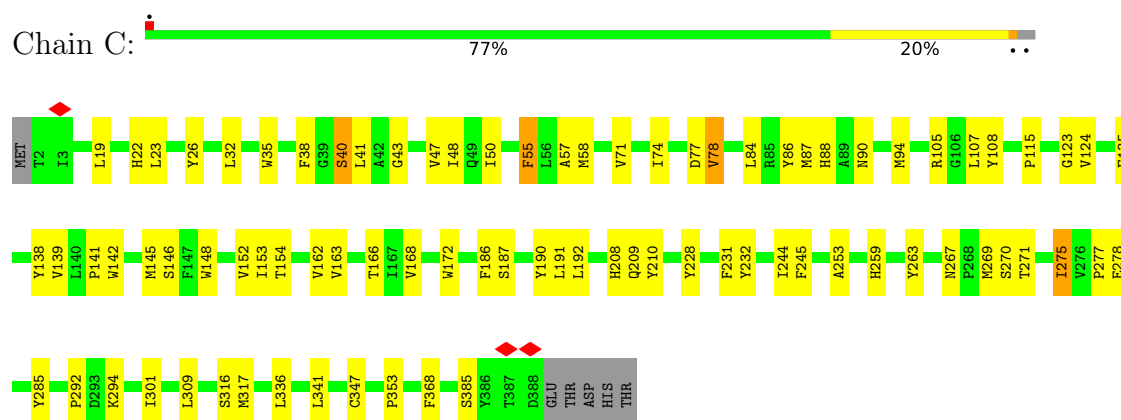
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Mol	Chain	Residues	Atoms		AltConf
18	R	2	Total 2	O 2	0
18	S	13	Total 13	O 13	0
18	T	1	Total 1	O 1	0

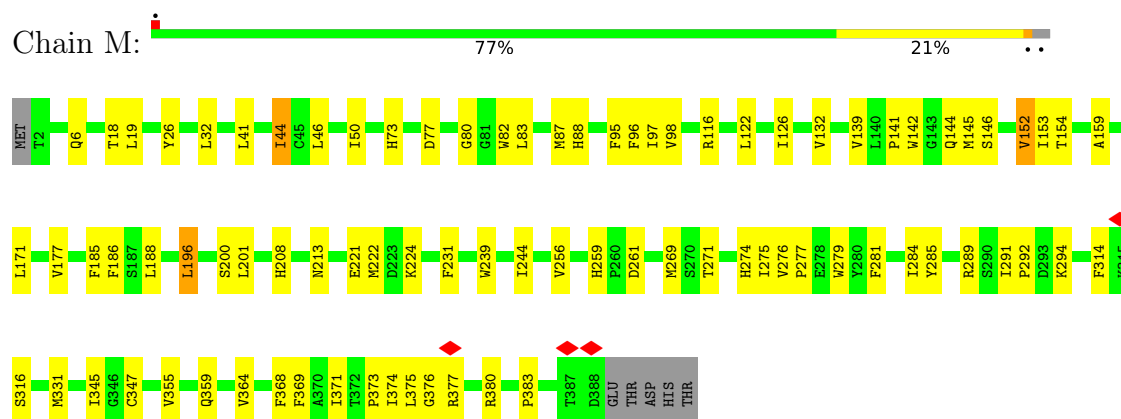
3 Residue-property plots

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.

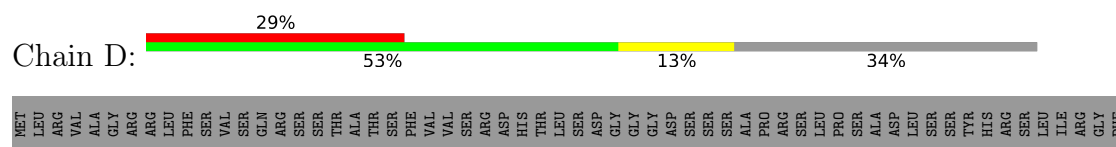
- Molecule 1: Cytochrome b

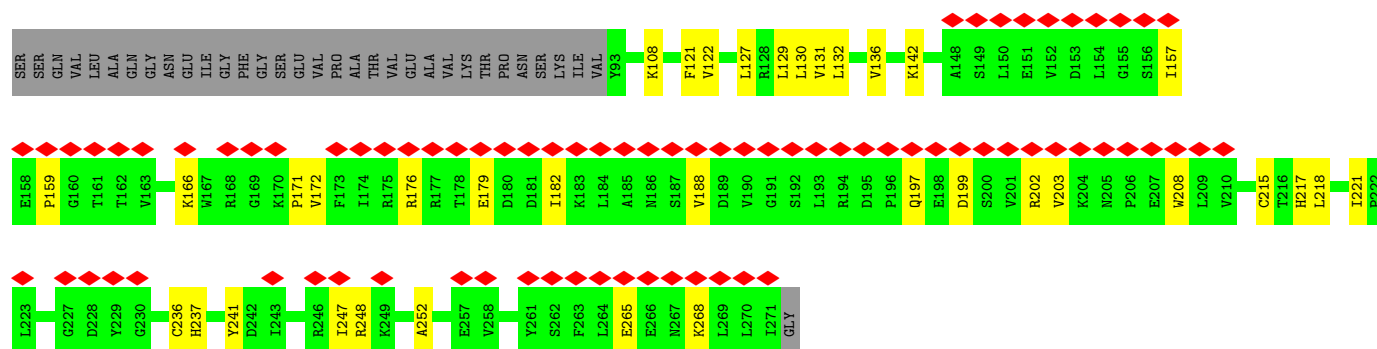


- Molecule 1: Cytochrome b

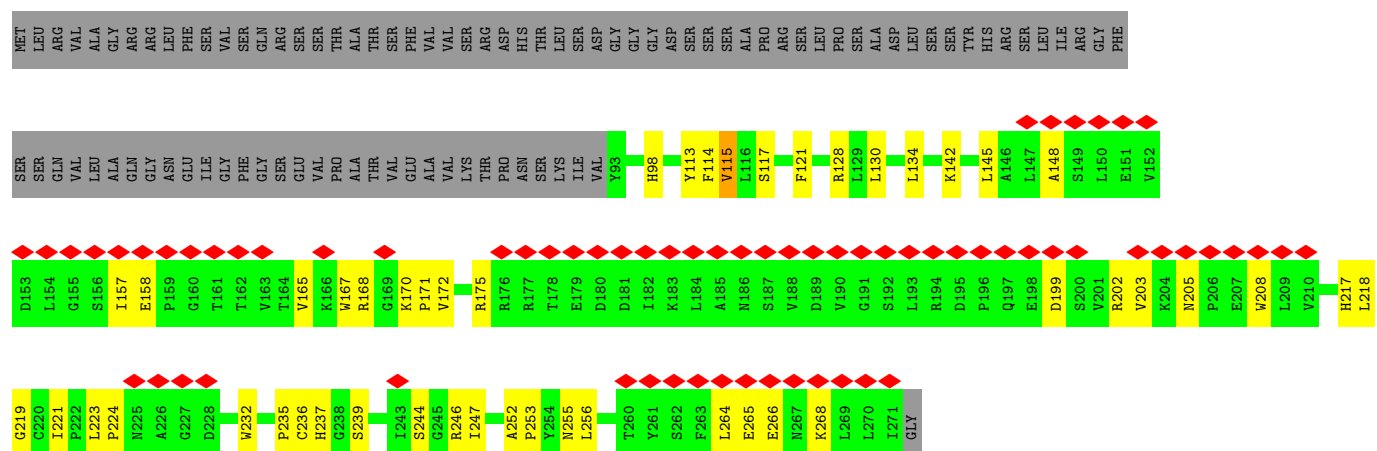


- Molecule 2: Cytochrome b-c1 complex subunit Rieske-1, mitochondrial

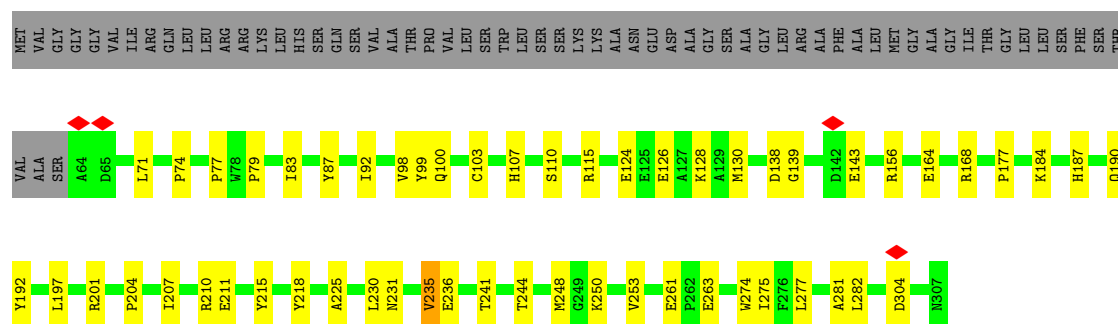




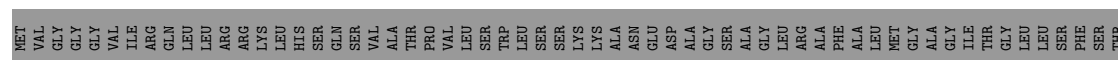
• Molecule 2: Cytochrome b-c1 complex subunit Rieske-1, mitochondrial

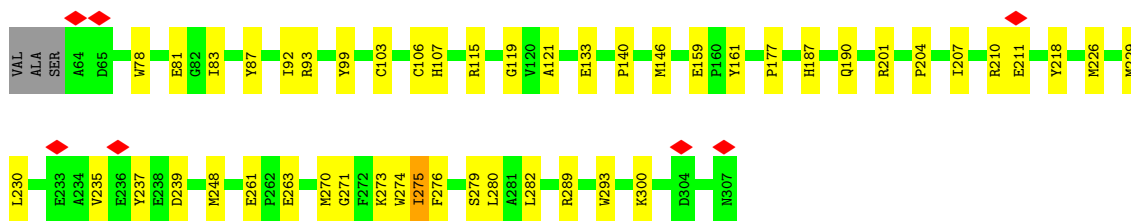


• Molecule 3: Cytochrome c1 2, heme protein, mitochondrial



• Molecule 3: Cytochrome c1 2, heme protein, mitochondrial

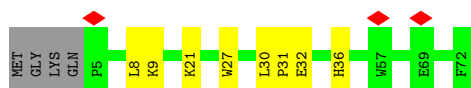
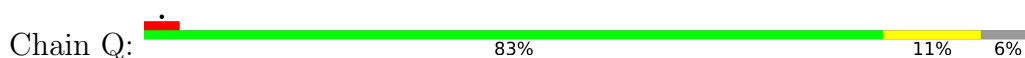




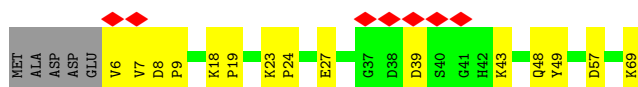
- Molecule 4: Cytochrome b-c1 complex subunit 8-1, mitochondrial



- Molecule 4: Cytochrome b-c1 complex subunit 8-1, mitochondrial



- Molecule 5: Cytochrome b-c1 complex subunit 6-1, mitochondrial



- Molecule 5: Cytochrome b-c1 complex subunit 6-1, mitochondrial



- Molecule 6: Cytochrome b-c1 complex subunit 9, mitochondrial

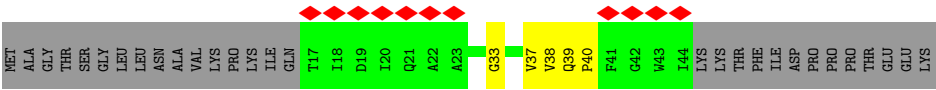
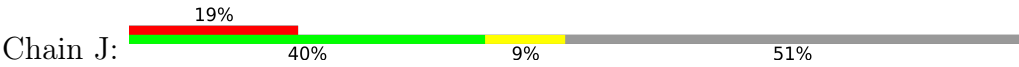


- Molecule 6: Cytochrome b-c1 complex subunit 9, mitochondrial

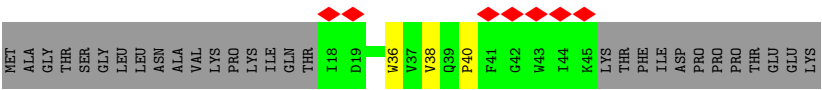
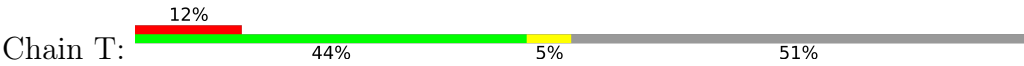




• Molecule 7: Cytochrome b-c1 complex subunit 10, mitochondrial



• Molecule 7: Cytochrome b-c1 complex subunit 10, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	213993	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	215000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	10.977	Depositor
Minimum map value	-3.645	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.288	Depositor
Recommended contour level	0.6	Depositor
Map size (Å)	145.542, 163.30501, 142.677	wwPDB
Map dimensions	249, 285, 254	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.573, 0.573, 0.573	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FES, PTY, HEM, 3PH, PC7, Q7G, UQ5, UQ7, CDL, PGT

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	C	0.68	13/3208 (0.4%)	0.75	8/4395 (0.2%)
1	M	0.63	7/3208 (0.2%)	0.77	5/4395 (0.1%)
2	D	0.34	0/1441	0.47	0/1961
2	N	0.48	0/1441	0.67	4/1961 (0.2%)
3	E	0.40	0/1968	0.57	2/2672 (0.1%)
3	O	0.44	0/1968	0.55	2/2672 (0.1%)
4	G	0.50	1/600 (0.2%)	0.47	1/815 (0.1%)
4	Q	0.37	0/591	0.69	0/802
5	H	0.26	0/531	0.43	0/713
5	R	0.64	2/524 (0.4%)	0.80	2/703 (0.3%)
6	I	0.96	4/488 (0.8%)	0.90	0/655
6	S	0.48	0/488	0.77	2/655 (0.3%)
7	J	0.66	0/210	1.14	4/290 (1.4%)
7	T	0.15	0/212	0.34	0/291
All	All	0.55	27/16878 (0.2%)	0.68	30/22980 (0.1%)

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	88	HIS	C-O	-9.52	1.13	1.24
1	C	192	LEU	C-O	-9.17	1.15	1.24
1	M	87	MET	C-O	-8.34	1.14	1.24
4	G	7	LYS	C-O	-7.99	1.14	1.24
1	C	190	TYR	C-O	-7.29	1.15	1.24
1	C	232	TYR	C-O	-7.01	1.16	1.24
1	C	263	TYR	C-O	-6.57	1.15	1.24
6	I	63	SER	CA-CB	-6.52	1.43	1.53
1	C	58	MET	C-O	-6.33	1.16	1.24
6	I	63	SER	C-O	-6.29	1.16	1.24
1	C	57	ALA	C-O	-6.24	1.16	1.24
1	M	188	LEU	C-O	-6.22	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	40	SER	C-O	-5.92	1.17	1.24
1	M	141	PRO	C-O	-5.79	1.16	1.24
1	M	95	PHE	C-O	-5.74	1.17	1.24
1	C	187	SER	C-O	-5.61	1.17	1.24
6	I	17	TYR	C-O	-5.56	1.17	1.24
6	I	61	ASP	C-O	-5.49	1.16	1.23
1	C	228	TYR	C-O	-5.48	1.16	1.24
1	M	88	HIS	C-O	-5.43	1.17	1.24
1	M	196	LEU	C-O	-5.38	1.17	1.24
1	M	185	PHE	C-O	-5.37	1.17	1.24
1	C	141	PRO	C-O	-5.28	1.17	1.24
5	R	62	PRO	C-O	-5.17	1.17	1.24
1	C	191	LEU	C-O	-5.16	1.18	1.24
5	R	66	ALA	C-O	-5.09	1.17	1.24
1	C	47	VAL	C-O	-5.05	1.18	1.24

