



Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 02:30 AM JST

PDB ID : 8IUJ / pdb_00008iuj
EMDB ID : EMD-35723
Title : Cryo-EM structure of Euglena gracilis super-complex III2+IV2, composite
Authors : Wu, M.C.; Tian, H.T.; He, Z.X.; Hu, Y.Q.; Zhou, L.
Deposited on : 2023-03-24
Resolution : 3.06 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.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
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) : 2.50

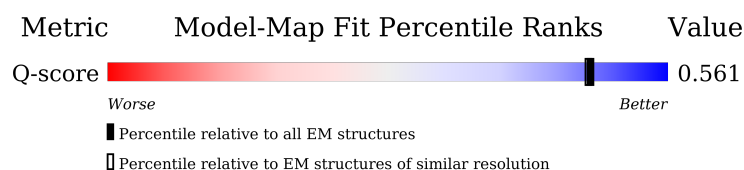
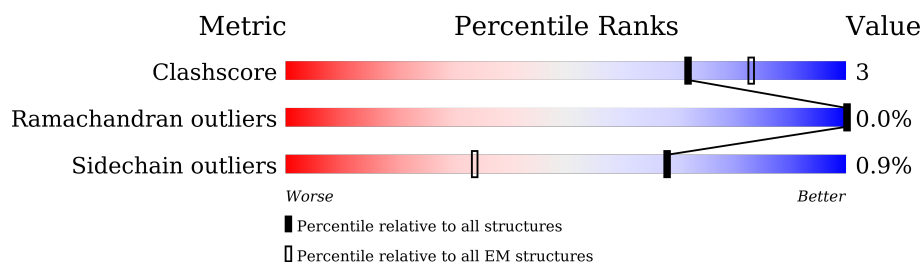
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.06 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.



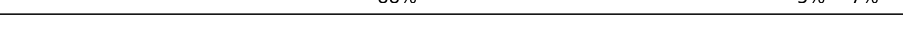
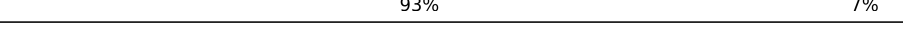
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13976 (2.56 - 3.56)

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	QA	479	
1	Qa	479	
2	QC	368	
2	Qc	368	

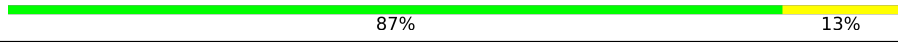
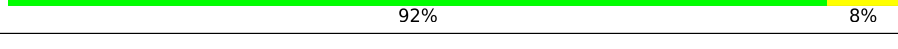
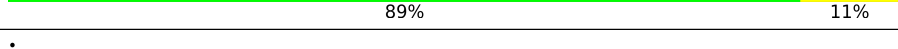
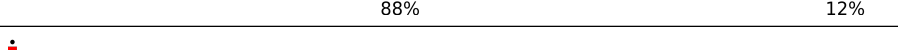
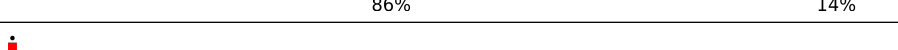
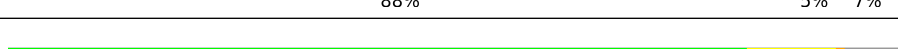
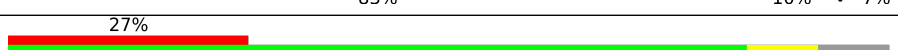
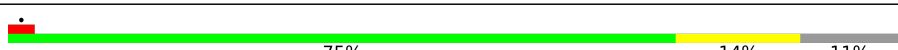
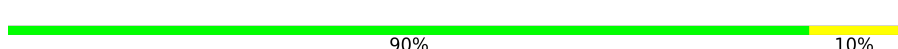
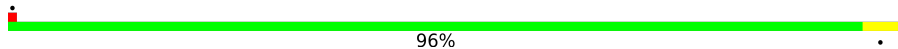
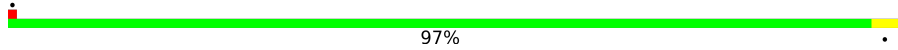
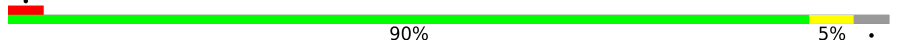
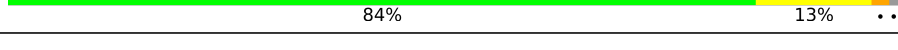
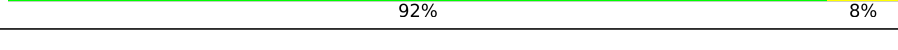
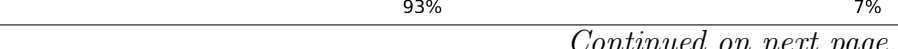
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Mol	Chain	Length	Quality of chain
3	QD	243	
3	Qd	243	
4	QH	86	
4	Qh	86	
5	QJ	154	
5	Qj	154	
6	QK	100	
6	Qk	100	
7	4A	246	
7	4a	246	
8	4C	139	
8	4c	139	
9	4E	165	
9	4e	165	
10	4H	221	
10	4h	221	
11	4J	88	
11	4j	88	
12	5C	208	
12	5c	208	
13	6A	112	
13	6a	112	
14	6B	287	
14	6b	287	
15	7C	171	

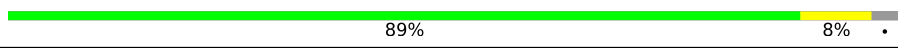
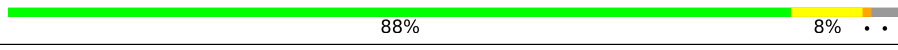
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Mol	Chain	Length	Quality of chain
15	7c	171	
16	C1	495	
16	c1	495	
17	C2	196	
17	c2	196	
18	C3	161	
18	c3	161	
19	DC	179	
19	dc	179	
20	QE	252	
20	Qe	252	
21	QF	72	
21	Qf	72	
22	QG	228	
22	Qg	228	
23	QI	70	
23	Qi	70	
24	QB	474	
24	Qb	474	
25	5B	174	
25	5b	174	
26	4D	174	
26	4d	174	
27	4F	75	
27	4f	75	

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Mol	Chain	Length	Quality of chain
28	4G	315	
28	4g	315	
29	4I	274	
29	4i	274	
30	7A	178	
30	7a	178	

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
33	HEC	QD	301	X	-	-	-
33	HEC	Qd	301	X	-	-	-

2 Entry composition

There are 42 unique types of molecules in this entry. The entry contains 200404 atoms, of which 99661 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 MPP-beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	QA	476	Total	C	H	N	O	S	2	0
			7408	2367	3658	655	713	15		
1	Qa	476	Total	C	H	N	O	S	2	0
			7408	2367	3658	655	713	15		

- Molecule 2 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	QC	364	Total	C	H	N	O	S	0	0
			6039	2005	3064	463	494	13		
2	Qc	364	Total	C	H	N	O	S	0	0
			6039	2005	3064	463	494	13		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
3	QD	241	Total	C	H	N	O	S	0	0
			3817	1261	1858	337	353	8		
3	Qd	241	Total	C	H	N	O	S	0	0
			3817	1261	1858	337	353	8		

- Molecule 4 is a protein called UQCRQ.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	QH	85	Total	C	H	N	O	S	0	0
			1393	447	692	131	120	3		
4	Qh	85	Total	C	H	N	O	S	0	0
			1393	447	692	131	120	3		

- Molecule 5 is a protein called UQCR10.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	QJ	149	Total	C	H	N	O	S	0	0
			2418	781	1212	220	204	1		
5	Qj	149	Total	C	H	N	O	S	0	0
			2418	781	1212	220	204	1		

- Molecule 6 is a protein called Ubiquinol-cytochrome-C reductase complex subunit IX, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	QK	61	Total	C	H	N	O	S	0	0
			984	325	499	79	78	3		
6	Qk	61	Total	C	H	N	O	S	0	0
			984	325	499	79	78	3		

- Molecule 7 is a protein called COXEG1.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	4a	204	Total	C	H	N	O	S	0	0
			3220	1054	1608	267	285	6		
7	4A	204	Total	C	H	N	O	S	0	0
			3220	1054	1608	267	285	6		

- Molecule 8 is a protein called COXEG3.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	4c	123	Total	C	H	N	O	S	0	0
			2049	670	1027	168	183	1		
8	4C	123	Total	C	H	N	O	S	0	0
			2049	670	1027	168	183	1		

- Molecule 9 is a protein called COXEG5.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	4e	160	Total	C	H	N	O	S	0	0
			2612	859	1279	220	247	7		
9	4E	160	Total	C	H	N	O	S	0	0
			2612	859	1279	220	247	7		

- Molecule 10 is a protein called COXEG8.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	4h	205	Total	C	H	N	O		0	0
			3250	1040	1644	260	306			

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	4H	205	Total	C	H	N	O	0	0
			3250	1040	1644	260	306		

- Molecule 11 is a protein called COXEG10.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	4j	88	Total	C	H	N	O	S	0	0
			1399	459	688	126	124	2		
11	4J	88	Total	C	H	N	O	S	0	0
			1399	459	688	126	124	2		

- Molecule 12 is a protein called COX5c.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	5c	196	Total	C	H	N	O	S	0	0
			3117	1026	1546	253	283	9		
12	5C	196	Total	C	H	N	O	S	0	0
			3117	1026	1546	253	283	9		

- Molecule 13 is a protein called COX6a.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	6a	91	Total	C	H	N	O	S	0	0
			1497	498	747	128	120	4		
13	6A	111	Total	C	H	N	O	S	0	0
			1829	608	909	157	150	5		

- Molecule 14 is a protein called COX6b-1.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	6b	282	Total	C	H	N	O	S	0	0
			4512	1455	2227	396	427	7		
14	6B	282	Total	C	H	N	O	S	0	0
			4514	1455	2229	396	427	7		

- Molecule 15 is a protein called COX7c.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	7c	151	Total	C	H	N	O	S	0	0
			2437	821	1183	204	226	3		
15	7C	151	Total	C	H	N	O	S	0	0
			2437	821	1183	204	226	3		

- Molecule 16 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	c1	495	Total	C	H	N	O	S	0	0
			7918	2635	3980	614	664	25		
16	C1	495	Total	C	H	N	O	S	0	0
			7918	2635	3980	614	664	25		

- Molecule 17 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	c2	196	Total	C	H	N	O	S	0	0
			3232	1046	1647	262	272	5		
17	C2	196	Total	C	H	N	O	S	0	0
			3232	1046	1647	262	272	5		

- Molecule 18 is a protein called Putative NADH dehydrogenase subunit 6.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	c3	161	Total	C	H	N	O	S	0	0
			2791	935	1413	213	226	4		
18	C3	161	Total	C	H	N	O	S	0	0
			2791	935	1413	213	226	4		

- Molecule 19 is a protein called COX4.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	dc	167	Total	C	H	N	O	S	0	0
			2728	887	1362	239	235	5		
19	DC	167	Total	C	H	N	O	S	0	0
			2728	887	1362	239	235	5		

- Molecule 20 is a protein called UQCRFS1.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	QE	231	Total	C	H	N	O	S	0	0
			3571	1143	1776	310	330	12		
20	Qe	231	Total	C	H	N	O	S	0	0
			3571	1143	1776	310	330	12		

- Molecule 21 is a protein called UQCRH.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	QF	64	Total	C	H	N	O	S	0	0
			1016	325	501	91	93	6		
21	Qf	64	Total	C	H	N	O	S	0	0
			1016	325	501	91	93	6		

- Molecule 22 is a protein called UQCRB.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	QG	228	Total	C	H	N	O	S	0	0
			3802	1232	1870	341	351	8		
22	Qg	228	Total	C	H	N	O	S	0	0
			3802	1232	1870	341	351	8		

- Molecule 23 is a protein called UQCR9.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	QI	70	Total	C	H	N	O	S	0	0
			741	290	292	77	81	1		
23	Qi	70	Total	C	H	N	O	S	0	0
			742	290	293	77	81	1		

- Molecule 24 is a protein called Ubiquinol-cytochrome-c reductase complex core protein 2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	Qb	455	Total	C	H	N	O	S	0	0
			6889	2205	3431	585	665	3		
24	QB	455	Total	C	H	N	O	S	0	0
			6889	2205	3431	585	665	3		

- Molecule 25 is a protein called COX5b-2.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	5B	157	Total	C	H	N	O	S	0	0
			2442	807	1184	208	237	6		
25	5b	157	Total	C	H	N	O	S	0	0
			2442	807	1184	208	237	6		

- Molecule 26 is a protein called COXEG4.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	4D	173	Total	C	H	N	O	S	0	0
			2708	863	1359	237	240	9		

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Mol	Chain	Residues	Atoms						AltConf	Trace
26	4d	173	Total	C	H	N	O	S	0	0
			2708	863	1359	237	240	9		

- Molecule 27 is a protein called COXEG6.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	4F	75	Total	C	H	N	O	S	0	0
			1246	418	626	98	103	1		
27	4f	75	Total	C	H	N	O	S	0	0
			1246	418	626	98	103	1		

- Molecule 28 is a protein called COXEG7.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	4G	297	Total	C	H	N	O	S	0	0
			4690	1478	2339	408	457	8		
28	4g	297	Total	C	H	N	O	S	0	0
			4690	1478	2339	408	457	8		

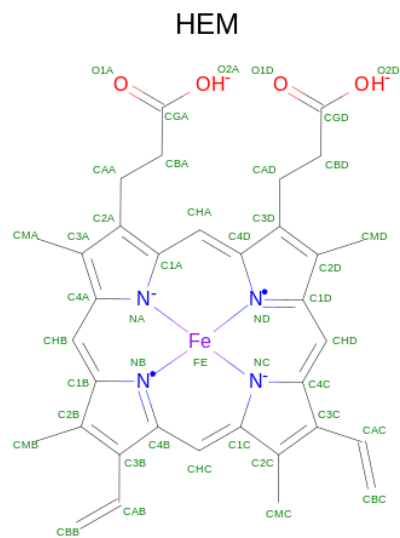
- Molecule 29 is a protein called COXEG9.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	4I	265	Total	C	H	N	O	S	0	0
			4224	1411	2046	374	388	5		
29	4i	265	Total	C	H	N	O	S	0	0
			4224	1411	2046	374	388	5		

- Molecule 30 is a protein called COX7a.

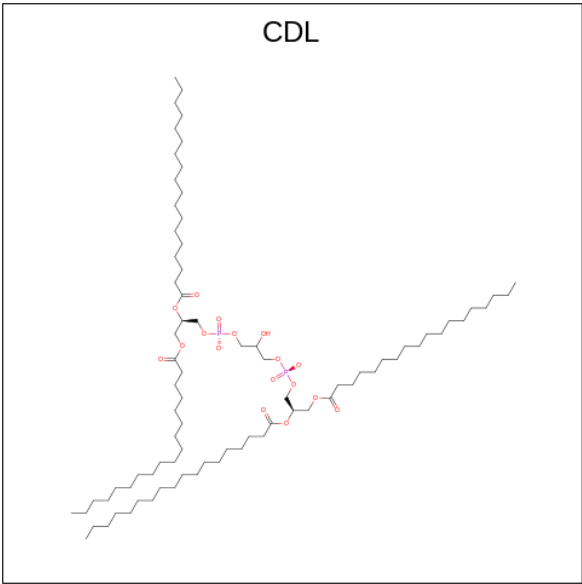
Mol	Chain	Residues	Atoms						AltConf	Trace
30	7a	165	Total	C	H	N	O	S	0	0
			2603	838	1284	248	226	7		
30	7A	165	Total	C	H	N	O	S	0	0
			2603	838	1284	248	226	7		

- Molecule 31 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄) (labeled as "Ligand of Interest" by depositor).



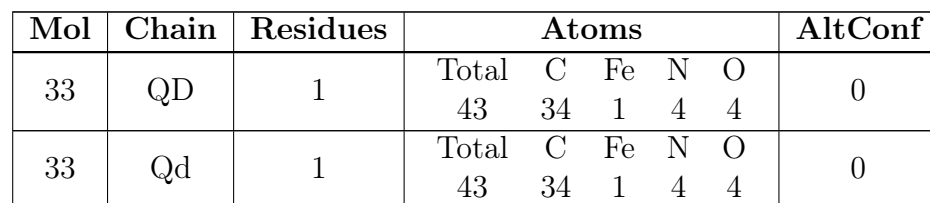
Mol	Chain	Residues	Atoms					AltConf
31	QC	1	Total 43	C 34	Fe 1	N 4	O 4	0
31	QC	1	Total 43	C 34	Fe 1	N 4	O 4	0
31	Qc	1	Total 43	C 34	Fe 1	N 4	O 4	0
31	Qc	1	Total 43	C 34	Fe 1	N 4	O 4	0

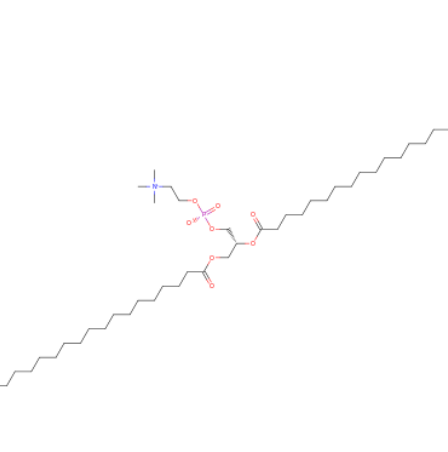
- Molecule 32 is CARDIOLIPIN (CCD ID: CDL) (formula: $\text{C}_{81}\text{H}_{156}\text{O}_{17}\text{P}_2$).



Mol	Chain	Residues	Atoms					AltConf
32	QC	1	Total	C	H	O	P	0
			112	37	56	17	2	
32	QD	1	Total	C	H	O	P	0
			151	50	82	17	2	
32	QH	1	Total	C	H	O	P	0
			175	57	99	17	2	
32	QJ	1	Total	C	H	O	P	0
			118	39	60	17	2	
32	Qc	1	Total	C	H	O	P	0
			106	35	52	17	2	
32	Qd	1	Total	C	H	O	P	0
			256	81	156	17	2	
32	Qh	1	Total	C	H	O	P	0
			139	46	74	17	2	
32	Qh	1	Total	C	H	O	P	0
			124	41	64	17	2	
32	Qj	1	Total	C	H	O	P	0
			88	29	40	17	2	
32	4c	1	Total	C	H	O	P	0
			157	51	87	17	2	
32	4e	1	Total	C	H	O	P	0
			163	53	91	17	2	
32	7c	1	Total	C	H	O	P	0
			220	71	130	17	2	
32	4E	1	Total	C	H	O	P	0
			163	53	91	17	2	
32	C1	1	Total	C	H	O	P	0
			220	71	130	17	2	
32	QE	1	Total	C	H	O	P	0
			124	41	64	17	2	

- Molecule 33 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



- PC1
- 
- The chemical structure of PC1 is a phosphazene-based polymer. It consists of a central phosphorus atom (P) bonded to two nitrogen atoms (N). Each nitrogen atom is part of a repeating unit that includes a long, zigzag alkyl chain and a phosphate group. The phosphate groups are linked together, forming a continuous backbone structure.

Mol	Chain	Residues	Atoms					AltConf	
34	QD	1	Total	C	H	N	O	P	0
			67	21	36	1	8	1	

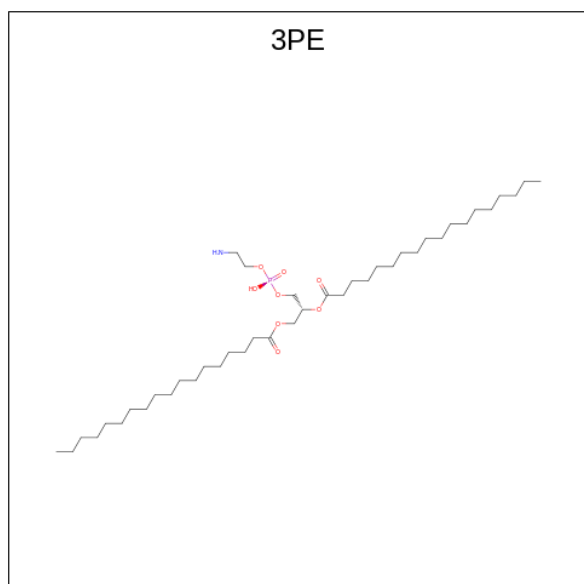


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Mol	Chain	Residues	Atoms						AltConf
34	Qc	1	Total	C	H	N	O	P	0
			82	26	46	1	8	1	
34	Qd	1	Total	C	H	N	O	P	0
			67	21	36	1	8	1	
34	Qj	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
34	4a	1	Total	C	H	N	O	P	0
			118	37	71	1	8	1	
34	4e	1	Total	C	H	N	O	P	0
			79	25	44	1	8	1	
34	7c	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
34	c1	1	Total	C	H	N	O	P	0
			127	40	77	1	8	1	
34	c1	1	Total	C	H	N	O	P	0
			82	26	46	1	8	1	
34	c3	1	Total	C	H	N	O	P	0
			130	41	79	1	8	1	
34	4A	1	Total	C	H	N	O	P	0
			118	37	71	1	8	1	
34	4A	1	Total	C	H	N	O	P	0
			112	36	66	1	8	1	
34	4E	1	Total	C	H	N	O	P	0
			79	25	44	1	8	1	
34	C1	1	Total	C	H	N	O	P	0
			127	40	77	1	8	1	
34	C1	1	Total	C	H	N	O	P	0
			82	26	46	1	8	1	
34	C3	1	Total	C	H	N	O	P	0
			130	41	79	1	8	1	
34	DC	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
34	QE	1	Total	C	H	N	O	P	0
			82	26	46	1	8	1	
34	Qe	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
34	Qe	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
34	Qe	1	Total	C	H	N	O	P	0
			82	26	46	1	8	1	
34	Qg	1	Total	C	H	N	O	P	0
			58	18	30	1	8	1	

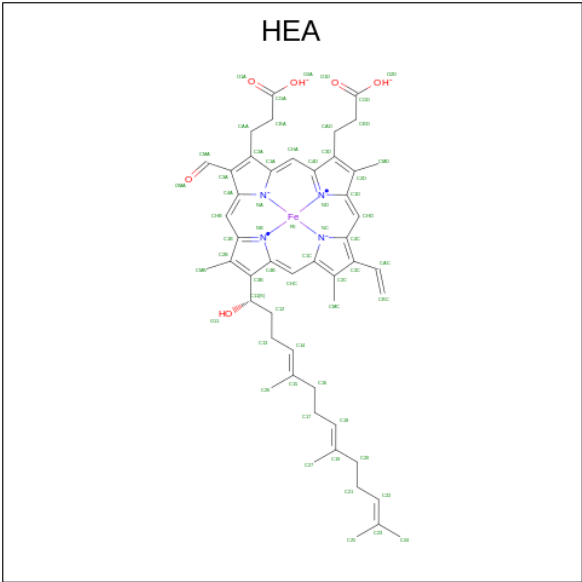
- ## PX2

- Molecule 36 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms						AltConf
36	4a	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
36	c1	1	Total 94	C 30	H 54	N 1	O 8	P 1	0
36	c1	1	Total 94	C 30	H 54	N 1	O 8	P 1	0
36	C1	1	Total 94	C 30	H 54	N 1	O 8	P 1	0
36	C1	1	Total 94	C 30	H 54	N 1	O 8	P 1	0
36	4D	1	Total 79	C 25	H 44	N 1	O 8	P 1	0
36	4F	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
36	7a	1	Total 100	C 31	H 59	N 1	O 8	P 1	0
36	4d	1	Total 79	C 25	H 44	N 1	O 8	P 1	0
36	4d	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
36	7A	1	Total 100	C 31	H 59	N 1	O 8	P 1	0

- Molecule 37 is HEME-A (CCD ID: HEA) (formula: C₄₉H₅₆FeN₄O₆).



Mol	Chain	Residues	Atoms					AltConf
37	c1	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
37	c1	1	Total 60	C 49	Fe 1	N 4	O 6	0
37	C1	1	Total 60	C 49	Fe 1	N 4	O 6	0
37	C1	1	Total 60	C 49	Fe 1	N 4	O 6	0

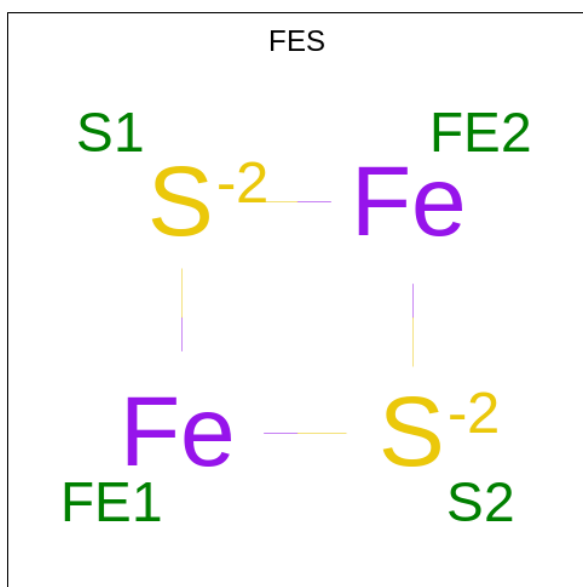
- Molecule 38 is COPPER (II) ION (CCD ID: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
38	c1	1	Total	Cu	0
			1	1	
38	c2	2	Total	Cu	0
			2	2	
38	C1	1	Total	Cu	0
			1	1	
38	C2	2	Total	Cu	0
			2	2	

- Molecule 39 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
39	c1	1	Total	Mg	0
			1	1	
39	C1	1	Total	Mg	0
			1	1	

- Molecule 40 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
40	QE	1	Total	Fe	S	0
			4	2	2	
40	Qe	1	Total	Fe	S	0
			4	2	2	

- Molecule 41 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
41	5B	1	Total	Zn	0
			1	1	
41	5b	1	Total	Zn	0
			1	1	

- Molecule 42 is O-[(S)-hydroxy{[(2S)-2-hydroxy-3-(octadec-9-enoyloxy)propyl]oxy}phosphoryl]-L-serine (CCD ID: S12) (formula: C₂₄H₄₆NO₉P).

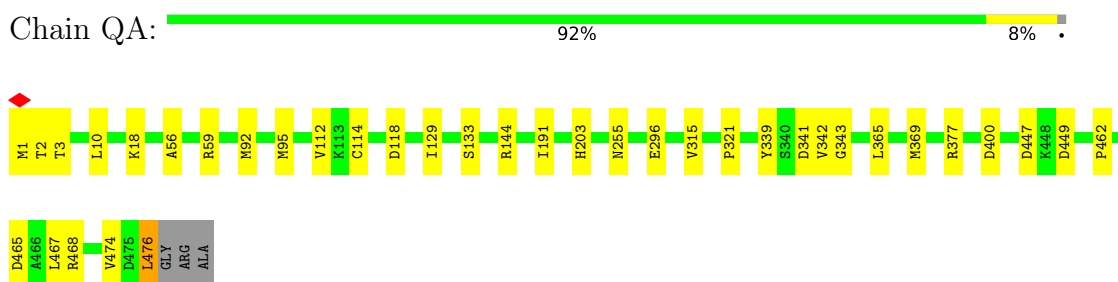


Mol	Chain	Residues	Atoms						AltConf
42	4F	1	Total	C	H	N	O	P	0
			79	24	44	1	9	1	
42	4d	1	Total	C	H	N	O	P	0
			79	24	44	1	9	1	

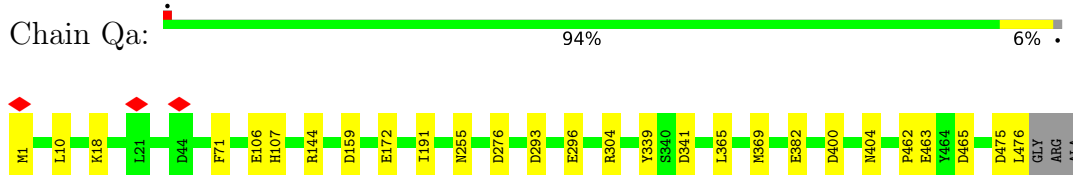
3 Residue-property plots [i](#)

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

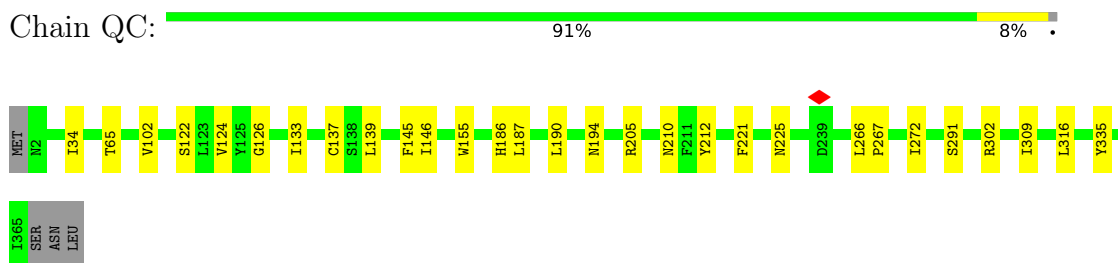
- Molecule 1: MPP-beta



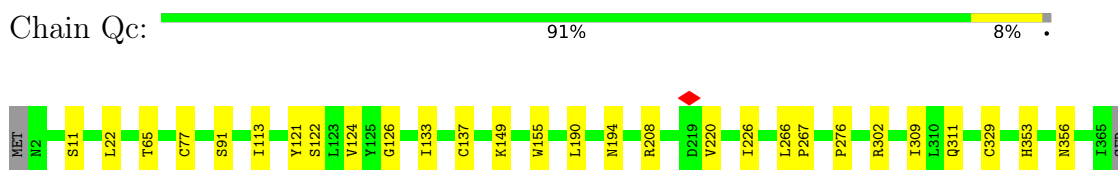
- Molecule 1: MPP-beta



- Molecule 2: Cytochrome b

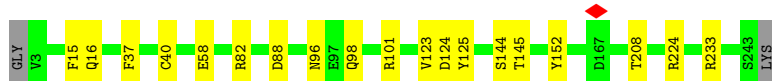


- Molecule 2: Cytochrome b



ASN
LEU

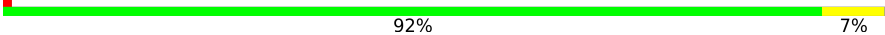
- Molecule 3: Cytochrome c1, heme protein

Chain QD:  91% 8%

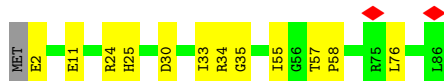
- Molecule 3: Cytochrome c1, heme protein

Chain Qd:  91% 9%

- Molecule 4: UQCRQ

Chain QH:  92% 7%

- Molecule 4: UQCRQ

Chain Qh:  85% 14%

- Molecule 5: UQCR10

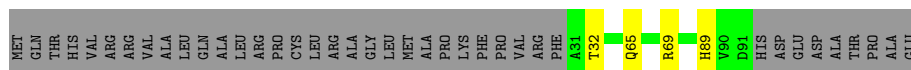
Chain QJ:  88% 8%

- Molecule 5: UQCR10

Chain Qj:  88% 8%

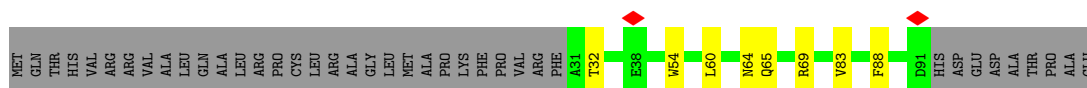
- Molecule 6: Ubiquinol-cytochrome-C reductase complex subunit IX, mitochondrial

Chain QK:  57% 39%



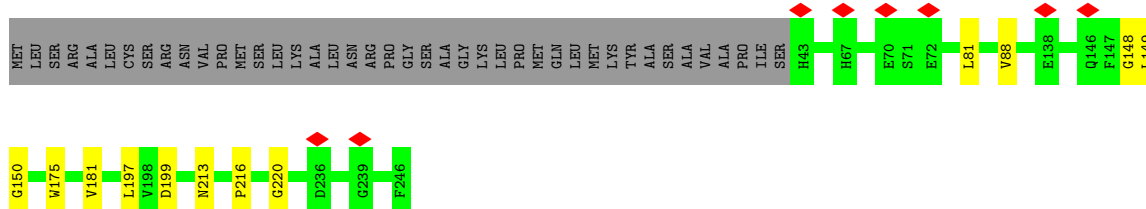
- Molecule 6: Ubiquinol-cytochrome-C reductase complex subunit IX, mitochondrial

Chain Qk:  53% 8% 39%



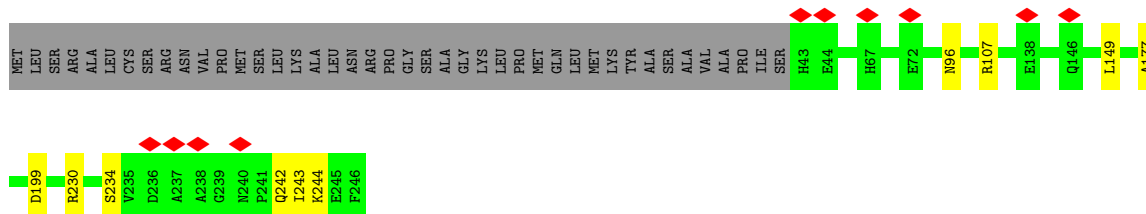
- Molecule 7: COXEG1

Chain 4a:  78% 5% 17%



- Molecule 7: COXEG1

Chain 4A:  79% 17%



- Molecule 8: COXEG3

Chain 4c:  81% 8% 12%

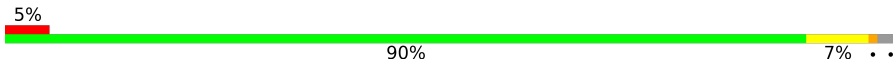


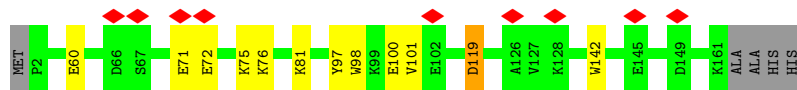
- Molecule 8: COXEG3

Chain 4C:  81% 7% 12%



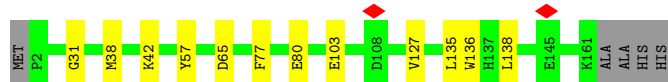
• Molecule 9: COXEG5

Chain 4e: 



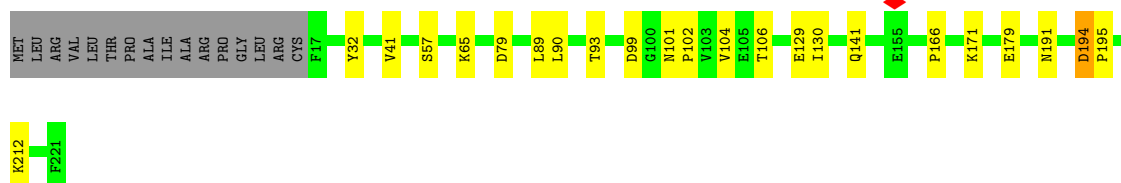
• Molecule 9: COXEG5

Chain 4E: 



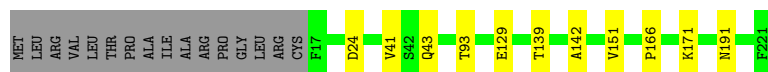
• Molecule 10: COXEG8

Chain 4h: 

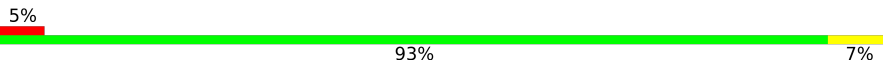


• Molecule 10: COXEG8

Chain 4H: 

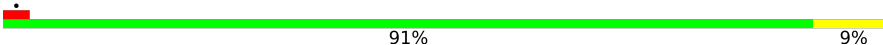


• Molecule 11: COXEG10

Chain 4j: 



• Molecule 11: COXEG10

Chain 4J: 



• Molecule 12: COX5c

Chain 5c: 



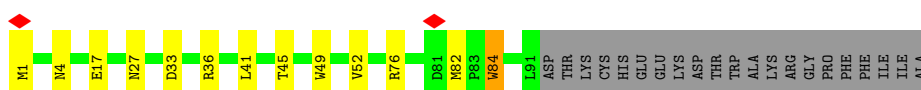
- Molecule 12: COX5c

Chain 5C: 87% 7% 6%



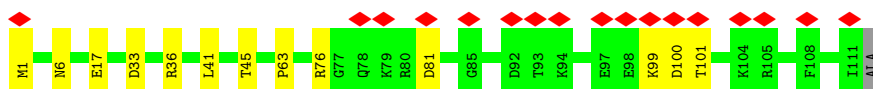
- Molecule 13: COX6a

Chain 6a: 70% 11% 19%



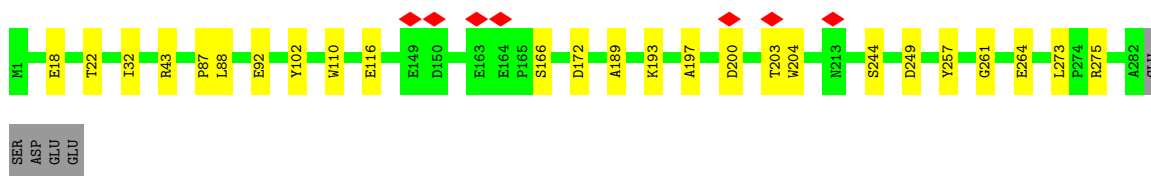
- Molecule 13: COX6a

Chain 6A: 15% 88% 12%



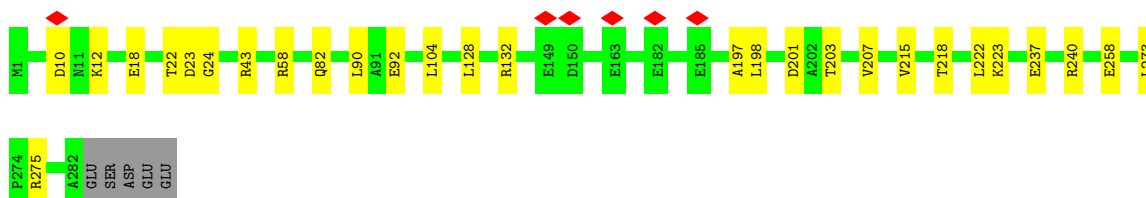
- Molecule 14: COX6b-1

Chain 6b: 90% 9%



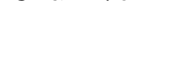
- Molecule 14: COX6b-1

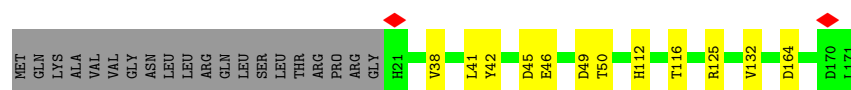
Chain 6B: 89% 10%



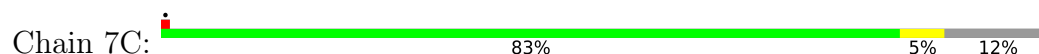
- Molecule 15: COX7c

Chain 7c: 81% 7% 12%

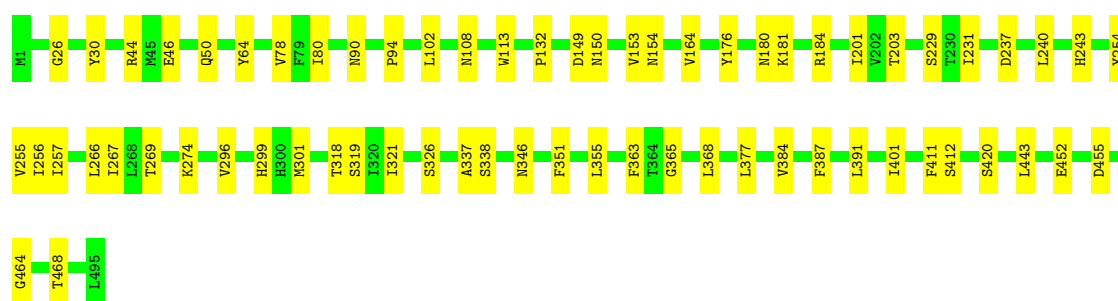




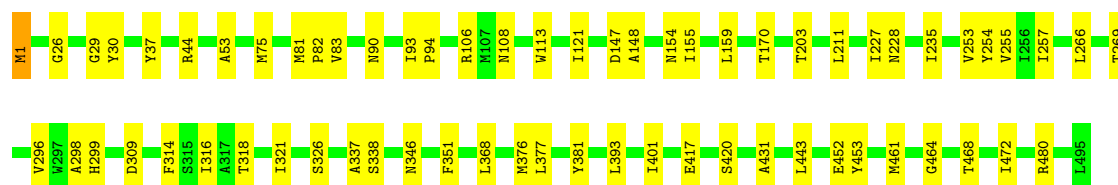
- Molecule 15: COX7c



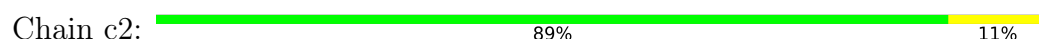
- Molecule 16: Cytochrome c oxidase subunit 1