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	175	ARG	CB-CA-C	-9.53	98.94	111.42
1	M	96	PHE	CA-C-O	-7.37	112.74	120.55
1	M	96	PHE	CB-CA-C	7.37	123.02	110.79
7	J	38	VAL	N-CA-C	-7.27	99.32	109.21
3	E	304	ASP	CA-CB-CG	6.38	118.98	112.60
1	M	152	VAL	N-CA-C	6.37	116.52	110.53
7	J	40	PRO	N-CA-CB	-6.19	98.67	102.81
2	N	114	PHE	CB-CA-C	6.16	121.16	110.68
3	O	271	GLY	CA-C-O	-5.72	114.85	120.75
1	C	86	TYR	CA-C-N	5.69	128.18	120.44
1	C	86	TYR	C-N-CA	5.69	128.18	120.44
1	C	86	TYR	CB-CA-C	5.67	121.12	110.63
3	O	275	ILE	CB-CA-C	5.67	120.04	112.22
1	C	86	TYR	CA-C-O	-5.64	113.72	120.10
5	R	65	PHE	CB-CA-C	5.53	121.87	110.31
6	S	43	ASP	CA-C-O	-5.52	114.67	120.63
2	N	115	VAL	N-CA-C	-5.38	105.29	110.72
1	C	71	VAL	O-C-N	5.33	127.45	121.90
1	C	55	PHE	CB-CA-C	5.33	119.91	110.85
1	C	84	LEU	CA-C-O	-5.27	115.29	120.82
7	J	38	VAL	CA-C-O	-5.18	114.94	121.11
1	C	87	MET	CA-C-O	-5.17	115.38	120.70
2	N	117	SER	N-CA-C	-5.14	105.76	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	S	27	TYR	CA-C-O	-5.04	115.18	120.63
3	E	235	VAL	CA-C-O	-5.04	116.53	121.67
4	G	7	LYS	CB-CA-C	5.03	118.83	110.78
1	M	383	PRO	N-CD-CG	-5.03	95.66	103.20
7	J	39	GLN	CB-CA-C	5.03	120.47	111.12
1	M	83	LEU	CA-C-O	-5.02	115.10	120.42
5	R	64	LEU	N-CA-C	5.00	116.73	111.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3093	0	3074	77	0
1	M	3093	0	3074	95	0
2	D	1404	0	1395	32	0
2	N	1404	0	1395	41	0
3	E	1917	0	1844	48	0
3	O	1917	0	1844	39	0
4	G	581	0	589	17	0
4	Q	572	0	582	9	0
5	H	518	0	518	14	0
5	R	511	0	511	13	0
6	I	476	0	469	11	0
6	S	476	0	469	14	0
7	J	203	0	197	1	0
7	T	205	0	203	4	0
8	C	86	0	60	2	0
8	E	43	0	30	5	0
8	M	86	0	60	1	0
8	O	43	0	30	6	0
9	C	76	0	100	17	0
9	M	38	0	50	8	0
10	C	33	0	38	1	0
10	G	33	0	39	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	I	32	0	37	3	0
10	M	44	0	64	6	0
10	T	89	0	133	2	0
11	C	92	0	133	10	0
11	G	51	0	78	2	0
11	M	37	0	47	4	0
12	C	166	0	232	19	0
12	G	85	0	120	6	0
12	M	77	0	98	8	0
12	N	81	0	112	3	0
12	O	88	0	123	7	0
12	Q	70	0	87	6	0
13	C	51	0	79	9	0
13	D	34	0	42	1	0
13	G	52	0	84	5	0
13	M	45	0	60	2	0
13	N	39	0	52	6	0
14	D	4	0	0	0	0
14	N	4	0	0	2	0
15	J	41	0	58	0	0
15	M	40	0	56	2	0
15	T	29	0	31	1	0
16	M	48	0	66	11	0
17	M	78	0	0	0	0
18	C	179	0	0	17	0
18	D	32	0	0	0	0
18	E	159	0	0	14	0
18	G	30	0	0	3	0
18	H	13	0	0	1	0
18	I	20	0	0	1	0
18	M	138	0	0	21	0
18	N	33	0	0	4	0
18	O	111	0	0	8	0
18	Q	13	0	0	1	0
18	R	2	0	0	2	0
18	S	13	0	0	5	0
18	T	1	0	0	0	0
All	All	18929	0	18363	430	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (430) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:316:SER:HB2	18:M:565:HOH:O	1.38	1.18
1:M:154:THR:HG22	1:M:171:LEU:HD21	1.18	1.13
1:M:154:THR:CG2	1:M:171:LEU:HD21	1.86	1.05
1:C:292:PRO:HA	18:N:425:HOH:O	1.57	1.01
1:M:154:THR:HG22	1:M:171:LEU:CD2	1.91	1.00
3:O:115:ARG:HD3	18:O:604:HOH:O	1.62	0.99
3:O:161:TYR:O	18:O:501:HOH:O	1.81	0.98
1:M:154:THR:CG2	1:M:171:LEU:CD2	2.44	0.94
1:C:107:LEU:HB3	18:C:615:HOH:O	1.68	0.93
4:G:28:LYS:HD2	18:G:223:HOH:O	1.72	0.90
5:H:6:VAL:HG12	5:H:7:VAL:H	1.35	0.90
1:M:274:HIS:CE1	1:M:276:VAL:CG1	2.57	0.88
3:E:77:PRO:O	18:E:501:HOH:O	1.92	0.87
5:H:6:VAL:HG12	5:H:7:VAL:N	1.87	0.87
1:M:6:GLN:HG2	18:M:625:HOH:O	1.73	0.87
1:M:369:PHE:CZ	18:M:626:HOH:O	2.29	0.84
5:H:6:VAL:HG12	5:H:7:VAL:HG22	1.60	0.84
1:C:294:LYS:HG2	2:N:217:HIS:HD2	1.42	0.83
1:M:316:SER:HA	18:M:565:HOH:O	1.79	0.81
1:M:316:SER:CA	18:M:565:HOH:O	2.26	0.81
1:M:18:THR:HG22	18:M:610:HOH:O	1.81	0.81
4:Q:32:GLU:O	4:Q:36:HIS:ND1	2.10	0.81
1:C:271:THR:OG1	18:C:501:HOH:O	1.98	0.80
1:M:213:ASN:HB2	18:M:609:HOH:O	1.81	0.80
1:M:154:THR:HB	1:M:171:LEU:HD22	1.62	0.80
1:M:274:HIS:CE1	1:M:276:VAL:HG13	2.16	0.80
1:M:274:HIS:CE1	1:M:276:VAL:HG11	2.18	0.79
3:E:74:PRO:HG3	5:H:57:ASP:HB3	1.63	0.79
1:C:26:TYR:HB3	9:C:403:UQ5:H3M1	1.66	0.78
3:E:138:ASP:OD1	3:E:139:GLY:N	2.17	0.78
1:C:259:HIS:CD2	18:E:540:HOH:O	2.36	0.78
1:C:186:PHE:HE2	1:M:186:PHE:HE2	1.31	0.77
1:M:77:ASP:OD1	18:M:501:HOH:O	2.02	0.77
2:D:265:GLU:HG2	2:D:268:LYS:HB2	1.66	0.77
11:M:406:PGT:H42	15:T:103:PTY:HC21	1.66	0.77
3:O:187:HIS:HB3	18:O:605:HOH:O	1.86	0.76
3:E:261:GLU:OE1	18:E:502:HOH:O	2.04	0.75
4:Q:9:LYS:O	18:Q:201:HOH:O	2.05	0.75
1:C:259:HIS:HD2	18:E:540:HOH:O	1.68	0.75
1:M:145:MET:HE1	1:M:276:VAL:H	1.51	0.75
1:M:153:ILE:HG21	16:M:404:UQ7:H161	1.69	0.74
5:R:58:LYS:HG3	18:R:102:HOH:O	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:C:408:CDL:H871	2:D:130:LEU:HD22	1.69	0.74
1:M:44:ILE:HG13	11:M:406:PGT:H252	1.69	0.74
1:M:259:HIS:CE1	1:M:276:VAL:HG21	2.23	0.74
3:O:261:GLU:OE2	18:O:502:HOH:O	2.04	0.74
1:M:259:HIS:NE2	1:M:276:VAL:HG23	2.03	0.73
1:C:77:ASP:OD2	18:C:502:HOH:O	2.06	0.73
2:N:202:ARG:NH1	2:N:244:SER:O	2.21	0.73
3:O:210:ARG:NH1	3:O:211:GLU:O	2.21	0.73
1:C:142:TRP:HA	18:C:563:HOH:O	1.89	0.72
3:E:253:VAL:HG12	18:E:630:HOH:O	1.89	0.71
2:N:265:GLU:HG2	2:N:266:GLU:H	1.54	0.71
12:M:408:CDL:H131	13:M:409:PC7:H381	1.72	0.71
3:E:190:GLN:N	3:E:190:GLN:OE1	2.22	0.70
1:M:316:SER:CB	18:M:565:HOH:O	2.07	0.70
3:O:280:LEU:HB3	12:Q:101:CDL:H371	1.73	0.70
1:M:73:HIS:NE2	18:M:503:HOH:O	2.24	0.70
3:O:300:LYS:HD3	18:O:529:HOH:O	1.90	0.70
12:M:408:CDL:HB22	18:M:580:HOH:O	1.91	0.70
1:M:259:HIS:NE2	1:M:276:VAL:CG2	2.55	0.69
1:C:259:HIS:NE2	18:C:507:HOH:O	2.25	0.69
3:O:78:TRP:HB2	3:O:81:GLU:HG2	1.72	0.69
1:M:213:ASN:CB	18:M:609:HOH:O	2.38	0.69
3:O:204:PRO:HG2	3:O:207:ILE:HG13	1.73	0.69
4:G:27:TRP:HB3	12:G:103:CDL:H321	1.75	0.68
1:M:154:THR:CB	1:M:171:LEU:HD22	2.23	0.68
1:C:347:CYS:SG	18:C:507:HOH:O	2.52	0.68
1:M:26:TYR:HD2	9:M:403:UQ5:H3M1	1.59	0.68
6:S:68:ARG:HD2	18:S:105:HOH:O	1.94	0.68
3:O:159:GLU:HB3	18:O:501:HOH:O	1.93	0.67
3:O:190:GLN:OE1	3:O:190:GLN:N	2.24	0.66
1:M:271:THR:CG2	1:M:275:ILE:HD11	2.25	0.66
3:E:210:ARG:NH1	3:E:211:GLU:O	2.29	0.66
1:M:269:MET:HE2	1:M:269:MET:HA	1.78	0.66
1:C:208:HIS:NE2	9:C:403:UQ5:H4M3	2.11	0.65
1:C:294:LYS:HG2	2:N:217:HIS:CD2	2.30	0.65
3:E:184:LYS:HG2	18:E:519:HOH:O	1.96	0.65
4:G:24:THR:O	18:G:201:HOH:O	2.15	0.65
1:C:163:VAL:HG12	10:T:101:3PH:H12	1.78	0.64
2:N:223:LEU:HD11	2:N:235:PRO:HG3	1.79	0.64
1:M:275:ILE:HB	18:M:534:HOH:O	1.97	0.63
12:C:408:CDL:H802	12:C:408:CDL:H201	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:218:LEU:HD13	1:M:152:VAL:HG13	1.81	0.62
1:C:253:ALA:HB2	11:C:407:PGT:H2	1.82	0.62
1:C:271:THR:HG21	2:N:221:ILE:O	1.99	0.62
2:N:202:ARG:NH2	2:N:256:LEU:O	2.32	0.62
1:M:144:GLN:NE2	18:M:506:HOH:O	2.32	0.62
3:E:282:LEU:HD23	12:G:103:CDL:H561	1.81	0.62
3:O:230:LEU:HD22	3:O:248:MET:HE3	1.80	0.62
1:M:222:MET:HE2	4:Q:8:LEU:HD23	1.80	0.62
1:M:285:TYR:CZ	1:M:289:ARG:HD3	2.35	0.62
3:E:190:GLN:NE2	18:E:502:HOH:O	2.30	0.61
2:N:223:LEU:CD1	2:N:235:PRO:HG3	2.30	0.61
12:C:408:CDL:H751	2:D:127:LEU:HB2	1.82	0.61
10:M:405:3PH:H3D1	3:O:275:ILE:HG22	1.81	0.61
13:N:303:PC7:H182	7:T:36:TRP:HZ3	1.64	0.61
4:Q:27:TRP:HA	4:Q:30:LEU:HD13	1.81	0.61
3:E:225:ALA:HB3	8:E:400:HEM:HBD2	1.83	0.61
1:M:154:THR:CG2	1:M:171:LEU:HD22	2.30	0.61
2:N:113:TYR:CZ	13:N:303:PC7:H63	2.36	0.61
3:E:235:VAL:HG12	3:E:248:MET:SD	2.42	0.60
1:C:139:VAL:HA	1:C:146:SER:HB3	1.83	0.60
1:C:48:ILE:HG12	12:C:408:CDL:H822	1.83	0.60
2:D:237:HIS:HD2	1:M:289:ARG:HG2	1.66	0.60
1:M:153:ILE:HD11	16:M:404:UQ7:C5	2.31	0.59
1:C:77:ASP:HA	2:D:142:LYS:HD2	1.84	0.59
10:I:101:3PH:H241	10:I:101:3PH:H341	1.85	0.59
3:O:103:CYS:SG	8:O:401:HEM:CAB	2.91	0.59
1:M:139:VAL:HA	1:M:146:SER:HB3	1.83	0.59
2:N:115:VAL:HG11	12:Q:101:CDL:H312	1.84	0.59
3:O:133:GLU:OE2	6:S:68:ARG:NH2	2.21	0.59
1:C:138:TYR:CE1	1:C:278:GLU:OE2	2.56	0.59
3:O:99:TYR:HA	3:O:103:CYS:SG	2.43	0.59
1:M:376:GLY:HA3	18:M:565:HOH:O	2.02	0.58
4:G:26:LEU:HD21	12:G:103:CDL:HB32	1.86	0.58
4:G:38:VAL:HG11	10:G:101:3PH:H321	1.84	0.58
6:S:19:LEU:HD22	6:S:26:VAL:HG21	1.85	0.58
4:G:4:GLN:NE2	4:G:5:PRO:O	2.36	0.58
3:E:241:THR:HG23	5:H:69:LYS:HE3	1.85	0.58
10:M:405:3PH:H3B1	3:O:276:PHE:HB2	1.85	0.58
2:N:134:LEU:HD11	12:N:302:CDL:H861	1.85	0.58
1:C:152:VAL:HG21	9:C:404:UQ5:O3	2.04	0.57
3:E:277:LEU:HD21	6:I:42:VAL:HG21	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:13:LEU:HD11	5:R:67:LYS:HD3	1.86	0.57
12:C:409:CDL:H172	13:C:410:PC7:H422	1.86	0.57
8:E:400:HEM:HMC1	8:E:400:HEM:HBC2	1.85	0.57
2:N:98:HIS:NE2	18:N:403:HOH:O	2.32	0.57
3:O:93:ARG:HB2	3:O:121:ALA:HB1	1.86	0.57
1:M:281:PHE:HB3	16:M:404:UQ7:H102	1.87	0.56
2:N:265:GLU:HG2	2:N:266:GLU:N	2.20	0.56
3:E:100:GLN:NE2	18:E:512:HOH:O	2.32	0.56
1:M:259:HIS:CE1	1:M:276:VAL:CG2	2.88	0.56
2:N:167:TRP:CG	2:N:168:ARG:H	2.23	0.56
6:S:62:ILE:HB	6:S:65:LEU:HB2	1.88	0.56
3:E:99:TYR:CD1	3:E:103:CYS:HB2	2.41	0.56
1:M:153:ILE:CG2	16:M:404:UQ7:H161	2.35	0.56
1:C:209:GLN:NE2	18:C:517:HOH:O	2.35	0.56
8:E:400:HEM:HMB1	8:E:400:HEM:HBB2	1.87	0.56
2:N:246:ARG:HA	2:N:255:ASN:HB3	1.88	0.56
3:O:99:TYR:CD1	3:O:103:CYS:HB2	2.40	0.56
1:M:145:MET:CE	1:M:276:VAL:H	2.19	0.56
3:O:270:MET:HG2	3:O:274:TRP:HD1	1.71	0.55
5:H:57:ASP:OD1	18:H:101:HOH:O	2.18	0.55
4:G:72:PHE:C	18:G:206:HOH:O	2.49	0.55
3:E:126:GLU:HG2	6:I:68:ARG:HB3	1.87	0.55
1:M:271:THR:HG23	1:M:275:ILE:HD11	1.88	0.55
2:D:131:VAL:HG13	16:M:404:UQ7:H361	1.88	0.55
12:M:408:CDL:H552	12:O:402:CDL:H202	1.89	0.55
4:G:36:HIS:O	4:G:40:GLU:HG3	2.07	0.55
1:C:26:TYR:CB	9:C:403:UQ5:H3M1	2.34	0.54
1:M:347:CYS:SG	18:M:632:HOH:O	2.57	0.54
1:C:154:THR:OG1	1:C:172:TRP:NE1	2.33	0.54
12:N:302:CDL:H752	12:N:302:CDL:H522	1.88	0.54
3:O:119:GLY:O	18:O:504:HOH:O	2.18	0.54
3:E:83:ILE:HD11	10:I:101:3PH:H332	1.90	0.54
3:O:270:MET:HG2	3:O:274:TRP:CD1	2.42	0.54
10:M:405:3PH:H3D2	3:O:276:PHE:HA	1.89	0.54
1:C:277:PRO:HB3	9:C:404:UQ5:C5	2.38	0.54
1:M:132:VAL:HG22	16:M:404:UQ7:H172	1.88	0.54
9:M:403:UQ5:H3M3	9:M:403:UQ5:H4M2	1.87	0.54
3:O:229:MET:HE2	8:O:401:HEM:HMC3	1.89	0.54
1:C:162:VAL:HG23	1:C:163:VAL:HG13	1.90	0.54
1:C:316:SER:HB2	18:C:631:HOH:O	2.07	0.53
1:C:277:PRO:HB3	9:C:404:UQ5:O5	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:115:VAL:CG1	12:Q:101:CDL:H312	2.37	0.53
2:N:247:ILE:HD13	2:N:252:ALA:HB3	1.89	0.53
5:R:10:LYS:HG3	5:R:64:LEU:HD22	1.90	0.53
6:S:44:TYR:CE1	6:S:48:LYS:HE2	2.44	0.53
2:D:121:PHE:HE1	6:I:31:ILE:HA	1.73	0.53
3:O:201:ARG:NH2	3:O:218:TYR:OH	2.41	0.53
1:C:368:PHE:HB2	11:G:102:PGT:H481	1.90	0.53
1:C:259:HIS:ND1	18:C:513:HOH:O	2.32	0.53
1:M:222:MET:CE	4:Q:8:LEU:HD23	2.38	0.53
3:E:184:LYS:CG	18:E:519:HOH:O	2.55	0.53
1:C:145:MET:HE1	1:C:275:ILE:HA	1.91	0.53
3:E:197:LEU:HB3	3:E:230:LEU:HD12	1.91	0.52
1:M:46:LEU:HD23	9:M:403:UQ5:H202	1.90	0.52
1:M:126:ILE:HD13	18:M:588:HOH:O	2.09	0.52
2:N:264:LEU:HB2	2:N:268:LYS:HB2	1.91	0.52
1:M:259:HIS:CD2	1:M:276:VAL:HG23	2.44	0.52
2:N:224:PRO:HA	2:N:232:TRP:CD1	2.45	0.52
1:C:50:ILE:HA	8:C:402:HEM:HAB	1.91	0.52
9:C:403:UQ5:H1M2	11:C:406:PGT:H392	1.91	0.52
1:M:239:TRP:HH2	11:M:406:PGT:H212	1.74	0.52
5:R:58:LYS:CG	18:R:102:HOH:O	2.51	0.52
1:M:244:ILE:HG21	12:O:402:CDL:H382	1.92	0.52
1:C:74:ILE:HA	1:C:78:VAL:HG13	1.92	0.52
12:C:409:CDL:H442	4:G:49:VAL:HG21	1.92	0.52
3:O:282:LEU:HD23	12:O:402:CDL:H342	1.92	0.51
12:M:408:CDL:H532	12:O:402:CDL:H181	1.91	0.51
2:D:157:ILE:H	2:D:208:TRP:HH2	1.58	0.51
7:J:33:GLY:O	7:J:37:VAL:HG23	2.10	0.51
1:C:385:SER:OG	18:C:505:HOH:O	2.18	0.51
1:C:275:ILE:HG21	2:N:236:CYS:SG	2.50	0.51
1:M:274:HIS:HE1	1:M:276:VAL:HG11	1.75	0.51
2:N:219:GLY:O	18:N:401:HOH:O	2.19	0.51
3:E:263:GLU:HA	18:E:588:HOH:O	2.11	0.51
1:C:267:ASN:OD1	1:C:270:SER:OG	2.29	0.51
4:G:56:TYR:O	4:G:60:GLN:HG2	2.11	0.51
12:C:409:CDL:O1	13:C:410:PC7:O31	2.29	0.51
3:E:192:TYR:OH	8:E:400:HEM:O1A	2.23	0.51
2:D:237:HIS:CD2	1:M:289:ARG:HG2	2.46	0.50
2:D:247:ILE:HD13	2:D:252:ALA:HB3	1.92	0.50
1:M:97:ILE:HG13	1:M:279:TRP:HH2	1.76	0.50
1:C:152:VAL:HG21	9:C:404:UQ5:C3	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:285:TYR:CE1	16:M:404:UQ7:HM32	2.46	0.50
9:C:403:UQ5:H18	11:C:406:PGT:C48	2.41	0.50
3:E:99:TYR:HA	3:E:103:CYS:SG	2.51	0.50
1:M:18:THR:HG23	1:M:19:LEU:HD22	1.92	0.50
4:G:30:LEU:O	4:G:34:ILE:HD12	2.11	0.50
5:H:6:VAL:CG1	5:H:7:VAL:H	2.06	0.50
3:E:244:THR:O	3:E:248:MET:HG3	2.11	0.50
1:C:245:PHE:HD1	11:C:407:PGT:H431	1.77	0.50
1:M:32:LEU:HB2	1:M:231:PHE:CE1	2.47	0.50
1:M:152:VAL:HG12	1:M:153:ILE:HD12	1.94	0.50
2:D:166:LYS:HG3	1:M:269:MET:SD	2.52	0.49
12:M:408:CDL:H712	12:M:408:CDL:H541	1.94	0.49
1:C:55:PHE:HZ	16:M:404:UQ7:H311	1.76	0.49
3:O:140:PRO:HG3	3:O:146:MET:HE1	1.95	0.49
1:M:371:ILE:O	1:M:374:ILE:HG13	2.12	0.49
1:C:336:LEU:HD11	13:C:410:PC7:H411	1.94	0.49
1:C:277:PRO:O	18:C:506:HOH:O	2.20	0.49
5:R:25:LEU:HD23	5:R:52:TYR:CE1	2.48	0.49
1:M:97:ILE:HG13	1:M:279:TRP:CH2	2.48	0.49
2:N:148:ALA:HA	2:N:168:ARG:HD2	1.95	0.49
13:N:303:PC7:H182	7:T:36:TRP:CZ3	2.47	0.48
2:D:121:PHE:CE1	6:I:31:ILE:HA	2.49	0.48
1:M:377:ARG:HA	1:M:380:ARG:HD2	1.95	0.48
11:C:406:PGT:H351	12:C:408:CDL:H112	1.95	0.48
2:N:237:HIS:HB2	14:N:301:FES:S2	2.53	0.48
12:C:409:CDL:H432	4:G:49:VAL:HG11	1.96	0.48
12:C:408:CDL:H742	2:D:127:LEU:HD22	1.96	0.48
5:R:10:LYS:O	5:R:14:GLU:HG2	2.12	0.48
12:C:408:CDL:H711	13:D:302:PC7:H142	1.96	0.48
3:O:103:CYS:SG	8:O:401:HEM:HAB	2.54	0.48
1:M:314:PHE:CD2	1:M:373:PRO:HG3	2.48	0.48
6:I:62:ILE:HA	18:I:214:HOH:O	2.13	0.47
6:S:68:ARG:HG2	18:S:105:HOH:O	2.14	0.47
12:C:409:CDL:H422	12:C:409:CDL:H391	1.65	0.47
2:D:171:PRO:HG2	2:D:221:ILE:HD13	1.96	0.47
1:M:80:GLY:C	18:M:551:HOH:O	2.57	0.47
1:M:50:ILE:HA	8:M:402:HEM:HAB	1.96	0.47
1:M:159:ALA:HA	1:M:294:LYS:HD3	1.96	0.47
10:M:405:3PH:H2C1	12:O:402:CDL:H232	1.95	0.47
5:H:27:GLU:HG3	5:H:48:GLN:HG2	1.95	0.47
3:O:226:MET:HB2	8:O:401:HEM:C1D	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:58:ARG:HB2	6:I:61:ASP:OD1	2.15	0.47
1:M:142:TRP:HH2	1:M:177:VAL:HG12	1.78	0.47
1:M:126:ILE:HG23	1:M:196:LEU:HD11	1.97	0.47
2:D:221:ILE:HB	1:M:271:THR:OG1	2.15	0.47
2:D:236:CYS:SG	1:M:275:ILE:HD12	2.55	0.47
3:E:143:GLU:CD	3:E:143:GLU:H	2.23	0.47
1:M:277:PRO:HB3	16:M:404:UQ7:H71	1.96	0.47
2:N:165:VAL:HG23	2:N:172:VAL:HB	1.97	0.47
12:C:409:CDL:H132	13:C:410:PC7:H152	1.97	0.47
1:M:116:ARG:HD2	18:M:609:HOH:O	2.14	0.47
2:D:188:VAL:HG11	2:D:248:ARG:NH2	2.30	0.46
16:M:404:UQ7:H322	16:M:404:UQ7:H28	1.60	0.46
2:D:159:PRO:HG3	2:D:176:ARG:HD3	1.98	0.46
2:D:179:GLU:HA	2:D:182:ILE:HD12	1.97	0.46
9:M:403:UQ5:H272	9:M:403:UQ5:H251	1.63	0.46
1:C:22:HIS:C	1:C:23:LEU:HD12	2.40	0.46
1:C:43:GLY:HA2	9:C:403:UQ5:H162	1.97	0.46
3:E:277:LEU:HD22	13:G:104:PC7:H242	1.98	0.46
1:M:26:TYR:CD2	9:M:403:UQ5:H3M1	2.47	0.46
1:M:154:THR:HG21	1:M:171:LEU:CD2	2.40	0.46
10:I:101:3PH:H321	10:I:101:3PH:H32	1.48	0.46
6:S:19:LEU:HB3	6:S:26:VAL:HG11	1.96	0.46
6:S:59:TYR:OH	18:S:101:HOH:O	2.20	0.46
1:M:239:TRP:CH2	11:M:406:PGT:H212	2.51	0.46
2:N:157:ILE:HG13	2:N:158:GLU:H	1.81	0.46
12:G:103:CDL:H572	12:G:103:CDL:H542	1.81	0.46
1:M:213:ASN:HB3	18:M:609:HOH:O	2.12	0.46
1:C:90:ASN:O	1:C:94:MET:HG2	2.16	0.46
1:C:317:MET:SD	18:C:589:HOH:O	2.61	0.46
3:O:237:TYR:HB3	3:O:239:ASP:OD1	2.15	0.46
1:C:35:TRP:HB3	1:C:105:ARG:HG3	1.98	0.45
3:E:164:GLU:CD	3:E:168:ARG:HE	2.24	0.45
2:N:121:PHE:HE1	6:S:31:ILE:HA	1.81	0.45
12:O:402:CDL:H621	4:Q:31:PRO:HG3	1.98	0.45
5:R:21:CYS:O	5:R:24:PRO:HD2	2.16	0.45
4:G:67:LYS:HB3	4:G:67:LYS:HE3	1.71	0.45
5:R:31:CYS:O	5:R:35:ILE:HG12	2.15	0.45
11:C:406:PGT:H431	11:C:406:PGT:H402	1.75	0.45
1:M:369:PHE:CE2	18:M:626:HOH:O	2.62	0.45
3:E:115:ARG:NH1	18:E:522:HOH:O	2.40	0.45
2:N:239:SER:OG	14:N:301:FES:S2	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:C:410:PC7:H41	13:C:410:PC7:H82	1.55	0.45
2:D:121:PHE:HE2	13:G:104:PC7:H442	1.82	0.45
3:E:143:GLU:CD	3:E:143:GLU:N	2.75	0.45
1:M:375:LEU:HD23	1:M:375:LEU:HA	1.79	0.45
13:G:104:PC7:H362	13:G:104:PC7:H142	1.99	0.45
2:N:205:ASN:HD22	2:N:208:TRP:HD1	1.65	0.45
1:C:35:TRP:CH2	12:C:409:CDL:H712	2.52	0.45
11:C:407:PGT:H212	11:C:407:PGT:H181	1.74	0.45
2:N:113:TYR:CE2	13:N:303:PC7:H63	2.51	0.45
6:S:68:ARG:CG	18:S:105:HOH:O	2.63	0.45
1:C:123:GLY:O	8:C:401:HEM:HMC3	2.17	0.45
13:G:104:PC7:H41	13:G:104:PC7:H62	1.58	0.45
5:R:44:HIS:CE1	5:R:46:THR:HB	2.52	0.45
6:I:60:GLU:CD	6:I:60:GLU:H	2.26	0.44
3:O:106:CYS:SG	8:O:401:HEM:CAC	3.05	0.44
12:O:402:CDL:H111	12:O:402:CDL:H141	1.62	0.44
9:C:403:UQ5:H222	9:C:403:UQ5:H262	1.87	0.44
3:E:87:TYR:HB3	3:E:92:ILE:HD11	1.99	0.44
3:E:201:ARG:NH2	3:E:218:TYR:OH	2.49	0.44
12:Q:101:CDL:H401	12:Q:101:CDL:H431	1.45	0.44
1:C:294:LYS:HD3	2:N:253:PRO:HG3	1.98	0.44
12:C:409:CDL:H271	12:C:409:CDL:H242	1.86	0.44
1:C:154:THR:O	1:C:168:VAL:HG22	2.17	0.44
3:E:204:PRO:HD3	3:E:215:TYR:CZ	2.53	0.44
1:M:82:TRP:CG	3:O:263:GLU:HG3	2.53	0.44
1:M:200:SER:HB3	9:M:403:UQ5:H161	1.98	0.44
2:N:128:ARG:HD2	7:T:36:TRP:CE2	2.52	0.44
5:H:39:ASP:HB2	5:H:43:LYS:HD2	1.98	0.44
1:C:115:PRO:HB2	1:C:210:TYR:CE2	2.53	0.44
3:O:289:ARG:HE	3:O:293:TRP:CD1	2.36	0.44
4:G:23:MET:HG3	13:G:104:PC7:H32	2.00	0.44
2:D:171:PRO:HG3	1:M:269:MET:HE2	2.00	0.43
1:C:108:TYR:CD1	13:C:410:PC7:H331	2.53	0.43
1:C:271:THR:CG2	2:N:221:ILE:O	2.66	0.43
11:C:407:PGT:H201	3:E:275:ILE:HG22	2.01	0.43
2:D:171:PRO:HG2	2:D:221:ILE:CD1	2.48	0.43
3:E:103:CYS:SG	8:E:400:HEM:CAB	3.06	0.43
3:E:207:ILE:HD13	3:E:207:ILE:HA	1.83	0.43
2:D:176:ARG:HB2	2:D:208:TRP:CZ3	2.53	0.43
3:O:107:HIS:HE1	3:O:177:PRO:HD2	1.83	0.43
4:Q:21:LYS:HB3	12:Q:101:CDL:HA21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:32:LEU:HB2	1:C:231:PHE:CE1	2.54	0.43
1:C:40:SER:HB3	9:C:403:UQ5:H71	2.01	0.43
3:E:231:ASN:O	3:E:248:MET:HE1	2.18	0.43
3:E:250:LYS:HE3	18:E:645:HOH:O	2.19	0.43
1:M:368:PHE:HB2	15:M:407:PTY:H441	2.00	0.43
3:E:98:VAL:HG22	3:E:235:VAL:HG11	2.00	0.43
1:C:163:VAL:O	1:C:166:THR:HG22	2.18	0.43
2:D:217:HIS:HD2	1:M:294:LYS:HB2	1.83	0.43
11:G:102:PGT:H242	11:G:102:PGT:H211	1.82	0.43
2:N:199:ASP:O	2:N:203:VAL:HG22	2.17	0.43
6:S:40:ARG:CZ	6:S:40:ARG:HA	2.48	0.43
1:C:19:LEU:HD13	1:C:23:LEU:HD13	2.01	0.43
1:C:38:PHE:HA	1:C:41:LEU:HB2	2.01	0.43
3:E:187:HIS:HB3	18:E:654:HOH:O	2.17	0.43
12:M:408:CDL:H541	12:M:408:CDL:H511	1.61	0.43
3:E:130:MET:HG3	6:I:68:ARG:CZ	2.49	0.43
1:M:208:HIS:NE2	9:M:403:UQ5:O3	2.52	0.43
1:M:277:PRO:HG3	16:M:404:UQ7:C1	2.49	0.43
2:N:142:LYS:HA	2:N:145:LEU:HD12	2.00	0.43
3:O:226:MET:HG3	8:O:401:HEM:C4C	2.53	0.43
6:S:48:LYS:HA	6:S:48:LYS:HD3	1.79	0.43
10:M:405:3PH:H3G1	3:O:279:SER:HB2	2.00	0.42
12:M:408:CDL:H422	12:M:408:CDL:H391	1.81	0.42
6:S:68:ARG:CD	18:S:105:HOH:O	2.62	0.42
7:T:38:VAL:O	7:T:40:PRO:HD3	2.19	0.42
1:C:48:ILE:CG1	12:C:408:CDL:H822	2.46	0.42
1:C:148:TRP:CH2	2:N:221:ILE:HG12	2.55	0.42
1:M:364:VAL:HG13	15:M:407:PTY:H422	2.01	0.42
12:M:408:CDL:H1	13:M:409:PC7:H42	2.01	0.42
5:R:23:LYS:HB2	5:R:24:PRO:HD3	2.00	0.42
1:C:353:PRO:HG3	4:G:62:PHE:CG	2.54	0.42
1:M:355:VAL:O	1:M:359:GLN:HG3	2.19	0.42
1:C:26:TYR:CD2	9:C:403:UQ5:H3M1	2.55	0.42
5:R:10:LYS:HG3	5:R:64:LEU:CD2	2.49	0.42
2:D:132:LEU:O	2:D:136:VAL:HG23	2.19	0.42
3:E:204:PRO:HG3	5:H:49:TYR:CG	2.55	0.42
5:R:23:LYS:HB2	5:R:23:LYS:HE2	1.76	0.42
3:E:79:PRO:HG3	18:E:645:HOH:O	2.19	0.42
1:C:142:TRP:CA	18:C:563:HOH:O	2.57	0.42
2:N:130:LEU:HB3	12:N:302:CDL:H862	2.02	0.42
13:N:303:PC7:H72	18:N:429:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:285:TYR:CZ	9:C:404:UQ5:H3M2	2.55	0.42
1:C:108:TYR:CG	13:C:410:PC7:H331	2.55	0.42
1:C:244:ILE:HG21	12:G:103:CDL:H602	2.02	0.42
13:C:410:PC7:H441	18:C:637:HOH:O	2.19	0.42
3:O:190:GLN:NE2	18:O:526:HOH:O	2.53	0.42
1:C:142:TRP:C	18:C:563:HOH:O	2.63	0.41
1:C:294:LYS:HB3	1:C:294:LYS:HE2	1.72	0.41
9:C:403:UQ5:H112	11:C:406:PGT:H462	2.02	0.41
3:E:124:GLU:HG2	3:E:128:LYS:HE3	2.01	0.41
12:G:103:CDL:H231	12:G:103:CDL:H262	1.80	0.41
1:M:291:ILE:HA	1:M:292:PRO:HD3	1.94	0.41
3:E:71:LEU:HD23	3:E:218:TYR:CE1	2.55	0.41
5:H:6:VAL:CG1	5:H:7:VAL:HG22	2.39	0.41
1:M:41:LEU:HD23	1:M:41:LEU:HA	1.89	0.41
1:C:124:VAL:HG11	1:C:309:LEU:HG	2.03	0.41
11:C:406:PGT:H471	11:C:406:PGT:H441	1.83	0.41
1:M:221:GLU:HA	1:M:224:LYS:HZ3	1.86	0.41
10:M:405:3PH:H322	10:M:405:3PH:H351	1.78	0.41
5:H:18:LYS:N	5:H:19:PRO:HD2	2.35	0.41
1:C:135:PHE:CZ	1:C:153:ILE:HB	2.56	0.41
9:C:403:UQ5:H1M1	9:C:403:UQ5:H72	1.66	0.41
12:C:409:CDL:H242	12:C:409:CDL:H211	1.78	0.41
3:E:107:HIS:HE1	3:E:177:PRO:HD2	1.86	0.41
4:G:61:TYR:O	4:G:65:GLN:HG2	2.21	0.41
5:H:23:LYS:HB3	5:H:24:PRO:HD3	2.02	0.41
9:C:404:UQ5:H151	9:C:404:UQ5:H171	1.82	0.41
12:C:409:CDL:H372	12:C:409:CDL:H341	1.93	0.41
2:D:197:GLN:HG2	2:D:202:ARG:HD2	2.03	0.41
2:D:199:ASP:O	2:D:203:VAL:HG12	2.21	0.41
5:H:8:ASP:HA	5:H:9:PRO:HD3	1.99	0.41
1:C:317:MET:HG2	18:C:572:HOH:O	2.20	0.41
1:C:341:LEU:HD21	4:G:52:VAL:HA	2.03	0.41
12:C:408:CDL:H851	2:D:130:LEU:HD13	2.03	0.41
2:D:215:CYS:SG	2:D:241:TYR:OH	2.76	0.41
13:N:303:PC7:H122	13:N:303:PC7:H32	1.65	0.41
10:T:101:3PH:H2A2	10:T:102:3PH:H371	2.03	0.41
1:M:145:MET:HG2	1:M:261:ASP:HB2	2.02	0.40
3:O:83:ILE:H	3:O:83:ILE:HG13	1.76	0.40
10:C:405:3PH:H221	10:C:405:3PH:H251	1.85	0.40
2:D:122:VAL:HG11	3:E:281:ALA:HB2	2.02	0.40
3:E:110:SER:O	3:E:156:ARG:HD2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:35:ILE:O	5:R:35:ILE:HG22	2.21	0.40
1:C:269:MET:HE3	2:N:171:PRO:HG3	2.03	0.40
6:I:23:ARG:HD3	6:I:23:ARG:HA	1.75	0.40
1:M:77:ASP:HA	2:N:142:LYS:HE3	2.02	0.40
4:Q:21:LYS:NZ	12:Q:101:CDL:OB4	2.53	0.40
1:C:41:LEU:HD23	1:C:41:LEU:HA	1.91	0.40
1:C:152:VAL:HG23	1:C:153:ILE:HD12	2.02	0.40
6:I:48:LYS:HD2	6:I:48:LYS:HA	1.57	0.40
1:M:201:LEU:HD23	9:M:403:UQ5:H152	2.04	0.40
2:N:167:TRP:CG	2:N:168:ARG:N	2.88	0.40
2:N:218:LEU:HD12	2:N:237:HIS:CE1	2.56	0.40
2:N:223:LEU:HA	2:N:224:PRO:HD3	1.96	0.40
4:Q:8:LEU:HD22	4:Q:9:LYS:N	2.36	0.40
6:S:59:TYR:O	6:S:65:LEU:HD22	2.21	0.40
1:C:316:SER:HB2	18:C:572:HOH:O	2.20	0.40
13:C:410:PC7:H322	13:C:410:PC7:H2	1.81	0.40
2:D:129:LEU:HD13	3:E:274:TRP:CZ2	2.56	0.40
6:I:58:ARG:HB2	6:I:58:ARG:HE	1.56	0.40
3:O:87:TYR:HB3	3:O:92:ILE:HD11	2.04	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	C	385/393 (98%)	376 (98%)	9 (2%)	0	100	100
1	M	385/393 (98%)	374 (97%)	11 (3%)	0	100	100
2	D	177/272 (65%)	168 (95%)	9 (5%)	0	100	100
2	N	177/272 (65%)	166 (94%)	11 (6%)	0	100	100
3	E	242/307 (79%)	238 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	O	242/307 (79%)	238 (98%)	4 (2%)	0	100	100
4	G	67/72 (93%)	67 (100%)	0	0	100	100
4	Q	66/72 (92%)	65 (98%)	1 (2%)	0	100	100
5	H	62/69 (90%)	61 (98%)	1 (2%)	0	100	100
5	R	61/69 (88%)	59 (97%)	2 (3%)	0	100	100
6	I	55/72 (76%)	53 (96%)	2 (4%)	0	100	100
6	S	55/72 (76%)	53 (96%)	2 (4%)	0	100	100
7	J	26/57 (46%)	25 (96%)	1 (4%)	0	100	100
7	T	26/57 (46%)	23 (88%)	3 (12%)	0	100	100
All	All	2026/2484 (82%)	1966 (97%)	60 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	330/336 (98%)	327 (99%)	3 (1%)	70	79
1	M	330/336 (98%)	323 (98%)	7 (2%)	47	58
2	D	155/232 (67%)	153 (99%)	2 (1%)	61	72
2	N	155/232 (67%)	154 (99%)	1 (1%)	78	84
3	E	200/247 (81%)	199 (100%)	1 (0%)	81	87
3	O	200/247 (81%)	198 (99%)	2 (1%)	68	77
4	G	63/65 (97%)	63 (100%)	0	100	100
4	Q	62/65 (95%)	62 (100%)	0	100	100
5	H	58/62 (94%)	58 (100%)	0	100	100
5	R	57/62 (92%)	56 (98%)	1 (2%)	51	63
6	I	48/59 (81%)	48 (100%)	0	100	100
6	S	48/59 (81%)	48 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	J	16/41 (39%)	16 (100%)	0	100	100
7	T	16/41 (39%)	16 (100%)	0	100	100
All	All	1738/2084 (83%)	1721 (99%)	17 (1%)	65	77

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	78	VAL
1	C	275	ILE
1	C	301	ILE
2	D	108	LYS
2	D	172	VAL
3	E	236	GLU
1	M	44	ILE
1	M	98	VAL
1	M	122	LEU
1	M	256	VAL
1	M	284	ILE
1	M	331	MET
1	M	345	ILE
2	N	170	LYS
3	O	235	VAL
3	O	273	LYS
5	R	27	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	348	GLN
4	G	70	HIS
1	M	144	GLN
1	M	274	HIS
2	N	96	HIS
3	O	163	ASN
5	R	54	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

39 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
13	PC7	C	410	-	50,50,51	0.99	4 (8%)	56,58,59	1.08	3 (5%)
11	PGT	M	406	-	36,36,50	1.22	4 (11%)	39,42,56	1.13	2 (5%)
8	HEM	C	401	1	50,50,50	1.48	8 (16%)	67,82,82	1.16	5 (7%)
9	UQ5	C	404	-	38,38,38	0.46	0	48,49,49	0.84	2 (4%)
10	3PH	M	405	-	43,43,47	0.66	1 (2%)	46,48,52	0.63	1 (2%)
11	PGT	G	102	-	50,50,50	1.09	4 (8%)	53,56,56	1.07	2 (3%)
15	PTY	M	407	-	39,39,49	0.99	4 (10%)	42,44,54	1.07	2 (4%)
12	CDL	N	302	-	80,80,99	0.97	8 (10%)	86,92,111	1.17	4 (4%)
9	UQ5	C	403	-	38,38,38	0.96	2 (5%)	48,49,49	0.91	1 (2%)
10	3PH	C	405	12	32,32,47	0.74	1 (3%)	35,37,52	0.78	1 (2%)
12	CDL	C	408	-	80,80,99	0.38	0	86,92,111	0.57	2 (2%)
14	FES	N	301	2	0,4,4	-	-	-	-	-
12	CDL	O	402	-	87,87,99	0.94	8 (9%)	93,99,111	1.12	4 (4%)
14	FES	D	301	2	0,4,4	-	-	-	-	-
12	CDL	M	408	-	76,76,99	1.01	8 (10%)	82,88,111	1.12	4 (4%)
15	PTY	T	103	-	28,28,49	1.14	4 (14%)	31,33,54	1.19	2 (6%)
11	PGT	C	406	-	40,40,50	0.39	0	43,46,56	0.44	0
13	PC7	M	409	-	43,43,51	1.05	4 (9%)	48,50,59	1.14	3 (6%)
10	3PH	T	102	-	47,47,47	0.64	1 (2%)	50,52,52	0.59	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	PC7	D	302	-	33,33,51	1.20	4 (12%)	39,41,59	1.09	2 (5%)
10	3PH	I	101	-	31,31,47	0.77	1 (3%)	34,36,52	0.77	2 (5%)
8	HEM	C	402	1	50,50,50	2.01	13 (26%)	67,82,82	1.62	11 (16%)
13	PC7	N	303	-	38,38,51	0.40	0	44,46,59	0.65	1 (2%)
10	3PH	T	101	-	40,40,47	0.68	1 (2%)	43,45,52	0.65	1 (2%)
12	CDL	C	409	10	84,84,99	0.96	8 (9%)	90,96,111	1.11	4 (4%)
17	Q7G	M	410	-	44,44,90	0.75	1 (2%)	64,68,138	1.40	12 (18%)
16	UQ7	M	404	-	48,48,48	0.67	2 (4%)	60,61,61	0.76	2 (3%)
12	CDL	Q	101	-	69,69,99	1.05	8 (11%)	75,81,111	1.18	5 (6%)
10	3PH	G	101	-	32,32,47	0.76	1 (3%)	35,37,52	0.68	1 (2%)
11	PGT	C	407	-	50,50,50	1.11	4 (8%)	53,56,56	1.05	2 (3%)
8	HEM	E	400	3	50,50,50	1.45	7 (14%)	67,82,82	1.17	8 (11%)
8	HEM	M	402	1	50,50,50	2.10	13 (26%)	67,82,82	1.68	16 (23%)
8	HEM	O	401	3	50,50,50	2.04	16 (32%)	67,82,82	2.04	20 (29%)
12	CDL	G	103	-	84,84,99	0.97	8 (9%)	90,96,111	1.12	4 (4%)
9	UQ5	M	403	-	38,38,38	0.49	0	48,49,49	0.62	1 (2%)
17	Q7G	M	411	-	44,44,90	0.79	1 (2%)	64,68,138	1.40	11 (17%)
8	HEM	M	401	1	50,50,50	2.02	18 (36%)	67,82,82	1.70	20 (29%)
13	PC7	G	104	-	51,51,51	0.99	4 (7%)	57,59,59	1.02	2 (3%)
15	PTY	J	101	-	40,40,49	0.34	0	43,45,54	0.38	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	PC7	C	410	-	-	19/54/54/55	-
11	PGT	M	406	-	-	20/41/41/55	-
8	HEM	C	401	1	-	2/14/54/54	-
9	UQ5	C	404	-	-	13/33/57/57	0/1/1/1
10	3PH	M	405	-	-	20/45/45/49	-
11	PGT	G	102	-	-	37/55/55/55	-
15	PTY	M	407	-	-	18/43/43/53	-
12	CDL	N	302	-	-	34/91/91/110	-
9	UQ5	C	403	-	-	11/33/57/57	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	3PH	C	405	12	-	17/34/34/49	-
12	CDL	C	408	-	-	47/91/91/110	-
14	FES	N	301	2	-	-	0/1/1/1
12	CDL	O	402	-	-	33/98/98/110	-
14	FES	D	301	2	-	-	0/1/1/1
12	CDL	M	408	-	-	42/87/87/110	-
15	PTY	T	103	-	-	17/32/32/53	-
11	PGT	C	406	-	-	12/45/45/55	-
13	PC7	M	409	-	-	19/45/45/55	-
10	3PH	T	102	-	-	13/49/49/49	-
13	PC7	D	302	-	-	15/37/37/55	-
10	3PH	I	101	-	-	15/33/33/49	-
8	HEM	C	402	1	-	6/14/54/54	-
13	PC7	N	303	-	-	10/42/42/55	-
10	3PH	T	101	-	-	14/42/42/49	-
12	CDL	C	409	10	-	40/95/95/110	-
17	Q7G	M	410	-	-	3/12/100/200	0/6/6/10
16	UQ7	M	404	-	-	19/45/69/69	0/1/1/1
12	CDL	Q	101	-	-	37/80/80/110	-
10	3PH	G	101	-	-	16/34/34/49	-
11	PGT	C	407	-	-	22/55/55/55	-
8	HEM	E	400	3	-	2/14/54/54	-
8	HEM	M	402	1	-	4/14/54/54	-
8	HEM	O	401	3	-	4/14/54/54	-
12	CDL	G	103	-	-	30/95/95/110	-
9	UQ5	M	403	-	-	9/33/57/57	0/1/1/1
17	Q7G	M	411	-	-	0/12/100/200	0/6/6/10
8	HEM	M	401	1	-	2/14/54/54	-
13	PC7	G	104	-	-	21/55/55/55	-
15	PTY	J	101	-	-	5/44/44/53	-