- Molecule 16: Cytochrome c oxidase subunit 1



- Molecule 17: Cytochrome c oxidase subunit 2



- Molecule 17: Cytochrome c oxidase subunit 2



- Molecule 18: Putative NADH dehydrogenase subunit 6

Chain c3:  86% 14%



- Molecule 18: Putative NADH dehydrogenase subunit 6

Chain C3:  88% 12%

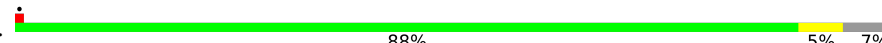


- Molecule 19: COX4

Chain dc:  83% 10% 7%



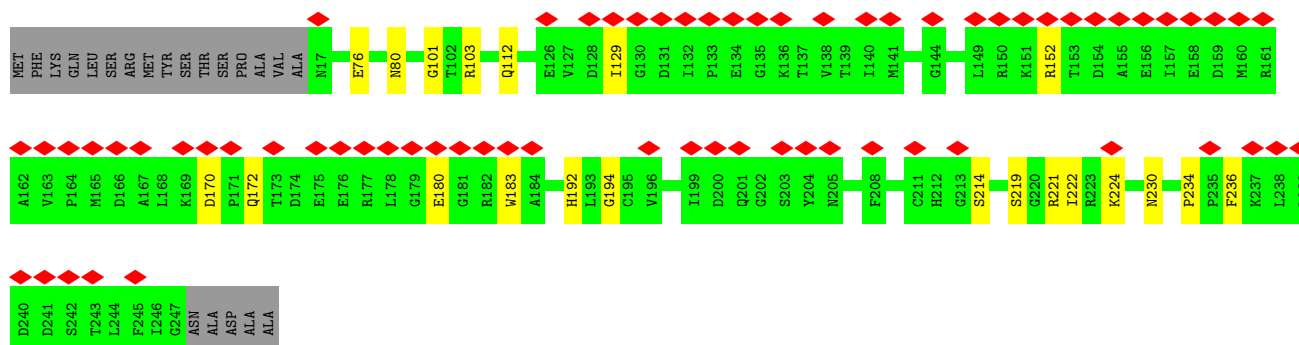
- Molecule 19: COX4

Chain DC:  88% 5% 7%



- Molecule 20: UQCRFS1

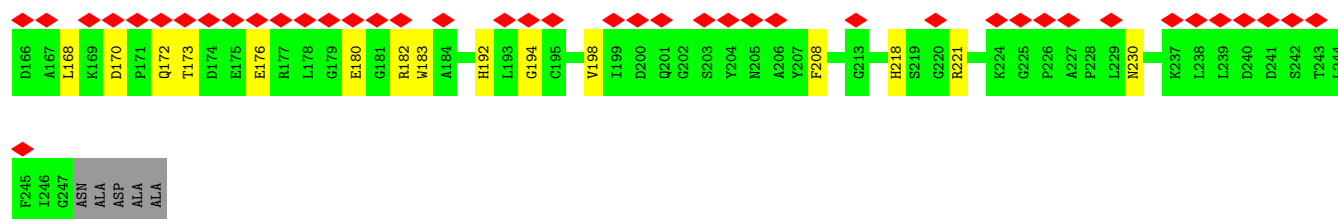
Chain QE:  27% 83% 8% 8%



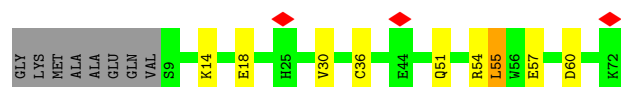
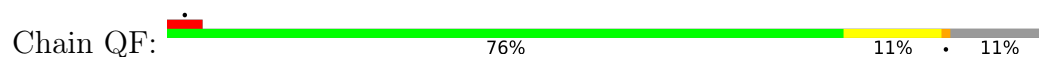
- Molecule 20: UQCRFS1

Chain Qe:  30% 81% 11% 8%

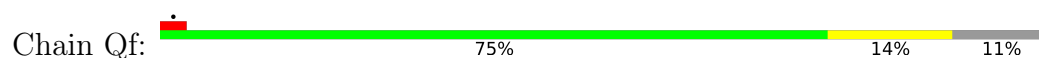




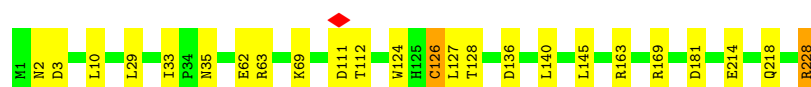
• Molecule 21: UQCRH



• Molecule 21: UQCRH



• Molecule 22: UQCRB



• Molecule 22: UQCRB



• Molecule 23: UQCR9

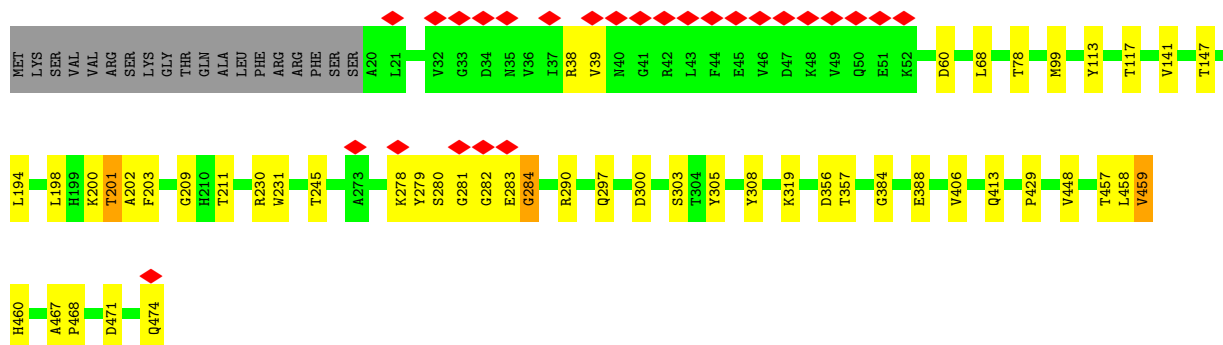
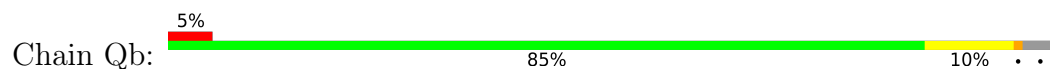


• Molecule 23: UQCR9

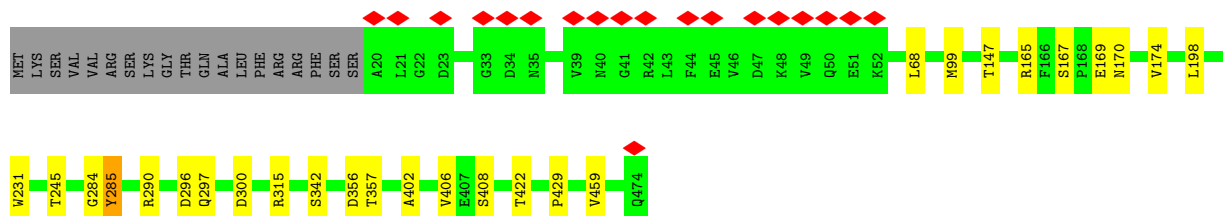




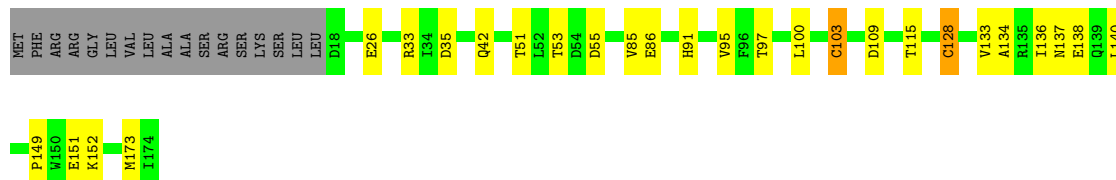
- Molecule 24: Ubiquinol-cytochrome-c reductase complex core protein 2, mitochondrial



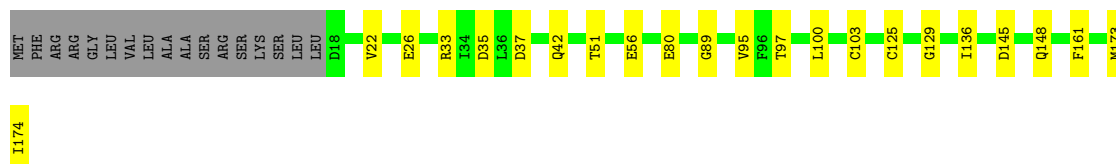
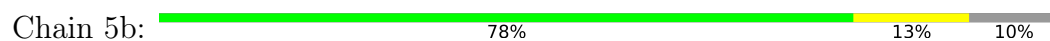
- Molecule 24: Ubiquinol-cytochrome-c reductase complex core protein 2, mitochondrial



- Molecule 25: COX5b-2



- Molecule 25: COX5b-2



- Molecule 26: COXEG4

Chain 4D:  89% 10% ..

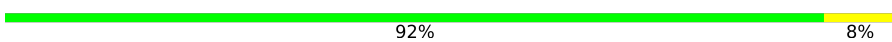


• Molecule 26: COXEG4

Chain 4d:  84% 13% ..



• Molecule 27: COXEG6

Chain 4F:  92% 8%



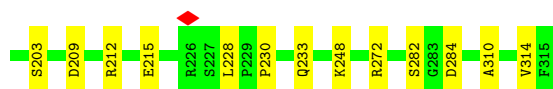
• Molecule 27: COXEG6

Chain 4f:  93% 7%



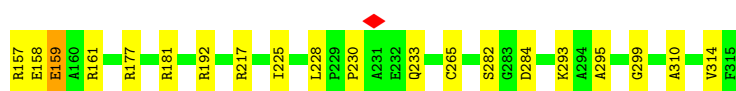
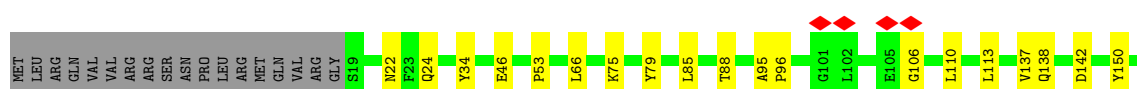
• Molecule 28: COXEG7

Chain 4G:  85% 10% 6%



• Molecule 28: COXEG7

Chain 4g:  82% 12% 6%



• Molecule 29: COXEG9

Chain 4I:  89% 8% .



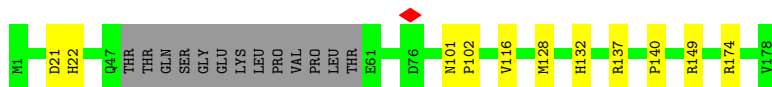
• Molecule 29: COXEG9

Chain 4i:  88% 8% . .



• Molecule 30: COX7a

Chain 7a:  87% 6% 7%



• Molecule 30: COX7a

Chain 7A:  84% 8% 7%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	135598	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 ($e^-/\text{\AA}^2$)	51.5	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	105000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	39.138	Depositor
Minimum map value	-21.701	Depositor
Average map value	-0.023	Depositor
Map value standard deviation	1.026	Depositor
Recommended contour level	4.8	Depositor
Map size ($\text{\AA}$)	537.60004, 537.60004, 537.60004	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.2, 1.2, 1.2	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PC1, HEA, HEM, CU, MG, CDL, 3PE, S12, FES, ZN, HEC, PX2

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	QA	0.21	0/3838	0.30	0/5193
1	Qa	0.21	0/3838	0.30	0/5193
2	QC	0.24	0/3058	0.31	0/4178
2	Qc	0.25	0/3058	0.33	0/4178
3	QD	0.24	0/2027	0.30	0/2760
3	Qd	0.24	0/2027	0.31	0/2760
4	QH	0.22	0/717	0.28	0/966
4	Qh	0.22	0/717	0.30	0/966
5	QJ	0.18	0/1243	0.26	0/1693
5	Qj	0.19	0/1243	0.26	0/1693
6	QK	0.20	0/498	0.27	0/677
6	Qk	0.19	0/498	0.25	0/677
7	4A	0.17	0/1650	0.25	0/2235
7	4a	0.18	0/1650	0.27	0/2235
8	4C	0.19	0/1051	0.27	0/1432
8	4c	0.19	0/1051	0.28	0/1432
9	4E	0.18	0/1376	0.25	0/1864
9	4e	0.16	0/1376	0.26	0/1864
10	4H	0.20	0/1640	0.29	0/2224
10	4h	0.18	0/1640	0.27	0/2224
11	4J	0.21	0/736	0.26	0/1008
11	4j	0.21	0/736	0.27	0/1008
12	5C	0.23	0/1616	0.29	0/2192
12	5c	0.23	0/1616	0.29	0/2192
13	6A	0.18	0/953	0.27	0/1292
13	6a	0.17	0/777	0.28	0/1055
14	6B	0.21	0/2343	0.26	0/3174
14	6b	0.21	0/2343	0.27	0/3174
15	7C	0.23	0/1299	0.28	0/1777
15	7c	0.23	0/1299	0.29	0/1777
16	C1	0.26	0/4054	0.36	0/5516
16	c1	0.29	0/4054	0.38	0/5516

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	C2	0.24	0/1620	0.34	0/2207
17	c2	0.26	0/1620	0.36	0/2207
18	C3	0.22	0/1416	0.30	0/1945
18	c3	0.23	0/1416	0.34	0/1945
19	DC	0.23	0/1410	0.29	0/1914
19	dc	0.23	0/1410	0.29	0/1914
20	QE	0.17	0/1842	0.28	0/2502
20	Qe	0.16	0/1842	0.28	0/2502
21	QF	0.16	0/526	0.25	0/702
21	Qf	0.17	0/526	0.26	0/702
22	QG	0.24	0/1987	0.33	0/2696
22	Qg	0.24	0/1987	0.32	0/2696
23	QI	0.21	0/251	0.25	0/340
23	Qi	0.21	0/251	0.26	0/340
24	QB	0.22	0/3532	0.31	0/4805
24	Qb	0.24	0/3532	0.37	0/4805
25	5B	0.25	0/1294	0.36	0/1759
25	5b	0.26	0/1294	0.32	0/1759
26	4D	0.22	0/1379	0.32	0/1867
26	4d	0.21	0/1379	0.33	0/1867
27	4F	0.19	0/641	0.28	0/867
27	4f	0.19	0/641	0.30	0/867
28	4G	0.20	0/2391	0.28	0/3240
28	4g	0.20	0/2391	0.28	0/3240
29	4I	0.25	0/2255	0.26	0/3059
29	4i	0.25	0/2255	0.28	0/3059
30	7A	0.20	0/1359	0.28	0/1835
30	7a	0.18	0/1359	0.29	0/1835
All	All	0.22	0/99828	0.30	0/135601

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

Mol	Chain	#Chirality outliers	#Planarity outliers
24	Qb	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
24	Qb	283	GLU	Peptide
24	Qb	284	GLY	Peptide

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	QA	3750	3658	3668	28	0
1	Qa	3750	3658	3668	19	0
2	QC	2975	3064	3076	19	0
2	Qc	2975	3064	3076	24	0
3	QD	1959	1858	1864	16	0
3	Qd	1959	1858	1864	15	0
4	QH	701	692	694	6	0
4	Qh	701	692	694	11	0
5	QJ	1206	1212	1216	10	0
5	Qj	1206	1212	1216	11	0
6	QK	485	499	500	3	0
6	Qk	485	499	500	7	0
7	4A	1612	1608	1617	6	0
7	4a	1612	1608	1617	12	0
8	4C	1022	1027	1029	8	0
8	4c	1022	1027	1029	9	0
9	4E	1333	1279	1283	9	0
9	4e	1333	1279	1283	5	0
10	4H	1606	1644	1648	7	0
10	4h	1606	1644	1648	16	0
11	4J	711	688	689	4	0
11	4j	711	688	689	5	0
12	5C	1571	1546	1550	11	0
12	5c	1571	1546	1550	11	0
13	6A	920	909	912	16	0
13	6a	750	747	749	13	0
14	6B	2285	2229	2239	23	0
14	6b	2285	2227	2237	18	0
15	7C	1254	1183	1190	7	0
15	7c	1254	1183	1190	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	C1	3938	3980	3999	44	0
16	c1	3938	3980	3999	47	0
17	C2	1585	1647	1652	13	0
17	c2	1585	1647	1652	16	0
18	C3	1378	1413	1419	15	0
18	c3	1378	1413	1419	19	0
19	DC	1366	1362	1366	8	0
19	dc	1366	1362	1366	13	0
20	QE	1795	1776	1780	14	0
20	Qe	1795	1776	1780	17	0
21	QF	515	501	507	5	0
21	Qf	515	501	507	5	0
22	QG	1932	1870	1880	18	0
22	Qg	1932	1870	1880	14	0
23	QI	449	292	292	2	0
23	Qi	449	293	294	1	0
24	QB	3458	3431	3443	20	0
24	Qb	3458	3431	3443	40	0
25	5B	1258	1184	1192	22	0
25	5b	1258	1184	1192	18	0
26	4D	1349	1359	1363	14	0
26	4d	1349	1359	1363	19	0
27	4F	620	626	627	3	0
27	4f	620	626	627	3	0
28	4G	2351	2339	2343	18	0
28	4g	2351	2339	2343	27	0
29	4I	2178	2046	2058	17	0
29	4i	2178	2046	2058	19	0
30	7A	1319	1284	1295	11	0
30	7a	1319	1284	1295	9	0
31	QC	86	0	60	4	0
31	Qc	86	0	60	7	0
32	4E	72	91	91	0	0
32	4c	70	87	87	0	0
32	4e	72	91	91	0	0
32	7c	90	130	130	0	0
32	C1	90	130	130	0	0
32	QC	56	56	56	1	0
32	QD	69	82	82	1	0
32	QE	60	64	64	0	0
32	QH	76	99	99	0	0
32	QJ	58	60	60	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	Qc	54	52	52	2	0
32	Qd	100	156	156	2	0
32	Qh	125	138	138	0	0
32	Qj	48	40	40	1	0
33	QD	43	0	31	6	0
33	Qd	43	0	31	2	0
34	4A	93	137	137	0	0
34	4E	35	44	44	1	0
34	4a	47	71	71	0	0
34	4e	35	44	44	1	0
34	7c	54	88	88	0	0
34	C1	86	123	123	1	0
34	C3	51	79	79	0	0
34	DC	54	88	88	1	0
34	QD	31	36	36	0	0
34	QE	36	46	46	1	0
34	Qc	36	46	46	0	0
34	Qd	31	36	36	0	0
34	Qe	144	222	222	4	0
34	Qg	28	30	30	0	0
34	Qj	54	88	88	0	0
34	c1	86	123	123	1	0
34	c3	51	79	79	0	0
35	4C	36	0	52	4	0
35	QD	36	0	52	3	0
35	QJ	36	0	52	2	0
36	4D	35	44	44	0	0
36	4F	51	82	82	1	0
36	4a	51	82	82	0	0
36	4d	86	126	126	0	0
36	7A	41	59	59	0	0
36	7a	41	59	59	0	0
36	C1	80	108	108	1	0
36	c1	80	108	108	1	0
37	C1	120	0	108	10	0
37	c1	120	0	108	18	0
38	C1	1	0	0	0	0
38	C2	2	0	0	0	0
38	c1	1	0	0	0	0
38	c2	2	0	0	0	0
39	C1	1	0	0	0	0
39	c1	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	QE	4	0	0	1	0
40	Qe	4	0	0	0	0
41	5B	1	0	0	0	0
41	5b	1	0	0	0	0
42	4F	35	44	44	1	0
42	4d	35	44	44	0	0
All	All	100743	99661	100585	689	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 3.

All (689) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:QD:40:CYS:SG	33:QD:301:HEC:CAC	2.02	1.48
2:QC:291:SER:OG	22:QG:35:ASN:O	1.89	0.89
24:Qb:460:HIS:NE2	24:Qb:468:PRO:O	2.06	0.88
5:Qj:54:ARG:NH2	32:Qj:202:CDL:OB3	2.08	0.85
13:6a:4:ASN:ND2	25:5b:148:GLN:OE1	2.08	0.85
5:Qj:47:PHE:O	5:Qj:54:ARG:NH1	2.11	0.83
24:QB:290:ARG:NH1	24:QB:300:ASP:O	2.12	0.83
16:c1:346:ASN:ND2	16:c1:420:SER:OG	2.12	0.82
5:QJ:54:ARG:NH2	32:QJ:202:CDL:OB3	2.13	0.81
1:QA:255:ASN:ND2	24:QB:297:GLN:OE1	2.13	0.81
2:Qc:208:ARG:NH1	4:Qh:11:GLU:OE2	2.16	0.79
21:QF:54:ARG:NH1	21:QF:57:GLU:OE1	2.16	0.78
12:5c:146:CYS:SG	12:5c:147:GLY:N	2.57	0.76
6:Qk:65:GLN:OE1	6:Qk:69:ARG:NH1	2.18	0.76
3:Qd:97:GLU:OE2	3:Qd:101:ARG:NH1	2.19	0.76
20:QE:214:SER:OG	40:QE:301:FES:S1	2.45	0.75
13:6a:1:MET:O	28:4g:161:ARG:NH2	2.20	0.74
5:Qj:115:GLY:O	22:QG:228:ARG:NH1	2.19	0.74
19:dc:127:GLU:N	19:dc:127:GLU:OE1	2.19	0.74
14:6B:58:ARG:NH2	18:C3:114:ASN:OD1	2.20	0.74
24:Qb:290:ARG:NH1	24:Qb:300:ASP:O	2.20	0.74
11:4j:29:THR:HG22	11:4j:30:SER:H	1.53	0.73
24:Qb:284:GLY:O	24:Qb:460:HIS:N	2.21	0.73
20:QE:170:ASP:OD2	20:QE:230:ASN:ND2	2.21	0.73
24:Qb:356:ASP:O	24:Qb:357:THR:OG1	2.05	0.72
1:QA:10:LEU:O	5:QJ:94:ARG:NH1	2.22	0.72
5:QJ:47:PHE:O	5:QJ:54:ARG:NH1	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:7c:46:GLU:O	15:7c:50:THR:OG1	2.08	0.71
26:4d:145:ASN:OD1	26:4d:148:ALA:N	2.24	0.71
3:Qd:70:ASP:OD1	3:Qd:81:LYS:NZ	2.23	0.71
24:Qb:198:LEU:HA	24:Qb:459:VAL:HG21	1.73	0.71
1:Qa:304:ARG:NH2	22:QG:218:GLN:OE1	2.23	0.71
5:QJ:79:ARG:NH2	22:Qg:61:ASP:OD1	2.23	0.71
12:5C:146:CYS:SG	12:5C:147:GLY:N	2.64	0.71
37:c1:501:HEA:HBC1	37:c1:501:HEA:HHD	1.71	0.71
22:Qg:181:ASP:OD1	22:Qg:185:ARG:NH1	2.23	0.71
13:6a:41:LEU:O	13:6a:45:THR:OG1	2.07	0.71
13:6A:41:LEU:O	13:6A:45:THR:OG1	2.09	0.70
3:QD:40:CYS:SG	33:QD:301:HEC:C3C	2.79	0.70
7:4a:199:ASP:OD2	18:c3:149:THR:OG1	2.08	0.70
28:4g:150:TYR:OH	25:5b:37:ASP:OD2	2.10	0.70
16:C1:346:ASN:ND2	16:C1:420:SER:OG	2.25	0.70
16:C1:381:TYR:OH	37:C1:502:HEA:O2A	2.06	0.70
27:4f:18:GLN:NE2	25:5b:56:GLU:OE2	2.24	0.69
16:c1:326:SER:HB2	37:c1:501:HEA:H202	1.73	0.69
13:6a:76:ARG:NH1	14:6b:92:GLU:OE2	2.24	0.69
35:4C:201:PX2:H45	12:5C:181:ALA:HB2	1.75	0.69
13:6A:33:ASP:OD1	13:6A:36:ARG:NH1	2.26	0.69
3:QD:152:TYR:OH	21:QF:60:ASP:OD2	2.11	0.68
5:Qj:14:ALA:N	24:Qb:60:ASP:OD1	2.26	0.68
4:Qh:57:THR:HG21	6:Qk:54:TRP:HE1	1.58	0.68
28:4G:181:ARG:NH2	29:4I:188:GLU:OE2	2.26	0.68
16:C1:452:GLU:OE2	17:C2:116:ARG:NH2	2.26	0.68
24:QB:356:ASP:O	24:QB:357:THR:OG1	2.09	0.68
8:4C:19:ARG:NH1	25:5B:109:ASP:OD1	2.26	0.67
13:6A:99:LYS:O	13:6A:101:THR:N	2.28	0.67
7:4A:230:ARG:NH2	14:6B:104:LEU:O	2.28	0.67
19:dc:100:ASN:O	19:dc:105:ARG:NH1	2.26	0.67
10:4H:24:ASP:OD2	28:4G:272:ARG:NH1	2.28	0.67
20:Qe:156:GLU:N	20:Qe:156:GLU:OE1	2.27	0.67
3:QD:101:ARG:NH2	20:Qe:194:GLY:O	2.29	0.66
4:QH:80:ARG:NH2	6:QK:89:HIS:O	2.29	0.66
14:6B:43:ARG:NE	26:4D:102:ASP:OD1	2.25	0.65
28:4g:228:LEU:O	28:4g:233:GLN:NE2	2.29	0.65
14:6b:43:ARG:NE	26:4d:102:ASP:OD1	2.28	0.65
3:QD:58:GLU:N	3:QD:58:GLU:OE1	2.29	0.65
25:5b:125:CYS:O	25:5b:129:GLY:N	2.29	0.65
12:5c:132:TYR:OH	29:4i:259:GLU:OE1	2.14	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:7C:46:GLU:O	15:7C:50:THR:OG1	2.15	0.65
2:Qc:137:CYS:SG	2:Qc:155:TRP:NE1	2.69	0.65
19:DC:127:GLU:N	19:DC:127:GLU:OE1	2.30	0.65
14:6b:249:ASP:OD2	26:4d:101:LYS:NZ	2.30	0.65
21:Qf:12:GLU:N	21:Qf:12:GLU:OE1	2.29	0.65
24:Qb:282:GLY:O	24:Qb:284:GLY:N	2.30	0.65
16:c1:411:PHE:O	16:c1:412:SER:OG	2.12	0.64
16:c1:455:ASP:OD1	17:c2:116:ARG:NH1	2.30	0.64
35:4C:201:PX2:H16	35:4C:201:PX2:H40	1.78	0.64
1:Qa:106:GLU:O	1:Qa:107:HIS:ND1	2.30	0.64
1:QA:59:ARG:NH2	1:QA:341:ASP:OD1	2.30	0.64
26:4d:38:ARG:NH2	25:5b:51:THR:O	2.31	0.64
9:4E:77:PHE:O	14:6B:132:ARG:NH2	2.31	0.64
35:4C:201:PX2:H13	17:C2:59:ILE:HG21	1.79	0.63
28:4G:75:LYS:O	28:4G:192:ARG:NH1	2.30	0.63
25:5B:26:GLU:O	25:5B:33:ARG:NH2	2.31	0.63
8:4C:94:ILE:HD11	8:4C:106:ILE:HD11	1.80	0.63
13:6a:33:ASP:OD2	18:c3:157:ARG:NH1	2.30	0.63
1:Qa:144:ARG:NH2	1:Qa:191:ILE:O	2.31	0.63
17:C2:108:GLU:OE1	17:C2:110:ARG:NH1	2.32	0.63
13:6A:1:MET:O	28:4G:161:ARG:NH2	2.32	0.63
24:Qb:202:ALA:O	24:Qb:280:SER:N	2.27	0.63
2:Qc:309:ILE:HG23	4:Qh:55:ILE:HG22	1.81	0.62
1:Qa:400:ASP:O	1:Qa:404:ASN:ND2	2.32	0.62
10:4h:179:GLU:OE2	29:4i:68:SER:OG	2.11	0.62
12:5c:144:ARG:NH2	19:dc:29:GLN:O	2.32	0.62
4:QH:19:LYS:NZ	24:QB:296:ASP:OD1	2.32	0.62
14:6b:166:SER:OG	14:6b:172:ASP:OD2	2.15	0.62
16:c1:326:SER:CB	37:c1:501:HEA:H202	2.29	0.62
14:6B:58:ARG:NH2	18:C3:116:ASN:OD1	2.33	0.62
13:6A:6:ASN:OD1	30:7A:115:ARG:NH2	2.34	0.61
20:QE:180:GLU:OE1	20:QE:183:TRP:N	2.33	0.61
9:4e:98:TRP:HA	9:4e:101:VAL:HG12	1.82	0.61
18:c3:107:TYR:OH	18:c3:128:ASN:ND2	2.32	0.61
10:4H:41:VAL:HG22	10:4H:129:GLU:OE1	1.99	0.61
19:dc:33:SER:O	19:dc:36:ARG:NH1	2.33	0.61
2:Qc:65:THR:OG1	20:Qe:112:GLN:NE2	2.33	0.61
7:4A:244:LYS:NZ	9:4E:103:GLU:OE2	2.32	0.61
14:6b:261:GLY:N	14:6b:264:GLU:OE1	2.34	0.61
16:c1:363:PHE:HE1	37:c1:501:HEA:H211	1.65	0.60
27:4f:6:THR:OG1	27:4f:24:ASP:OD1	2.14	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:QC:137:CYS:SG	2:QC:155:TRP:NE1	2.74	0.60
4:QH:14:VAL:O	22:QG:169:ARG:NH2	2.35	0.60
16:C1:203:THR:HG23	16:C1:255:VAL:HG13	1.84	0.60
16:C1:337:ALA:O	16:C1:338:SER:OG	2.20	0.60
13:6a:82:MET:SD	13:6a:84:TRP:NE1	2.74	0.60
16:C1:346:ASN:ND2	16:C1:417:GLU:OE1	2.34	0.60
20:Qe:152:ARG:NH2	20:Qe:218:HIS:O	2.35	0.60
5:Qj:78:ARG:NH2	22:QG:10:LEU:O	2.34	0.60
14:6b:197:ALA:O	14:6b:203:THR:OG1	2.19	0.60
16:c1:368:LEU:HB3	37:c1:501:HEA:HMA	1.84	0.60
24:Qb:282:GLY:O	24:Qb:458:LEU:O	2.19	0.59
16:C1:368:LEU:HB3	37:C1:501:HEA:HMA	1.84	0.59
28:4G:228:LEU:O	28:4G:233:GLN:NE2	2.36	0.59
8:4c:100:GLU:N	8:4c:100:GLU:OE1	2.34	0.59
16:c1:50:GLN:OE1	19:dc:109:GLN:NE2	2.34	0.59
27:4F:6:THR:OG1	27:4F:24:ASP:OD1	2.15	0.59
15:7C:125:ARG:NH2	19:DC:101:ALA:O	2.36	0.59
24:Qb:202:ALA:HA	24:Qb:281:GLY:N	2.17	0.59
24:QB:167:SER:OG	24:QB:169:GLU:OE1	2.21	0.59
37:c1:501:HEA:HHD	37:c1:501:HEA:CBC	2.33	0.58
10:4H:166:PRO:O	10:4H:171:LYS:NZ	2.35	0.58
12:5C:140:GLU:OE1	19:DC:26:ARG:NH2	2.36	0.58
15:7C:39:GLU:OE1	30:7A:137:ARG:NH1	2.36	0.58
24:Qb:459:VAL:HG12	24:Qb:459:VAL:O	2.02	0.58
18:C3:157:ARG:NH1	13:6A:33:ASP:OD2	2.36	0.58
14:6b:273:LEU:O	14:6b:275:ARG:NH1	2.35	0.58
8:4c:16:TYR:N	26:4d:22:ASN:OD1	2.37	0.58
16:c1:351:PHE:HA	16:c1:401:ILE:HD11	1.85	0.58
22:Qg:163:ARG:NH2	22:Qg:214:GLU:OE2	2.37	0.58
16:c1:90:ASN:ND2	16:c1:176:TYR:OH	2.37	0.58
21:Qf:51:GLN:N	21:Qf:51:GLN:OE1	2.37	0.58
28:4g:181:ARG:NH2	29:4i:188:GLU:OE2	2.36	0.58
3:Qd:165:THR:O	3:Qd:179:VAL:HG22	2.04	0.58
14:6B:207:VAL:HG21	26:4D:170:VAL:HG22	1.84	0.58
24:Qb:78:THR:OG1	24:Qb:413:GLN:NE2	2.37	0.58
8:4c:114:ALA:HB1	26:4d:167:LEU:HD23	1.86	0.57
11:4j:27:LYS:NZ	29:4i:35:GLY:O	2.37	0.57
16:C1:75:MET:HE1	37:C1:502:HEA:H172	1.86	0.57
3:Qd:204:LEU:O	3:Qd:208:THR:HG23	2.05	0.57
15:7c:132:VAL:O	19:dc:105:ARG:NH2	2.34	0.57
1:Qa:255:ASN:ND2	24:Qb:297:GLN:OE1	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:4I:69:ALA:O	29:4I:73:VAL:HG23	2.03	0.57
1:QA:144:ARG:NH2	1:QA:191:ILE:O	2.37	0.57
2:QC:205:ARG:NH2	2:QC:210:ASN:OD1	2.37	0.57
2:Qc:77:CYS:HB2	31:Qc:401:HEM:HBC2	1.87	0.57
16:c1:149:ASP:OD1	16:c1:150:ASN:ND2	2.37	0.57
2:QC:309:ILE:HG23	4:QH:55:ILE:HG22	1.87	0.57
26:4d:35:GLU:O	26:4d:39:GLY:N	2.38	0.56
22:Qg:116:THR:HG22	22:Qg:117:PRO:HD2	1.87	0.56
14:6b:200:ASP:OD1	14:6b:203:THR:OG1	2.23	0.56
16:c1:181:LYS:NZ	34:c1:508:PC1:O32	2.37	0.56
18:c3:30:TYR:OH	18:c3:40:ASN:OD1	2.17	0.56
8:4C:18:THR:OG1	25:5B:109:ASP:OD2	2.23	0.56
16:C1:326:SER:CB	37:C1:501:HEA:H202	2.35	0.56
21:Qf:14:LYS:NZ	21:Qf:18:GLU:OE2	2.39	0.56
30:7a:101:ASN:ND2	30:7a:102:PRO:O	2.37	0.56
3:Qd:208:THR:HG22	34:Qe:302:PC1:H351	1.87	0.56
1:QA:129:ILE:O	1:QA:133:SER:OG	2.22	0.56
5:QJ:115:GLY:O	22:Qg:228:ARG:NH1	2.39	0.56
12:5c:69:ASP:OD2	28:4g:217:ARG:NE	2.38	0.56
26:4D:173:ARG:O	26:4D:173:ARG:NH1	2.38	0.56
2:QC:190:LEU:O	2:QC:194:ASN:N	2.37	0.55
24:Qb:39:VAL:HG12	28:4g:113:LEU:HD13	1.87	0.55
1:Qa:18:LYS:H	24:Qb:147:THR:HG22	1.71	0.55
21:QF:51:GLN:N	21:QF:51:GLN:OE1	2.38	0.55
28:4G:66:LEU:O	28:4G:198:GLN:NE2	2.38	0.55
29:4i:21:LYS:O	29:4i:27:LYS:NZ	2.39	0.55
10:4h:166:PRO:O	10:4h:171:LYS:NZ	2.40	0.55
3:QD:37:PHE:HD2	33:QD:301:HEC:HAB	1.71	0.55
16:c1:30:TYR:CE2	37:c1:502:HEA:H22	2.41	0.55
16:C1:1:MET:SD	16:C1:1:MET:N	2.78	0.55
20:Qe:152:ARG:N	20:Qe:182:ARG:O	2.40	0.55
22:Qg:111:ASP:O	22:Qg:112:THR:OG1	2.25	0.55
25:5B:51:THR:O	26:4D:38:ARG:NH2	2.39	0.55
7:4a:213:ASN:ND2	18:c3:130:ASN:O	2.38	0.55
4:Qh:57:THR:HG21	6:Qk:54:TRP:NE1	2.21	0.55
16:C1:106:ARG:NH1	34:C1:505:PC1:O14	2.39	0.55
25:5B:86:GLU:OE1	25:5B:137:ASN:ND2	2.40	0.55
16:c1:44:ARG:HB3	16:c1:468:THR:HG21	1.89	0.54
16:c1:243:HIS:ND1	16:c1:301:MET:HE1	2.22	0.54
18:c3:33:TYR:OH	30:7a:174:ARG:NH2	2.39	0.54
35:4C:201:PX2:H13	17:C2:59:ILE:CG2	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:c3:9:TYR:OH	18:c3:65:GLU:OE2	2.25	0.54
16:C1:464:GLY:O	16:C1:468:THR:HG23	2.07	0.54
18:C3:1:MET:HB3	25:5B:140:LEU:HD22	1.88	0.54
16:c1:266:LEU:O	16:c1:269:THR:OG1	2.21	0.54
17:c2:5:ASN:OD1	17:c2:6:ARG:N	2.40	0.54
1:QA:1:MET:HE2	1:QA:3:THR:HB	1.89	0.54
16:c1:90:ASN:OD1	16:c1:108:ASN:ND2	2.38	0.54
3:QD:233:ARG:NH1	22:QG:181:ASP:OD1	2.41	0.54
2:QC:302:ARG:NH1	22:QG:33:ILE:O	2.34	0.54
37:C1:501:HEA:H243	17:C2:25:ILE:CD1	2.38	0.54
28:4g:158:GLU:OE1	28:4g:158:GLU:N	2.40	0.54
30:7A:101:ASN:ND2	30:7A:102:PRO:O	2.40	0.54
9:4e:60:GLU:OE2	9:4e:97:TYR:OH	2.26	0.53
37:c1:501:HEA:HMA	37:c1:501:HEA:HBA2	1.91	0.53
21:QF:14:LYS:NZ	21:QF:18:GLU:OE2	2.39	0.53
22:QG:163:ARG:NH2	22:QG:214:GLU:OE2	2.41	0.53
28:4g:138:GLN:NE2	28:4g:142:ASP:OD1	2.39	0.53
16:c1:464:GLY:O	16:c1:468:THR:HG23	2.07	0.53
28:4g:295:ALA:O	28:4g:299:GLY:N	2.41	0.53
1:QA:365:LEU:HD12	1:QA:462:PRO:HD2	1.90	0.53
1:Qa:10:LEU:O	5:Qj:94:ARG:NH1	2.42	0.53
30:7A:128:MET:O	30:7A:132:HIS:N	2.40	0.53
3:Qd:224:ARG:NH1	4:Qh:33:ILE:O	2.42	0.53
28:4g:22:ASN:OD1	28:4g:24:GLN:NE2	2.40	0.53
14:6B:197:ALA:O	14:6B:203:THR:OG1	2.25	0.53
3:QD:37:PHE:CD2	33:QD:301:HEC:HAB	2.43	0.53
12:5c:140:GLU:OE1	19:dc:26:ARG:NH2	2.42	0.53
12:5C:43:ILE:HG23	29:4I:109:LEU:HD21	1.91	0.53
14:6B:92:GLU:OE2	13:6A:76:ARG:NH1	2.40	0.53
18:C3:73:ASN:O	18:C3:77:ASN:ND2	2.40	0.53
17:c2:38:ARG:O	17:c2:42:ASN:ND2	2.36	0.53
8:4C:54:VAL:O	8:4C:56:PRO:HD3	2.08	0.53
15:7C:116:THR:HG21	16:C1:53:ALA:HB1	1.90	0.52
16:C1:44:ARG:HB3	16:C1:468:THR:HG21	1.91	0.52
1:QA:447:ASP:OD2	23:QI:10:TYR:OH	2.25	0.52
13:6a:27:ASN:ND2	30:7a:21:ASP:O	2.42	0.52
14:6B:237:GLU:OE2	14:6B:240:ARG:NH2	2.39	0.52
30:7a:128:MET:O	30:7a:132:HIS:N	2.39	0.52
2:Qc:11:SER:OG	4:Qh:2:GLU:OE2	2.24	0.52
26:4D:105:ASP:O	26:4D:106:SER:OG	2.24	0.52
28:4g:106:GLY:HA3	28:4g:110:LEU:HD22	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:1:MET:SD	24:QB:165:ARG:NH1	2.83	0.52
2:QC:221:PHE:O	2:QC:225:ASN:ND2	2.35	0.52
16:c1:337:ALA:O	16:c1:338:SER:OG	2.27	0.52
37:C1:502:HEA:HBA2	37:C1:502:HEA:CMA	2.40	0.52
18:C3:66:TYR:OH	25:5B:26:GLU:OE2	2.22	0.52
16:c1:391:LEU:CD2	37:c1:501:HEA:HBC2	2.40	0.52
14:6b:87:PRO:HG2	17:c2:96:ILE:HD11	1.92	0.52
26:4D:86:GLN:N	26:4D:87:PRO:HD2	2.25	0.52
20:Qe:137:THR:OG1	20:Qe:150:ARG:NH1	2.43	0.51
18:C3:131:THR:OG1	13:6A:63:PRO:O	2.27	0.51
12:5c:198:THR:OG1	12:5c:202:SER:O	2.28	0.51
20:Qe:180:GLU:OE1	20:Qe:183:TRP:N	2.40	0.51
24:Qb:281:GLY:HA3	24:Qb:457:THR:OG1	2.11	0.51
16:c1:365:GLY:O	37:c1:501:HEA:HMB3	2.11	0.51
12:5c:43:ILE:HG23	29:4i:109:LEU:HD21	1.92	0.51
20:QE:76:GLU:N	20:QE:76:GLU:OE1	2.43	0.51
9:4e:72:GLU:O	9:4e:76:LYS:N	2.39	0.51
16:c1:254:TYR:HA	16:c1:257:ILE:HG22	1.92	0.51
28:4G:76:GLU:OE2	28:4G:84:ARG:NH2	2.40	0.51
2:Qc:124:VAL:O	2:Qc:126:GLY:N	2.42	0.51
9:4e:71:GLU:O	9:4e:75:LYS:N	2.44	0.51
22:Qg:53:ARG:NH2	22:Qg:56:GLU:OE2	2.43	0.51
1:QA:18:LYS:O	24:QB:147:THR:OG1	2.27	0.51
32:Qc:404:CDL:O1	34:Qe:304:PC1:O14	2.29	0.50
13:6a:1:MET:SD	28:4g:150:TYR:HA	2.51	0.50
12:5C:68:LYS:NZ	28:4G:89:GLU:OE2	2.41	0.50
14:6B:43:ARG:NH1	26:4D:94:GLN:O	2.43	0.50
3:QD:96:ASN:ND2	3:QD:98:GLN:OE1	2.42	0.50
29:4I:235:LYS:NZ	29:4I:242:GLU:OE2	2.44	0.50
16:C1:326:SER:HB2	37:C1:501:HEA:H202	1.93	0.50
1:QA:365:LEU:HD13	1:QA:467:LEU:HD21	1.94	0.50
1:Qa:365:LEU:HD12	1:Qa:462:PRO:HD2	1.93	0.50
6:Qk:32:THR:OG1	22:Qg:2:ASN:ND2	2.44	0.50
7:4a:81:LEU:HB3	15:7c:41:LEU:HD23	1.92	0.50
12:5C:18:GLY:O	15:7C:27:ASN:ND2	2.44	0.50
25:5B:103:CYS:HB2	25:5B:128:CYS:CB	2.41	0.50
5:QJ:85:SER:O	5:QJ:87:ASN:N	2.42	0.50
14:6b:244:SER:O	26:4d:92:ASN:ND2	2.39	0.50
11:4J:4:GLU:OE1	11:4J:79:ARG:NH2	2.43	0.50
24:QB:198:LEU:HA	24:QB:459:VAL:HG21	1.92	0.50
26:4D:5:LEU:O	26:4D:9:GLY:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:4a:148:GLY:O	7:4a:149:LEU:C	2.55	0.50
3:QD:82:ARG:NH1	3:QD:88:ASP:OD2	2.44	0.50
4:Qh:30:ASP:OD1	20:Qe:80:ASN:ND2	2.44	0.50
9:4E:38:MET:HE3	9:4E:42:LYS:HD2	1.94	0.50
16:C1:90:ASN:OD1	16:C1:108:ASN:ND2	2.44	0.50
24:Qb:388:GLU:N	24:Qb:388:GLU:OE1	2.41	0.50
2:QC:124:VAL:O	2:QC:126:GLY:N	2.44	0.49
2:Qc:190:LEU:O	2:Qc:194:ASN:N	2.43	0.49
3:Qd:101:ARG:NH2	20:QE:194:GLY:O	2.45	0.49
37:c1:501:HEA:HBA2	37:c1:501:HEA:CMA	2.41	0.49
10:4h:41:VAL:HG22	10:4h:129:GLU:OE1	2.13	0.49
24:Qb:39:VAL:HG21	28:4g:110:LEU:HG	1.94	0.49
30:7a:22:HIS:O	30:7a:22:HIS:ND1	2.45	0.49
28:4g:265:CYS:O	28:4g:293:LYS:NZ	2.34	0.49
1:QA:296:GLU:OE1	22:Qg:218:GLN:NE2	2.45	0.49
11:4j:29:THR:HG22	11:4j:30:SER:N	2.26	0.49
16:c1:132:PRO:HA	16:c1:154:ASN:HD21	1.77	0.49
22:QG:111:ASP:O	22:QG:112:THR:OG1	2.25	0.49
24:Qb:460:HIS:CE1	24:Qb:467:ALA:HB1	2.47	0.49
25:5B:103:CYS:HB2	25:5B:128:CYS:HB3	1.93	0.49
30:7a:132:HIS:NE2	25:5b:145:ASP:OD2	2.43	0.49
13:6a:1:MET:HG2	28:4g:157:ARG:CZ	2.43	0.49
13:6a:17:GLU:OE1	13:6a:17:GLU:N	2.42	0.49
16:c1:80:ILE:HG21	16:c1:256:ILE:HG23	1.93	0.49
20:Qe:172:GLN:NE2	20:Qe:176:GLU:OE2	2.46	0.49
25:5b:26:GLU:O	25:5b:33:ARG:NH2	2.46	0.49
35:QD:304:PX2:O8	35:QD:304:PX2:H35	2.11	0.49
24:Qb:202:ALA:O	24:Qb:279:TYR:HA	2.13	0.49
2:QC:190:LEU:HD22	31:QC:402:HEM:CAA	2.43	0.49
19:DC:108:THR:O	19:DC:114:LYS:NZ	2.45	0.49
23:QI:21:ILE:HB	23:QI:22:PRO:HD3	1.95	0.49
35:QD:304:PX2:H25	20:QE:101:GLY:HA3	1.95	0.49
2:Qc:190:LEU:HD22	31:Qc:402:HEM:HAA2	1.94	0.49
37:C1:501:HEA:H18	37:C1:501:HEA:H261	1.95	0.49
5:Qj:56:ARG:O	5:Qj:60:THR:OG1	2.19	0.48
10:4h:191:ASN:O	11:4j:17:TRP:NE1	2.46	0.48
16:C1:326:SER:HB3	37:C1:501:HEA:H202	1.95	0.48
29:4I:109:LEU:O	29:4I:116:LYS:NZ	2.44	0.48
28:4g:85:LEU:O	28:4g:88:THR:OG1	2.27	0.48
2:Qc:77:CYS:CB	31:Qc:401:HEM:HBC2	2.43	0.48
18:c3:12:ARG:NH2	25:5b:174:ILE:O	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:4E:80:GLU:OE1	9:4E:80:GLU:N	2.36	0.48
16:C1:227:ILE:HG22	16:C1:227:ILE:O	2.14	0.48
19:DC:154:ARG:O	19:DC:155:LYS:HB2	2.12	0.48
30:7a:116:VAL:HG21	25:5b:22:VAL:HG21	1.94	0.48
3:Qd:15:PHE:O	3:Qd:16:GLN:HB2	2.14	0.48
18:c3:20:ILE:HB	18:c3:21:PRO:HD3	1.95	0.48
16:C1:316:ILE:HG23	42:4F:102:S12:H28	1.96	0.48
20:Qe:101:GLY:HA3	34:Qe:302:PC1:H392	1.95	0.48
24:Qb:308:TYR:OH	24:Qb:474:GLN:NE2	2.47	0.48
19:dc:120:ASP:OD2	19:dc:122:ARG:NE	2.44	0.48
15:7C:112:HIS:O	15:7C:116:THR:HG23	2.14	0.48
16:C1:351:PHE:HA	16:C1:401:ILE:HD11	1.96	0.48
34:DC:201:PC1:C1	34:DC:201:PC1:O22	2.62	0.48
24:Qb:68:LEU:O	24:Qb:245:THR:O	2.32	0.48
21:Qf:44:GLU:OE1	21:Qf:44:GLU:N	2.41	0.48
1:Qa:296:GLU:OE1	22:QG:218:GLN:NE2	2.39	0.48
29:4i:244:PHE:O	29:4i:247:ASN:ND2	2.43	0.48
37:c1:502:HEA:CMA	37:c1:502:HEA:HBA2	2.44	0.48
7:4A:107:ARG:NH2	7:4A:177:ALA:O	2.46	0.48
1:QA:449:ASP:OD1	1:QA:468:ARG:NE	2.46	0.48
1:Qa:276:ASP:OD1	10:4h:212:LYS:NZ	2.43	0.48
2:Qc:311:GLN:OE1	2:Qc:356:ASN:ND2	2.45	0.48
10:4H:41:VAL:HG22	10:4H:129:GLU:CD	2.39	0.48
11:4J:11:ASN:O	11:4J:15:GLY:N	2.47	0.48
17:C2:38:ARG:O	17:C2:42:ASN:ND2	2.44	0.48
18:C3:42:ILE:HD12	30:7A:161:PHE:CD2	2.49	0.48
20:QE:129:ILE:HB	20:QE:183:TRP:CZ2	2.49	0.48
28:4G:282:SER:OG	28:4G:284:ASP:OD2	2.29	0.48
27:4F:72:GLY:HA2	27:4F:75:VAL:HG23	1.95	0.47
3:QD:125:TYR:OH	33:QD:301:HEC:O2A	2.27	0.47
11:4j:38:ASP:OD1	11:4j:39:ASN:N	2.43	0.47
24:QB:356:ASP:C	24:QB:357:THR:HG1	2.16	0.47
1:QA:1:MET:O	1:QA:2:THR:OG1	2.27	0.47
16:c1:267:ILE:HD13	16:c1:401:ILE:HG22	1.96	0.47
18:c3:5:THR:OG1	25:5b:173:MET:O	2.32	0.47
24:Qb:198:LEU:O	24:Qb:202:ALA:HB2	2.15	0.47
15:7c:45:ASP:O	15:7c:49:ASP:OD1	2.33	0.47
16:C1:266:LEU:O	16:C1:269:THR:OG1	2.31	0.47
24:Qb:282:GLY:C	24:Qb:284:GLY:N	2.73	0.47
25:5B:53:THR:OG1	25:5B:55:ASP:OD1	2.28	0.47
8:4c:77:TRP:NE1	14:6b:257:TYR:O	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:6B:10:ASP:OD1	14:6B:12:LYS:N	2.47	0.47
16:C1:443:LEU:HB3	19:DC:163:THR:HG22	1.95	0.47
18:C3:20:ILE:HB	18:C3:21:PRO:HD3	1.96	0.47
22:QG:136:ASP:OD1	22:QG:136:ASP:N	2.45	0.47
25:5B:35:ASP:HA	25:5B:42:GLN:HG3	1.97	0.47
3:Qd:32:VAL:HG22	3:Qd:169:ILE:HD11	1.96	0.47
26:4d:81:ILE:CG2	26:4d:85:LEU:HB2	2.45	0.47
34:4E:201:PC1:O14	13:6A:36:ARG:NH2	2.48	0.47
18:C3:5:THR:OG1	25:5B:173:MET:O	2.28	0.47
10:4h:99:ASP:OD2	10:4h:101:ASN:ND2	2.47	0.47
16:C1:170:THR:HG23	16:C1:211:LEU:HD13	1.97	0.47
16:C1:309:ASP:OD1	17:C2:80:TYR:OH	2.33	0.47
25:5b:95:VAL:HG22	25:5b:136:ILE:HG13	1.97	0.47
10:4h:141:GLN:OE1	10:4h:141:GLN:N	2.46	0.46
12:5C:198:THR:OG1	12:5C:202:SER:O	2.31	0.46
16:C1:480:ARG:NH2	29:4I:31:TRP:O	2.46	0.46
2:QC:102:VAL:HG12	2:QC:186:HIS:CE1	2.51	0.46
2:QC:190:LEU:HD22	31:QC:402:HEM:HAA1	1.97	0.46
19:dc:136:ASP:OD1	19:dc:136:ASP:N	2.47	0.46
13:6A:1:MET:SD	28:4G:150:TYR:HA	2.55	0.46
24:QB:99:MET:HE1	24:QB:231:TRP:HB2	1.97	0.46
28:4G:138:GLN:NE2	28:4G:142:ASP:OD1	2.47	0.46
4:Qh:24:ARG:NH1	4:Qh:25:HIS:O	2.48	0.46