All (171) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	402	HEM	FE-NB	7.17	2.17	1.94
8	M	402	HEM	C1B-NB	-6.33	1.29	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	402	HEM	FE-NB	6.13	2.13	1.94
8	C	402	HEM	FE-NC	5.81	2.14	1.95
8	O	401	HEM	C1B-NB	-5.52	1.30	1.40
8	M	401	HEM	FE-NC	5.30	2.12	1.95
8	O	401	HEM	FE-NB	5.19	2.10	1.94
8	M	401	HEM	FE-NB	5.03	2.10	1.94
8	M	402	HEM	FE-NC	4.84	2.11	1.95
8	M	401	HEM	C1B-NB	-4.78	1.32	1.40
8	O	401	HEM	FE-NC	4.32	2.09	1.95
8	C	402	HEM	C1B-NB	-4.08	1.33	1.40
8	C	401	HEM	FE-ND	4.04	2.07	1.94
8	M	401	HEM	C4D-ND	-3.96	1.33	1.40
8	M	402	HEM	C4D-ND	-3.93	1.33	1.40
8	C	401	HEM	FE-NB	3.92	2.07	1.94
8	O	401	HEM	C4B-NB	-3.91	1.31	1.38
8	C	402	HEM	C4D-ND	-3.87	1.33	1.40
8	E	400	HEM	FE-NA	3.84	2.07	1.95
8	M	402	HEM	C4B-NB	-3.83	1.31	1.38
8	O	401	HEM	C4D-ND	-3.62	1.34	1.40
8	C	402	HEM	C4B-NB	-3.60	1.31	1.38
8	E	400	HEM	FE-NC	3.52	2.06	1.95
8	O	401	HEM	C1C-C2C	-3.49	1.38	1.45
8	M	401	HEM	O2A-CGA	-3.42	1.19	1.30
8	M	402	HEM	C1D-ND	-3.35	1.32	1.38
10	T	102	3PH	P-O11	3.33	1.70	1.60
9	C	403	UQ5	C3-C2	-3.31	1.39	1.48
10	M	405	3PH	P-O11	3.31	1.70	1.60
10	G	101	3PH	P-O11	3.31	1.70	1.60
10	T	101	3PH	P-O11	3.30	1.70	1.60
10	I	101	3PH	P-O11	3.29	1.70	1.60
10	C	405	3PH	P-O11	3.28	1.70	1.60
11	G	102	PGT	O3-C11	3.17	1.42	1.33
8	E	400	HEM	CAC-C3C	3.10	1.55	1.47
11	C	407	PGT	O3-C11	3.10	1.42	1.33
8	C	401	HEM	CAC-C3C	3.08	1.55	1.47
11	M	406	PGT	O3-C11	3.08	1.42	1.33
8	C	401	HEM	CAB-C3B	3.06	1.55	1.47
8	C	402	HEM	C1C-NC	-3.06	1.33	1.39
8	O	401	HEM	O2A-CGA	-3.06	1.20	1.30
11	C	407	PGT	O2-C31	3.05	1.42	1.34
8	M	401	HEM	C1C-C2C	-3.05	1.39	1.45
8	C	402	HEM	O2D-CGD	-3.02	1.20	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	M	406	PGT	O2-C31	3.01	1.42	1.34
8	O	401	HEM	C1D-ND	-2.98	1.33	1.38
8	O	401	HEM	C3C-C4C	-2.96	1.40	1.46
12	M	408	CDL	OA6-CA4	-2.95	1.39	1.46
8	M	401	HEM	C3C-C4C	-2.92	1.40	1.46
8	M	402	HEM	O2A-CGA	-2.91	1.21	1.30
8	E	400	HEM	CAB-C3B	2.90	1.55	1.47
11	G	102	PGT	O2-C31	2.89	1.42	1.34
12	Q	101	CDL	OA6-CA4	-2.89	1.39	1.46
8	M	401	HEM	C1D-ND	-2.86	1.33	1.38
8	E	400	HEM	FE-ND	2.85	2.03	1.94
13	C	410	PC7	O2-C2	-2.84	1.39	1.46
8	C	402	HEM	C1D-ND	-2.83	1.33	1.38
8	C	401	HEM	FE-NC	2.81	2.04	1.95
12	G	103	CDL	OB6-CB4	-2.80	1.40	1.46
13	G	104	PC7	O2-C2	-2.77	1.40	1.46
8	M	401	HEM	C1C-NC	-2.77	1.34	1.39
8	C	401	HEM	FE-NA	2.76	2.04	1.95
8	O	401	HEM	C1A-C2A	-2.76	1.39	1.44
13	D	302	PC7	O2-C2	-2.75	1.40	1.46
12	G	103	CDL	OA6-CA4	-2.74	1.40	1.46
12	O	402	CDL	OB6-CB4	-2.74	1.40	1.46
12	Q	101	CDL	OB6-CB4	-2.74	1.40	1.46
8	C	402	HEM	O2A-CGA	-2.72	1.21	1.30
8	M	401	HEM	C1A-C2A	-2.70	1.39	1.44
12	C	409	CDL	OA6-CA4	-2.69	1.40	1.46
8	E	400	HEM	FE-NB	2.68	2.03	1.94
15	M	407	PTY	O7-C6	-2.67	1.40	1.46
8	O	401	HEM	C4A-NA	-2.66	1.34	1.39
15	T	103	PTY	O7-C6	-2.65	1.40	1.46
12	N	302	CDL	OB6-CB4	-2.64	1.40	1.46
13	M	409	PC7	O2-C2	-2.63	1.40	1.46
8	O	401	HEM	FE-ND	-2.60	1.86	1.94
17	M	411	Q7G	C11-C08	-2.59	1.51	1.56
12	N	302	CDL	OA6-CA4	-2.58	1.40	1.46
9	C	403	UQ5	C4-C5	-2.58	1.41	1.48
8	M	401	HEM	O2D-CGD	-2.56	1.22	1.30
8	O	401	HEM	O2D-CGD	-2.55	1.22	1.30
8	M	402	HEM	C1A-C2A	-2.55	1.39	1.44
8	M	401	HEM	C4B-NB	-2.52	1.33	1.38
8	C	402	HEM	C1C-C2C	-2.52	1.40	1.45
12	N	302	CDL	OA8-CA7	2.49	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	Q	101	CDL	OA8-CA7	2.49	1.40	1.33
12	G	103	CDL	OA8-CA7	2.49	1.40	1.33
12	M	408	CDL	OB8-CB7	2.48	1.40	1.33
12	C	409	CDL	OA8-CA7	2.48	1.40	1.33
8	M	401	HEM	C4C-NC	-2.48	1.35	1.39
12	M	408	CDL	OA8-CA7	2.46	1.40	1.33
12	G	103	CDL	OB8-CB7	2.46	1.40	1.33
12	Q	101	CDL	OB8-CB7	2.46	1.40	1.33
12	C	409	CDL	OB6-CB4	-2.46	1.40	1.46
8	M	402	HEM	O2D-CGD	-2.43	1.22	1.30
16	M	404	UQ7	C3-C4	-2.43	1.41	1.48
12	O	402	CDL	OA8-CA7	2.43	1.40	1.33
8	M	401	HEM	C3D-C2D	-2.42	1.31	1.36
12	C	409	CDL	OB8-CB7	2.42	1.40	1.33
12	O	402	CDL	OB8-CB7	2.41	1.40	1.33
8	O	401	HEM	C4C-NC	-2.40	1.35	1.39
17	M	410	Q7G	C11-C08	-2.39	1.52	1.56
8	M	401	HEM	C4A-NA	-2.38	1.35	1.39
12	N	302	CDL	OB8-CB7	2.38	1.40	1.33
13	G	104	PC7	O3-C11	2.38	1.40	1.33
13	D	302	PC7	O3-C11	2.37	1.40	1.33
8	C	402	HEM	C4A-NA	-2.36	1.35	1.39
12	M	408	CDL	OB6-CB5	2.36	1.40	1.34
15	T	103	PTY	O4-C30	2.35	1.40	1.33
15	M	407	PTY	O4-C30	2.35	1.40	1.33
8	C	402	HEM	C4C-NC	-2.34	1.35	1.39
11	C	407	PGT	P-O3P	2.34	1.68	1.59
12	O	402	CDL	OA6-CA5	2.32	1.40	1.34
13	M	409	PC7	O3-C3	-2.32	1.40	1.45
12	M	408	CDL	OB6-CB4	-2.31	1.41	1.46
11	M	406	PGT	P-O3P	2.30	1.68	1.59
12	O	402	CDL	OA6-CA4	-2.30	1.41	1.46
13	D	302	PC7	O3-C3	-2.30	1.40	1.45
13	C	410	PC7	O3-C3	-2.29	1.40	1.45
8	M	402	HEM	C3C-C4C	-2.28	1.42	1.46
15	T	103	PTY	O4-C1	-2.26	1.40	1.45
13	M	409	PC7	O3-C11	2.25	1.39	1.33
13	C	410	PC7	O3-C11	2.25	1.39	1.33
11	G	102	PGT	P-O3P	2.24	1.68	1.59
8	O	401	HEM	C1C-NC	-2.23	1.35	1.39
13	G	104	PC7	O3-C3	-2.23	1.40	1.45
12	O	402	CDL	OA8-CA6	-2.22	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	409	CDL	OB6-CB5	2.21	1.40	1.34
12	N	302	CDL	OA6-CA5	2.20	1.40	1.34
12	M	408	CDL	OB8-CB6	-2.20	1.40	1.45
8	M	402	HEM	C4A-NA	-2.19	1.35	1.39
13	M	409	PC7	O2-C31	2.19	1.40	1.34
8	C	401	HEM	CMB-C2B	2.19	1.55	1.50
12	Q	101	CDL	OA8-CA6	-2.18	1.40	1.45
12	N	302	CDL	OB8-CB6	-2.18	1.40	1.45
15	M	407	PTY	O4-C1	-2.17	1.40	1.45
15	M	407	PTY	O7-C8	2.17	1.40	1.34
12	G	103	CDL	OA8-CA6	-2.17	1.40	1.45
12	O	402	CDL	OB8-CB6	-2.17	1.40	1.45
12	G	103	CDL	OB8-CB6	-2.17	1.40	1.45
15	T	103	PTY	O7-C8	2.17	1.40	1.34
8	M	401	HEM	C1B-C2B	-2.16	1.40	1.44
12	Q	101	CDL	OB8-CB6	-2.16	1.40	1.45
8	M	402	HEM	C1C-C2C	-2.15	1.41	1.45
8	C	402	HEM	FE-NA	2.15	2.02	1.95
12	G	103	CDL	OA6-CA5	2.15	1.40	1.34
16	M	404	UQ7	C2-C1	-2.14	1.42	1.48
8	M	401	HEM	C4A-C3A	-2.14	1.38	1.43
12	C	409	CDL	OA6-CA5	2.13	1.40	1.34
12	Q	101	CDL	OA6-CA5	2.13	1.40	1.34
8	M	401	HEM	C1A-NA	-2.12	1.35	1.39
12	O	402	CDL	OB6-CB5	2.11	1.40	1.34
13	G	104	PC7	O2-C31	2.11	1.40	1.34
12	Q	101	CDL	OB6-CB5	2.11	1.40	1.34
12	G	103	CDL	OB6-CB5	2.10	1.40	1.34
12	N	302	CDL	OB6-CB5	2.10	1.40	1.34
12	C	409	CDL	OA8-CA6	-2.09	1.40	1.45
13	C	410	PC7	O2-C31	2.09	1.40	1.34
8	O	401	HEM	C1B-C2B	-2.08	1.40	1.44
12	N	302	CDL	OA8-CA6	-2.07	1.40	1.45
11	M	406	PGT	O2-C2	-2.06	1.41	1.46
8	C	401	HEM	CMA-C3A	2.05	1.55	1.50
12	M	408	CDL	OA8-CA6	-2.05	1.40	1.45
8	M	402	HEM	C3B-C4B	2.05	1.48	1.44
11	G	102	PGT	O2-C2	-2.05	1.41	1.46
13	D	302	PC7	O2-C31	2.05	1.40	1.34
12	M	408	CDL	OA6-CA5	2.03	1.40	1.34
12	C	409	CDL	OB8-CB6	-2.02	1.40	1.45
11	C	407	PGT	O2-C2	-2.02	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	E	400	HEM	CMC-C2C	2.01	1.54	1.50

All (164) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	O	401	HEM	CHC-C4B-NB	8.02	133.06	124.42
8	M	402	HEM	C1B-NB-C4B	5.26	111.44	105.21
8	O	401	HEM	CHD-C1D-ND	5.22	130.04	124.42
8	C	402	HEM	C1B-NB-C4B	5.21	111.38	105.21
8	O	401	HEM	C1B-NB-C4B	4.81	110.91	105.21
8	C	402	HEM	C3B-C4B-NB	-4.72	106.08	109.47
8	M	402	HEM	CHC-C4B-NB	4.71	129.49	124.42
8	C	402	HEM	CHC-C4B-NB	4.69	129.47	124.42
8	O	401	HEM	O2A-CGA-O1A	-4.61	111.48	123.33
12	C	409	CDL	OB6-CB5-C51	4.53	121.29	111.48
13	M	409	PC7	O2-C31-C32	4.47	121.16	111.48
13	C	410	PC7	O2-C31-C32	4.34	120.88	111.48
12	G	103	CDL	OA6-CA5-C11	4.30	120.78	111.48
12	O	402	CDL	OA6-CA5-C11	4.29	120.76	111.48
12	N	302	CDL	OB6-CB5-C51	4.29	120.75	111.48
12	N	302	CDL	OA6-CA5-C11	4.20	120.57	111.48
8	M	401	HEM	CHC-C4B-NB	4.18	128.93	124.42
12	M	408	CDL	OB6-CB5-C51	4.11	120.37	111.48
11	M	406	PGT	O2-C31-C32	4.04	120.22	111.48
15	T	103	PTY	O7-C8-C11	4.00	120.13	111.48
12	Q	101	CDL	OA6-CA5-C11	3.96	120.04	111.48
11	C	407	PGT	O2-C31-C32	3.91	119.95	111.48
12	C	409	CDL	OA6-CA5-C11	3.91	119.94	111.48
12	O	402	CDL	OB6-CB5-C51	3.89	119.90	111.48
12	G	103	CDL	OB6-CB5-C51	3.88	119.89	111.48
12	Q	101	CDL	OB6-CB5-C51	3.87	119.85	111.48
11	G	102	PGT	O2-C31-C32	3.84	119.78	111.48
8	M	401	HEM	C1B-NB-C4B	3.84	109.75	105.21
13	G	104	PC7	O2-C31-C32	3.82	119.74	111.48
15	M	407	PTY	O7-C8-C11	3.82	119.74	111.48
13	D	302	PC7	O2-C31-C32	3.74	119.57	111.48
9	C	404	UQ5	C7-C6-C5	-3.73	114.18	118.52
8	M	402	HEM	CHA-C4D-ND	3.71	128.96	124.37
17	M	410	Q7G	C02-C06-C07	-3.68	109.19	114.41
8	O	401	HEM	C3B-C4B-NB	-3.65	106.85	109.47
12	M	408	CDL	OA6-CA5-C11	3.59	119.26	111.48
8	M	401	HEM	O2A-CGA-O1A	-3.48	114.38	123.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	401	HEM	CHD-C1D-ND	3.44	128.13	124.42
17	M	411	Q7G	C12-C11-C08	-3.43	107.81	111.66
8	M	401	HEM	CMD-C2D-C1D	3.36	130.28	125.03
9	C	403	UQ5	C7-C6-C1	-3.26	119.31	124.89
8	O	401	HEM	CHD-C1D-C2D	-3.21	119.95	125.03
8	C	402	HEM	O2D-CGD-O1D	-3.20	115.11	123.33
8	O	401	HEM	O2A-CGA-CBA	3.15	123.96	114.00
17	M	410	Q7G	C02-C03-C74	-3.14	111.21	120.50
8	M	401	HEM	C2A-C1A-NA	-3.12	106.69	110.15
8	M	402	HEM	O2D-CGD-O1D	-3.12	115.31	123.33
17	M	410	Q7G	C17-C16-C13	-3.08	106.90	111.45
8	M	402	HEM	C4D-ND-C1D	3.03	108.80	105.21
8	M	402	HEM	CHD-C1D-ND	3.03	127.68	124.42
17	M	411	Q7G	C76-C73-C74	-3.02	110.19	115.66
13	M	409	PC7	O3-C11-C12	3.02	121.03	111.83
17	M	410	Q7G	C12-C11-C08	-3.02	108.28	111.66
11	G	102	PGT	O3-C11-C12	2.97	120.90	111.83
8	O	401	HEM	CHA-C4D-ND	2.97	128.03	124.37
8	M	401	HEM	CHA-C4D-ND	2.93	127.99	124.37
8	C	402	HEM	CHA-C4D-ND	2.89	127.94	124.37
17	M	411	Q7G	C77-C76-C73	-2.86	107.45	111.93
8	M	401	HEM	C3B-C4B-NB	-2.83	107.43	109.47
17	M	410	Q7G	C76-C73-C74	-2.81	110.57	115.66
8	C	401	HEM	C4D-ND-C1D	2.80	108.52	105.21
8	O	401	HEM	O2D-CGD-O1D	-2.79	116.16	123.33
12	M	408	CDL	OA8-CA7-C31	2.75	120.20	111.83
8	C	402	HEM	CHD-C1D-ND	2.74	127.37	124.42
8	C	401	HEM	C1B-NB-C4B	2.74	108.45	105.21
12	N	302	CDL	OB8-CB7-C71	2.73	120.16	111.83
13	D	302	PC7	O3-C11-C12	2.73	120.15	111.83
12	G	103	CDL	OA8-CA7-C31	2.72	120.14	111.83
8	M	402	HEM	O2D-CGD-CBD	2.72	122.60	114.00
13	C	410	PC7	O3-C11-C12	2.71	120.11	111.83
12	G	103	CDL	OB8-CB7-C71	2.71	120.10	111.83
12	C	409	CDL	OA8-CA7-C31	2.71	120.10	111.83
8	M	401	HEM	O2D-CGD-CBD	2.68	122.48	114.00
12	O	402	CDL	OA8-CA7-C31	2.66	119.95	111.83
11	C	407	PGT	O3-C11-C12	2.64	119.89	111.83
12	Q	101	CDL	OB8-CB7-C71	2.63	119.85	111.83
15	M	407	PTY	O4-C30-C31	2.63	119.84	111.83
12	N	302	CDL	OA8-CA7-C31	2.61	119.79	111.83
12	Q	101	CDL	OA8-CA7-C31	2.61	119.79	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	401	HEM	CHB-C1B-NB	2.60	127.59	124.37
8	O	401	HEM	C1A-CHA-C4D	-2.60	120.14	126.25
13	G	104	PC7	O3-C11-C12	2.59	119.74	111.83
12	M	408	CDL	OB8-CB7-C71	2.59	119.73	111.83
8	M	402	HEM	O2A-CGA-O1A	-2.58	116.70	123.33
11	M	406	PGT	O3-C11-C12	2.58	119.69	111.83
8	M	401	HEM	CBD-CAD-C3D	-2.57	105.43	112.53
17	M	411	Q7G	C75-C74-C03	-2.56	109.38	114.50
15	T	103	PTY	O4-C30-C31	2.56	119.64	111.83
12	O	402	CDL	OB8-CB7-C71	2.55	119.62	111.83
8	M	402	HEM	C4B-C3B-C2B	-2.55	104.94	107.28
8	E	400	HEM	CAA-CBA-CGA	-2.54	106.92	113.67
8	O	401	HEM	CHA-C1A-NA	2.51	128.41	123.86
8	O	401	HEM	CHC-C4B-C3B	-2.50	120.08	125.07
8	C	401	HEM	C2A-C1A-NA	-2.48	107.40	110.15
17	M	411	Q7G	C09-C10-C02	-2.48	108.56	112.74
8	M	401	HEM	CHD-C1D-C2D	-2.47	121.13	125.03
8	C	402	HEM	C4C-NC-C1C	2.46	109.83	105.82
12	C	409	CDL	OB8-CB7-C71	2.45	119.31	111.83
8	M	402	HEM	CBD-CAD-C3D	-2.45	105.76	112.53
17	M	410	Q7G	C19-C11-C08	2.44	111.96	108.74
8	C	402	HEM	CBD-CAD-C3D	-2.42	105.84	112.53
8	M	402	HEM	C3B-C4B-NB	-2.40	107.74	109.47
8	M	401	HEM	O2A-CGA-CBA	2.40	121.57	114.00
8	E	400	HEM	C1B-NB-C4B	2.40	108.04	105.21
17	M	411	Q7G	C02-C03-C74	-2.38	113.47	120.50
8	E	400	HEM	C3B-C2B-C1B	2.37	108.19	106.41
8	M	401	HEM	O2D-CGD-O1D	-2.37	117.23	123.33
17	M	411	Q7G	C08-C07-C06	-2.37	105.99	109.09
12	C	408	CDL	OB6-CB4-CB3	2.37	116.83	108.34
12	Q	101	CDL	CA4-OA6-CA5	-2.36	112.14	117.80
10	M	405	3PH	O13-P-O11	-2.34	100.56	106.67
10	C	405	3PH	O13-P-O11	-2.33	100.58	106.67
17	M	410	Q7G	C11-C08-C07	-2.33	109.30	112.71
12	C	408	CDL	OB6-CB5-C51	2.32	116.50	111.48
16	M	404	UQ7	C7-C6-C5	-2.31	120.93	124.89
17	M	410	Q7G	C09-C10-C02	-2.30	108.86	112.74
8	E	400	HEM	C4D-ND-C1D	2.29	107.92	105.21
16	M	404	UQ7	C17-C16-C14	2.29	120.78	113.19
17	M	411	Q7G	C02-C06-C07	-2.29	111.17	114.41
17	M	410	Q7G	C75-C74-C03	-2.29	109.93	114.50
8	E	400	HEM	C3D-C4D-ND	-2.26	107.69	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	401	HEM	CHD-C4C-NC	2.26	126.91	124.45
8	O	401	HEM	CHD-C4C-NC	2.26	126.91	124.45
17	M	410	Q7G	C75-C74-C73	-2.25	111.30	114.94
17	M	411	Q7G	C19-C11-C08	2.25	111.71	108.74
8	M	401	HEM	CHA-C1A-NA	2.24	127.93	123.86
8	O	401	HEM	CHB-C1B-NB	2.24	127.14	124.37
8	O	401	HEM	C1C-CHC-C4B	-2.22	121.29	126.02
8	C	401	HEM	C3D-C4D-ND	-2.21	107.75	110.17
8	M	401	HEM	C4A-NA-C1A	2.20	109.40	105.82
10	I	101	3PH	O13-P-O11	-2.20	100.94	106.67
10	T	101	3PH	O13-P-O11	-2.19	100.96	106.67
8	C	402	HEM	CHB-C1B-NB	2.19	127.07	124.37
8	M	402	HEM	O2A-CGA-CBA	2.17	120.86	114.00
8	M	401	HEM	C4B-C3B-C2B	-2.16	105.29	107.28
17	M	411	Q7G	C15-C14-C13	-2.15	121.39	125.02
8	M	401	HEM	C4C-NC-C1C	2.14	109.32	105.82
10	T	102	3PH	O13-P-O11	-2.14	101.08	106.67
13	N	303	PC7	O2-C2-C1	2.13	115.99	108.34
8	O	401	HEM	C4D-ND-C1D	2.13	107.73	105.21
8	M	402	HEM	CAA-C2A-C1A	2.13	129.09	124.94
10	G	101	3PH	O13-P-O11	-2.12	101.13	106.67
8	E	400	HEM	C2A-C1A-NA	-2.12	107.80	110.15
8	O	401	HEM	CBD-CAD-C3D	-2.12	106.68	112.53
9	M	403	UQ5	C6-C1-C2	2.11	120.84	119.17
17	M	410	Q7G	C09-C08-C11	-2.11	110.48	113.08
8	C	402	HEM	C2A-C1A-NA	-2.11	107.81	110.15
17	M	410	Q7G	C07-C15-C14	-2.10	109.86	112.76
9	C	404	UQ5	C12-C13-C14	2.09	132.41	127.62
8	O	401	HEM	C2A-C1A-NA	-2.09	107.83	110.15
8	O	401	HEM	CBA-CAA-C2A	2.09	118.30	112.53
17	M	411	Q7G	C19-C18-C17	2.08	113.73	110.33
8	E	400	HEM	CBD-CAD-C3D	-2.08	106.79	112.53
10	I	101	3PH	C3-C2-C1	2.08	116.62	111.78
8	M	401	HEM	CAD-C3D-C4D	2.07	128.31	124.70
8	M	402	HEM	CHA-C4D-C3D	-2.07	121.40	125.23
8	O	401	HEM	CAA-CBA-CGA	-2.07	108.18	113.67
8	E	400	HEM	CHC-C4B-NB	2.07	126.65	124.42
13	C	410	PC7	O2-C31-O31	-2.06	118.88	123.70
13	M	409	PC7	O2-C31-O31	-2.03	118.95	123.70
8	M	402	HEM	CMC-C2C-C1C	2.02	128.28	124.73
8	M	402	HEM	C4C-NC-C1C	2.01	109.10	105.82
8	C	401	HEM	C3B-C4B-NB	-2.01	108.03	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	402	HEM	C4A-NA-C1A	2.01	109.10	105.82

There are no chirality outliers.

All (648) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	M	402	HEM	C2C-C3C-CAC-CBC
9	C	403	UQ5	C17-C18-C19-C20
9	C	403	UQ5	C17-C18-C19-C21
10	C	405	3PH	C1-O11-P-O13
10	C	405	3PH	C1-O11-P-O14
10	C	405	3PH	C22-C21-O21-C2
10	G	101	3PH	C1-O11-P-O13
10	G	101	3PH	C1-O11-P-O14
10	G	101	3PH	C2-C1-O11-P
10	I	101	3PH	C1-O11-P-O13
10	I	101	3PH	C1-O11-P-O14
10	I	101	3PH	C32-C31-O31-C3
10	T	101	3PH	C1-O11-P-O13
11	C	406	PGT	C1-O3P-P-O1P
11	C	407	PGT	C32-C31-O2-C2
11	C	407	PGT	C4-C5-C6-O6
11	G	102	PGT	C1-O3P-P-O2P
11	G	102	PGT	C1-O3P-P-O4P
11	G	102	PGT	C4-O4P-P-O2P
11	M	406	PGT	C32-C31-O2-C2
11	M	406	PGT	O2-C2-C3-O3
11	M	406	PGT	C2-C1-O3P-P
11	M	406	PGT	C1-O3P-P-O1P
11	M	406	PGT	C1-O3P-P-O2P
11	M	406	PGT	C1-O3P-P-O4P
12	C	408	CDL	CA2-OA2-PA1-OA4
12	C	408	CDL	CA2-OA2-PA1-OA5
12	C	408	CDL	CA3-OA5-PA1-OA2
12	C	408	CDL	CB2-OB2-PB2-OB4
12	C	408	CDL	C51-CB5-OB6-CB4
12	C	409	CDL	CA2-OA2-PA1-OA3
12	G	103	CDL	OA7-CA5-OA6-CA4
12	G	103	CDL	C11-CA5-OA6-CA4
12	G	103	CDL	CB3-OB5-PB2-OB2
12	G	103	CDL	CB3-OB5-PB2-OB4
12	M	408	CDL	C11-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
12	M	408	CDL	CB2-OB2-PB2-OB4
12	M	408	CDL	CB2-OB2-PB2-OB5
12	M	408	CDL	C51-CB5-OB6-CB4
12	N	302	CDL	OA7-CA5-OA6-CA4
12	N	302	CDL	C11-CA5-OA6-CA4
12	N	302	CDL	OB5-CB3-CB4-OB6
12	O	402	CDL	CA6-CA4-OA6-CA5
12	O	402	CDL	C11-CA5-OA6-CA4
12	O	402	CDL	CB3-OB5-PB2-OB2
12	O	402	CDL	CB3-OB5-PB2-OB3
12	O	402	CDL	CB3-OB5-PB2-OB4
12	Q	101	CDL	CA3-OA5-PA1-OA3
12	Q	101	CDL	CA3-OA5-PA1-OA4
12	Q	101	CDL	C11-CA5-OA6-CA4
12	Q	101	CDL	CB2-OB2-PB2-OB5
12	Q	101	CDL	CB4-CB3-OB5-PB2
13	C	410	PC7	C32-C31-O2-C2
13	C	410	PC7	O31-C31-O2-C2
13	D	302	PC7	O31-C31-O2-C2
13	D	302	PC7	C4-O4P-P-O3P
13	G	104	PC7	C32-C31-O2-C2
13	M	409	PC7	C32-C31-O2-C2
13	M	409	PC7	O2-C2-C3-O3
13	M	409	PC7	C1-O3P-P-O1P
13	M	409	PC7	C1-O3P-P-O4P
13	M	409	PC7	C21-C22-C23-C24
13	N	303	PC7	C32-C31-O2-C2
15	J	101	PTY	C11-C8-O7-C6
15	M	407	PTY	N1-C2-C3-O11
15	M	407	PTY	C3-O11-P1-O12
15	M	407	PTY	C3-O11-P1-O14
15	T	103	PTY	N1-C2-C3-O11
16	M	404	UQ7	C17-C18-C19-C20
16	M	404	UQ7	C17-C18-C19-C21
10	I	101	3PH	O32-C31-O31-C3
12	C	409	CDL	OB9-CB7-OB8-CB6
13	N	303	PC7	O11-C11-O3-C3
15	T	103	PTY	O30-C30-O4-C1
11	C	406	PGT	C12-C11-O3-C3
12	C	409	CDL	C71-CB7-OB8-CB6
13	N	303	PC7	C12-C11-O3-C3
15	T	103	PTY	C31-C30-O4-C1

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Mol	Chain	Res	Type	Atoms
10	M	405	3PH	O32-C31-O31-C3
10	T	101	3PH	O32-C31-O31-C3
11	C	406	PGT	O11-C11-O3-C3
11	G	102	PGT	O11-C11-O3-C3
12	G	103	CDL	OA9-CA7-OA8-CA6
12	Q	101	CDL	OB9-CB7-OB8-CB6
12	G	103	CDL	OB9-CB7-OB8-CB6
10	C	405	3PH	O22-C21-O21-C2
11	C	407	PGT	O31-C31-O2-C2
12	C	408	CDL	OA7-CA5-OA6-CA4
12	C	408	CDL	OB7-CB5-OB6-CB4
12	M	408	CDL	OA7-CA5-OA6-CA4
12	M	408	CDL	OB7-CB5-OB6-CB4
12	Q	101	CDL	OA7-CA5-OA6-CA4
13	G	104	PC7	O31-C31-O2-C2
13	M	409	PC7	O31-C31-O2-C2
13	N	303	PC7	O31-C31-O2-C2
15	J	101	PTY	O10-C8-O7-C6
10	T	101	3PH	C32-C31-O31-C3
12	Q	101	CDL	C71-CB7-OB8-CB6
13	D	302	PC7	C32-C31-O2-C2
16	M	404	UQ7	C20-C19-C21-C22
16	M	404	UQ7	C18-C19-C21-C22
10	M	405	3PH	C32-C31-O31-C3
11	G	102	PGT	C12-C11-O3-C3
12	G	103	CDL	C31-CA7-OA8-CA6
12	G	103	CDL	C71-CB7-OB8-CB6
11	M	406	PGT	O31-C31-O2-C2
12	O	402	CDL	OA7-CA5-OA6-CA4
12	O	402	CDL	O1-C1-CA2-OA2
12	Q	101	CDL	O1-C1-CA2-OA2
12	C	408	CDL	C11-CA5-OA6-CA4
9	C	403	UQ5	C12-C11-C9-C10
16	M	404	UQ7	C25-C24-C26-C27
9	C	403	UQ5	C12-C11-C9-C8
16	M	404	UQ7	C23-C24-C26-C27
9	C	404	UQ5	C14-C16-C17-C18
9	C	404	UQ5	C19-C21-C22-C23
9	C	404	UQ5	C24-C26-C27-C28
9	M	403	UQ5	C9-C11-C12-C13
9	M	403	UQ5	C19-C21-C22-C23
12	C	408	CDL	C1-CB2-OB2-PB2