19:dc:32:ARG:NH1	29:4i:134:LEU:O	2.43	0.46
25:5B:55:ASP:OD1	25:5B:55:ASP:N	2.47	0.46
29:4I:91:PHE:CD1	29:4I:91:PHE:C	2.94	0.46
2:Qc:121:TYR:HA	31:Qc:401:HEM:HAD2	1.98	0.46
15:7c:112:HIS:O	15:7c:116:THR:HG23	2.15	0.46
16:C1:453:TYR:CZ	16:C1:461:MET:HG3	2.50	0.46
1:QA:377:ARG:HD3	1:QA:476:LEU:HD11	1.97	0.46
5:Qj:94:ARG:O	22:QG:63:ARG:NH1	2.46	0.46
7:4a:149:LEU:HD23	16:c1:231:ILE:HD11	1.98	0.46
12:5c:206:ARG:NH2	17:c2:9:GLU:OE1	2.48	0.46
10:4H:151:VAL:HG21	26:4D:7:ILE:HG13	1.96	0.46
24:Qb:200:LYS:HE2	24:Qb:211:THR:HG22	1.97	0.46
16:c1:203:THR:HG23	16:c1:255:VAL:HG13	1.98	0.46
24:Qb:203:PHE:HA	24:Qb:278:LYS:O	2.16	0.46
1:QA:1:MET:HE3	1:QA:1:MET:HA	1.97	0.46
2:Qc:122:SER:HB3	2:Qc:133:ILE:HD11	1.98	0.46
8:4c:114:ALA:CB	26:4d:166:ILE:HD11	2.46	0.46
17:C2:142:ILE:HG22	17:C2:180:GLU:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:4d:5:LEU:O	26:4d:9:GLY:N	2.48	0.46
1:QA:400:ASP:OD2	24:QB:408:SER:OG	2.33	0.46
20:Qe:170:ASP:OD2	20:Qe:230:ASN:ND2	2.48	0.46
24:Qb:202:ALA:HA	24:Qb:281:GLY:CA	2.46	0.46
25:5B:97:THR:HA	29:4I:150:VAL:O	2.15	0.46
28:4G:199:VAL:O	28:4G:203:SER:OG	2.29	0.46
30:7A:22:HIS:O	30:7A:22:HIS:ND1	2.49	0.46
25:5B:133:VAL:HG11	29:4I:209:TRP:HB2	1.99	0.46
28:4g:159:GLU:N	28:4g:159:GLU:OE1	2.49	0.46
6:QK:65:GLN:OE1	6:QK:69:ARG:NH1	2.48	0.45
1:Qa:172:GLU:OE2	3:Qd:234:ARG:NH2	2.42	0.45
2:Qc:220:VAL:HG21	32:Qc:404:CDL:H322	1.98	0.45
16:c1:164:VAL:HG13	18:c3:28:PHE:HE2	1.81	0.45
16:c1:274:LYS:NZ	16:c1:337:ALA:O	2.49	0.45
29:4i:150:VAL:O	25:5b:97:THR:HA	2.16	0.45
2:QC:139:LEU:HD11	2:QC:272:ILE:HG12	1.98	0.45
5:QJ:60:THR:O	30:7A:149:ARG:NH2	2.49	0.45
6:QK:32:THR:OG1	22:QG:2:ASN:ND2	2.49	0.45
7:4a:197:LEU:CD1	18:c3:86:ILE:HG23	2.46	0.45
15:7c:125:ARG:NH2	19:dc:101:ALA:O	2.50	0.45
18:C3:134:CYS:SG	18:C3:137:ILE:HB	2.56	0.45
22:Qg:33:ILE:HB	22:Qg:34:PRO:HA	1.99	0.45
1:QA:95:MET:HE3	1:QA:118:ASP:HB3	1.98	0.45
14:6b:102:TYR:O	14:6b:110:TRP:NE1	2.48	0.45
10:4H:139:THR:HG23	10:4H:142:ALA:H	1.82	0.45
1:QA:112:VAL:HG12	1:QA:114:CYS:SG	2.57	0.45
16:c1:318:THR:O	16:c1:321:ILE:HG22	2.17	0.45
2:QC:65:THR:OG1	20:QE:112:GLN:NE2	2.43	0.45
25:5b:80:GLU:OE1	25:5b:80:GLU:N	2.49	0.45
3:Qd:165:THR:OG1	3:Qd:166:ASP:N	2.50	0.45
14:6b:88:LEU:HD22	17:c2:139:LEU:HD13	1.98	0.45
16:c1:26:GLY:O	16:c1:30:TYR:HD1	2.00	0.45
37:c1:502:HEA:H272	37:c1:502:HEA:H261	1.98	0.45
24:Qb:38:ARG:NH1	29:4i:74:ASN:OD1	2.50	0.45
24:QB:284:GLY:O	24:QB:459:VAL:HA	2.17	0.45
29:4i:155:GLU:OE1	29:4i:155:GLU:N	2.50	0.45
2:QC:187:LEU:HD21	31:QC:402:HEM:CMA	2.47	0.45
9:4E:38:MET:HE2	9:4E:127:VAL:HG21	1.97	0.45
9:4E:135:LEU:HA	9:4E:138:LEU:HD13	1.99	0.45
16:C1:298:ALA:HB3	16:C1:314:PHE:CZ	2.52	0.45
34:QE:303:PC1:H142	34:QE:303:PC1:O13	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:1:MET:HE1	24:QB:167:SER:HA	1.98	0.45
1:QA:377:ARG:CD	1:QA:476:LEU:HD21	2.47	0.45
1:Qa:1:MET:O	22:QG:163:ARG:NH1	2.50	0.45
6:Qk:60:LEU:O	6:Qk:64:ASN:ND2	2.50	0.45
16:C1:113:TRP:HB2	18:C3:21:PRO:HG2	1.98	0.45
24:QB:406:VAL:HG22	24:QB:429:PRO:HB2	1.99	0.45
26:4d:105:ASP:O	26:4d:106:SER:OG	2.28	0.45
28:4g:177:ARG:NH2	29:4i:203:GLN:O	2.50	0.45
5:QJ:147:ARG:O	20:QE:103:ARG:NH1	2.50	0.45
16:c1:377:LEU:HD21	16:c1:443:LEU:HD23	1.98	0.45
16:c1:452:GLU:OE2	17:c2:116:ARG:NH2	2.50	0.45
22:QG:126:CYS:SG	22:QG:127:LEU:N	2.89	0.45
12:5C:36:GLU:OE2	19:DC:26:ARG:NH1	2.50	0.44
28:4g:79:TYR:CE1	28:4g:137:VAL:HG11	2.52	0.44
4:QH:30:ASP:OD1	20:QE:80:ASN:ND2	2.51	0.44
7:4a:88:VAL:HG21	15:7c:38:VAL:HG21	1.99	0.44
14:6b:18:GLU:O	14:6b:22:THR:OG1	2.36	0.44
7:4A:234:SER:O	7:4A:242:GLN:N	2.47	0.44
3:QD:144:SER:OG	3:QD:145:THR:N	2.50	0.44
1:Qa:463:GLU:OE1	1:Qa:463:GLU:N	2.50	0.44
8:4c:43:SER:OG	12:5c:185:VAL:HG12	2.16	0.44
17:C2:60:TRP:CD1	17:C2:60:TRP:C	2.95	0.44
20:Qe:129:ILE:HB	20:Qe:183:TRP:CZ2	2.53	0.44
1:QA:465:ASP:N	1:QA:465:ASP:OD1	2.51	0.44
2:Qc:22:LEU:HD21	32:Qd:302:CDL:H622	1.99	0.44
10:4h:79:ASP:OD2	12:5c:107:LYS:NZ	2.51	0.44
24:Qb:194:LEU:HD22	24:Qb:305:TYR:HB3	1.99	0.44
16:C1:318:THR:O	16:C1:321:ILE:HG22	2.17	0.44
2:QC:335:TYR:HB3	4:QH:77:GLU:HG3	2.00	0.44
2:Qc:302:ARG:NH1	22:Qg:33:ILE:O	2.47	0.44
4:Qh:57:THR:OG1	4:Qh:58:PRO:HD3	2.17	0.44
16:c1:180:ASN:HB3	16:c1:201:ILE:HD11	2.00	0.44
15:7C:123:TYR:HB3	19:DC:105:ARG:O	2.17	0.44
1:QA:339:TYR:O	1:QA:341:ASP:N	2.50	0.44
3:QD:15:PHE:O	3:QD:16:GLN:NE2	2.50	0.44
25:5b:35:ASP:HA	25:5b:42:GLN:HG3	2.00	0.44
18:C3:135:LEU:HD12	18:C3:135:LEU:H	1.83	0.44
28:4G:230:PRO:O	28:4G:233:GLN:HB2	2.18	0.44
28:4g:95:ALA:N	28:4g:96:PRO:HD2	2.33	0.44
29:4i:234:VAL:HG23	25:5b:125:CYS:HA	1.98	0.44
3:Qd:109:PRO:HG3	33:Qd:301:HEC:HMD3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:4c:67:ALA:HB1	14:6b:32:ILE:HD11	2.00	0.44
9:4e:119:ASP:OD1	9:4e:119:ASP:N	2.50	0.44
16:C1:26:GLY:O	16:C1:30:TYR:HD1	2.01	0.44
16:C1:81:MET:HB2	16:C1:82:PRO:HD3	2.00	0.44
20:QE:172:GLN:O	20:QE:221:ARG:NH1	2.43	0.44
12:5c:44:TYR:N	12:5c:45:PRO:CD	2.81	0.43
16:C1:155:ILE:O	16:C1:159:LEU:HG	2.17	0.43
26:4d:86:GLN:N	26:4d:87:PRO:HD2	2.33	0.43
19:dc:25:VAL:HG12	19:dc:26:ARG:N	2.32	0.43
8:4C:94:ILE:HG21	14:6B:222:LEU:HD11	2.00	0.43
16:C1:254:TYR:HA	16:C1:257:ILE:HG22	1.99	0.43
25:5B:85:VAL:HG23	25:5B:134:ALA:HA	1.99	0.43
28:4G:310:ALA:O	28:4G:314:VAL:N	2.51	0.43
2:Qc:276:PRO:HG3	6:Qk:83:VAL:HG11	2.01	0.43
5:QJ:113:VAL:HG12	5:QJ:114:LYS:H	1.83	0.43
33:Qd:301:HEC:HBB3	33:Qd:301:HEC:HMB3	2.00	0.43
8:4c:126:LYS:NZ	8:4c:138:GLU:OE2	2.37	0.43
10:4h:65:LYS:HA	28:4g:53:PRO:HB3	2.00	0.43
16:c1:46:GLU:HG2	16:c1:64:TYR:CD1	2.53	0.43
37:c1:501:HEA:H251	17:c2:68:LEU:HD13	2.00	0.43
17:c2:98:ASN:ND2	17:c2:103:ILE:HD12	2.33	0.43
24:QB:68:LEU:O	24:QB:245:THR:O	2.37	0.43
1:Qa:365:LEU:O	1:Qa:369:MET:HG2	2.19	0.43
7:4a:216:PRO:O	7:4a:220:GLY:N	2.51	0.43
18:C3:128:ASN:O	18:C3:129:ASN:ND2	2.51	0.43
20:Qe:134:GLU:HA	20:Qe:151:LYS:HB3	2.01	0.43
29:4I:217:GLU:OE2	29:4I:219:THR:OG1	2.34	0.43
2:QC:266:LEU:N	2:QC:267:PRO:HD2	2.34	0.43
3:QD:123:VAL:HG23	3:QD:124:ASP:N	2.34	0.43
17:c2:142:ILE:HG22	17:c2:180:GLU:HG2	2.01	0.43
29:4I:67:SER:OG	29:4I:68:SER:N	2.51	0.43
17:C2:77:THR:HG21	36:4F:101:3PE:H272	2.00	0.43
25:5B:100:LEU:H	29:4I:153:ASN:HD21	1.67	0.43
28:4g:230:PRO:O	28:4g:233:GLN:HB2	2.19	0.43
1:Qa:465:ASP:N	1:Qa:465:ASP:OD1	2.52	0.43
16:c1:78:VAL:HG12	16:c1:78:VAL:O	2.19	0.43
22:Qg:126:CYS:SG	22:Qg:127:LEU:N	2.91	0.43
26:4D:173:ARG:O	26:4D:174:VAL:C	2.62	0.43
26:4d:44:PHE:CZ	27:4f:28:TRP:HB3	2.53	0.43
37:c1:501:HEA:HBC1	37:c1:501:HEA:CHD	2.45	0.42
12:5C:44:TYR:N	12:5C:45:PRO:CD	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Qb:99:MET:HE1	24:Qb:231:TRP:HB2	2.01	0.42
24:QB:285:TYR:C	24:QB:285:TYR:CD1	2.97	0.42
29:4I:73:VAL:HG12	29:4I:75:TRP:H	1.84	0.42
26:4d:24:PHE:CE1	25:5b:100:LEU:HD11	2.54	0.42
1:QA:56:ALA:HB2	1:QA:203:HIS:HB3	2.01	0.42
1:Qa:475:ASP:O	1:Qa:476:LEU:CB	2.67	0.42
2:Qc:226:ILE:HD11	32:Qd:302:CDL:H632	2.00	0.42
12:5C:59:ASN:OD1	12:5C:63:ASN:ND2	2.52	0.42
20:QE:222:ILE:HD11	20:QE:224:LYS:O	2.18	0.42
24:Qb:282:GLY:O	24:Qb:458:LEU:C	2.62	0.42
1:QA:342:VAL:HG22	1:QA:343:GLY:H	1.84	0.42
8:4c:111:ARG:HD3	14:6b:204:TRP:CD2	2.55	0.42
10:4h:57:SER:OG	29:4i:181:VAL:N	2.48	0.42
37:c1:501:HEA:H261	37:c1:501:HEA:C18	2.50	0.42
24:Qb:406:VAL:HG22	24:Qb:429:PRO:HB2	2.00	0.42
26:4D:173:ARG:O	26:4D:173:ARG:CZ	2.68	0.42
26:4d:77:LEU:HB3	26:4d:81:ILE:HD13	2.01	0.42
33:QD:301:HEC:HHA	33:QD:301:HEC:HBD1	2.02	0.42
18:c3:134:CYS:SG	18:c3:137:ILE:HB	2.59	0.42
16:C1:37:TYR:OH	16:C1:472:ILE:HA	2.19	0.42
37:C1:502:HEA:CMA	37:C1:502:HEA:CBA	2.97	0.42
20:QE:234:PRO:O	20:QE:236:PHE:N	2.48	0.42
24:Qb:113:TYR:O	24:Qb:117:THR:OG1	2.29	0.42
29:4i:109:LEU:O	29:4i:116:LYS:NZ	2.53	0.42
29:4i:236:ASN:O	29:4i:237:ALA:HB3	2.19	0.42
3:QD:208:THR:HG22	35:QD:304:PX2:H13	2.02	0.42
3:Qd:32:VAL:HG11	3:Qd:186:VAL:CG2	2.49	0.42
13:6a:49:TRP:O	13:6a:52:VAL:HG22	2.19	0.42
19:dc:108:THR:O	19:dc:114:LYS:NZ	2.52	0.42
9:4E:65:ASP:N	9:4E:65:ASP:OD1	2.53	0.42
13:6A:1:MET:SD	25:5B:152:LYS:HA	2.59	0.42
24:Qb:201:THR:C	24:Qb:281:GLY:HA2	2.44	0.42
16:C1:29:GLY:HA3	16:C1:83:VAL:HG23	2.01	0.42
24:Qb:99:MET:HE3	24:Qb:230:ARG:HG2	2.02	0.42
26:4d:105:ASP:OD1	26:4d:105:ASP:N	2.52	0.42
29:4i:67:SER:OG	29:4i:68:SER:N	2.53	0.42
5:QJ:19:ALA:O	5:QJ:20:ASP:HB2	2.19	0.42
16:c1:113:TRP:HB2	18:c3:21:PRO:HG2	2.01	0.42
17:c2:60:TRP:CD1	17:c2:60:TRP:C	2.98	0.42
18:c3:61:VAL:HG12	30:7a:140:PRO:HG2	2.02	0.42
24:Qb:471:ASP:OD1	24:Qb:471:ASP:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:QB:402:ALA:O	24:QB:406:VAL:HG23	2.19	0.42
29:4i:146:PHE:CG	25:5b:89:GLY:HA2	2.55	0.42
1:Qa:159:ASP:OD1	1:Qa:159:ASP:N	2.51	0.42
1:Qa:339:TYR:O	1:Qa:341:ASP:N	2.53	0.42
5:Qj:60:THR:O	30:7a:149:ARG:NH1	2.53	0.42
10:4h:93:THR:HG22	10:4h:102:PRO:HB2	2.01	0.42
16:c1:387:PHE:HB2	37:c1:501:HEA:CMD	2.50	0.42
17:c2:143:HIS:CE1	17:c2:189:MET:HE1	2.54	0.42
16:C1:147:ASP:OD1	16:C1:148:ALA:N	2.53	0.42
17:C2:61:THR:HG23	26:4D:49:LEU:HD22	2.00	0.42
24:Qb:457:THR:HG23	24:Qb:459:VAL:HG23	2.01	0.42
26:4d:165:LEU:HD12	26:4d:166:ILE:HG23	2.01	0.42
28:4g:34:TYR:CE2	29:4i:174:VAL:HG23	2.55	0.42
28:4g:75:LYS:O	28:4g:192:ARG:NH1	2.52	0.42
35:QJ:201:PX2:H46	35:QJ:201:PX2:H41	1.81	0.42
2:Qc:266:LEU:N	2:Qc:267:PRO:HD2	2.35	0.42
7:4a:175:TRP:HB3	7:4a:181:VAL:HG23	2.01	0.42
10:4h:32:TYR:CE1	10:4h:130:ILE:HD11	2.55	0.42
7:4a:197:LEU:HD12	18:c3:86:ILE:HG23	2.02	0.42
34:4e:201:PC1:O14	13:6a:36:ARG:NH2	2.49	0.42
18:c3:1:MET:HG2	25:5b:161:PHE:HB3	2.01	0.42
16:C1:480:ARG:NH1	29:4I:34:GLY:HA2	2.35	0.42
24:QB:285:TYR:C	24:QB:285:TYR:HD1	2.28	0.42
1:QA:92:MET:HE1	1:QA:112:VAL:HG11	2.00	0.41
2:Qc:113:ILE:HD11	31:Qc:402:HEM:HBB1	2.01	0.41
3:Qd:123:VAL:O	3:Qd:124:ASP:C	2.63	0.41
5:Qj:85:SER:O	5:Qj:87:ASN:N	2.51	0.41
16:c1:94:PRO:HG3	16:c1:102:LEU:HD23	2.01	0.41
9:4E:31:GLY:O	9:4E:136:TRP:O	2.38	0.41
11:4J:66:ALA:HB1	11:4J:78:VAL:HG21	2.02	0.41
16:C1:93:ILE:HB	16:C1:94:PRO:HD3	2.02	0.41
20:Qe:153:THR:OG1	20:Qe:154:ASP:N	2.53	0.41
16:c1:181:LYS:O	16:c1:184:ARG:NH1	2.53	0.41
17:c2:117:ILE:O	17:c2:117:ILE:HG22	2.20	0.41
8:4C:43:SER:OG	12:5C:185:VAL:HG12	2.20	0.41
14:6B:23:ASP:OD1	14:6B:24:GLY:N	2.53	0.41
20:Qe:134:GLU:OE2	20:Qe:182:ARG:NH1	2.52	0.41
2:Qc:91:SER:HB2	31:Qc:402:HEM:HMD3	2.03	0.41
2:Qc:353:HIS:NE2	22:Qg:44:PHE:O	2.51	0.41
10:4h:90:LEU:O	10:4h:93:THR:HG23	2.19	0.41
15:7c:41:LEU:HD12	15:7c:42:TYR:CD1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:4H:191:ASN:O	11:4J:17:TRP:CD1	2.73	0.41
14:6B:203:THR:O	14:6B:207:VAL:HG23	2.20	0.41
22:Qg:83:TYR:O	22:Qg:84:SER:C	2.63	0.41
25:5B:95:VAL:HG22	25:5B:136:ILE:HG13	2.01	0.41
1:Qa:475:ASP:O	1:Qa:476:LEU:HB2	2.20	0.41
36:c1:506:3PE:O22	36:c1:506:3PE:C3	2.68	0.41
14:6B:18:GLU:O	14:6B:22:THR:OG1	2.35	0.41
17:C2:144:SER:HB3	17:C2:178:CYS:O	2.21	0.41
24:QB:170:ASN:O	24:QB:174:VAL:HG23	2.21	0.41
30:7A:110:SER:O	30:7A:115:ARG:NH1	2.53	0.41
2:QC:34:ILE:HD13	31:QC:401:HEM:HAB	2.02	0.41
35:QJ:201:PX2:H31	2:Qc:149:LYS:HB3	2.02	0.41
4:Qh:76:LEU:HD21	6:Qk:88:PHE:HA	2.03	0.41
8:4C:118:ILE:HD12	14:6B:198:LEU:HD12	2.03	0.41
16:C1:377:LEU:HD21	16:C1:443:LEU:HD23	2.02	0.41
13:6A:1:MET:HA	28:4G:157:ARG:HD3	2.01	0.41
22:QG:124:TRP:O	22:QG:128:THR:HG22	2.20	0.41
25:5B:91:HIS:N	25:5B:138:GLU:OE2	2.47	0.41
13:6a:45:THR:HG22	18:c3:147:TYR:OH	2.20	0.41
13:6A:17:GLU:OE1	13:6A:17:GLU:N	2.53	0.41
13:6A:101:THR:HG22	13:6A:101:THR:O	2.21	0.41
24:Qb:202:ALA:HA	24:Qb:281:GLY:H	1.85	0.41
24:Qb:203:PHE:O	24:Qb:209:GLY:HA3	2.21	0.41
1:QA:315:VAL:HG12	1:QA:321:PRO:HB3	2.03	0.41
5:Qj:102:GLU:O	5:Qj:106:ASN:N	2.54	0.41
14:6B:82:GLN:HA	14:6B:90:LEU:HD11	2.03	0.41
10:4h:89:LEU:HD22	10:4h:106:THR:HG21	2.03	0.41
36:C1:507:3PE:O22	36:C1:507:3PE:H31	2.20	0.41
3:Qd:45:PHE:HB2	3:Qd:113:SER:OG	2.21	0.41
16:c1:319:SER:HB3	17:c2:68:LEU:HD21	2.03	0.41
7:4A:96:ASN:OD1	30:7A:129:ARG:NH1	2.54	0.41
20:Qe:198:VAL:N	20:Qe:208:PHE:O	2.53	0.41
22:QG:3:ASP:OD2	22:QG:69:LYS:NZ	2.32	0.41
22:QG:140:LEU:HD13	22:QG:145:LEU:HD21	2.03	0.41
24:Qb:384:GLY:CA	24:Qb:448:VAL:HG21	2.51	0.41
25:5B:115:THR:OG1	29:4I:127:ARG:NH1	2.54	0.41
28:4g:225:ILE:HG23	28:4g:233:GLN:HA	2.03	0.41
28:4g:310:ALA:O	28:4g:314:VAL:N	2.53	0.41
1:QA:365:LEU:O	1:QA:369:MET:HG2	2.21	0.41
14:6b:189:ALA:O	14:6b:193:LYS:HG2	2.20	0.41
16:c1:384:VAL:HA	16:c1:387:PHE:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:QF:30:VAL:HG22	21:QF:55:LEU:HD11	2.03	0.41
24:QB:315:ARG:NH1	24:QB:422:THR:HG21	2.35	0.41
30:7A:141:GLU:HG2	30:7A:142:PHE:N	2.36	0.41
2:QC:122:SER:HB3	2:QC:133:ILE:HD11	2.03	0.40
4:Qh:34:ARG:O	4:Qh:35:GLY:C	2.63	0.40
7:4a:148:GLY:O	7:4a:150:GLY:N	2.54	0.40
14:6b:116:GLU:OE1	14:6b:116:GLU:N	2.49	0.40
16:c1:237:ASP:HB3	16:c1:240:LEU:HB3	2.03	0.40
14:6B:201:ASP:OD1	14:6B:201:ASP:N	2.54	0.40
14:6B:218:THR:O	14:6B:222:LEU:HG	2.22	0.40
20:Qe:168:LEU:HD13	20:Qe:221:ARG:HD2	2.03	0.40
23:Qi:13:PHE:O	23:Qi:19:THR:OG1	2.31	0.40
29:4I:87:PHE:O	29:4I:91:PHE:HB3	2.21	0.40
28:4g:282:SER:OG	28:4g:284:ASP:OD2	2.29	0.40
10:4h:194:ASP:CG	10:4h:195:PRO:HD2	2.46	0.40
8:4C:107:LEU:HD21	14:6B:215:VAL:HG21	2.02	0.40
14:6B:258:GLU:HG2	26:4D:148:ALA:HB3	2.03	0.40
16:C1:296:VAL:O	16:C1:299:HIS:CD2	2.75	0.40
16:C1:393:LEU:HD21	16:C1:431:ALA:HB3	2.03	0.40
20:QE:152:ARG:HH22	20:QE:219:SER:HA	1.85	0.40
28:4G:95:ALA:N	28:4G:96:PRO:HD2	2.36	0.40
28:4G:215:GLU:OE2	28:4G:248:LYS:NZ	2.45	0.40
15:7c:164:ASP:N	15:7c:164:ASP:OD1	2.53	0.40
16:c1:153:VAL:HG21	18:c3:36:TYR:HB2	2.03	0.40
7:4A:199:ASP:OD2	18:C3:149:THR:OG1	2.22	0.40
13:6A:1:MET:HE2	25:5B:149:PRO:HB2	2.02	0.40
28:4G:209:ASP:OD1	28:4G:212:ARG:NH2	2.43	0.40
2:QC:212:TYR:OH	32:QC:403:CDL:OB7	2.37	0.40
3:QD:224:ARG:HB2	32:QD:302:CDL:OA9	2.21	0.40
2:Qc:77:CYS:SG	31:Qc:401:HEM:CBC	3.10	0.40
7:4a:149:LEU:HD22	16:c1:229:SER:CB	2.51	0.40
16:c1:30:TYR:CD2	37:c1:502:HEA:H22	2.56	0.40
16:c1:296:VAL:O	16:c1:299:HIS:CD2	2.75	0.40
17:c2:170:THR:O	17:c2:174:TYR:OH	2.30	0.40
16:C1:228:ASN:ND2	13:6A:81:ASP:O	2.54	0.40
16:C1:376:MET:SD	17:C2:8:ILE:HD11	2.62	0.40
34:Qe:301:PC1:O22	34:Qe:301:PC1:H11	2.20	0.40
10:4h:93:THR:HA	10:4h:104:VAL:HG22	2.02	0.40
17:c2:7:GLU:HB3	17:c2:82:LEU:HD22	2.02	0.40
9:4E:57:TYR:HB3	14:6B:128:LEU:HD11	2.03	0.40
14:6B:273:LEU:O	14:6B:275:ARG:NH1	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:C1:121:ILE:HG12	30:7A:166:TYR:OH	2.21	0.40
21:Qf:25:HIS:ND1	21:Qf:62:CYS:SG	2.95	0.40
26:4D:105:ASP:O	26:4D:106:SER:CB	2.69	0.40
27:4F:4:SER:O	27:4F:8:PRO:HD2	2.21	0.40
29:4I:235:LYS:HG2	29:4I:236:ASN:N	2.36	0.40
26:4d:47:PHE:O	26:4d:47:PHE:CG	2.74	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	QA	476/479 (99%)	460 (97%)	16 (3%)	0	100	100
1	Qa	476/479 (99%)	462 (97%)	14 (3%)	0	100	100
2	QC	362/368 (98%)	354 (98%)	7 (2%)	1 (0%)	36	63
2	Qc	362/368 (98%)	350 (97%)	12 (3%)	0	100	100
3	QD	239/243 (98%)	225 (94%)	14 (6%)	0	100	100
3	Qd	239/243 (98%)	218 (91%)	21 (9%)	0	100	100
4	QH	83/86 (96%)	81 (98%)	2 (2%)	0	100	100
4	Qh	83/86 (96%)	78 (94%)	5 (6%)	0	100	100
5	QJ	147/154 (96%)	141 (96%)	6 (4%)	0	100	100
5	Qj	147/154 (96%)	139 (95%)	8 (5%)	0	100	100
6	QK	59/100 (59%)	59 (100%)	0	0	100	100
6	Qk	59/100 (59%)	59 (100%)	0	0	100	100
7	4A	202/246 (82%)	195 (96%)	7 (4%)	0	100	100
7	4a	202/246 (82%)	191 (95%)	11 (5%)	0	100	100
8	4C	121/139 (87%)	115 (95%)	6 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	4c	121/139 (87%)	118 (98%)	3 (2%)	0	100	100
9	4E	158/165 (96%)	154 (98%)	4 (2%)	0	100	100
9	4e	158/165 (96%)	154 (98%)	4 (2%)	0	100	100
10	4H	203/221 (92%)	200 (98%)	3 (2%)	0	100	100
10	4h	203/221 (92%)	197 (97%)	6 (3%)	0	100	100
11	4J	86/88 (98%)	83 (96%)	3 (4%)	0	100	100
11	4j	86/88 (98%)	84 (98%)	2 (2%)	0	100	100
12	5C	194/208 (93%)	189 (97%)	5 (3%)	0	100	100
12	5c	194/208 (93%)	185 (95%)	9 (5%)	0	100	100
13	6A	109/112 (97%)	101 (93%)	7 (6%)	1 (1%)	14	39
13	6a	89/112 (80%)	86 (97%)	3 (3%)	0	100	100
14	6B	280/287 (98%)	274 (98%)	6 (2%)	0	100	100
14	6b	280/287 (98%)	271 (97%)	9 (3%)	0	100	100
15	7C	149/171 (87%)	143 (96%)	6 (4%)	0	100	100
15	7c	149/171 (87%)	142 (95%)	7 (5%)	0	100	100
16	C1	493/495 (100%)	479 (97%)	14 (3%)	0	100	100
16	c1	493/495 (100%)	473 (96%)	20 (4%)	0	100	100
17	C2	194/196 (99%)	184 (95%)	10 (5%)	0	100	100
17	c2	194/196 (99%)	180 (93%)	14 (7%)	0	100	100
18	C3	159/161 (99%)	152 (96%)	7 (4%)	0	100	100
18	c3	159/161 (99%)	151 (95%)	8 (5%)	0	100	100
19	DC	165/179 (92%)	159 (96%)	6 (4%)	0	100	100
19	dc	165/179 (92%)	157 (95%)	8 (5%)	0	100	100
20	QE	229/252 (91%)	219 (96%)	10 (4%)	0	100	100
20	Qe	229/252 (91%)	216 (94%)	13 (6%)	0	100	100
21	QF	62/72 (86%)	62 (100%)	0	0	100	100
21	Qf	62/72 (86%)	61 (98%)	1 (2%)	0	100	100
22	QG	226/228 (99%)	220 (97%)	6 (3%)	0	100	100
22	Qg	226/228 (99%)	219 (97%)	7 (3%)	0	100	100
23	QI	28/70 (40%)	28 (100%)	0	0	100	100
23	Qi	28/70 (40%)	27 (96%)	1 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	QB	453/474 (96%)	438 (97%)	15 (3%)	0	100	100
24	Qb	453/474 (96%)	429 (95%)	24 (5%)	0	100	100
25	5B	155/174 (89%)	149 (96%)	6 (4%)	0	100	100
25	5b	155/174 (89%)	148 (96%)	7 (4%)	0	100	100
26	4D	171/174 (98%)	157 (92%)	14 (8%)	0	100	100
26	4d	171/174 (98%)	161 (94%)	10 (6%)	0	100	100
27	4F	73/75 (97%)	70 (96%)	3 (4%)	0	100	100
27	4f	73/75 (97%)	67 (92%)	6 (8%)	0	100	100
28	4G	295/315 (94%)	286 (97%)	9 (3%)	0	100	100
28	4g	295/315 (94%)	283 (96%)	12 (4%)	0	100	100
29	4I	263/274 (96%)	255 (97%)	8 (3%)	0	100	100
29	4i	263/274 (96%)	252 (96%)	11 (4%)	0	100	100
30	7A	161/178 (90%)	155 (96%)	6 (4%)	0	100	100
30	7a	161/178 (90%)	156 (97%)	5 (3%)	0	100	100
All	All	11970/12768 (94%)	11501 (96%)	467 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	6A	100	ASP
2	QC	145	PHE