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Mol	Chain	Res	Type	Atoms
12	Q	101	CDL	CB2-C1-CA2-OA2
12	C	408	CDL	C71-CB7-OB8-CB6
12	M	408	CDL	C31-CA7-OA8-CA6
9	M	403	UQ5	C25-C24-C26-C27
16	M	404	UQ7	C15-C14-C16-C17
9	M	403	UQ5	C23-C24-C26-C27
16	M	404	UQ7	C13-C14-C16-C17
12	C	409	CDL	C11-C12-C13-C14
15	T	103	PTY	C11-C8-O7-C6
12	M	408	CDL	OB6-CB4-CB6-OB8
12	C	409	CDL	C31-CA7-OA8-CA6
9	C	403	UQ5	C12-C13-C14-C15
11	C	407	PGT	O5-C5-C6-O6
12	C	408	CDL	C31-CA7-OA8-CA6
10	M	405	3PH	C21-C22-C23-C24
12	M	408	CDL	C51-C52-C53-C54
16	M	404	UQ7	C29-C31-C32-C33
11	C	406	PGT	C40-C41-C42-C43
10	T	102	3PH	C31-C32-C33-C34
12	C	408	CDL	CA5-C11-C12-C13
12	M	408	CDL	CB5-C51-C52-C53
10	C	405	3PH	C21-C22-C23-C24
10	T	101	3PH	C21-C22-C23-C24
12	Q	101	CDL	C40-C41-C42-C43
12	Q	101	CDL	C31-CA7-OA8-CA6
12	C	408	CDL	OB9-CB7-OB8-CB6
12	M	408	CDL	OA9-CA7-OA8-CA6
13	N	303	PC7	C11-C12-C13-C14
11	C	406	PGT	C32-C31-O2-C2
12	C	409	CDL	OA9-CA7-OA8-CA6
15	T	103	PTY	O10-C8-O7-C6
11	G	102	PGT	O4P-C4-C5-C6
12	O	402	CDL	CB2-C1-CA2-OA2
12	C	408	CDL	C16-C17-C18-C19
9	M	403	UQ5	C12-C11-C9-C10
12	C	409	CDL	C11-CA5-OA6-CA4
12	C	409	CDL	OA7-CA5-OA6-CA4
9	M	403	UQ5	C14-C16-C17-C18
9	M	403	UQ5	C24-C26-C27-C28
11	C	407	PGT	O4P-C4-C5-O5
11	G	102	PGT	O4P-C4-C5-O5
12	Q	101	CDL	OA9-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
11	G	102	PGT	C4-C5-C6-O6
10	C	405	3PH	C3-C2-O21-C21
12	M	408	CDL	CB3-CB4-OB6-CB5
12	N	302	CDL	C56-C57-C58-C59
12	C	408	CDL	OA9-CA7-OA8-CA6
11	C	406	PGT	O31-C31-O2-C2
11	G	102	PGT	C2-C3-O3-C11
12	N	302	CDL	C51-CB5-OB6-CB4
13	M	409	PC7	C4-C5-N-C7
11	C	407	PGT	C15-C16-C17-C18
12	C	409	CDL	C37-C38-C39-C40
15	M	407	PTY	C34-C35-C36-C37
11	M	406	PGT	C15-C16-C17-C18
12	O	402	CDL	C15-C16-C17-C18
13	C	410	PC7	C32-C33-C34-C35
11	G	102	PGT	C42-C43-C44-C45
12	C	409	CDL	C31-C32-C33-C34
12	N	302	CDL	C59-C60-C61-C62
10	I	101	3PH	C33-C34-C35-C36
11	C	407	PGT	C40-C41-C42-C43
11	G	102	PGT	O5-C5-C6-O6
12	O	402	CDL	C12-C13-C14-C15
13	G	104	PC7	C21-C22-C23-C24
12	M	408	CDL	C73-C74-C75-C76
12	C	409	CDL	C58-C59-C60-C61
12	M	408	CDL	C56-C57-C58-C59
10	G	101	3PH	C24-C25-C26-C27
10	I	101	3PH	C22-C23-C24-C25
12	C	408	CDL	C54-C55-C56-C57
13	G	104	PC7	C39-C40-C41-C42
12	Q	101	CDL	CB7-C71-C72-C73
12	N	302	CDL	C71-CB7-OB8-CB6
10	I	101	3PH	C38-C39-C3A-C3B
10	T	101	3PH	C22-C23-C24-C25
11	C	407	PGT	C18-C19-C20-C21
11	G	102	PGT	C37-C38-C39-C40
10	I	101	3PH	C36-C37-C38-C39
11	C	407	PGT	O4P-C4-C5-C6
12	M	408	CDL	CA7-C31-C32-C33
12	O	402	CDL	CB7-C71-C72-C73
11	G	102	PGT	C16-C17-C18-C19
12	C	409	CDL	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
12	G	103	CDL	C20-C21-C22-C23
12	O	402	CDL	C19-C20-C21-C22
13	C	410	PC7	C16-C17-C18-C19
12	M	408	CDL	C11-C12-C13-C14
11	M	406	PGT	C17-C18-C19-C20
12	C	409	CDL	C19-C20-C21-C22
11	G	102	PGT	C40-C41-C42-C43
12	C	409	CDL	CA7-C31-C32-C33
12	G	103	CDL	CB7-C71-C72-C73
11	C	407	PGT	C13-C14-C15-C16
12	C	408	CDL	C76-C77-C78-C79
13	M	409	PC7	C14-C15-C16-C17
12	C	408	CDL	C57-C58-C59-C60
12	C	408	CDL	C83-C84-C85-C86
12	N	302	CDL	OB7-CB5-OB6-CB4
12	G	103	CDL	C36-C37-C38-C39
16	M	404	UQ7	C12-C13-C14-C16
9	M	403	UQ5	C12-C11-C9-C8
13	C	410	PC7	C15-C16-C17-C18
11	C	407	PGT	C19-C20-C21-C22
12	G	103	CDL	C32-C33-C34-C35
12	C	408	CDL	C55-C56-C57-C58
12	C	408	CDL	C58-C59-C60-C61
12	C	409	CDL	C57-C58-C59-C60
13	D	302	PC7	C13-C14-C15-C16
11	C	407	PGT	C33-C34-C35-C36
12	N	302	CDL	OB9-CB7-OB8-CB6
12	C	409	CDL	C36-C37-C38-C39
16	M	404	UQ7	C37-C38-C39-C40
12	C	408	CDL	C80-C81-C82-C83
12	N	302	CDL	C16-C17-C18-C19
12	N	302	CDL	C80-C81-C82-C83
10	G	101	3PH	C22-C21-O21-C2
10	I	101	3PH	C22-C21-O21-C2
9	C	403	UQ5	C6-C7-C8-C9
12	C	408	CDL	CB7-C71-C72-C73
12	C	408	CDL	C75-C76-C77-C78
10	G	101	3PH	O22-C21-O21-C2
13	C	410	PC7	C18-C19-C20-C21
15	J	101	PTY	C16-C17-C18-C19
15	M	407	PTY	C40-C41-C42-C43
13	C	410	PC7	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
13	M	409	PC7	C4-C5-N-C8
13	M	409	PC7	C4-C5-N-C6
13	C	410	PC7	C34-C35-C36-C37
12	C	408	CDL	C12-C13-C14-C15
10	M	405	3PH	C31-C32-C33-C34
12	N	302	CDL	CA5-C11-C12-C13
15	T	103	PTY	C30-C31-C32-C33
12	C	408	CDL	OB5-CB3-CB4-OB6
8	M	402	HEM	C4C-C3C-CAC-CBC
12	G	103	CDL	C35-C36-C37-C38
13	M	409	PC7	C33-C34-C35-C36
12	G	103	CDL	CA5-C11-C12-C13
12	C	408	CDL	OB6-CB4-CB6-OB8
10	M	405	3PH	C33-C34-C35-C36
12	G	103	CDL	C11-C12-C13-C14
12	N	302	CDL	C74-C75-C76-C77
11	G	102	PGT	C36-C37-C38-C39
10	M	405	3PH	C34-C35-C36-C37
13	G	104	PC7	C20-C21-C22-C23
13	N	303	PC7	C12-C13-C14-C15
10	I	101	3PH	O22-C21-O21-C2
12	O	402	CDL	C79-C80-C81-C82
13	C	410	PC7	C14-C15-C16-C17
15	M	407	PTY	C13-C14-C15-C16
13	N	303	PC7	C33-C34-C35-C36
15	J	101	PTY	C31-C32-C33-C34
10	G	101	3PH	C29-C2A-C2B-C2C
12	G	103	CDL	C13-C14-C15-C16
13	D	302	PC7	C35-C36-C37-C38
11	C	407	PGT	C43-C44-C45-C46
10	T	102	3PH	C32-C33-C34-C35
13	C	410	PC7	C19-C20-C21-C22
12	G	103	CDL	CA7-C31-C32-C33
12	C	409	CDL	C13-C14-C15-C16
12	M	408	CDL	CB3-CB4-CB6-OB8
12	N	302	CDL	CA3-CA4-CA6-OA8
12	O	402	CDL	CA3-CA4-CA6-OA8
12	Q	101	CDL	CB3-CB4-CB6-OB8
13	D	302	PC7	C1-C2-C3-O3
13	M	409	PC7	C1-C2-C3-O3
16	M	404	UQ7	C9-C11-C12-C13
11	G	102	PGT	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
12	M	408	CDL	C35-C36-C37-C38
13	G	104	PC7	C14-C15-C16-C17
12	N	302	CDL	C73-C74-C75-C76
9	C	403	UQ5	C27-C28-C29-C30
12	M	408	CDL	C40-C41-C42-C43
9	C	404	UQ5	C18-C19-C21-C22
12	C	409	CDL	C55-C56-C57-C58
10	C	405	3PH	C1-O11-P-O12
10	G	101	3PH	C1-O11-P-O12
10	I	101	3PH	C1-O11-P-O12
12	C	409	CDL	C53-C54-C55-C56
10	T	102	3PH	C32-C31-O31-C3
13	M	409	PC7	C35-C36-C37-C38
10	G	101	3PH	C32-C33-C34-C35
12	Q	101	CDL	C38-C39-C40-C41
11	G	102	PGT	O3P-C1-C2-O2
11	C	406	PGT	C33-C34-C35-C36
13	G	104	PC7	C32-C33-C34-C35
13	M	409	PC7	C40-C41-C42-C43
11	C	407	PGT	C32-C33-C34-C35
12	M	408	CDL	C13-C14-C15-C16
16	M	404	UQ7	C11-C12-C13-C14
12	C	409	CDL	C16-C17-C18-C19
13	D	302	PC7	C31-C32-C33-C34
15	T	103	PTY	O4-C1-C6-O7
16	M	404	UQ7	C37-C38-C39-C41
12	C	408	CDL	C32-C31-CA7-OA8
11	M	406	PGT	C20-C21-C22-C23
13	G	104	PC7	C15-C16-C17-C18
11	C	406	PGT	C45-C46-C47-C48
13	C	410	PC7	C44-C45-C46-C47
10	T	102	3PH	C23-C24-C25-C26
11	C	407	PGT	C42-C43-C44-C45
12	C	409	CDL	C74-C75-C76-C77
12	N	302	CDL	C81-C82-C83-C84
11	C	407	PGT	C31-C32-C33-C34
12	C	409	CDL	C15-C16-C17-C18
9	C	404	UQ5	C20-C19-C21-C22
13	M	409	PC7	C16-C17-C18-C19
11	G	102	PGT	C21-C22-C23-C24
13	M	409	PC7	C32-C33-C34-C35
12	C	409	CDL	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
10	T	102	3PH	C35-C36-C37-C38
11	M	406	PGT	C12-C11-O3-C3
10	T	101	3PH	C35-C36-C37-C38
12	M	408	CDL	C57-C58-C59-C60
10	G	101	3PH	O11-C1-C2-C3
12	C	408	CDL	OB5-CB3-CB4-CB6
12	C	409	CDL	OA5-CA3-CA4-CA6
9	C	404	UQ5	C12-C11-C9-C10
12	O	402	CDL	C11-C12-C13-C14
10	G	101	3PH	C25-C26-C27-C28
11	C	406	PGT	C41-C42-C43-C44
11	G	102	PGT	C32-C31-O2-C2
15	T	103	PTY	C11-C12-C13-C14
10	C	405	3PH	C1-C2-C3-O31
11	M	406	PGT	C1-C2-C3-O3
12	C	408	CDL	CA3-CA4-CA6-OA8
13	N	303	PC7	C1-C2-C3-O3
10	M	405	3PH	C2B-C2C-C2D-C2E
12	G	103	CDL	C53-C54-C55-C56
12	M	408	CDL	C55-C56-C57-C58
13	N	303	PC7	C17-C18-C19-C20
12	N	302	CDL	C11-C12-C13-C14
15	J	101	PTY	C34-C35-C36-C37
15	M	407	PTY	C11-C12-C13-C14
13	M	409	PC7	C31-C32-C33-C34
9	C	404	UQ5	C12-C11-C9-C8
10	T	102	3PH	O32-C31-O31-C3
10	C	405	3PH	O11-C1-C2-O21
10	G	101	3PH	O11-C1-C2-O21
12	G	103	CDL	C41-C42-C43-C44
12	C	408	CDL	OA6-CA4-CA6-OA8
12	Q	101	CDL	OB6-CB4-CB6-OB8
13	C	410	PC7	O2-C2-C3-O3
13	D	302	PC7	O2-C2-C3-O3
11	C	407	PGT	C34-C35-C36-C37
12	O	402	CDL	C52-C53-C54-C55
10	T	101	3PH	C36-C37-C38-C39
11	G	102	PGT	C41-C42-C43-C44
17	M	410	Q7G	C22-CG1-O20-C17
10	G	101	3PH	C33-C34-C35-C36
12	C	409	CDL	C17-C18-C19-C20
11	G	102	PGT	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
13	C	410	PC7	C13-C14-C15-C16
12	C	408	CDL	C72-C71-CB7-OB8
12	M	408	CDL	C31-C32-C33-C34
10	C	405	3PH	C37-C38-C39-C3A
12	O	402	CDL	C18-C19-C20-C21
13	G	104	PC7	C17-C18-C19-C20
12	M	408	CDL	OB5-CB3-CB4-CB6
12	N	302	CDL	OB5-CB3-CB4-CB6
12	Q	101	CDL	OA5-CA3-CA4-CA6
15	T	103	PTY	O14-C5-C6-C1
13	G	104	PC7	C16-C17-C18-C19
16	M	404	UQ7	C12-C13-C14-C15
12	N	302	CDL	C53-C54-C55-C56
8	O	401	HEM	C2B-C3B-CAB-CBB
12	G	103	CDL	C74-C75-C76-C77
12	Q	101	CDL	C41-C42-C43-C44
11	M	406	PGT	O11-C11-O3-C3
12	Q	101	CDL	C43-C44-C45-C46
11	G	102	PGT	O31-C31-O2-C2
10	T	102	3PH	O11-C1-C2-O21
12	C	409	CDL	OA5-CA3-CA4-OA6
12	C	409	CDL	C33-C34-C35-C36
11	G	102	PGT	C1-C2-C3-O3
12	C	409	CDL	CA3-CA4-CA6-OA8
12	M	408	CDL	CA3-CA4-CA6-OA8
13	C	410	PC7	C1-C2-C3-O3
11	G	102	PGT	C17-C18-C19-C20
12	Q	101	CDL	C51-C52-C53-C54
15	M	407	PTY	C2-C3-O11-P1
10	C	405	3PH	O21-C2-C3-O31
11	G	102	PGT	O2-C2-C3-O3
12	M	408	CDL	OA6-CA4-CA6-OA8
12	O	402	CDL	OB6-CB4-CB6-OB8
10	C	405	3PH	C25-C26-C27-C28
12	G	103	CDL	C19-C20-C21-C22
12	Q	101	CDL	CB4-CB6-OB8-CB7
9	C	403	UQ5	C27-C28-C29-C31
12	C	409	CDL	C59-C60-C61-C62
10	C	405	3PH	C39-C3A-C3B-C3C
10	C	405	3PH	C22-C23-C24-C25
9	C	404	UQ5	C25-C24-C26-C27
10	M	405	3PH	C39-C3A-C3B-C3C

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Mol	Chain	Res	Type	Atoms
10	C	405	3PH	O11-C1-C2-C3
10	T	102	3PH	O11-C1-C2-C3
11	G	102	PGT	O3P-C1-C2-C3
12	C	408	CDL	OA5-CA3-CA4-CA6
12	Q	101	CDL	C13-C14-C15-C16
12	M	408	CDL	C74-C75-C76-C77
12	Q	101	CDL	C31-C32-C33-C34
11	M	406	PGT	C22-C23-C24-C25
10	T	101	3PH	C33-C34-C35-C36
12	C	408	CDL	OA5-CA3-CA4-OA6
12	M	408	CDL	OA5-CA3-CA4-OA6
12	M	408	CDL	OB5-CB3-CB4-OB6
12	Q	101	CDL	OA5-CA3-CA4-OA6
15	T	103	PTY	O14-C5-C6-O7
12	N	302	CDL	C77-C78-C79-C80
10	M	405	3PH	O21-C2-C3-O31
12	C	409	CDL	OA6-CA4-CA6-OA8
12	N	302	CDL	OA6-CA4-CA6-OA8
12	O	402	CDL	OA6-CA4-CA6-OA8
12	C	409	CDL	C44-C45-C46-C47
15	T	103	PTY	O4-C1-C6-C5
17	M	410	Q7G	CG1-C22-C23-C24
17	M	410	Q7G	CG1-C22-C23-C48
10	M	405	3PH	C36-C37-C38-C39
12	C	409	CDL	C56-C57-C58-C59
12	G	103	CDL	C22-C23-C24-C25
11	M	406	PGT	C23-C24-C25-C26
9	C	404	UQ5	C2-C3-O3-C3M
12	C	409	CDL	C20-C21-C22-C23
11	C	406	PGT	C4-O4P-P-O1P
11	G	102	PGT	C1-O3P-P-O1P
11	G	102	PGT	C4-O4P-P-O3P
11	G	102	PGT	C4-O4P-P-O1P
11	M	406	PGT	C4-O4P-P-O3P
11	M	406	PGT	C4-O4P-P-O2P
12	C	408	CDL	CA3-OA5-PA1-OA3
12	C	408	CDL	CA3-OA5-PA1-OA4
12	C	408	CDL	CB2-OB2-PB2-OB5
12	G	103	CDL	CB3-OB5-PB2-OB3
12	N	302	CDL	CA2-OA2-PA1-OA3
12	N	302	CDL	CB2-OB2-PB2-OB3
12	N	302	CDL	CB2-OB2-PB2-OB5

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Mol	Chain	Res	Type	Atoms
12	Q	101	CDL	CA3-OA5-PA1-OA2
12	Q	101	CDL	CB2-OB2-PB2-OB3
13	D	302	PC7	C4-O4P-P-O2P
13	G	104	PC7	C4-O4P-P-O2P
15	M	407	PTY	C3-O11-P1-O13
15	T	103	PTY	C3-O11-P1-O13
15	T	103	PTY	C5-O14-P1-O13
13	G	104	PC7	C13-C14-C15-C16
9	C	404	UQ5	C15-C14-C16-C17
10	I	101	3PH	C2-C1-O11-P
11	G	102	PGT	C5-C4-O4P-P
12	C	408	CDL	CB4-CB3-OB5-PB2
12	O	402	CDL	CB4-CB3-OB5-PB2
10	T	101	3PH	C1-O11-P-O12
11	C	407	PGT	C35-C36-C37-C38
11	G	102	PGT	C31-C32-C33-C34
12	C	408	CDL	O1-C1-CB2-OB2
12	N	302	CDL	CA6-CA4-OA6-CA5
9	C	403	UQ5	C14-C16-C17-C18
12	M	408	CDL	C16-C17-C18-C19
12	M	408	CDL	OA5-CA3-CA4-CA6
12	C	409	CDL	C72-C73-C74-C75
12	Q	101	CDL	CA2-C1-CB2-OB2
12	C	409	CDL	C23-C24-C25-C26
15	M	407	PTY	C41-C42-C43-C44
16	M	404	UQ7	C4-C3-O3-CM3
11	G	102	PGT	C19-C20-C21-C22
13	N	303	PC7	O2-C2-C3-O3
12	N	302	CDL	C78-C79-C80-C81
10	T	101	3PH	C22-C21-O21-C2
15	T	103	PTY	C8-C11-C12-C13
12	O	402	CDL	C38-C39-C40-C41
10	T	101	3PH	O22-C21-O21-C2
15	T	103	PTY	C33-C34-C35-C36
12	G	103	CDL	C12-C13-C14-C15
12	G	103	CDL	C17-C18-C19-C20
10	G	101	3PH	C28-C29-C2A-C2B
13	C	410	PC7	C4-C5-N-C8
12	M	408	CDL	CA2-C1-CB2-OB2
12	C	408	CDL	C19-C20-C21-C22
9	C	403	UQ5	C2-C3-O3-C3M
8	C	402	HEM	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
12	N	302	CDL	C63-C64-C65-C66
12	C	409	CDL	OB5-CB3-CB4-OB6
8	O	401	HEM	C4B-C3B-CAB-CBB
12	C	409	CDL	C43-C44-C45-C46
12	N	302	CDL	C58-C59-C60-C61
11	G	102	PGT	C11-C12-C13-C14
10	T	102	3PH	C29-C2A-C2B-C2C
10	C	405	3PH	C3A-C3B-C3C-C3D
8	M	402	HEM	CAD-CBD-CGD-O2D
11	G	102	PGT	C15-C16-C17-C18
12	M	408	CDL	C72-C73-C74-C75
10	C	405	3PH	C33-C34-C35-C36
8	M	402	HEM	CAD-CBD-CGD-O1D
8	C	402	HEM	CAD-CBD-CGD-O2D
12	O	402	CDL	C78-C79-C80-C81
12	C	409	CDL	CB7-C71-C72-C73
11	C	406	PGT	C44-C45-C46-C47
8	O	401	HEM	CAA-CBA-CGA-O2A
12	G	103	CDL	C54-C55-C56-C57
12	M	408	CDL	C52-C53-C54-C55
8	E	400	HEM	CAA-CBA-CGA-O1A
8	M	401	HEM	CAA-CBA-CGA-O1A
10	M	405	3PH	C32-C33-C34-C35
16	M	404	UQ7	C26-C27-C28-C29
8	O	401	HEM	CAA-CBA-CGA-O1A
13	C	410	PC7	C41-C42-C43-C44
12	G	103	CDL	OB6-CB4-CB6-OB8
8	C	402	HEM	CAD-CBD-CGD-O1D
13	G	104	PC7	C12-C11-O3-C3
10	T	102	3PH	C26-C27-C28-C29
12	G	103	CDL	C16-C17-C18-C19
8	M	401	HEM	CAA-CBA-CGA-O2A
12	C	408	CDL	C60-C61-C62-C63
10	T	102	3PH	C39-C3A-C3B-C3C
10	M	405	3PH	O22-C21-O21-C2
10	T	102	3PH	O22-C21-O21-C2
15	M	407	PTY	O10-C8-O7-C6
12	N	302	CDL	C83-C84-C85-C86
12	N	302	CDL	C14-C15-C16-C17
8	E	400	HEM	CAA-CBA-CGA-O2A
9	C	404	UQ5	C23-C24-C26-C27
11	M	406	PGT	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
8	C	401	HEM	CAA-CBA-CGA-O2A
12	C	408	CDL	C32-C31-CA7-OA9
10	M	405	3PH	C37-C38-C39-C3A
12	C	409	CDL	C38-C39-C40-C41
10	M	405	3PH	O11-C1-C2-O21
12	Q	101	CDL	OB5-CB3-CB4-OB6
12	O	402	CDL	C37-C38-C39-C40
12	O	402	CDL	C34-C35-C36-C37
13	C	410	PC7	C35-C36-C37-C38
12	N	302	CDL	CB2-C1-CA2-OA2
11	C	407	PGT	C36-C37-C38-C39
15	M	407	PTY	C39-C40-C41-C42
12	Q	101	CDL	OB5-CB3-CB4-CB6
10	T	102	3PH	C22-C21-O21-C2
11	C	407	PGT	C41-C42-C43-C44
12	C	408	CDL	CA4-CA3-OA5-PA1
15	M	407	PTY	C12-C13-C14-C15
10	M	405	3PH	C3F-C3G-C3H-C3I
10	M	405	3PH	C22-C23-C24-C25
12	O	402	CDL	C77-C78-C79-C80
12	M	408	CDL	O1-C1-CB2-OB2
12	Q	101	CDL	O1-C1-CB2-OB2
13	G	104	PC7	O11-C11-O3-C3
12	G	103	CDL	C71-C72-C73-C74
10	T	101	3PH	C1-O11-P-O14
12	C	408	CDL	C17-C18-C19-C20
12	Q	101	CDL	C11-C12-C13-C14
8	C	402	HEM	C2B-C3B-CAB-CBB
15	M	407	PTY	C16-C17-C18-C19
12	N	302	CDL	O1-C1-CA2-OA2
9	C	404	UQ5	C13-C14-C16-C17
12	C	408	CDL	C15-C16-C17-C18
8	C	401	HEM	CAA-CBA-CGA-O1A
13	C	410	PC7	C4-C5-N-C6
12	C	408	CDL	CB3-CB4-CB6-OB8
12	G	103	CDL	CB3-CB4-CB6-OB8
8	C	402	HEM	C4B-C3B-CAB-CBB
12	Q	101	CDL	C36-C37-C38-C39
12	O	402	CDL	C76-C77-C78-C79
12	N	302	CDL	C51-C52-C53-C54
12	C	408	CDL	C72-C71-CB7-OB9
10	M	405	3PH	C22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
10	M	405	3PH	O11-C1-C2-C3
11	M	406	PGT	C18-C19-C20-C21
9	C	404	UQ5	C4-C3-O3-C3M
13	C	410	PC7	C4-C5-N-C7
13	D	302	PC7	C4-C5-N-C7
13	G	104	PC7	O4P-C4-C5-N
13	D	302	PC7	O3-C11-C12-C13
15	M	407	PTY	C11-C8-O7-C6
15	T	103	PTY	C12-C11-C8-O7
10	G	101	3PH	O21-C21-C22-C23
12	M	408	CDL	C12-C11-CA5-OA6
12	Q	101	CDL	C32-C31-CA7-OA8
12	M	408	CDL	C58-C59-C60-C61
12	O	402	CDL	C32-C31-CA7-OA8
12	Q	101	CDL	C72-C71-CB7-OB8
10	I	101	3PH	O31-C31-C32-C33
10	I	101	3PH	C1-C2-C3-O31
10	M	405	3PH	C1-C2-C3-O31
12	O	402	CDL	CB3-CB4-CB6-OB8
16	M	404	UQ7	C14-C16-C17-C18
13	G	104	PC7	O2-C31-C32-C33
15	M	407	PTY	O4-C30-C31-C32
10	T	101	3PH	C37-C38-C39-C3A
13	G	104	PC7	O3-C11-C12-C13
12	M	408	CDL	C15-C16-C17-C18
11	C	407	PGT	C39-C40-C41-C42
15	M	407	PTY	C33-C34-C35-C36
16	M	404	UQ7	C2-C3-O3-CM3
12	M	408	CDL	OB9-CB7-OB8-CB6
11	G	102	PGT	C44-C45-C46-C47
12	C	409	CDL	OB7-CB5-OB6-CB4
12	M	408	CDL	C71-CB7-OB8-CB6
13	G	104	PC7	C43-C44-C45-C46
13	G	104	PC7	C22-C23-C24-C25
10	G	101	3PH	O22-C21-C22-C23
12	Q	101	CDL	C72-C71-CB7-OB9
13	D	302	PC7	O11-C11-C12-C13
12	O	402	CDL	C13-C14-C15-C16
11	M	406	PGT	O2-C31-C32-C33
12	O	402	CDL	C72-C71-CB7-OB8
9	M	403	UQ5	C16-C17-C18-C19
10	T	101	3PH	C39-C3A-C3B-C3C

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Mol	Chain	Res	Type	Atoms
13	D	302	PC7	C4-C5-N-C8
13	D	302	PC7	C4-C5-N-C6
11	C	407	PGT	C20-C21-C22-C23
9	C	403	UQ5	C12-C13-C14-C16
12	Q	101	CDL	C32-C31-CA7-OA9
13	G	104	PC7	O31-C31-C32-C33
13	M	409	PC7	O11-C11-O3-C3
13	G	104	PC7	O11-C11-C12-C13
15	T	103	PTY	C12-C11-C8-O10
11	C	406	PGT	C39-C40-C41-C42
12	M	408	CDL	C12-C11-CA5-OA7
10	M	405	3PH	O21-C21-C22-C23
15	M	407	PTY	O30-C30-C31-C32
12	M	408	CDL	C34-C35-C36-C37
8	C	402	HEM	C2C-C3C-CAC-CBC
12	N	302	CDL	C12-C13-C14-C15
10	I	101	3PH	O32-C31-C32-C33
12	O	402	CDL	C59-C60-C61-C62
11	G	102	PGT	C45-C46-C47-C48
13	M	409	PC7	C12-C11-O3-C3
13	D	302	PC7	O2-C31-C32-C33
12	O	402	CDL	C32-C31-CA7-OA9
12	O	402	CDL	CB5-C51-C52-C53
11	G	102	PGT	C12-C13-C14-C15

There are no ring outliers.

34 monomers are involved in 142 short contacts:

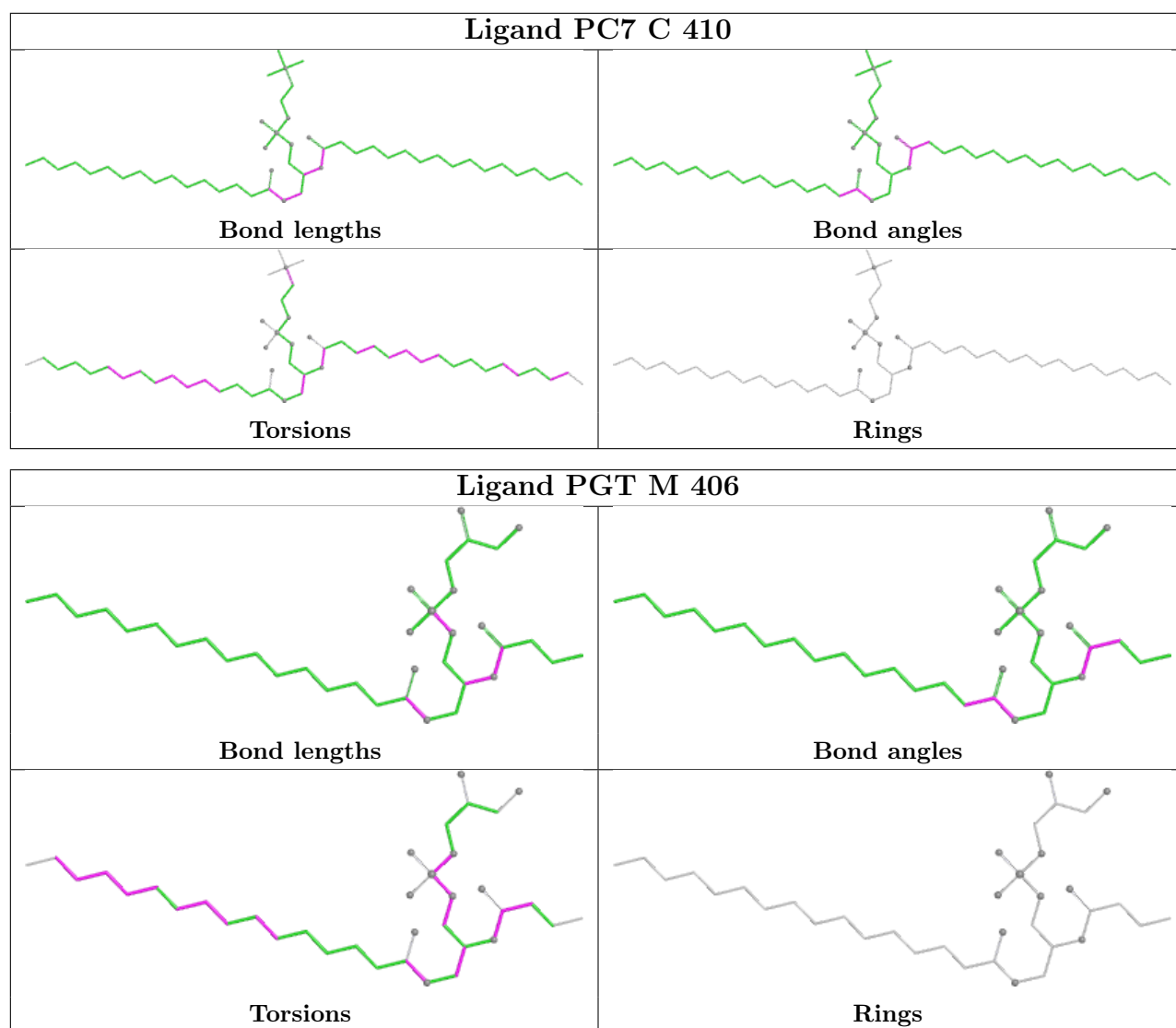
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	C	410	PC7	9	0
11	M	406	PGT	4	0
8	C	401	HEM	1	0
9	C	404	UQ5	6	0
10	M	405	3PH	6	0
11	G	102	PGT	2	0
15	M	407	PTY	2	0
12	N	302	CDL	3	0
9	C	403	UQ5	11	0
10	C	405	3PH	1	0
12	C	408	CDL	9	0
14	N	301	FES	2	0
12	O	402	CDL	7	0

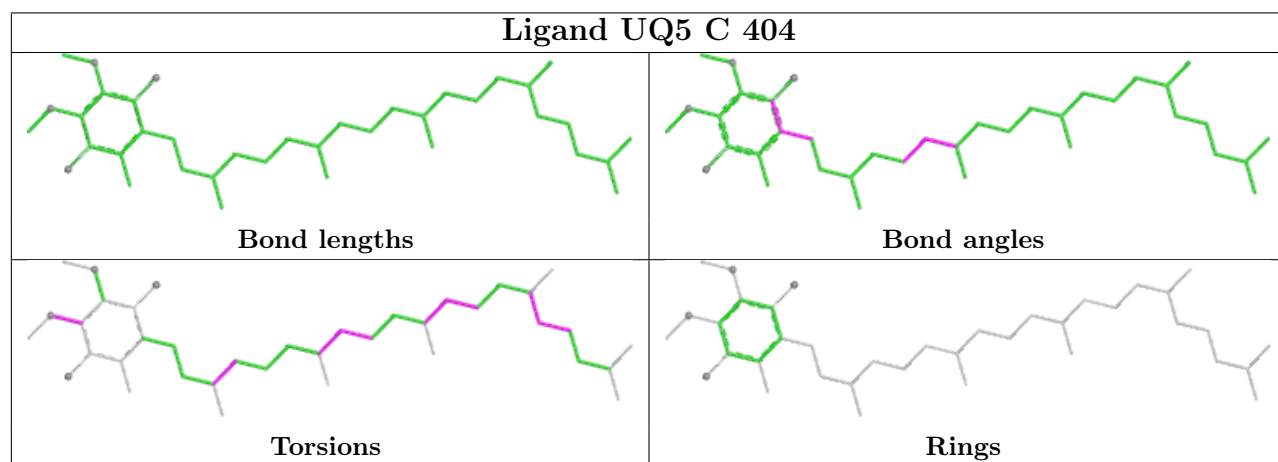
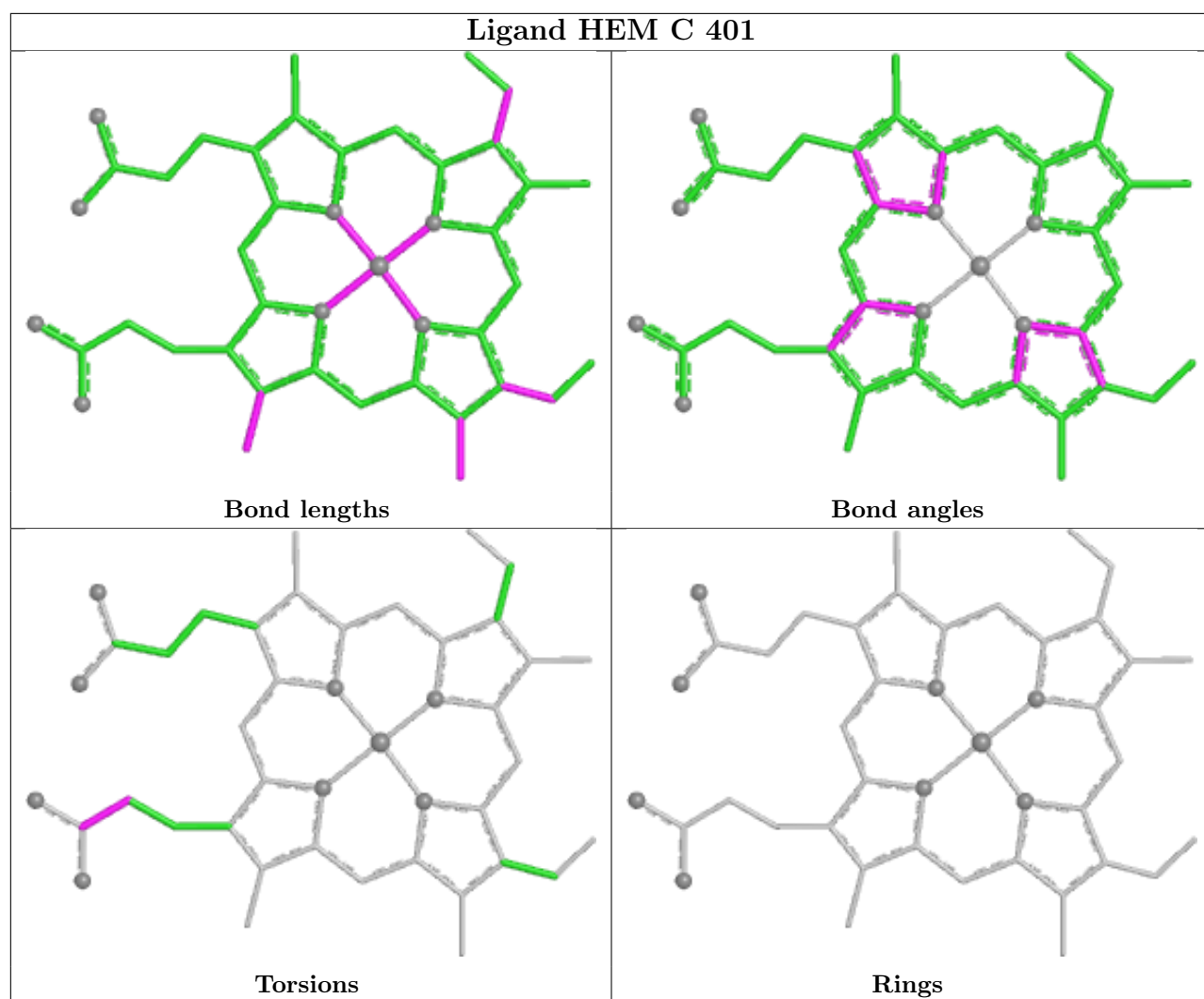
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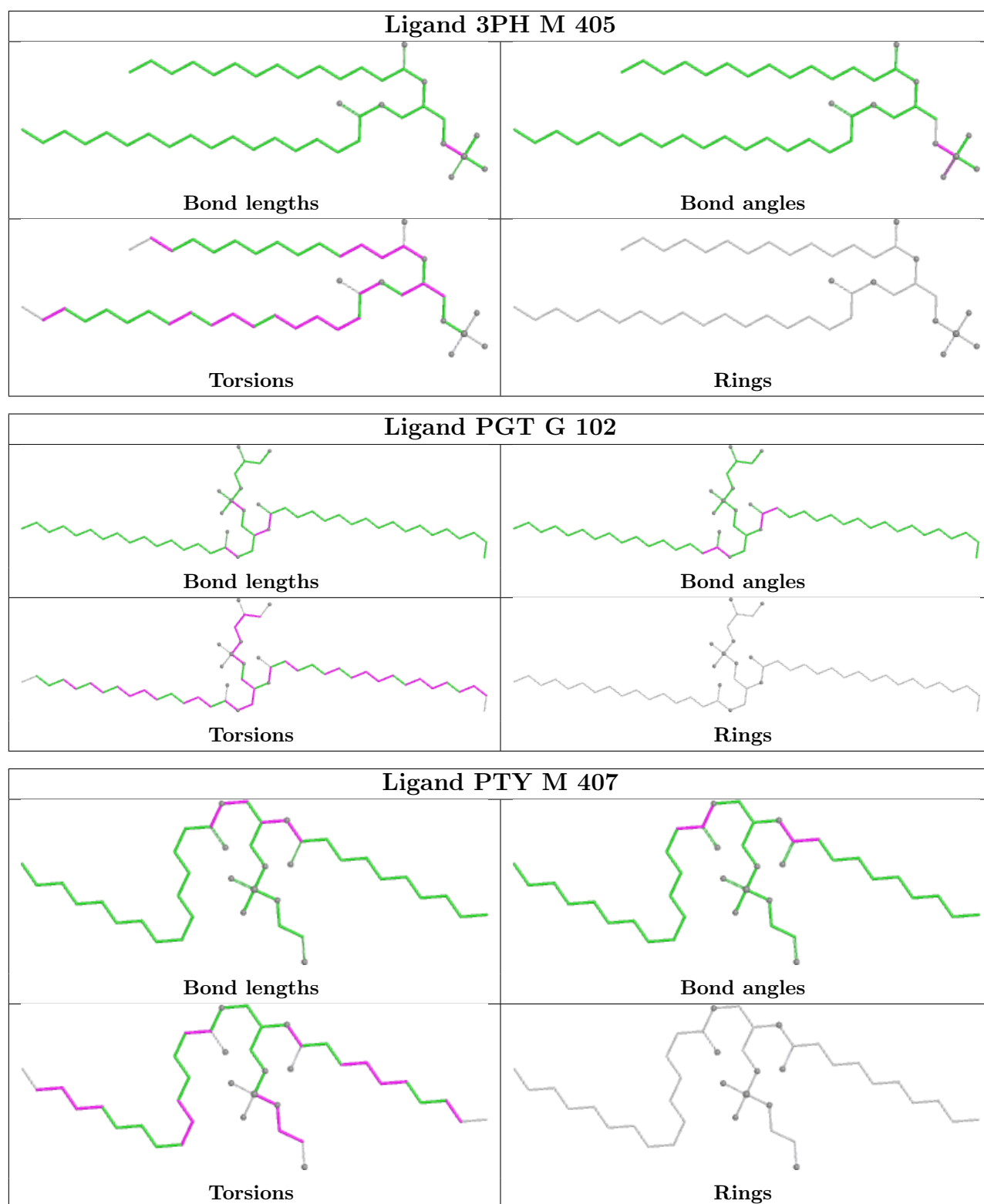
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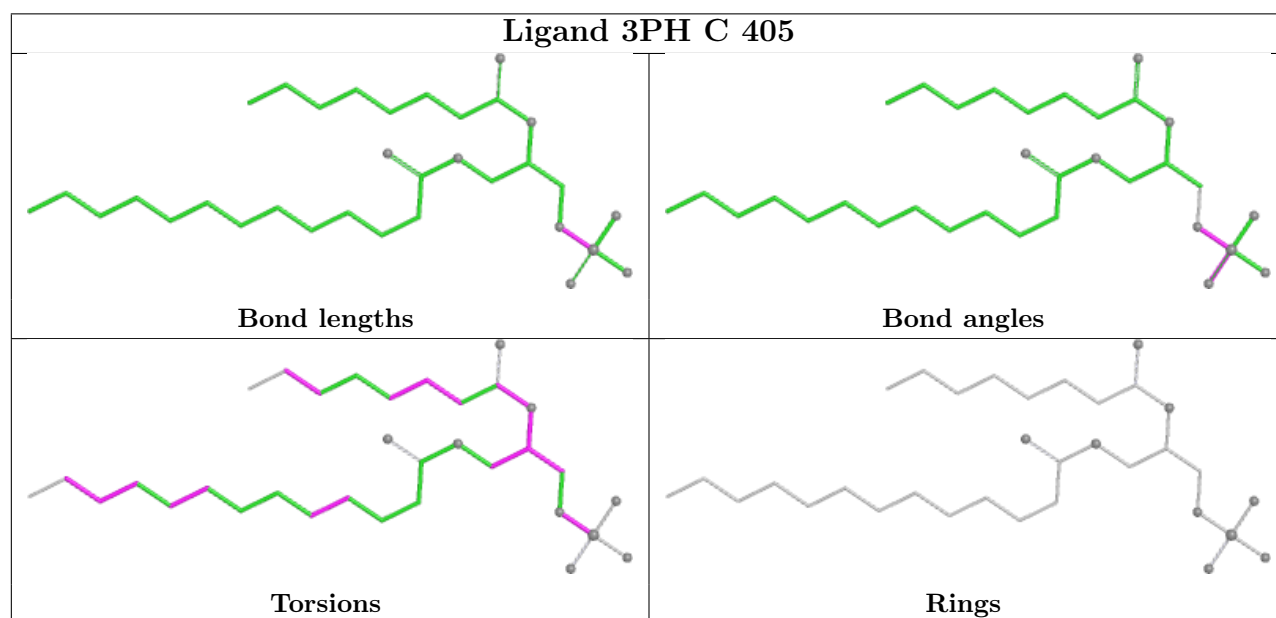
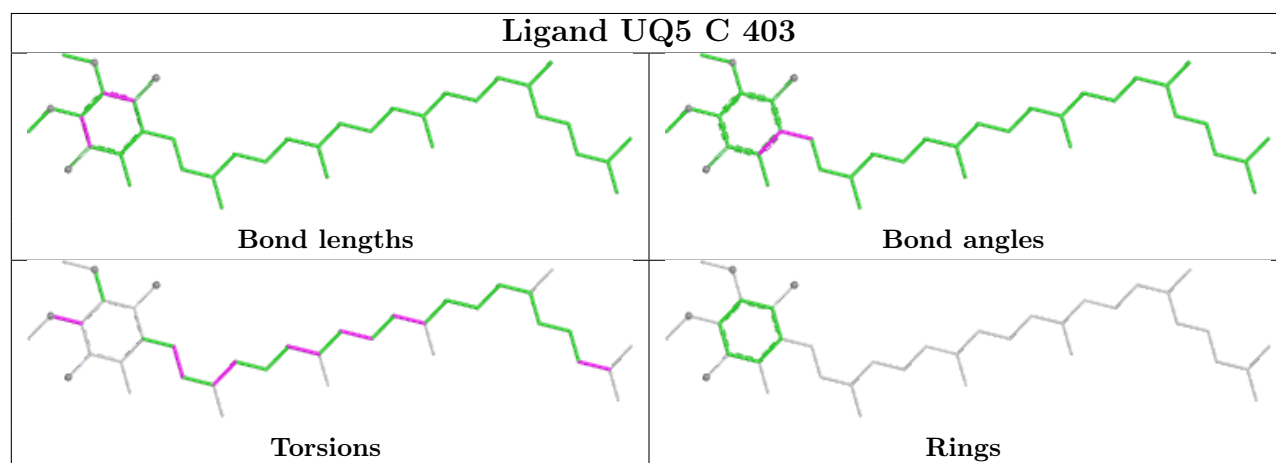
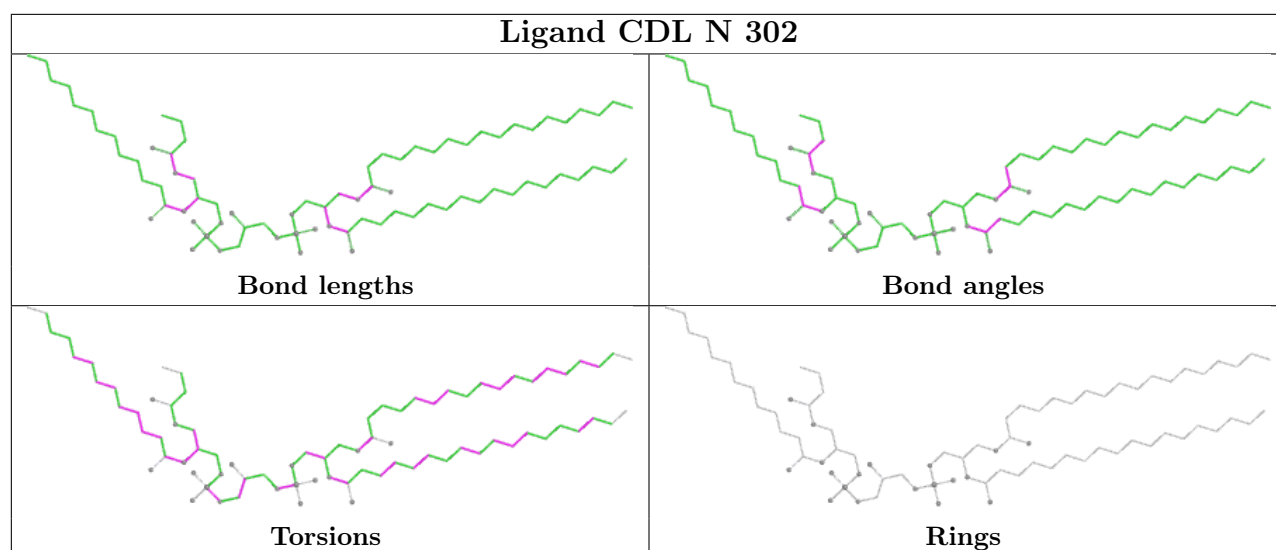
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	M	408	CDL	8	0
15	T	103	PTY	1	0
11	C	406	PGT	6	0
13	M	409	PC7	2	0
10	T	102	3PH	1	0
13	D	302	PC7	1	0
10	I	101	3PH	3	0
8	C	402	HEM	1	0
13	N	303	PC7	6	0
10	T	101	3PH	2	0
12	C	409	CDL	10	0
16	M	404	UQ7	11	0
12	Q	101	CDL	6	0
10	G	101	3PH	1	0
11	C	407	PGT	4	0
8	E	400	HEM	5	0
8	M	402	HEM	1	0
8	O	401	HEM	6	0
12	G	103	CDL	6	0
9	M	403	UQ5	8	0
13	G	104	PC7	5	0

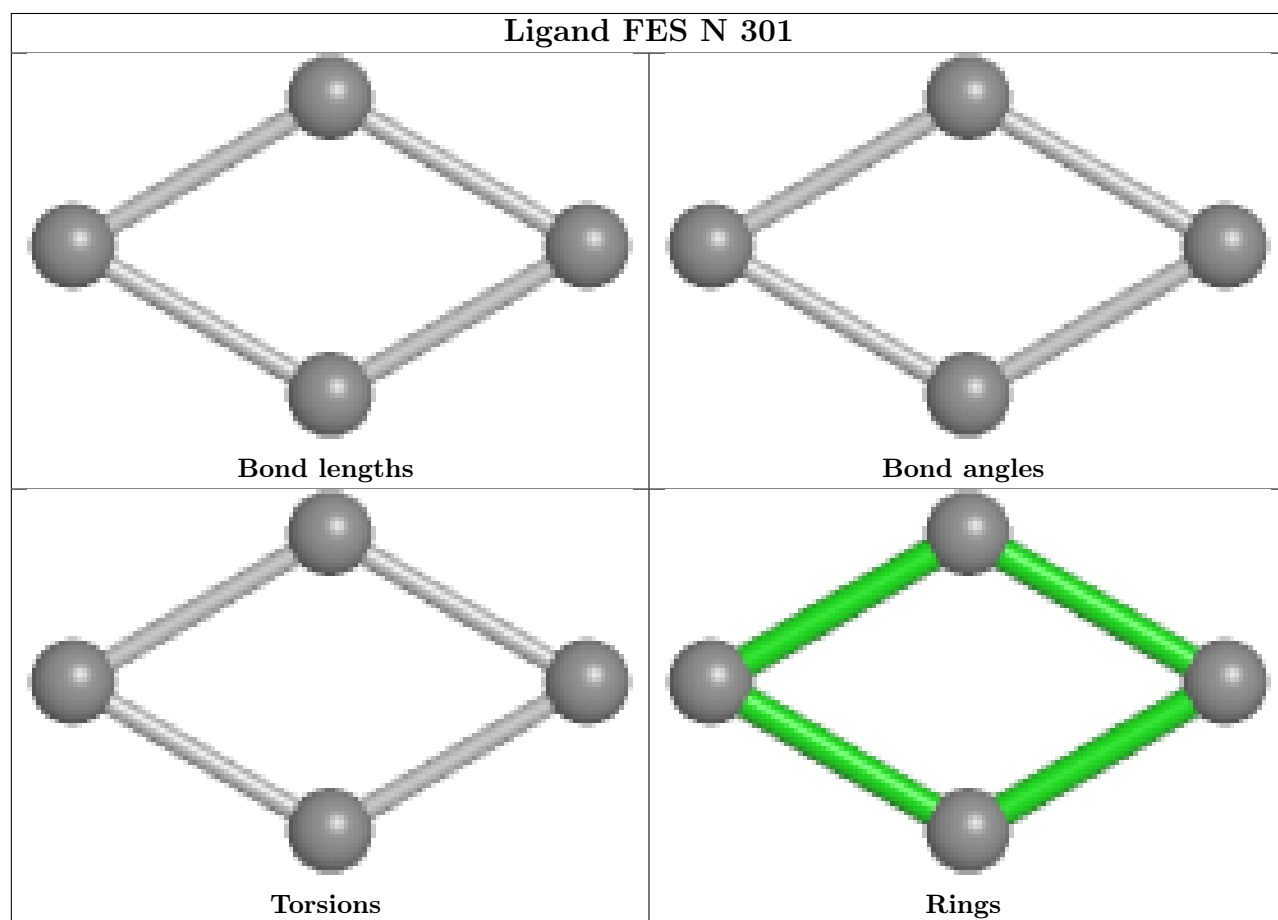
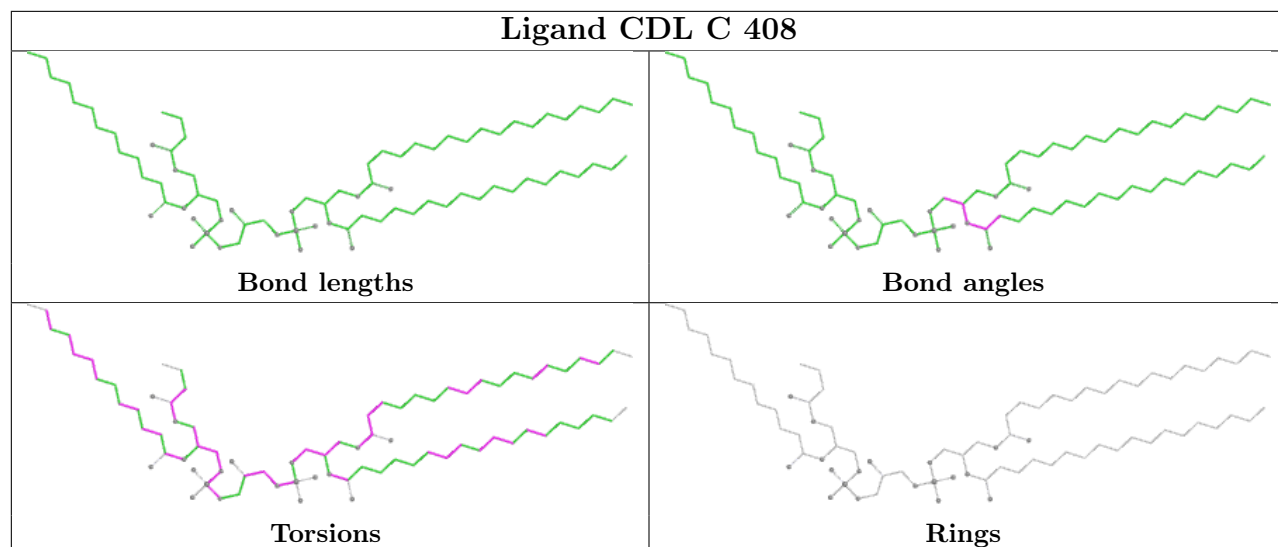
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

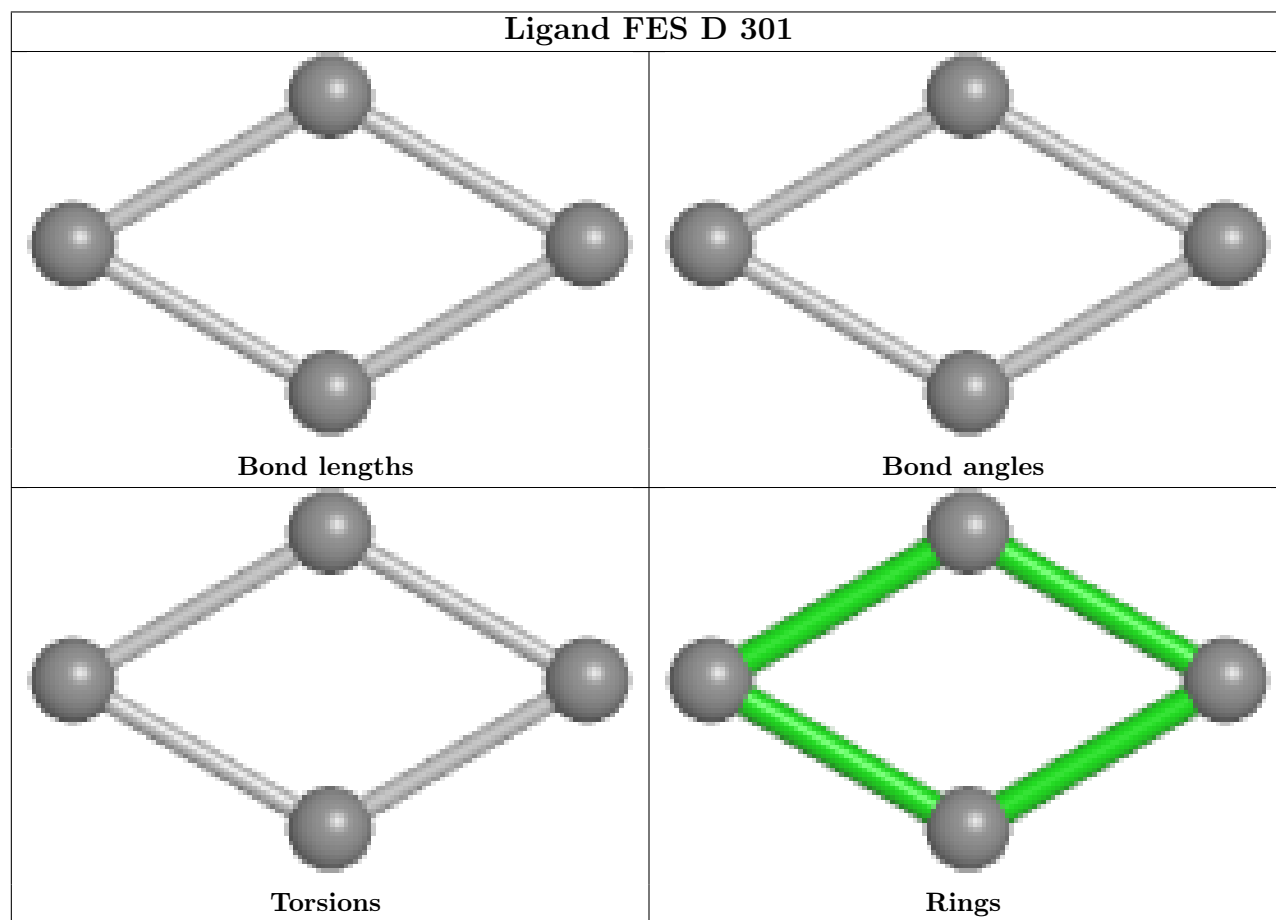
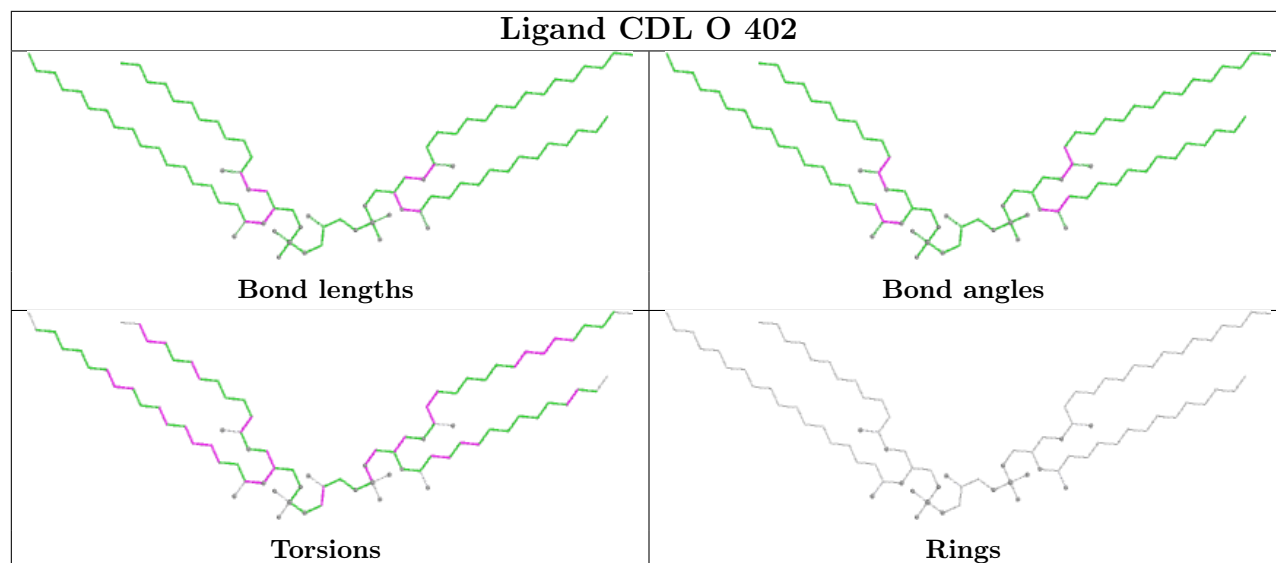