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	QA	400/401 (100%)	398 (100%)	2 (0%)	81	82
1	Qa	400/401 (100%)	397 (99%)	3 (1%)	73	79
2	QC	337/341 (99%)	335 (99%)	2 (1%)	78	81
2	Qc	337/341 (99%)	336 (100%)	1 (0%)	86	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	QD	206/207 (100%)	206 (100%)	0	100	100
3	Qd	206/207 (100%)	206 (100%)	0	100	100
4	QH	71/72 (99%)	71 (100%)	0	100	100
4	Qh	71/72 (99%)	71 (100%)	0	100	100
5	QJ	124/128 (97%)	124 (100%)	0	100	100
5	Qj	124/128 (97%)	123 (99%)	1 (1%)	73	79
6	QK	50/82 (61%)	50 (100%)	0	100	100
6	Qk	50/82 (61%)	50 (100%)	0	100	100
7	4A	173/207 (84%)	171 (99%)	2 (1%)	63	75
7	4a	173/207 (84%)	173 (100%)	0	100	100
8	4C	112/127 (88%)	111 (99%)	1 (1%)	70	78
8	4c	112/127 (88%)	110 (98%)	2 (2%)	51	70
9	4E	142/145 (98%)	142 (100%)	0	100	100
9	4e	142/145 (98%)	138 (97%)	4 (3%)	38	63
10	4H	176/189 (93%)	174 (99%)	2 (1%)	65	76
10	4h	176/189 (93%)	175 (99%)	1 (1%)	78	81
11	4J	75/75 (100%)	74 (99%)	1 (1%)	61	74
11	4j	75/75 (100%)	75 (100%)	0	100	100
12	5C	167/178 (94%)	165 (99%)	2 (1%)	63	75
12	5c	167/178 (94%)	167 (100%)	0	100	100
13	6A	97/97 (100%)	97 (100%)	0	100	100
13	6a	79/97 (81%)	78 (99%)	1 (1%)	61	74
14	6B	238/243 (98%)	237 (100%)	1 (0%)	84	84
14	6b	238/243 (98%)	238 (100%)	0	100	100
15	7C	135/152 (89%)	134 (99%)	1 (1%)	76	80
15	7c	135/152 (89%)	135 (100%)	0	100	100
16	C1	438/438 (100%)	434 (99%)	4 (1%)	70	78
16	c1	438/438 (100%)	437 (100%)	1 (0%)	87	87
17	C2	178/178 (100%)	177 (99%)	1 (1%)	78	81
17	c2	178/178 (100%)	176 (99%)	2 (1%)	65	76
18	C3	155/155 (100%)	154 (99%)	1 (1%)	78	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	c3	155/155 (100%)	155 (100%)	0	100	100
19	DC	148/153 (97%)	148 (100%)	0	100	100
19	dc	148/153 (97%)	144 (97%)	4 (3%)	39	64
20	QE	193/209 (92%)	192 (100%)	1 (0%)	81	82
20	Qe	193/209 (92%)	191 (99%)	2 (1%)	68	77
21	QF	58/63 (92%)	56 (97%)	2 (3%)	32	59
21	Qf	58/63 (92%)	55 (95%)	3 (5%)	21	48
22	QG	207/207 (100%)	203 (98%)	4 (2%)	50	69
22	Qg	207/207 (100%)	204 (99%)	3 (1%)	59	73
23	QI	27/27 (100%)	27 (100%)	0	100	100
23	Qi	27/27 (100%)	27 (100%)	0	100	100
24	QB	369/386 (96%)	367 (100%)	2 (0%)	81	82
24	Qb	369/386 (96%)	364 (99%)	5 (1%)	59	73
25	5B	134/148 (90%)	131 (98%)	3 (2%)	45	67
25	5b	134/148 (90%)	133 (99%)	1 (1%)	76	80
26	4D	146/147 (99%)	141 (97%)	5 (3%)	32	59
26	4d	146/147 (99%)	139 (95%)	7 (5%)	23	50
27	4F	62/62 (100%)	62 (100%)	0	100	100
27	4f	62/62 (100%)	61 (98%)	1 (2%)	55	72
28	4G	247/264 (94%)	246 (100%)	1 (0%)	84	84
28	4g	247/264 (94%)	244 (99%)	3 (1%)	63	75
29	4I	230/238 (97%)	230 (100%)	0	100	100
29	4i	230/238 (97%)	227 (99%)	3 (1%)	61	74
30	7A	138/150 (92%)	136 (99%)	2 (1%)	59	73
30	7a	138/150 (92%)	137 (99%)	1 (1%)	76	80
All	All	10448/10938 (96%)	10359 (99%)	89 (1%)	68	78