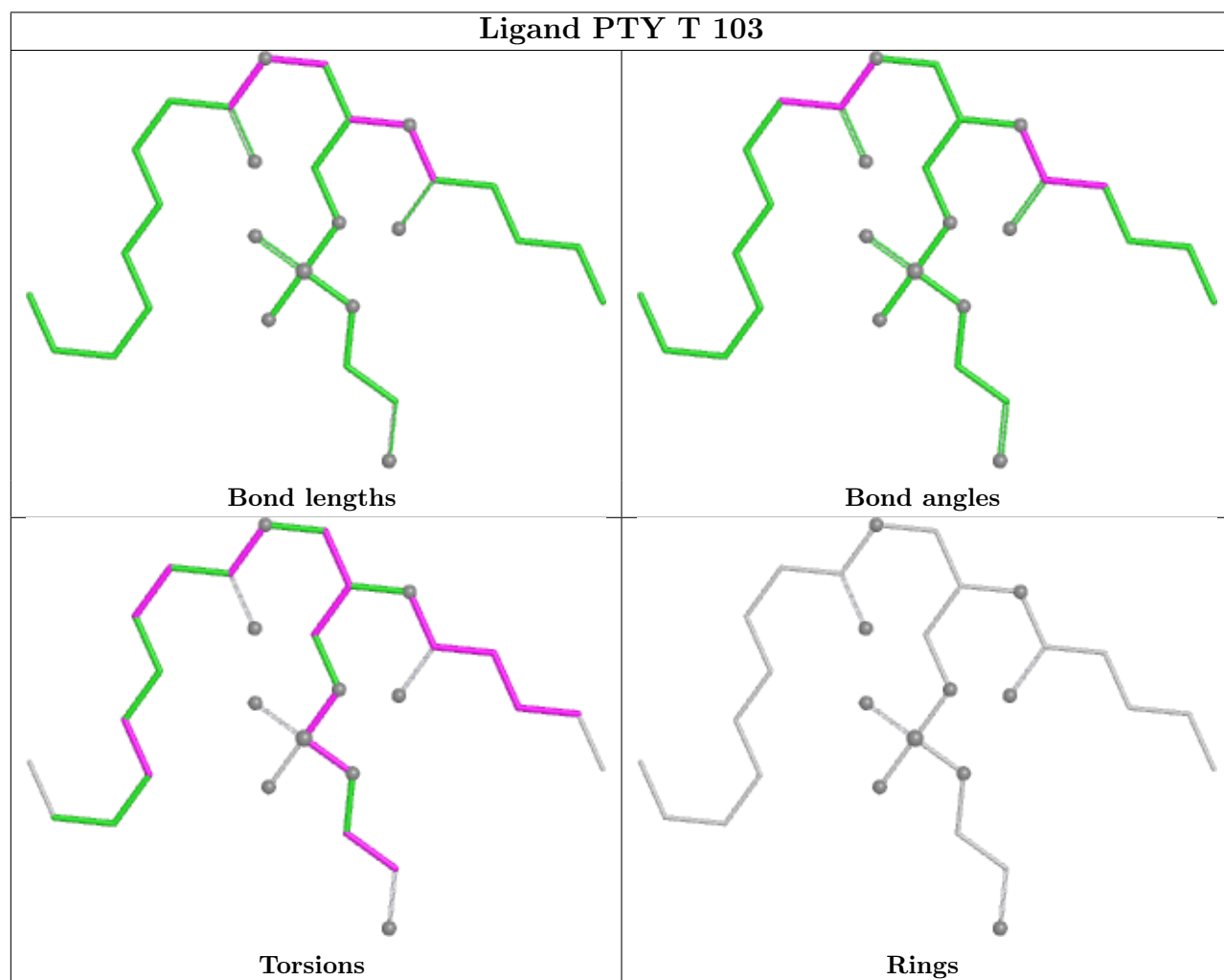
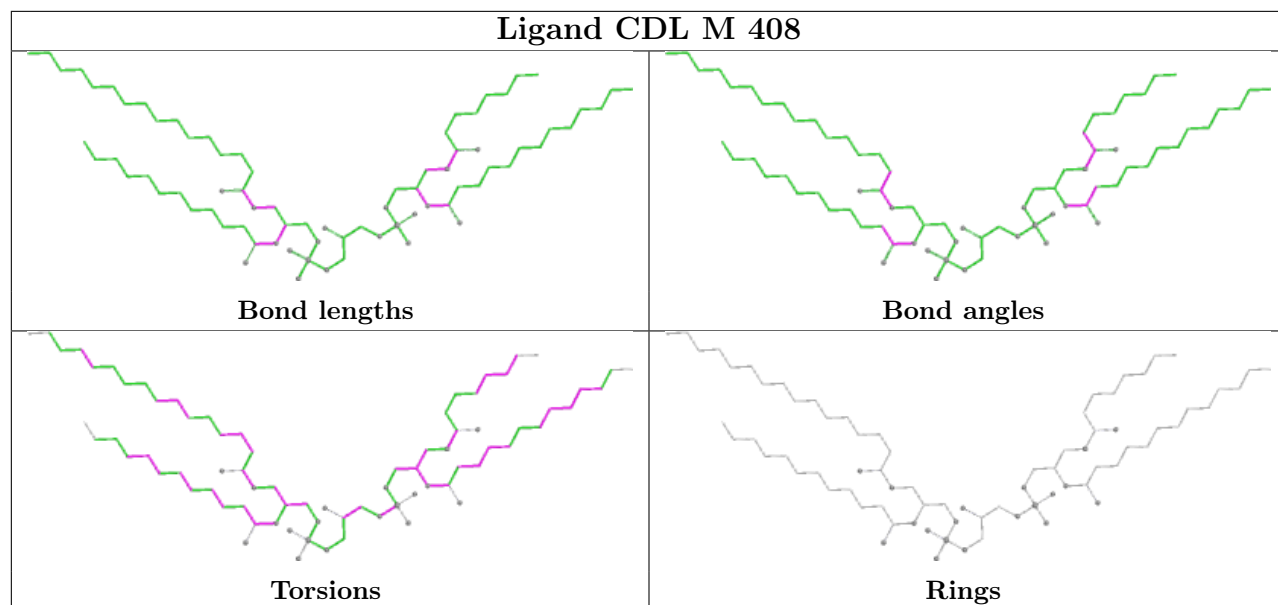


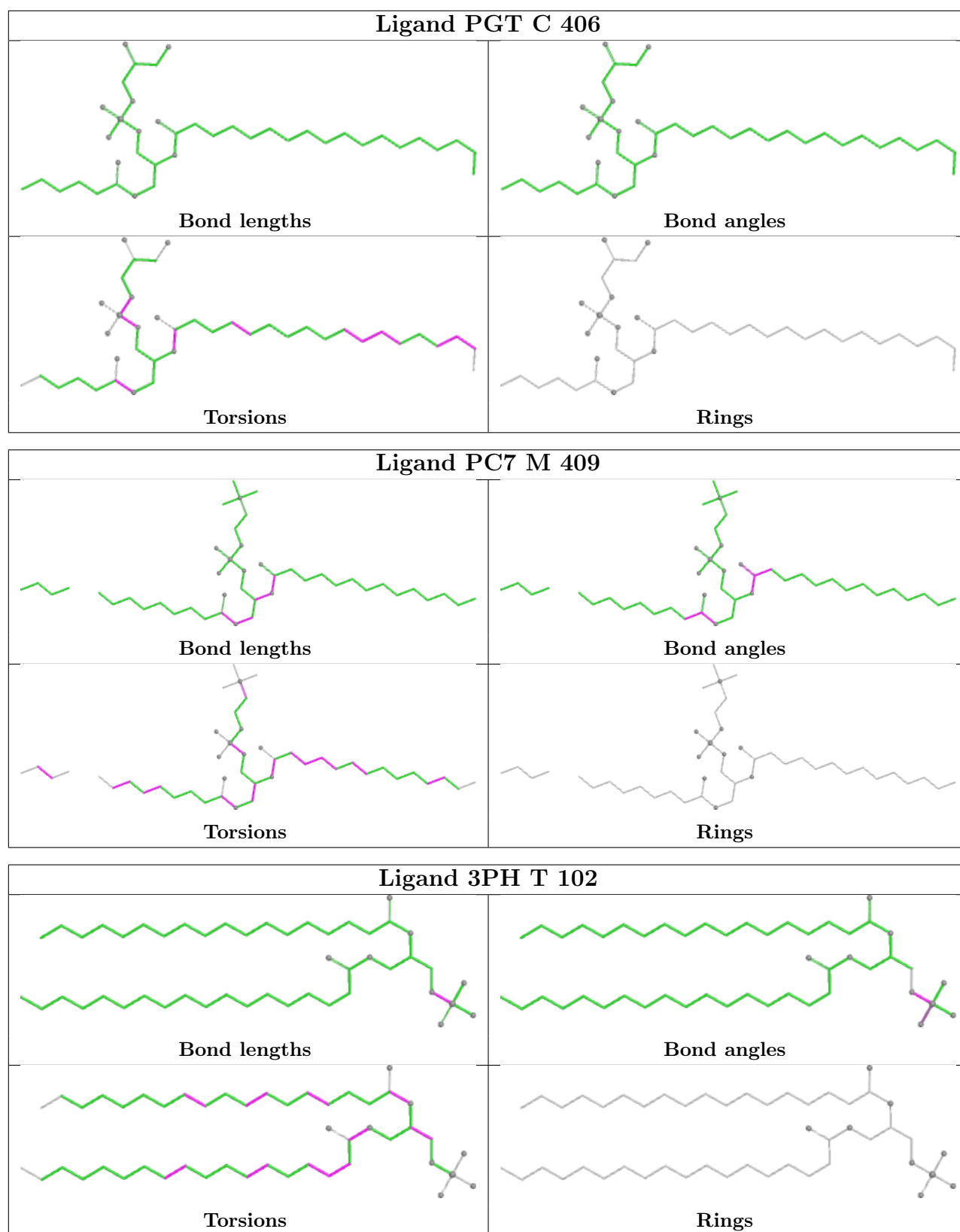


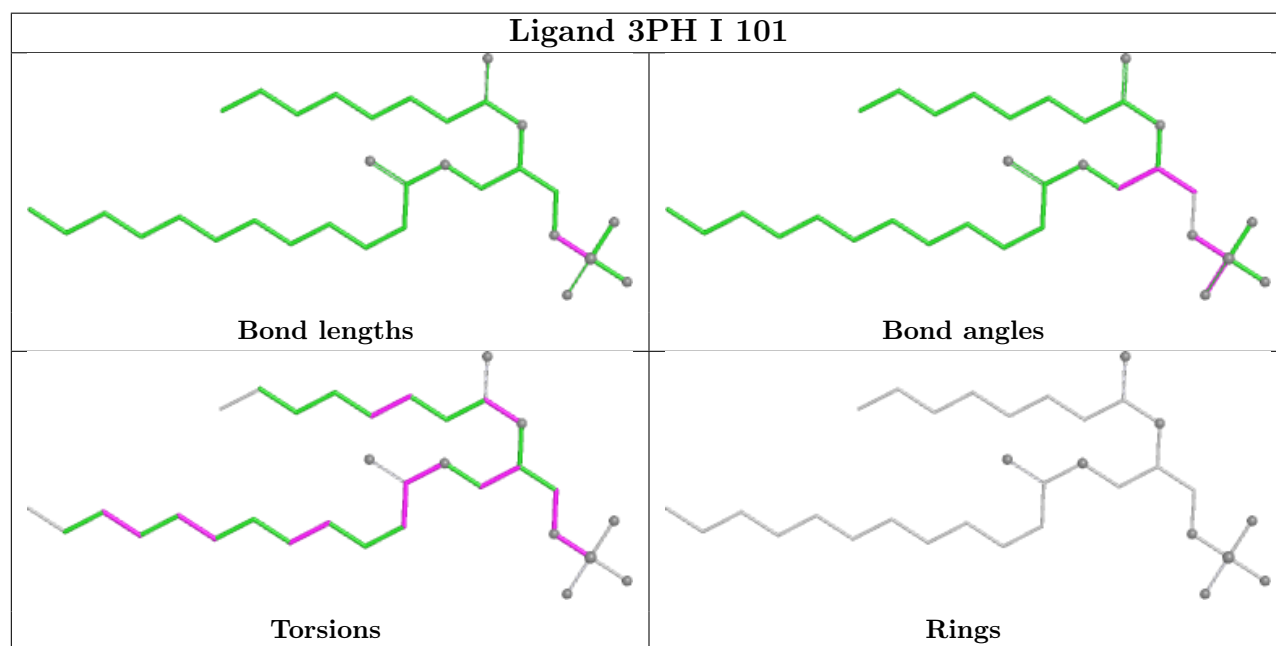
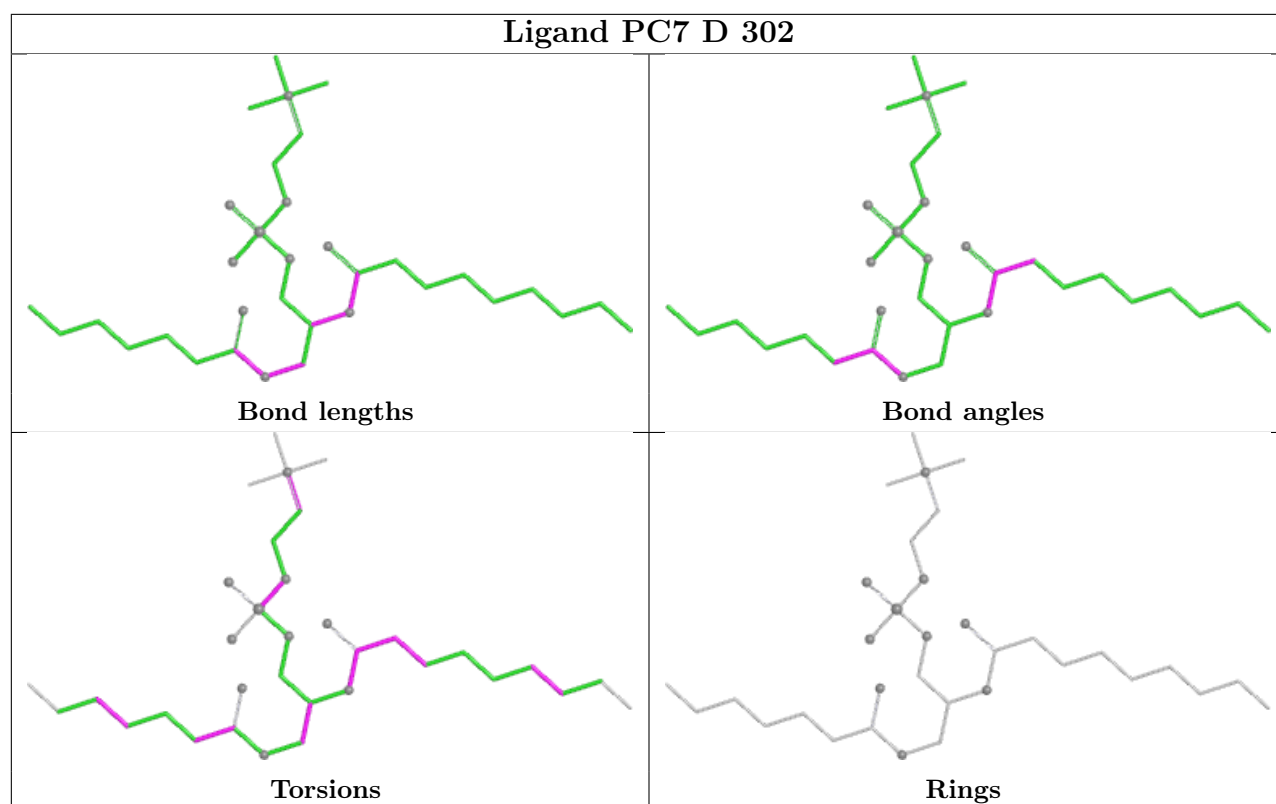


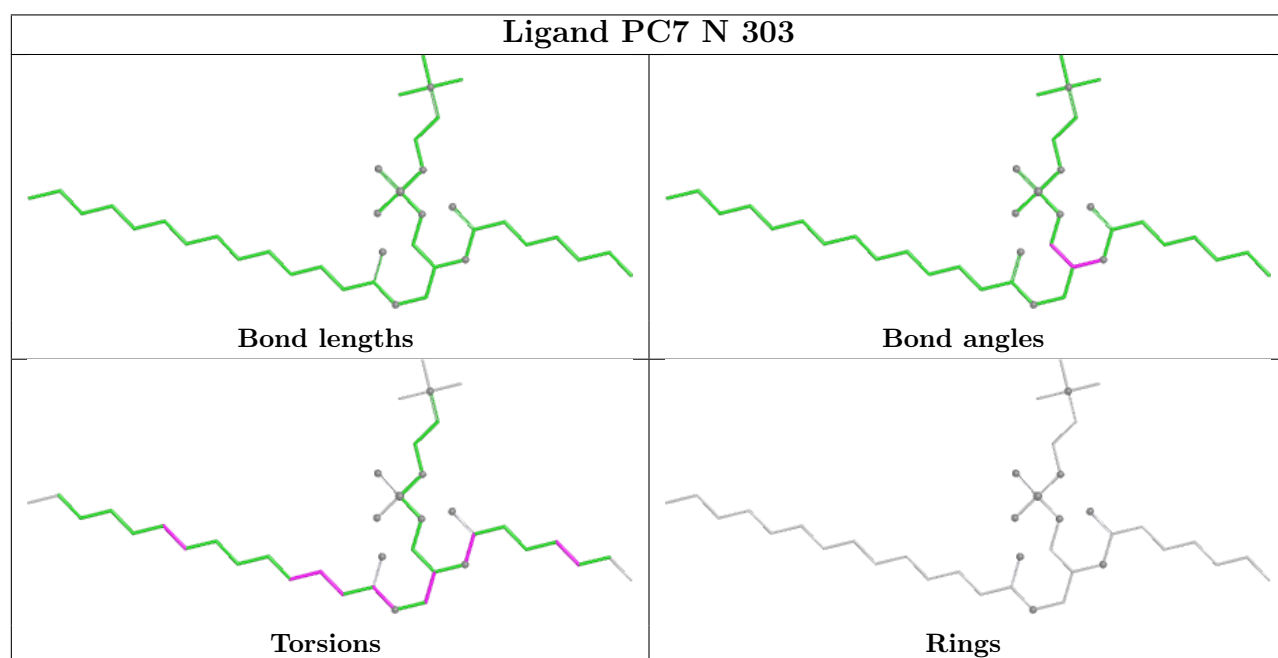
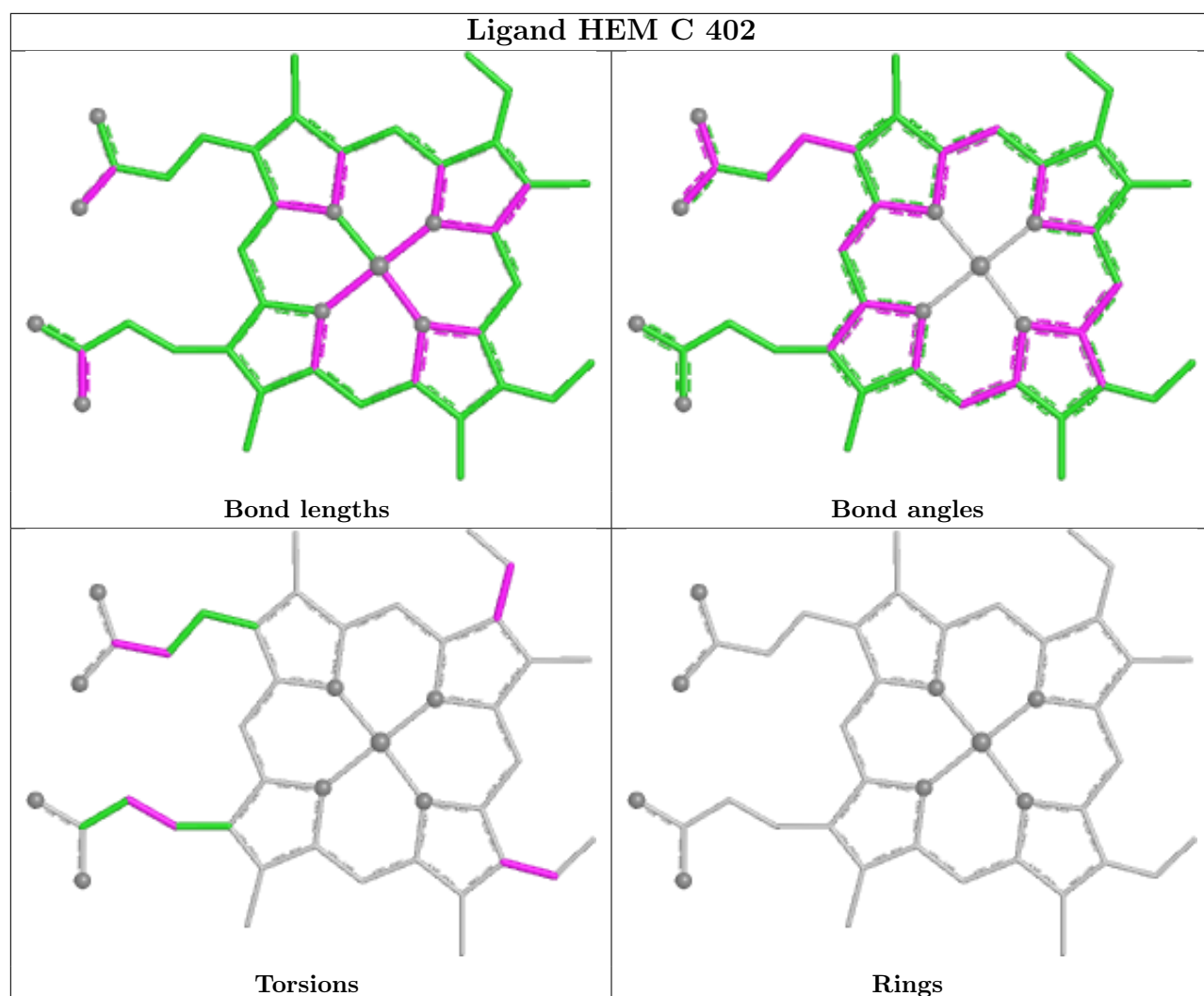


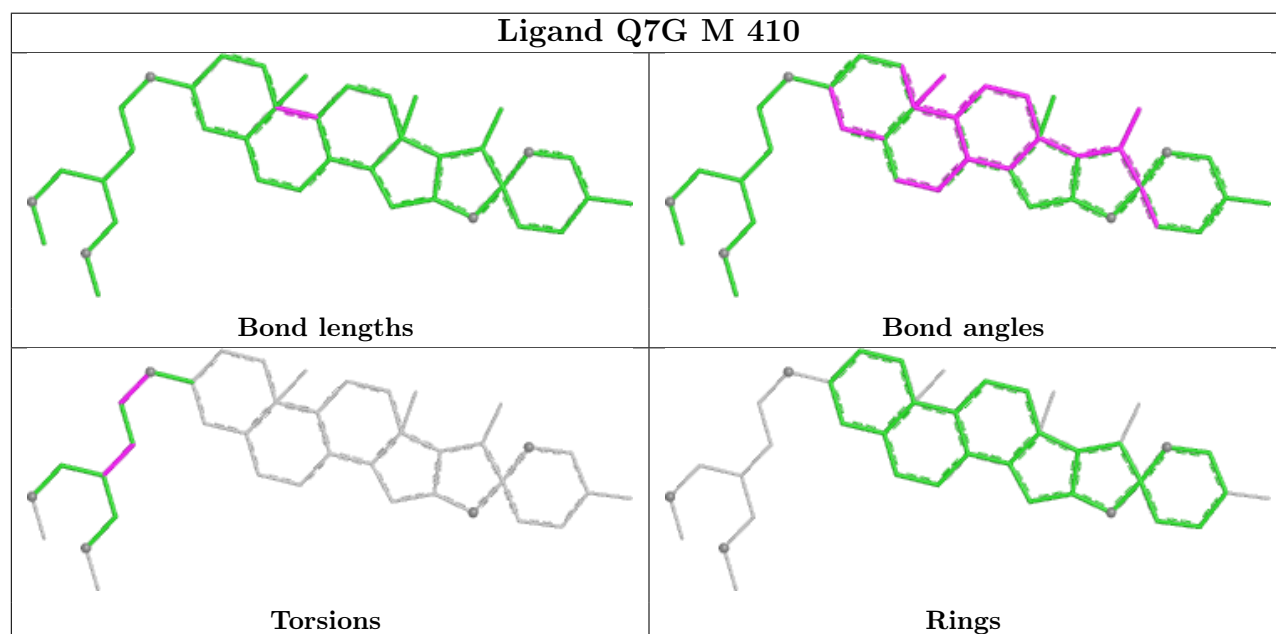
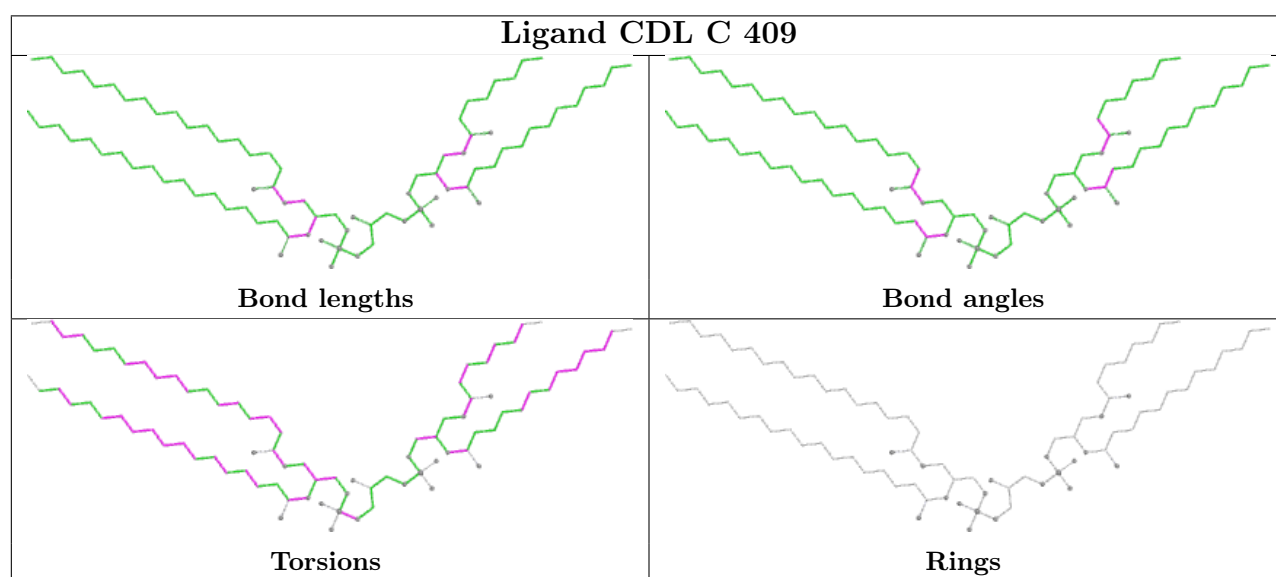
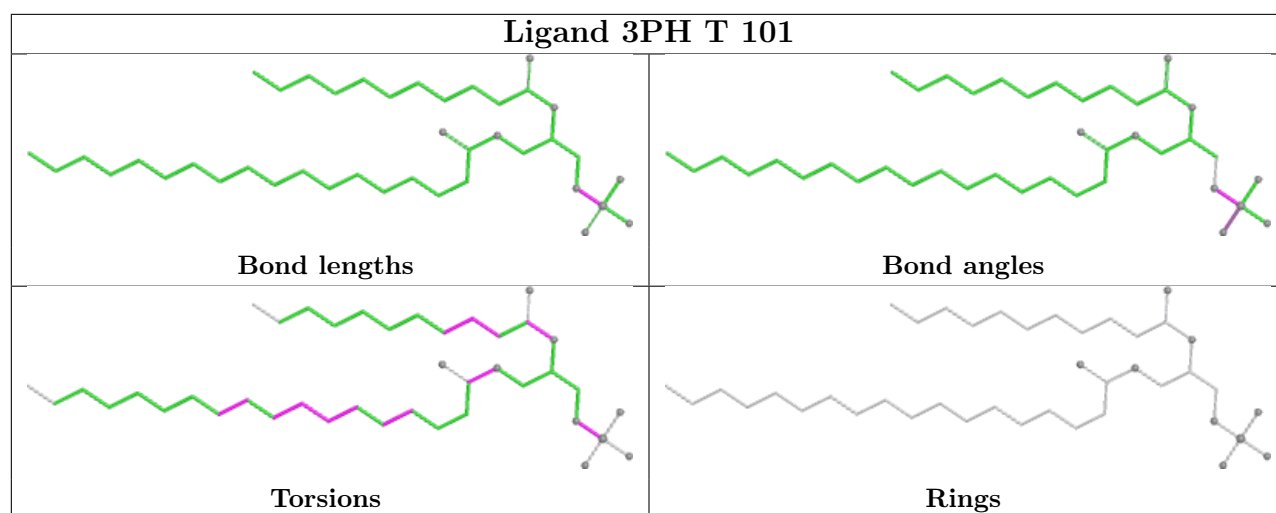


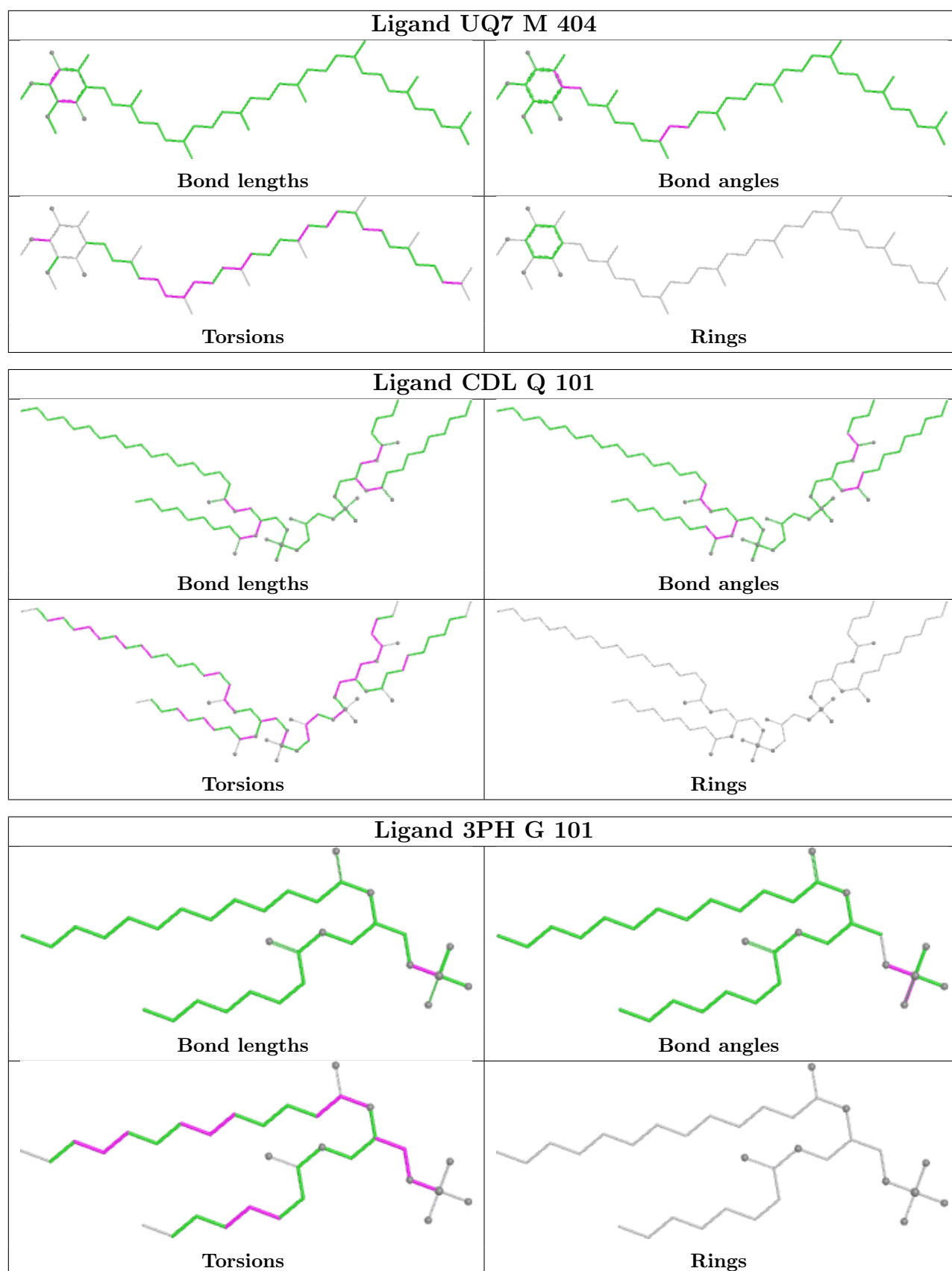


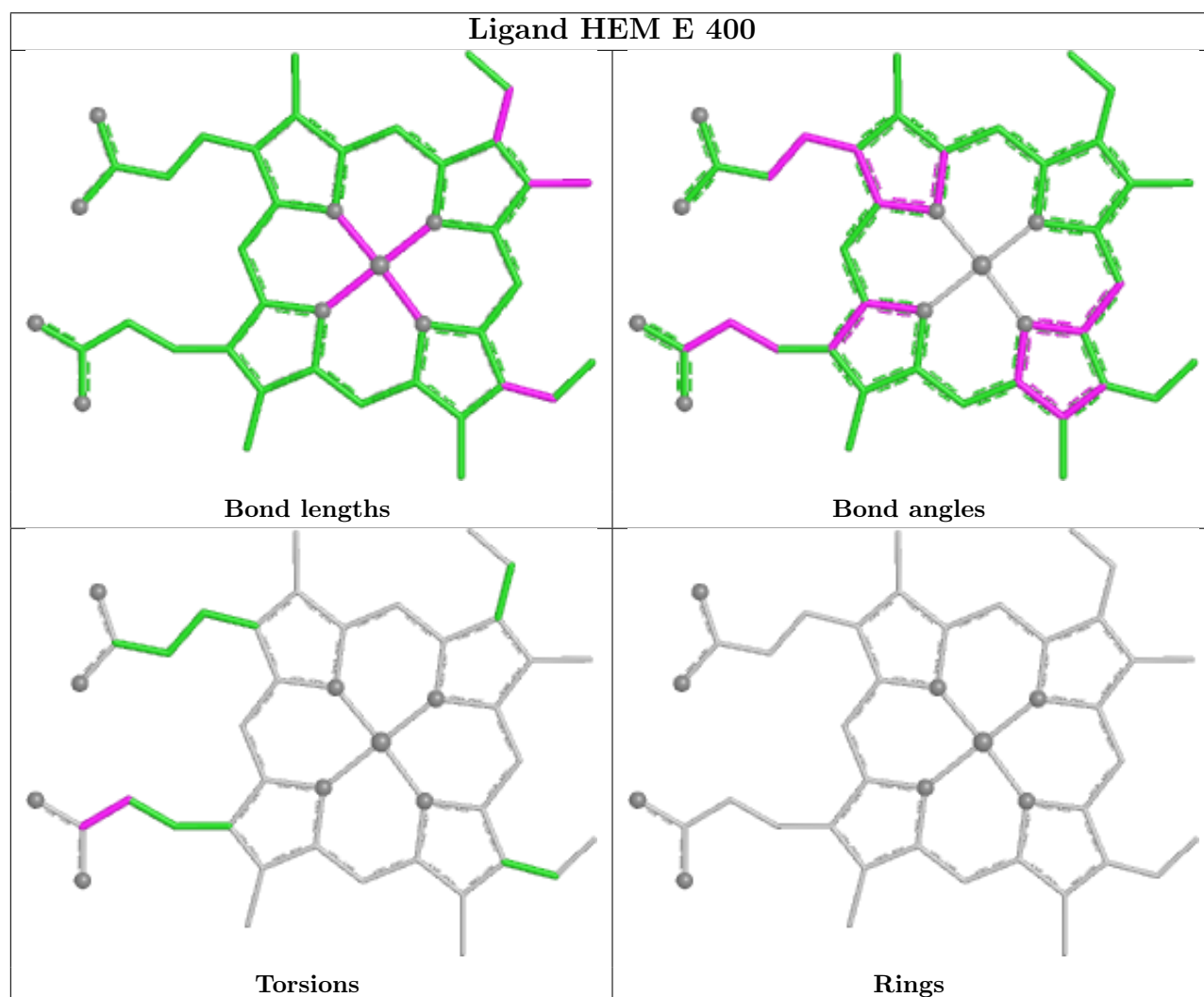
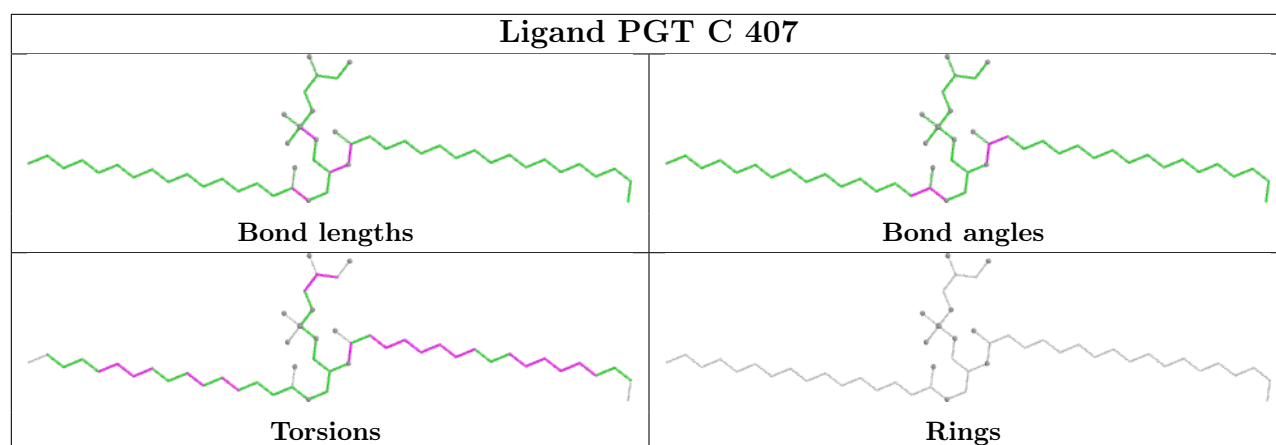


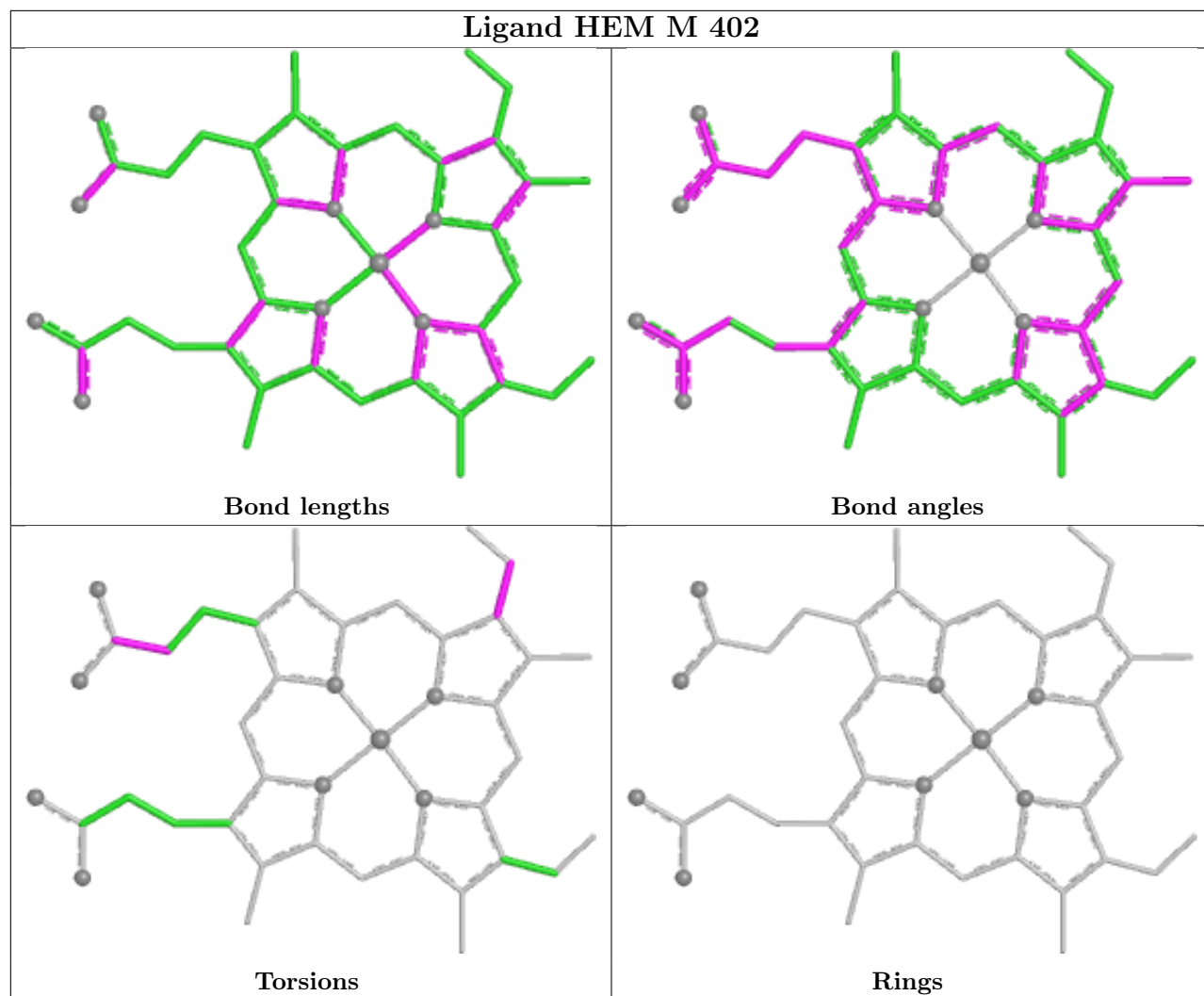


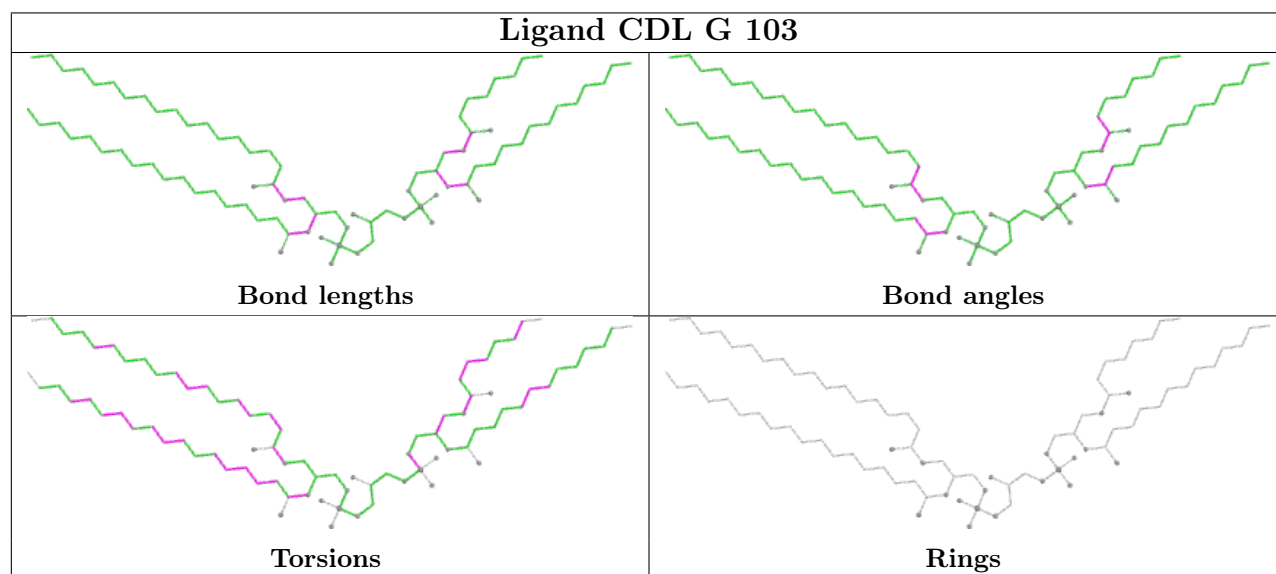
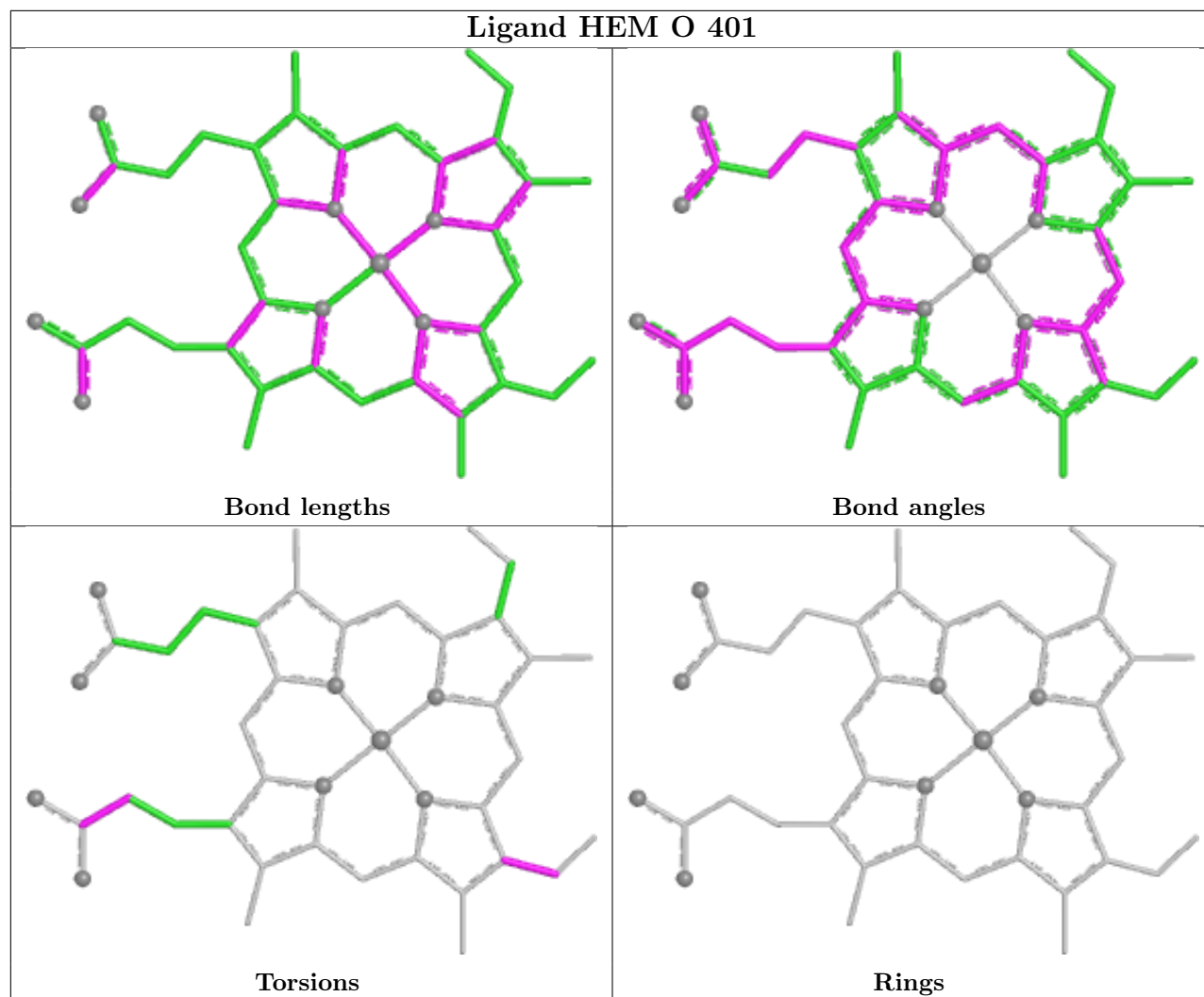


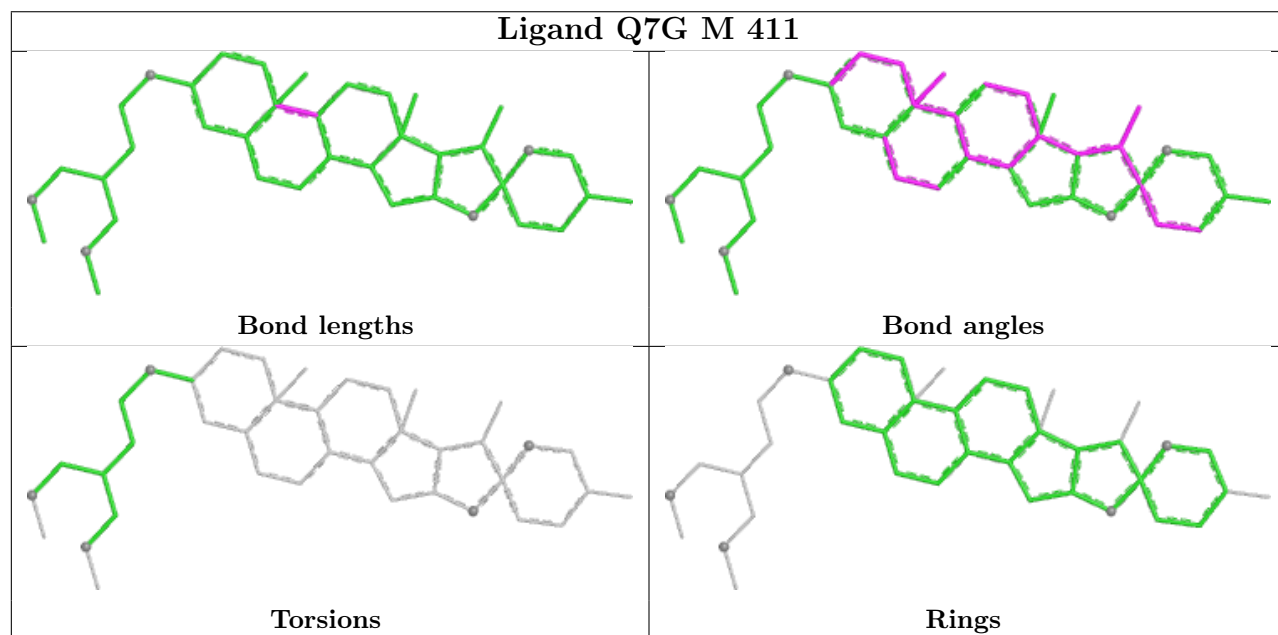
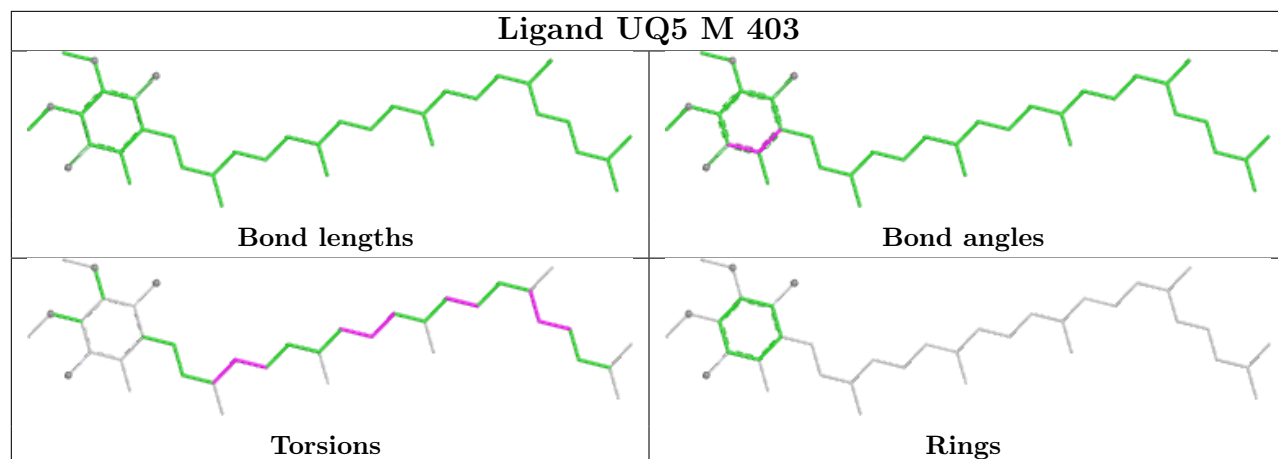




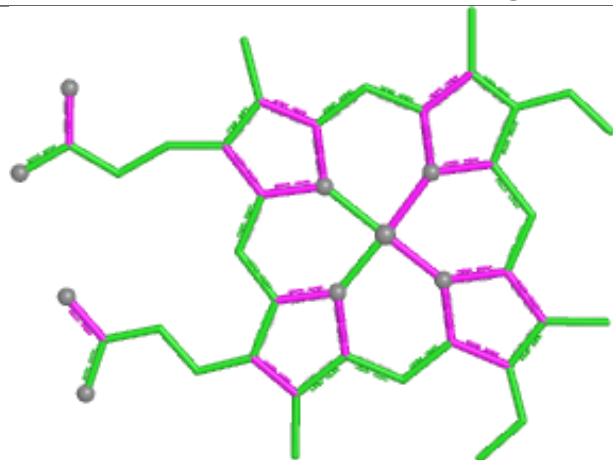




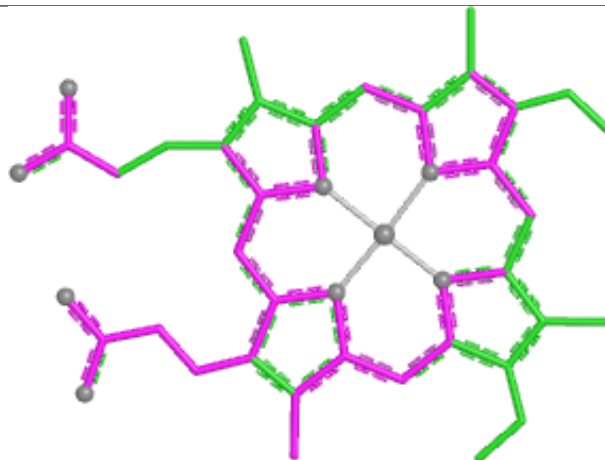




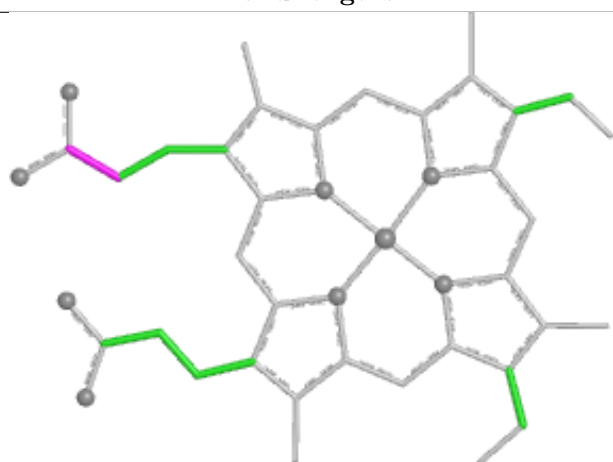
Ligand HEM M 401



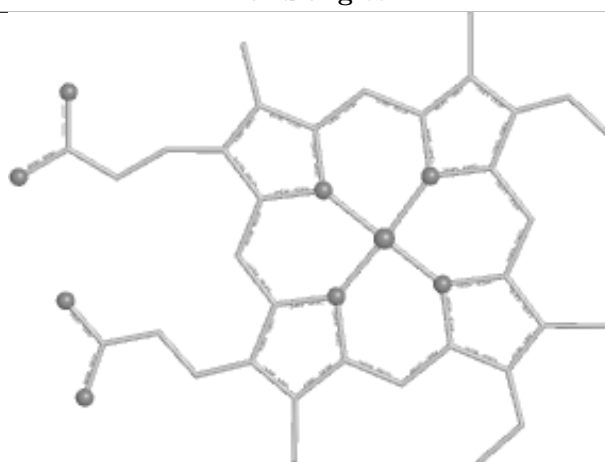
Bond lengths



Bond angles

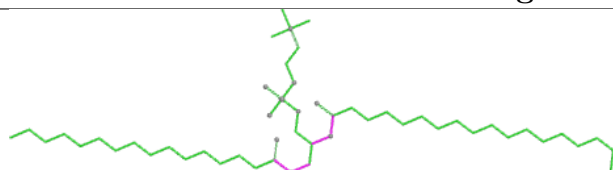


Torsions

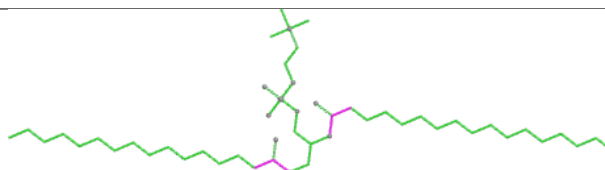


Rings

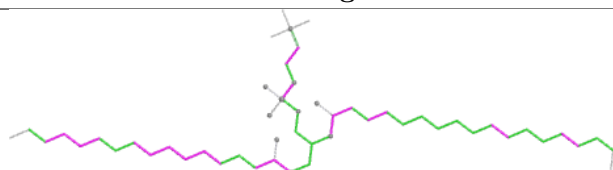
Ligand PC7 G 104



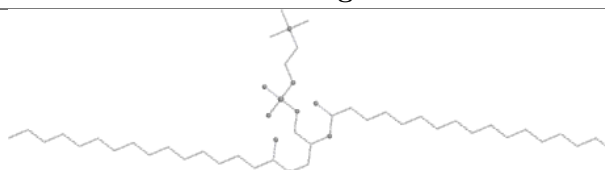
Bond lengths



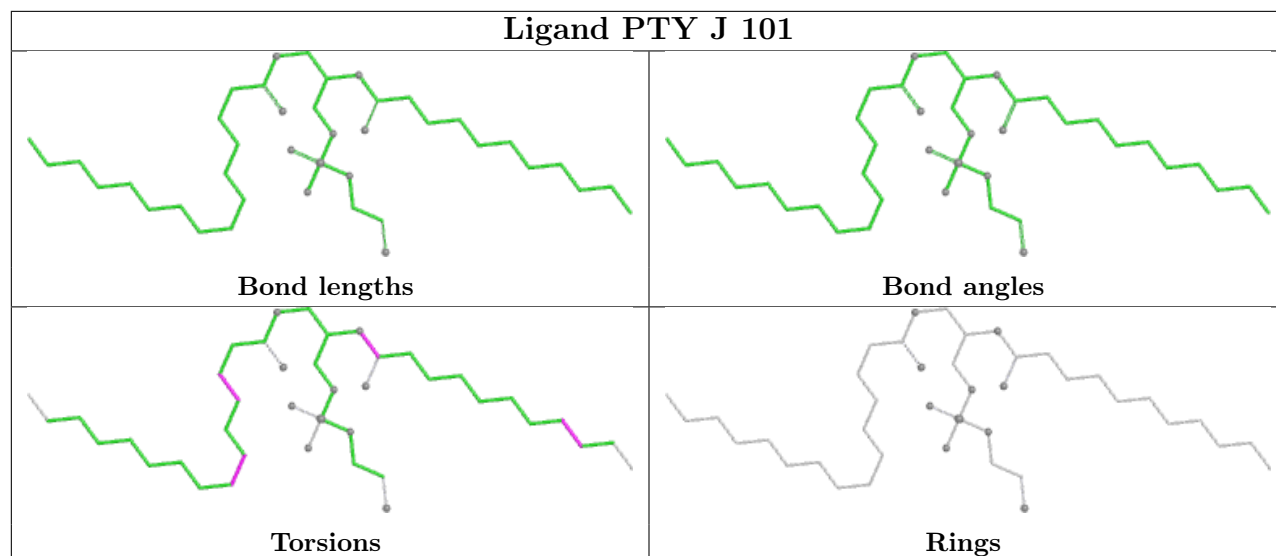
Bond angles



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.

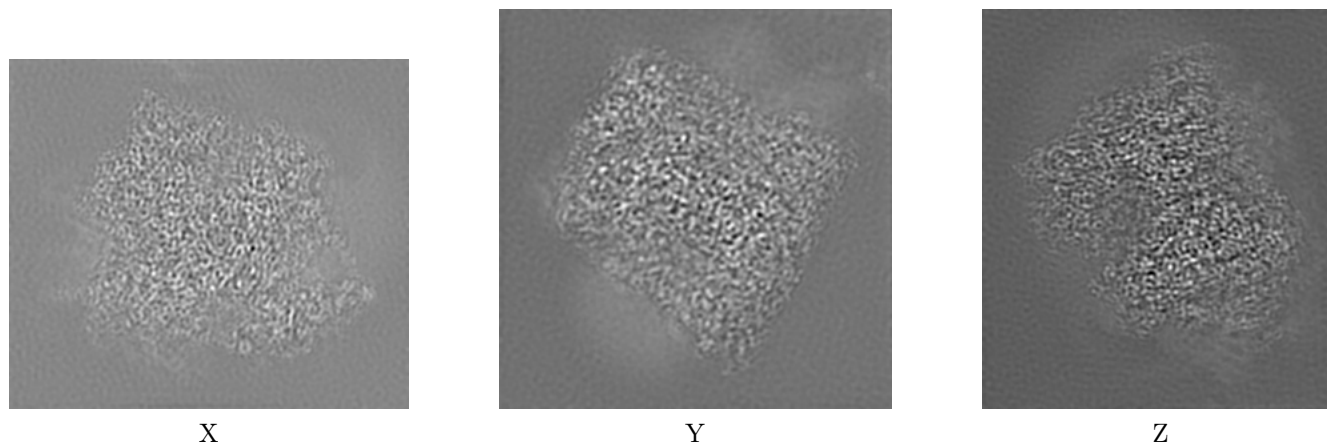
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16007. These allow visual inspection of the internal detail of the map and identification of artifacts.