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	QA	474	VAL
1	QA	476	LEU
2	QC	146	ILE

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Mol	Chain	Res	Type
2	QC	316	LEU
1	Qa	71	PHE
1	Qa	293	ASP
1	Qa	382	GLU
2	Qc	329	CYS
5	Qj	62	ASN
8	4c	55	ARG
8	4c	109	TRP
9	4e	81	LYS
9	4e	100	GLU
9	4e	119	ASP
9	4e	142	TRP
10	4h	194	ASP
13	6a	84	TRP
16	c1	355	LEU
17	c2	60	TRP
17	c2	133	HIS
19	dc	13	LEU
19	dc	14	HIS
19	dc	92	THR
19	dc	100	ASN
7	4A	149	LEU
7	4A	243	ILE
8	4C	55	ARG
10	4H	43	GLN
10	4H	93	THR
11	4J	29	THR
12	5C	115	GLN
12	5C	146	CYS
14	6B	223	LYS
15	7C	40	GLN
16	C1	1	MET
16	C1	154	ASN
16	C1	235	ILE
16	C1	253	VAL
17	C2	60	TRP
18	C3	136	TYR
20	QE	192	HIS
20	Qe	173	THR
20	Qe	192	HIS
21	QF	36	CYS
21	QF	55	LEU

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Mol	Chain	Res	Type
22	QG	29	LEU
22	QG	62	GLU
22	QG	126	CYS
22	QG	228	ARG
24	Qb	141	VAL
24	Qb	201	THR
24	Qb	303	SER
24	Qb	319	LYS
24	Qb	459	VAL
21	Qf	47	ASN
21	Qf	54	ARG
21	Qf	71	LEU
22	Qg	16	ASN
22	Qg	101	GLU
22	Qg	126	CYS
24	QB	285	TYR
24	QB	342	SER
25	5B	103	CYS
25	5B	128	CYS
25	5B	151	GLU
26	4D	81	ILE
26	4D	126	VAL
26	4D	168	ASP
26	4D	169	ASP
26	4D	173	ARG
28	4G	45	LEU
30	7a	137	ARG
26	4d	81	ILE
26	4d	126	VAL
26	4d	165	LEU
26	4d	166	ILE
26	4d	167	LEU
26	4d	171	GLN
26	4d	172	LYS
27	4f	64	VAL
28	4g	46	GLU
28	4g	66	LEU
28	4g	159	GLU
29	4i	116	LYS
29	4i	155	GLU
29	4i	269	LYS
25	5b	103	CYS

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Mol	Chain	Res	Type
30	7A	137	ARG
30	7A	175	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (202) such sidechains are listed below:

Mol	Chain	Res	Type
1	QA	29	GLN
1	QA	70	HIS
1	QA	167	HIS
1	QA	268	GLN
1	QA	333	ASN
1	QA	398	GLN
1	QA	442	HIS
2	QC	56	HIS
2	QC	158	ASN
2	QC	204	ASN
3	QD	14	HIS
3	QD	16	GLN
3	QD	19	GLN
3	QD	241	ASN
4	QH	25	HIS
4	QH	36	ASN
6	QK	89	HIS
1	Qa	70	HIS
1	Qa	167	HIS
1	Qa	268	GLN
1	Qa	317	GLN
2	Qc	33	GLN
2	Qc	73	HIS
2	Qc	94	HIS
2	Qc	352	HIS
3	Qd	19	GLN
3	Qd	147	GLN
4	Qh	15	ASN
4	Qh	18	GLN
4	Qh	25	HIS
5	Qj	30	HIS
7	4a	43	HIS
7	4a	137	HIS
8	4c	25	HIS
9	4e	95	ASN
11	4j	23	GLN

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Mol	Chain	Res	Type
11	4j	31	GLN
12	5c	22	GLN
12	5c	63	ASN
12	5c	81	GLN
13	6a	68	ASN
14	6b	71	ASN
14	6b	83	GLN
14	6b	101	HIS
14	6b	105	GLN
14	6b	111	ASN
14	6b	252	HIS
15	7c	32	ASN
15	7c	78	ASN
15	7c	112	HIS
15	7c	134	GLN
16	c1	7	HIS
16	c1	18	HIS
16	c1	154	ASN
16	c1	194	ASN
16	c1	299	HIS
16	c1	346	ASN
16	c1	423	HIS
16	c1	466	HIS
16	c1	484	GLN
16	c1	488	HIS
17	c2	98	ASN
17	c2	105	ASN
18	c3	8	ASN
18	c3	106	HIS
18	c3	124	HIS
18	c3	127	HIS
18	c3	128	ASN
18	c3	129	ASN
18	c3	130	ASN
19	dc	29	GLN
19	dc	35	HIS
19	dc	54	HIS
19	dc	76	ASN
7	4A	130	ASN
7	4A	186	HIS
7	4A	213	ASN
10	4H	74	GLN

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Mol	Chain	Res	Type
10	4H	92	HIS
11	4J	3	HIS
11	4J	31	GLN
11	4J	65	ASN
12	5C	22	GLN
12	5C	63	ASN
12	5C	79	GLN
12	5C	115	GLN
14	6B	64	GLN
14	6B	71	ASN
14	6B	83	GLN
14	6B	101	HIS
14	6B	105	GLN
14	6B	252	HIS
14	6B	256	ASN
15	7C	24	ASN
15	7C	32	ASN
15	7C	112	HIS
15	7C	120	GLN
15	7C	134	GLN
16	C1	126	ASN
16	C1	154	ASN
16	C1	192	ASN
16	C1	242	GLN
16	C1	346	ASN
16	C1	386	HIS
16	C1	423	HIS
17	C2	94	ASN
17	C2	98	ASN
17	C2	167	ASN
18	C3	8	ASN
18	C3	106	HIS
18	C3	124	HIS
18	C3	160	GLN
19	DC	29	GLN
19	DC	54	HIS
13	6A	60	ASN
13	6A	68	ASN
13	6A	72	ASN
20	QE	112	GLN
20	Qe	112	GLN
20	Qe	192	HIS