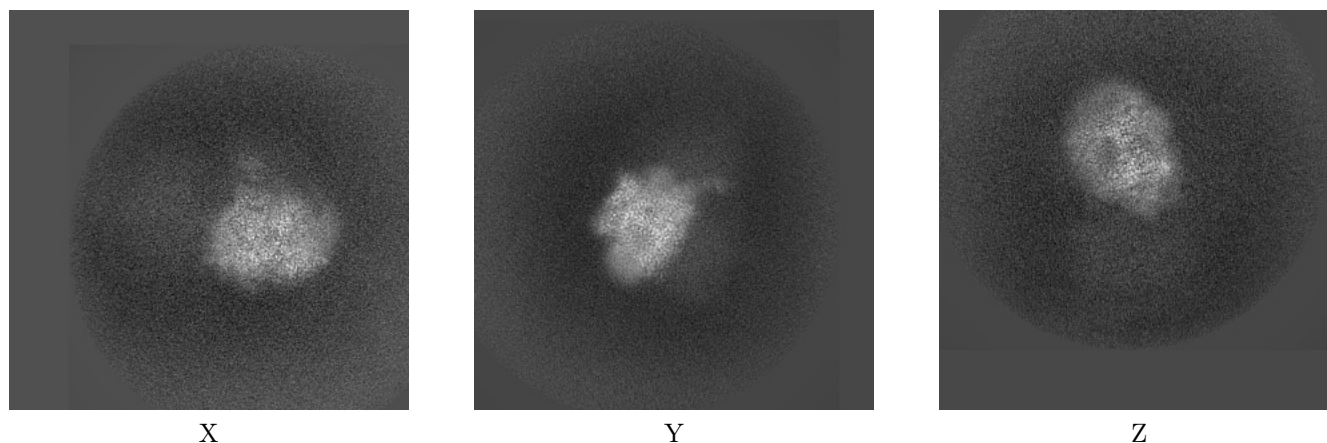
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



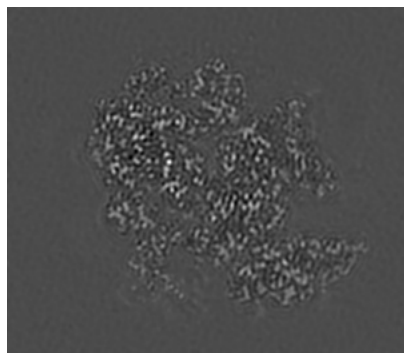
6.1.2 Raw map



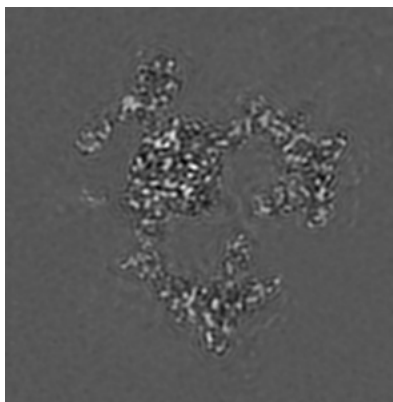
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

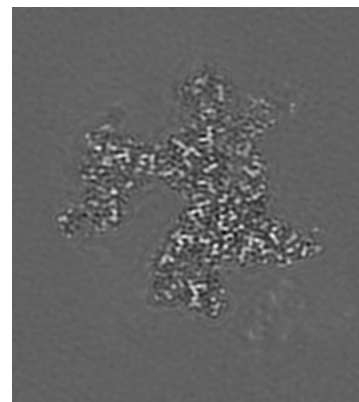
6.2.1 Primary map



X Index: 127

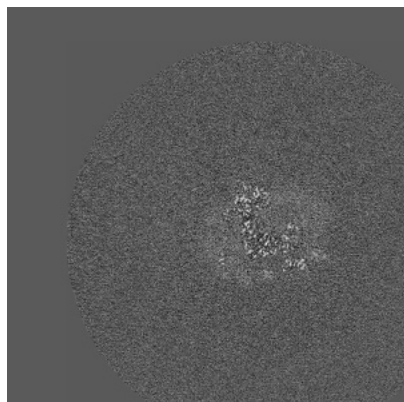


Y Index: 142

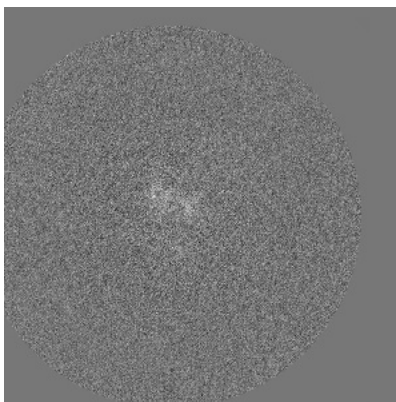


Z Index: 124

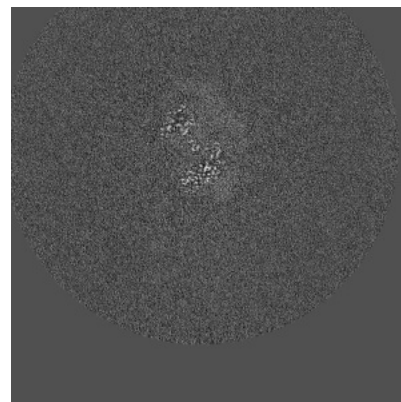
6.2.2 Raw map



X Index: 375



Y Index: 375

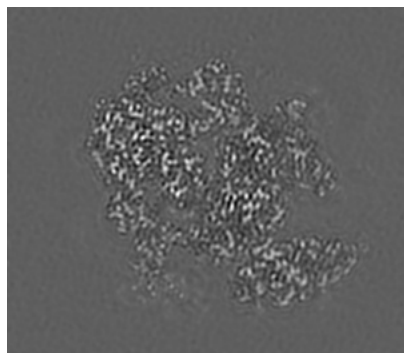


Z Index: 375

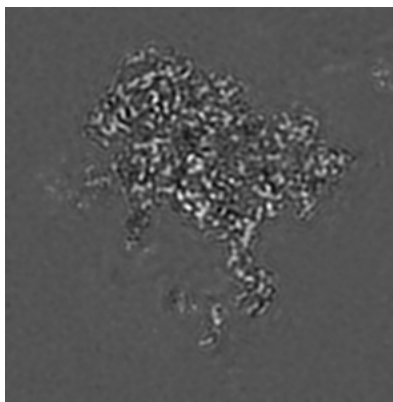
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

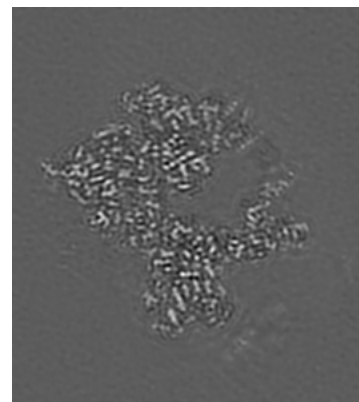
6.3.1 Primary map



X Index: 126

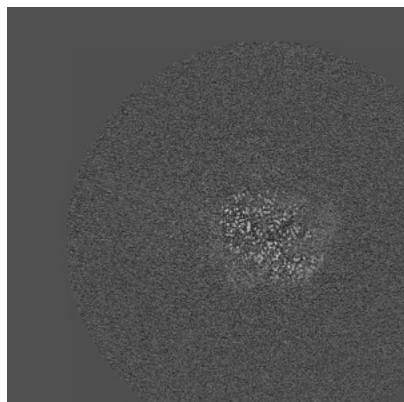


Y Index: 121

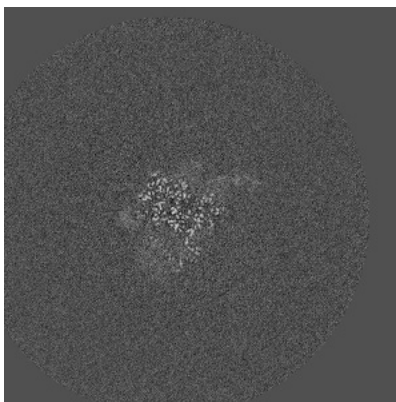


Z Index: 146

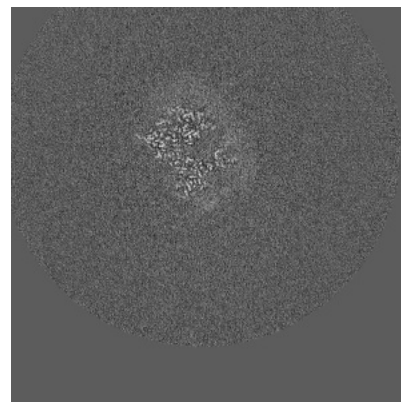
6.3.2 Raw map



X Index: 343



Y Index: 458

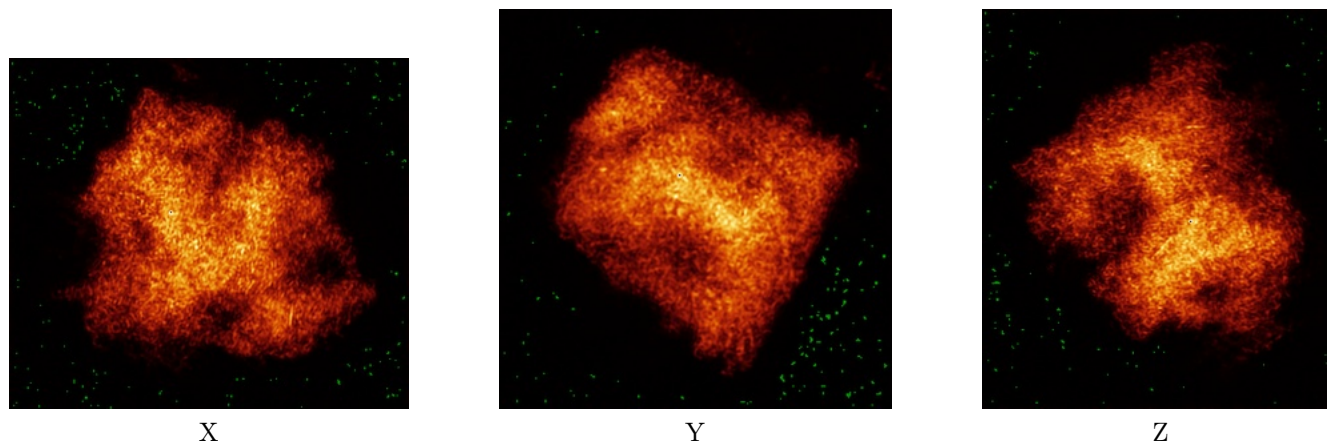


Z Index: 344

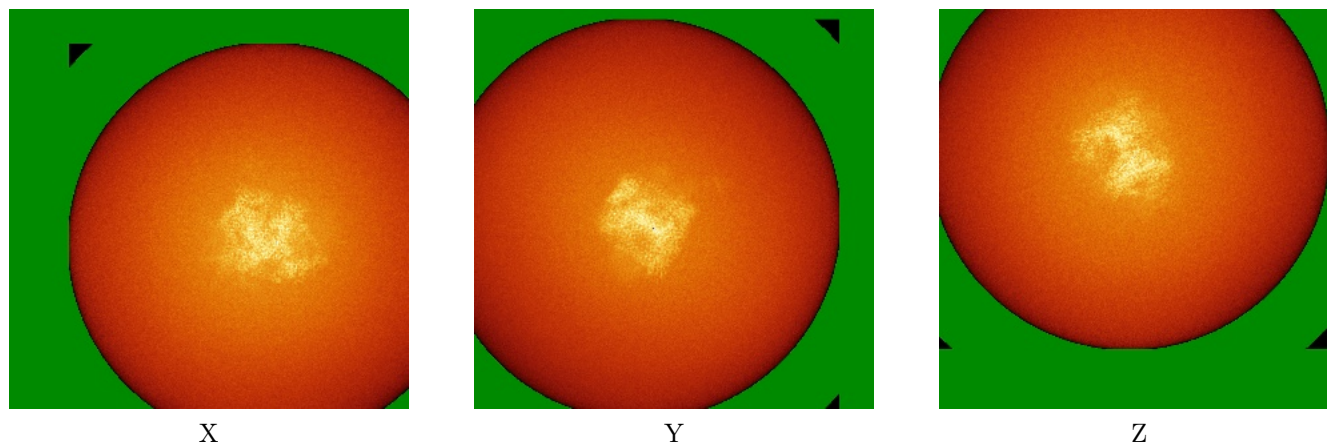
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

6.4.1 Primary map



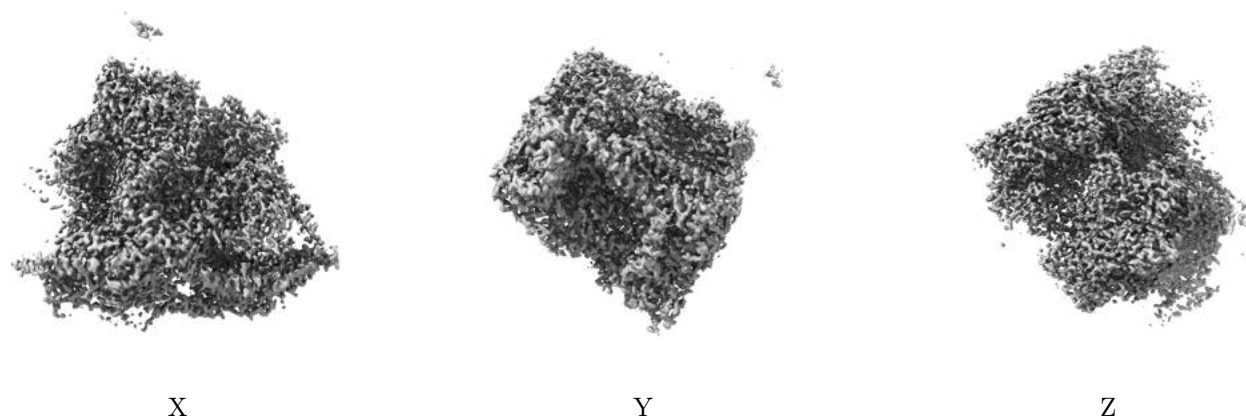
6.4.2 Raw map



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.

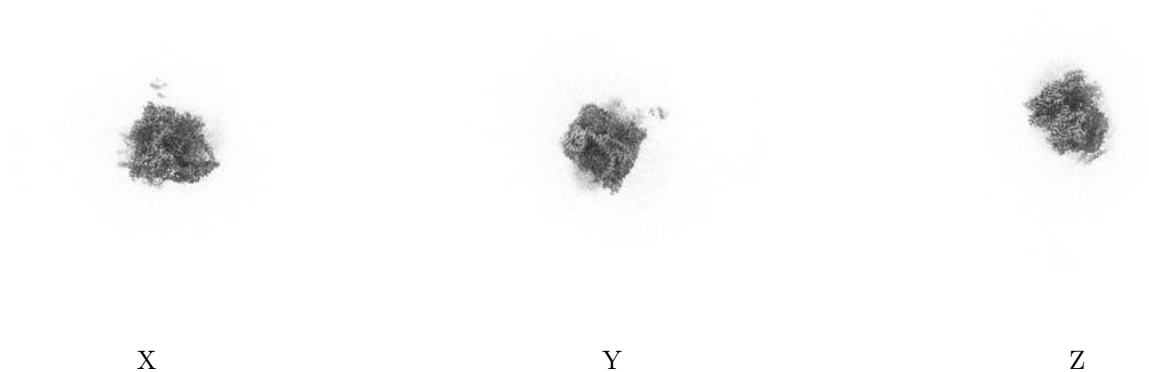
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.6. 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



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.

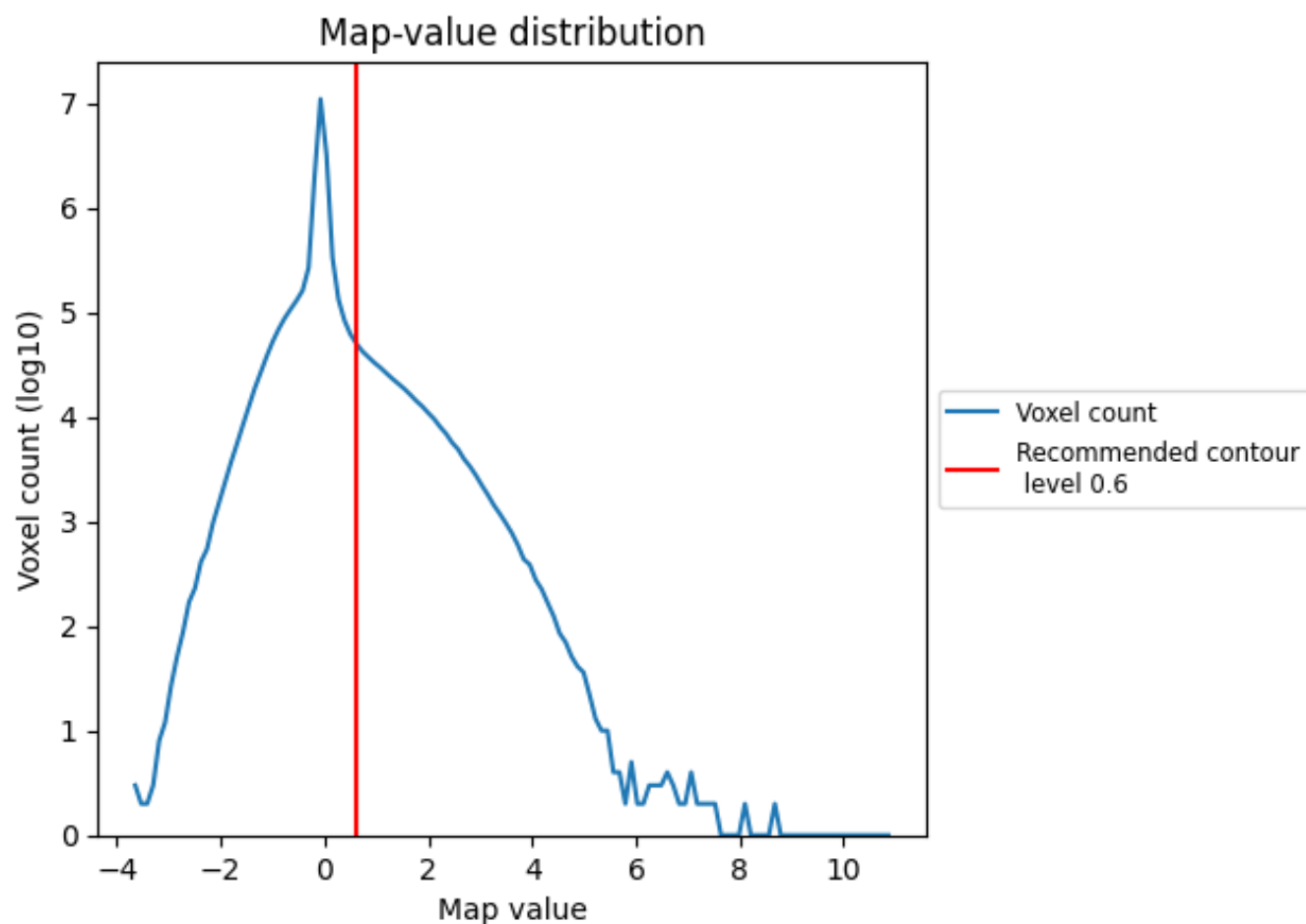
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

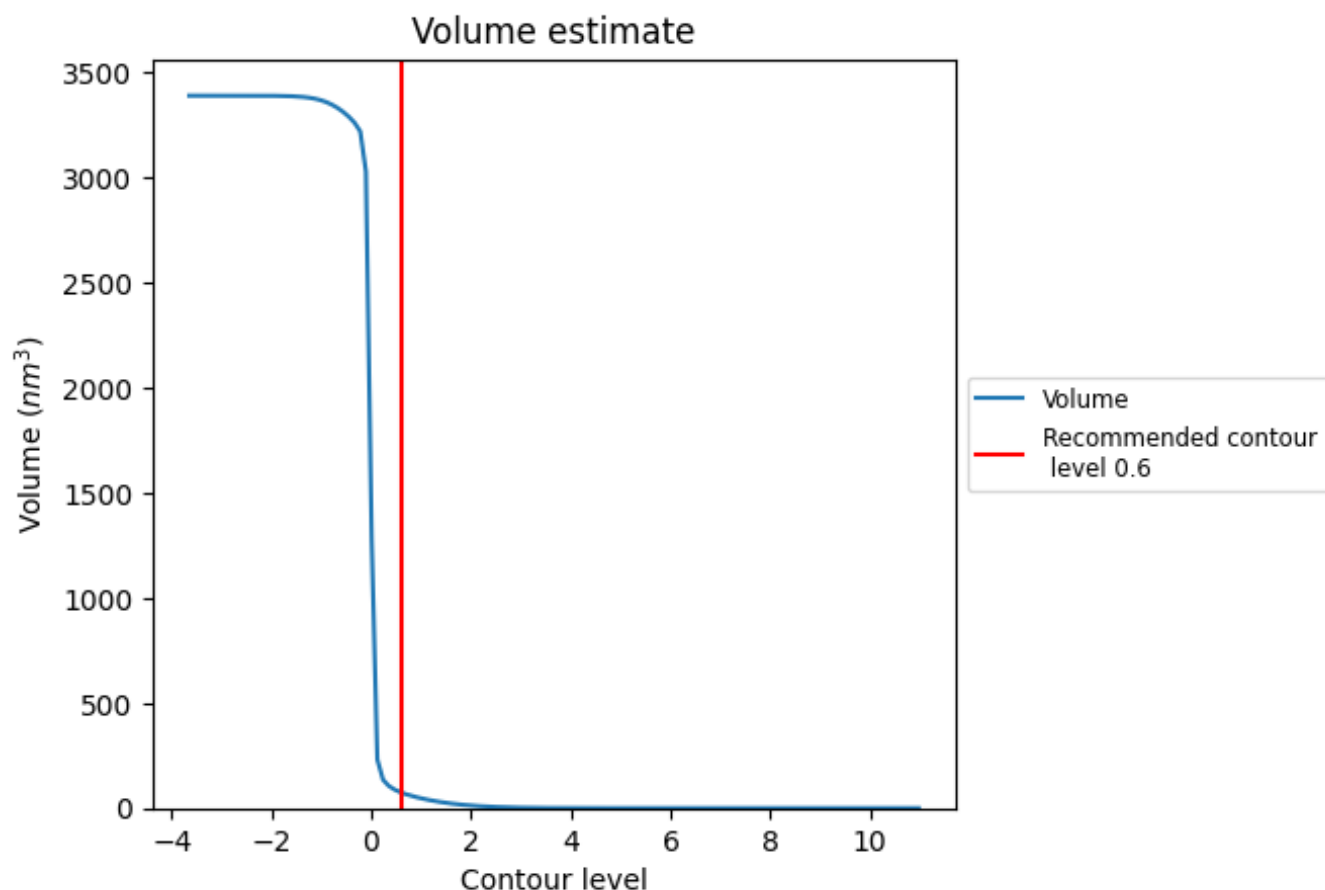
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

7.2 Volume estimate [i](#)



The volume at the recommended contour level is 75 nm³; this corresponds to an approximate mass of 68 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.

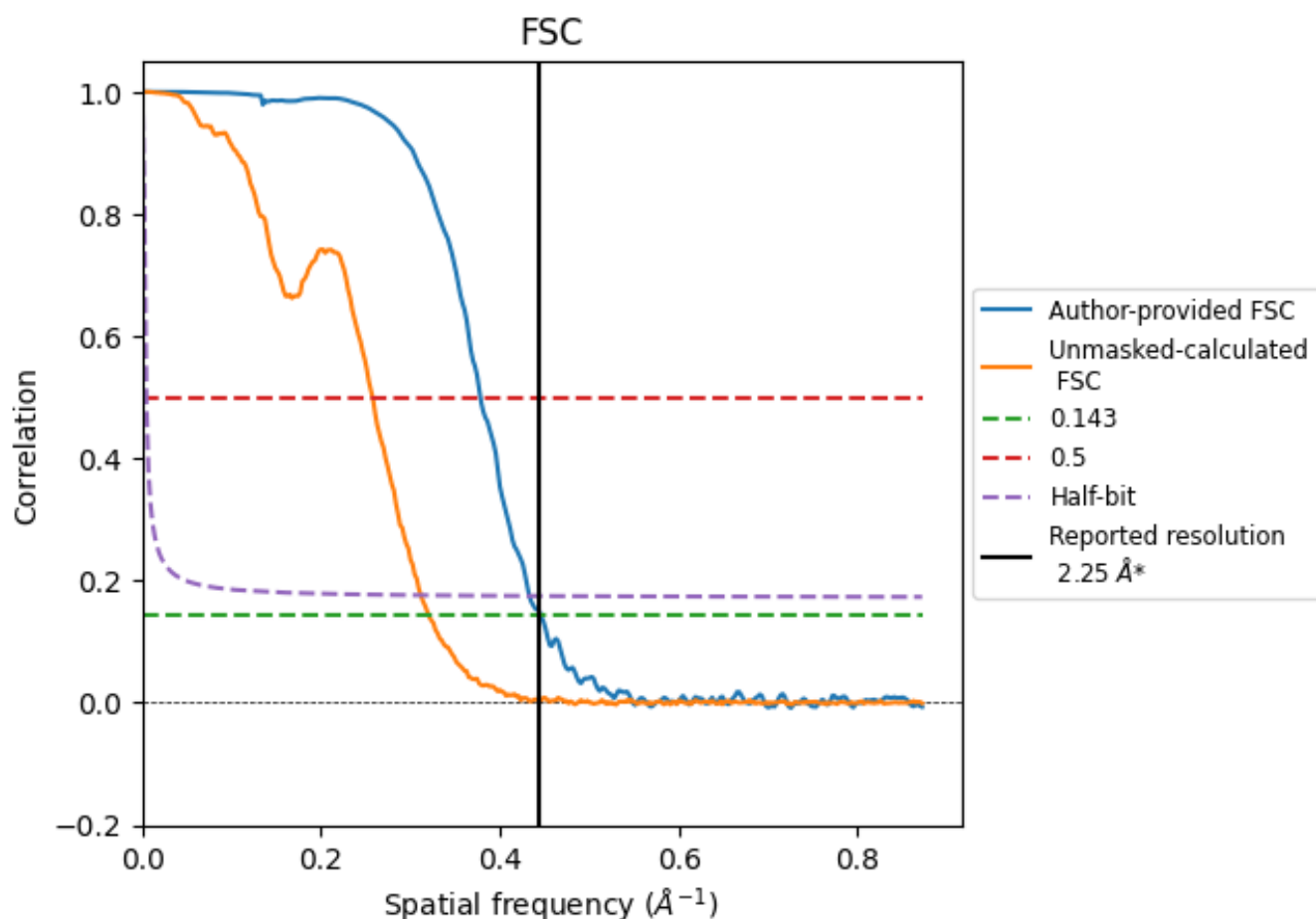
7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.444 Å⁻¹

8.2 Resolution estimates [i](#)

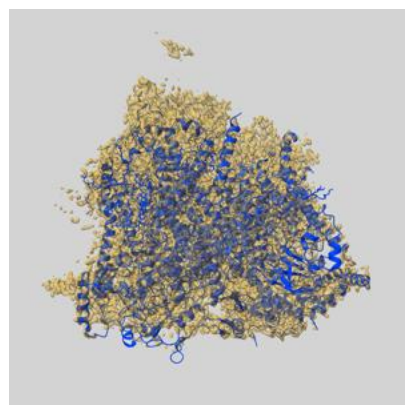
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.25	-	-
Author-provided FSC curve	2.24	2.64	2.31
Unmasked-calculated*	3.12	3.88	3.21

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.12 differs from the reported value 2.25 by more than 10 %

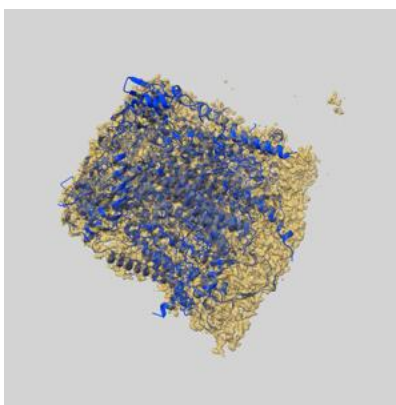
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-16007 and PDB model 8BEL. Per-residue inclusion information can be found in [section 3](#) on [page 15](#).

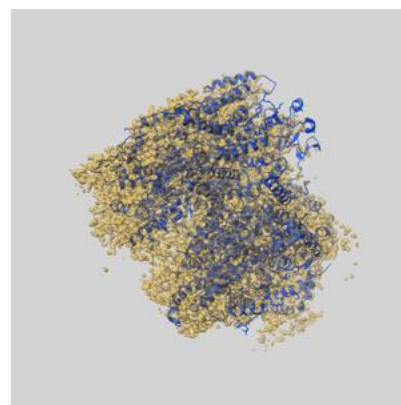
9.1 Map-model overlay [i](#)



X



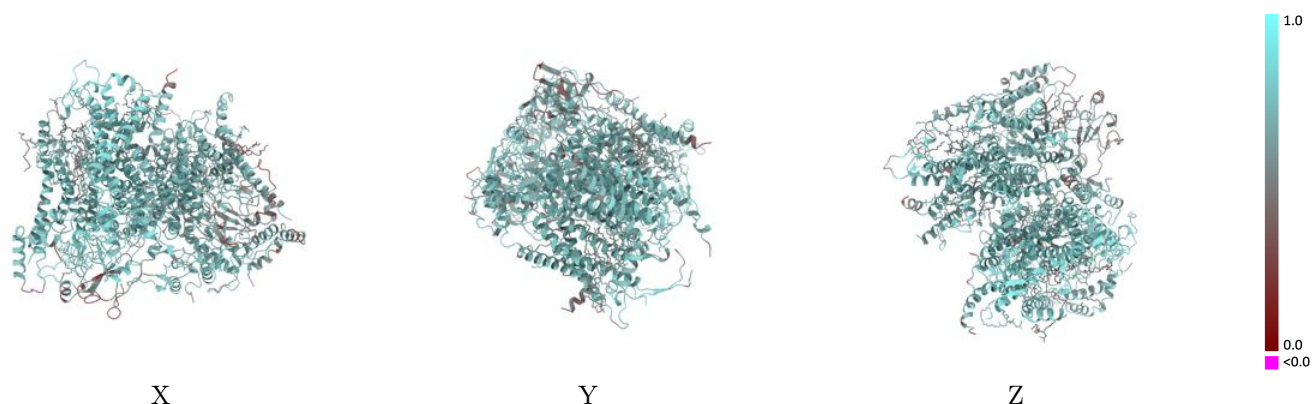
Y



Z

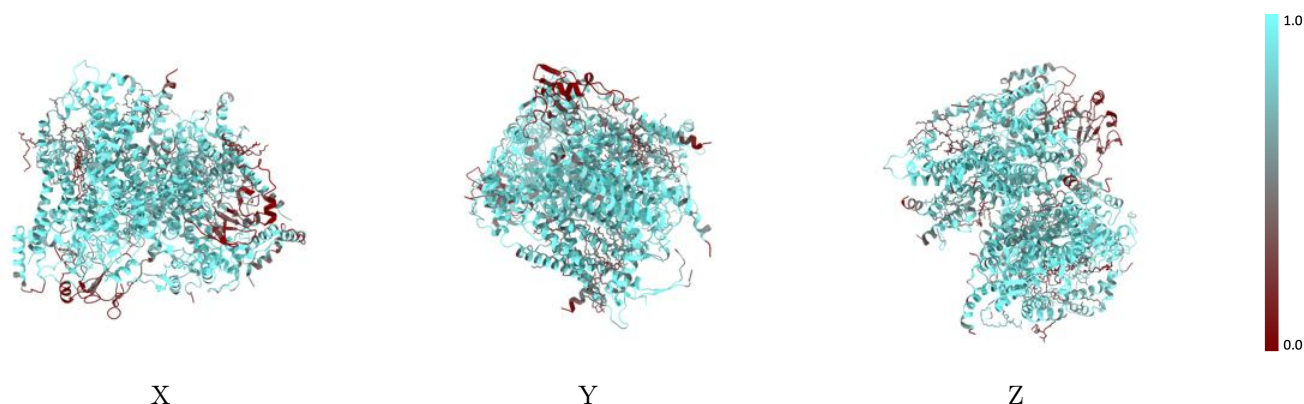
The images above show the 3D surface view of the map at the recommended contour level 0.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



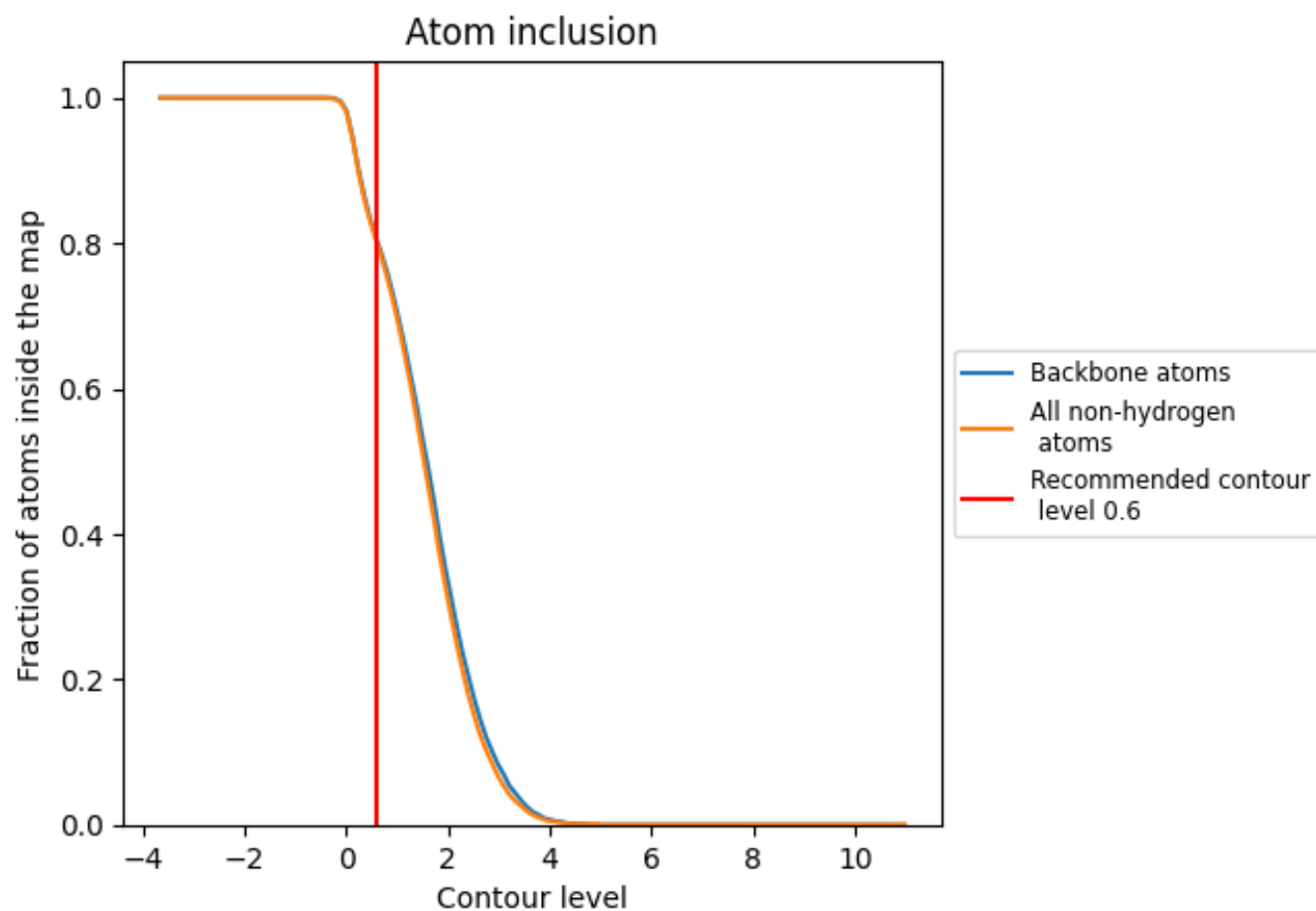
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (0.6).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 80% 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 (0.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8020	 0.6820
C	 0.9050	 0.7310
D	 0.5210	 0.5940
E	 0.9330	 0.7410
G	 0.7630	 0.6610
H	 0.7980	 0.6640
I	 0.8270	 0.7040
J	 0.4560	 0.5700
M	 0.8830	 0.7050
N	 0.5570	 0.5950
O	 0.8840	 0.7010
Q	 0.7650	 0.6440
R	 0.6490	 0.5850
S	 0.7690	 0.6440
T	 0.5490	 0.6090