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Mol	Chain	Res	Type
22	QG	2	ASN
22	QG	25	HIS
22	QG	96	HIS
22	QG	196	HIS
22	QG	205	HIS
22	QG	219	HIS
23	QI	15	GLN
24	Qb	40	ASN
24	Qb	76	GLN
24	Qb	133	ASN
24	Qb	195	GLN
24	Qb	199	HIS
24	Qb	321	HIS
24	Qb	372	GLN
24	Qb	405	ASN
24	Qb	413	GLN
22	Qg	2	ASN
22	Qg	21	GLN
22	Qg	25	HIS
22	Qg	96	HIS
22	Qg	196	HIS
22	Qg	219	HIS
24	QB	29	GLN
24	QB	50	GLN
24	QB	101	HIS
24	QB	199	HIS
24	QB	266	HIS
24	QB	289	HIS
24	QB	461	HIS
25	5B	21	HIS
25	5B	47	GLN
25	5B	131	HIS
26	4D	64	HIS
26	4D	94	GLN
26	4D	118	HIS
26	4D	125	HIS
26	4D	133	ASN
26	4D	171	GLN
28	4G	24	GLN
28	4G	97	HIS
28	4G	141	ASN
28	4G	197	GLN

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Mol	Chain	Res	Type
28	4G	198	GLN
28	4G	266	ASN
29	4I	62	HIS
29	4I	74	ASN
29	4I	90	HIS
29	4I	153	ASN
29	4I	164	GLN
29	4I	167	HIS
29	4I	199	ASN
29	4I	223	HIS
29	4I	243	HIS
30	7a	15	HIS
30	7a	19	HIS
30	7a	30	GLN
30	7a	84	GLN
30	7a	101	ASN
30	7a	138	HIS
26	4d	22	ASN
26	4d	30	GLN
26	4d	37	GLN
26	4d	94	GLN
26	4d	118	HIS
26	4d	120	ASN
28	4g	22	ASN
28	4g	24	GLN
28	4g	141	ASN
28	4g	197	GLN
28	4g	243	ASN
28	4g	266	ASN
28	4g	276	HIS
29	4i	153	ASN
29	4i	167	HIS
29	4i	260	HIS
25	5b	21	HIS
25	5b	42	GLN
25	5b	47	GLN
25	5b	131	HIS
30	7A	15	HIS
30	7A	30	GLN
30	7A	84	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 75 ligands modelled in this entry, 10 are monoatomic - leaving 65 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
32	CDL	Qd	302	-	99,99,99	0.31	0	105,111,111	0.30	0
33	HEC	QD	301	3	50,50,50	1.30	4 (8%)	68,82,82	1.20	6 (8%)
34	PC1	c1	508	-	35,35,53	0.36	0	41,43,61	0.31	0
34	PC1	QE	303	-	35,35,53	0.35	0	41,43,61	0.37	0
40	FES	Qe	303	20	0,4,4	-	-	-	-	-
31	HEM	QC	402	2	50,50,50	1.34	7 (14%)	66,82,82	1.73	15 (22%)
32	CDL	QE	302	-	59,59,99	0.38	0	65,71,111	0.33	0
34	PC1	4a	301	-	46,46,53	0.32	0	52,54,61	0.31	0
34	PC1	Qe	301	-	53,53,53	0.30	0	59,61,61	0.35	0
36	3PE	C1	507	-	39,39,50	0.36	0	42,44,55	0.35	0
36	3PE	7A	201	-	40,40,50	0.34	0	43,45,55	0.30	0
37	HEA	c1	501	16	66,67,67	2.20	24 (36%)	78,103,103	2.70	31 (39%)
32	CDL	4c	201	-	69,69,99	0.35	0	75,81,111	0.32	0
31	HEM	Qc	402	2	50,50,50	1.33	7 (14%)	66,82,82	1.74	14 (21%)
36	3PE	c1	506	-	39,39,50	0.35	0	42,44,55	0.39	0
37	HEA	c1	502	16	66,67,67	2.24	24 (36%)	78,103,103	2.60	26 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	PC1	Qc	403	-	35,35,53	0.36	0	41,43,61	0.34	0
34	PC1	c3	201	-	50,50,53	0.31	0	56,58,61	0.29	0
32	CDL	7c	201	-	89,89,99	0.32	0	95,101,111	0.35	0
34	PC1	Qe	302	-	53,53,53	0.30	0	59,61,61	0.29	0
34	PC1	4E	201	-	34,34,53	0.36	0	40,42,61	0.33	0
40	FES	QE	301	20	0,4,4	-	-	-	-	-
32	CDL	4E	202	-	71,71,99	0.36	0	77,83,111	0.34	0
35	PX2	4C	201	-	35,35,35	0.99	4 (11%)	39,40,40	1.06	2 (5%)
34	PC1	4A	302	-	45,45,53	0.32	0	51,53,61	0.33	0
34	PC1	Qg	301	-	27,27,53	0.40	0	33,35,61	0.35	0
36	3PE	4d	201	-	34,34,50	0.37	0	37,39,55	0.34	0
32	CDL	Qh	102	-	59,59,99	0.38	0	65,71,111	0.37	0
36	3PE	4d	202	-	50,50,50	0.31	0	53,55,55	0.27	0
34	PC1	4A	301	-	46,46,53	0.32	0	52,54,61	0.33	0
37	HEA	C1	501	16	66,67,67	2.22	25 (37%)	78,103,103	2.69	28 (35%)
36	3PE	7a	201	-	40,40,50	0.34	0	43,45,55	0.29	0
32	CDL	Qj	202	-	47,47,99	0.43	0	53,59,111	0.37	0
36	3PE	C1	508	-	39,39,50	0.35	0	42,44,55	0.34	0
34	PC1	Qd	303	-	30,30,53	0.38	0	36,38,61	0.34	0
42	S12	4F	102	-	33,34,34	0.79	0	36,40,40	1.18	2 (5%)
35	PX2	QJ	201	-	35,35,35	0.98	3 (8%)	39,40,40	1.11	2 (5%)
32	CDL	QH	101	-	75,75,99	0.34	0	81,87,111	0.32	0
34	PC1	C3	201	-	50,50,53	0.32	0	56,58,61	0.30	0
34	PC1	Qe	304	-	35,35,53	0.35	0	41,43,61	0.36	0
36	3PE	4a	302	-	50,50,50	0.31	0	53,55,55	0.42	0
31	HEM	QC	401	2	50,50,50	1.33	8 (16%)	66,82,82	1.74	14 (21%)
34	PC1	C1	505	-	49,49,53	0.32	0	55,57,61	0.32	0
34	PC1	4e	201	-	34,34,53	0.36	0	40,42,61	0.32	0
32	CDL	C1	506	-	89,89,99	0.32	0	95,101,111	0.28	0
34	PC1	C1	509	-	35,35,53	0.37	0	41,43,61	0.32	0
36	3PE	4F	101	-	50,50,50	0.31	0	53,55,55	0.32	0
37	HEA	C1	502	16	66,67,67	2.23	24 (36%)	78,103,103	2.57	29 (37%)
31	HEM	Qc	401	2	50,50,50	1.34	8 (16%)	66,82,82	1.79	15 (22%)
35	PX2	QD	304	-	35,35,35	0.99	4 (11%)	39,40,40	1.02	2 (5%)
42	S12	4d	203	-	33,34,34	0.77	0	36,40,40	1.10	3 (8%)
32	CDL	Qc	404	-	53,53,99	0.40	0	59,65,111	0.34	0
34	PC1	QD	303	-	30,30,53	0.38	0	36,38,61	0.37	0
32	CDL	Qh	101	-	64,64,99	0.37	0	70,76,111	0.32	0
32	CDL	QJ	202	-	57,57,99	0.39	0	63,69,111	0.33	0
32	CDL	QD	302	-	68,68,99	0.38	0	74,80,111	0.37	0
33	HEC	Qd	301	3	50,50,50	1.31	5 (10%)	68,82,82	1.19	4 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	PC1	c1	505	-	49,49,53	0.31	0	55,57,61	0.31	0
36	3PE	c1	507	-	39,39,50	0.34	0	42,44,55	0.33	0
32	CDL	4e	202	-	71,71,99	0.36	0	77,83,111	0.33	0
34	PC1	Qj	201	-	53,53,53	0.30	0	59,61,61	0.28	0
34	PC1	7c	202	-	53,53,53	0.30	0	59,61,61	0.30	0
34	PC1	DC	201	-	53,53,53	0.32	0	59,61,61	0.51	1 (1%)
32	CDL	QC	403	-	55,55,99	0.40	0	61,67,111	0.33	0
36	3PE	4D	201	-	34,34,50	0.37	0	37,39,55	0.34	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
32	CDL	Qd	302	-	-	28/110/110/110	-
33	HEC	QD	301	3	1/1/3/7	2/14/54/54	-
34	PC1	c1	508	-	-	6/39/39/57	-
34	PC1	QE	303	-	-	10/39/39/57	-
40	FES	Qe	303	20	-	-	0/1/1/1
31	HEM	QC	402	2	-	6/14/54/54	-
32	CDL	QE	302	-	-	24/70/70/110	-
34	PC1	4a	301	-	-	14/50/50/57	-
34	PC1	Qe	301	-	-	17/57/57/57	-
36	3PE	C1	507	-	-	17/43/43/54	-
36	3PE	7A	201	-	-	8/44/44/54	-
37	HEA	c1	501	16	-	13/36/76/76	-
32	CDL	4c	201	-	-	25/80/80/110	-
31	HEM	Qc	402	2	-	6/14/54/54	-
36	3PE	c1	506	-	-	19/43/43/54	-
37	HEA	c1	502	16	-	15/36/76/76	-
34	PC1	Qc	403	-	-	12/39/39/57	-
34	PC1	c3	201	-	-	16/54/54/57	-
32	CDL	7c	201	-	-	18/100/100/110	-
34	PC1	Qe	302	-	-	15/57/57/57	-
34	PC1	4E	201	-	-	5/38/38/57	-
40	FES	QE	301	20	-	-	0/1/1/1
32	CDL	4E	202	-	-	24/82/82/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	PX2	4C	201	-	-	16/37/37/37	-
34	PC1	4A	302	-	-	15/49/49/57	-
34	PC1	Qg	301	-	-	5/31/31/57	-
36	3PE	4d	201	-	-	5/38/38/54	-
32	CDL	Qh	102	-	-	15/70/70/110	-
36	3PE	4d	202	-	-	19/54/54/54	-
34	PC1	4A	301	-	-	12/50/50/57	-
37	HEA	C1	501	16	-	15/36/76/76	-
36	3PE	7a	201	-	-	9/44/44/54	-
32	CDL	Qj	202	-	-	11/58/58/110	-
36	3PE	C1	508	-	-	6/43/43/54	-
34	PC1	Qd	303	-	-	6/34/34/57	-
42	S12	4F	102	-	-	20/38/38/38	-
35	PX2	QJ	201	-	-	18/37/37/37	-
32	CDL	QH	101	-	-	17/86/86/110	-
34	PC1	C3	201	-	-	16/54/54/57	-
34	PC1	Qe	304	-	-	8/39/39/57	-
36	3PE	4a	302	-	-	23/54/54/54	-
31	HEM	QC	401	2	-	5/14/54/54	-
34	PC1	C1	505	-	-	13/53/53/57	-
34	PC1	4e	201	-	-	3/38/38/57	-
32	CDL	C1	506	-	-	19/100/100/110	-
34	PC1	C1	509	-	-	8/39/39/57	-
36	3PE	4F	101	-	-	21/54/54/54	-
37	HEA	C1	502	16	-	13/36/76/76	-
31	HEM	Qc	401	2	-	6/14/54/54	-
35	PX2	QD	304	-	-	15/37/37/37	-
42	S12	4d	203	-	-	24/38/38/38	-
32	CDL	Qc	404	-	-	12/64/64/110	-
34	PC1	QD	303	-	-	17/34/34/57	-
32	CDL	Qh	101	-	-	18/75/75/110	-
32	CDL	QJ	202	-	-	17/68/68/110	-
33	HEC	Qd	301	3	1/1/3/7	3/14/54/54	-
32	CDL	QD	302	-	-	22/79/79/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	PC1	c1	505	-	-	16/53/53/57	-
36	3PE	c1	507	-	-	14/43/43/54	-
32	CDL	4e	202	-	-	23/82/82/110	-
34	PC1	Qj	201	-	-	8/57/57/57	-
34	PC1	7c	202	-	-	26/57/57/57	-
34	PC1	DC	201	-	-	29/57/57/57	-
32	CDL	QC	403	-	-	13/66/66/110	-
36	3PE	4D	201	-	-	6/38/38/54	-

All (147) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	c1	502	HEA	C3B-C2B	5.42	1.46	1.34
37	C1	502	HEA	C3B-C2B	5.27	1.46	1.34
37	C1	501	HEA	C3B-C2B	5.12	1.46	1.34
37	c1	501	HEA	C3B-C2B	5.07	1.46	1.34
37	C1	501	HEA	FE-ND	5.02	2.10	1.94
37	C1	502	HEA	FE-NB	4.98	2.10	1.94
37	c1	501	HEA	FE-ND	4.78	2.09	1.94
37	c1	502	HEA	C3A-C2A	4.75	1.46	1.36
37	c1	502	HEA	FE-ND	4.73	2.09	1.94
37	C1	502	HEA	C4B-NB	-4.65	1.32	1.40
37	C1	502	HEA	C3A-C2A	4.65	1.46	1.36
37	c1	501	HEA	C4B-NB	-4.58	1.32	1.40
37	C1	501	HEA	FE-NB	4.54	2.08	1.94
37	c1	502	HEA	C4B-NB	-4.46	1.32	1.40
37	C1	501	HEA	FE-NC	4.45	2.10	1.95
37	C1	502	HEA	FE-NC	4.40	2.10	1.95
37	C1	502	HEA	FE-ND	4.38	2.08	1.94
37	c1	501	HEA	FE-NC	4.37	2.10	1.95
37	c1	502	HEA	FE-NC	4.37	2.10	1.95
37	c1	502	HEA	FE-NB	4.37	2.08	1.94
37	c1	501	HEA	FE-NB	4.25	2.08	1.94
37	c1	502	HEA	C1D-ND	-4.24	1.33	1.40
37	c1	501	HEA	C3A-C2A	4.22	1.45	1.36
37	C1	501	HEA	C1D-ND	-4.09	1.33	1.40
37	C1	501	HEA	C3A-C2A	4.09	1.45	1.36
37	C1	501	HEA	C4B-NB	-4.09	1.33	1.40
31	QC	401	HEM	C4D-ND	-3.95	1.33	1.40
37	c1	501	HEA	C1D-ND	-3.95	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	C1	501	HEA	C3D-C2D	3.93	1.45	1.36
37	C1	502	HEA	CHC-C4B	3.87	1.46	1.38
37	C1	502	HEA	C3D-C2D	3.86	1.44	1.36
31	Qc	402	HEM	C4D-ND	-3.83	1.33	1.40
31	QC	402	HEM	C4D-ND	-3.82	1.33	1.40
37	c1	501	HEA	C3D-C2D	3.82	1.44	1.36
37	c1	502	HEA	CHC-C4B	3.79	1.46	1.38
37	C1	501	HEA	CHC-C4B	3.79	1.46	1.38
37	c1	502	HEA	C3D-C2D	3.76	1.44	1.36
37	C1	501	HEA	CHA-C1A	3.72	1.45	1.38
37	c1	501	HEA	C4C-NC	-3.71	1.32	1.39
37	c1	502	HEA	C4C-NC	-3.70	1.32	1.39
31	Qc	401	HEM	C4D-ND	-3.70	1.33	1.40
37	c1	501	HEA	CHD-C1D	3.64	1.45	1.38
37	C1	502	HEA	C1D-ND	-3.53	1.34	1.40
37	c1	502	HEA	CHA-C1A	3.47	1.45	1.38
37	c1	501	HEA	CHC-C4B	3.46	1.45	1.38
37	C1	501	HEA	C4C-NC	-3.44	1.33	1.39
31	Qc	401	HEM	C1B-NB	-3.42	1.34	1.40
37	C1	502	HEA	CHA-C1A	3.39	1.45	1.38
37	C1	502	HEA	C1C-NC	-3.35	1.33	1.39
33	QD	301	HEC	CBC-CAC	-3.34	1.36	1.51
33	Qd	301	HEC	CBC-CAC	-3.32	1.36	1.51
37	C1	501	HEA	CHD-C1D	3.30	1.45	1.38
37	c1	501	HEA	C1B-NB	-3.26	1.32	1.38
37	c1	502	HEA	C1C-NC	-3.25	1.33	1.39
37	C1	502	HEA	C4C-NC	-3.24	1.33	1.39
37	C1	502	HEA	C1B-NB	-3.23	1.32	1.38
31	QC	401	HEM	C1B-NB	-3.21	1.34	1.40
31	Qc	402	HEM	C1B-NB	-3.20	1.34	1.40
37	c1	501	HEA	CHA-C1A	3.19	1.44	1.38
37	C1	502	HEA	CHC-C1C	3.18	1.46	1.39
31	QC	402	HEM	C1B-NB	-3.16	1.34	1.40
37	C1	502	HEA	CHD-C1D	3.11	1.44	1.38
37	c1	501	HEA	C1C-NC	-3.10	1.33	1.39
37	c1	502	HEA	CHD-C1D	3.09	1.44	1.38
37	C1	501	HEA	C1C-NC	-3.04	1.33	1.39
37	C1	501	HEA	CHC-C1C	3.00	1.46	1.39
31	Qc	401	HEM	C1C-C2C	-2.97	1.39	1.45
37	C1	501	HEA	CHD-C4C	2.89	1.45	1.39
37	C1	502	HEA	CHB-C4A	2.89	1.44	1.38
37	c1	502	HEA	CHC-C1C	2.88	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	c1	501	HEA	CHC-C1C	2.86	1.45	1.39
37	c1	501	HEA	CHD-C4C	2.84	1.45	1.39
37	c1	502	HEA	CHB-C4A	2.82	1.43	1.38
31	QC	402	HEM	C1C-C2C	-2.81	1.39	1.45
37	c1	502	HEA	C1B-NB	-2.78	1.33	1.38
31	Qc	402	HEM	C1C-C2C	-2.78	1.39	1.45
37	C1	501	HEA	CHA-C4D	2.77	1.45	1.39
37	c1	502	HEA	CHB-C1B	2.77	1.45	1.39
37	C1	502	HEA	CHA-C4D	2.76	1.45	1.39
35	QD	304	PX2	O7-C2	-2.76	1.39	1.46
31	QC	401	HEM	C1D-ND	-2.72	1.33	1.38
35	4C	201	PX2	O7-C2	-2.70	1.39	1.46
37	C1	501	HEA	C1B-NB	-2.70	1.33	1.38
37	c1	501	HEA	C4A-NA	2.68	1.44	1.39
37	C1	502	HEA	C1A-NA	2.68	1.44	1.39
31	Qc	402	HEM	C1D-ND	-2.68	1.33	1.38
37	c1	502	HEA	CHA-C4D	2.67	1.45	1.39
33	Qd	301	HEC	CAC-C3C	2.67	1.58	1.51
33	QD	301	HEC	CAC-C3C	2.67	1.58	1.51
31	QC	402	HEM	C1D-ND	-2.67	1.33	1.38
37	c1	502	HEA	C4D-ND	-2.65	1.33	1.38
35	QJ	201	PX2	O7-C2	-2.63	1.40	1.46
37	C1	502	HEA	CHB-C1B	2.61	1.45	1.39
31	QC	401	HEM	C1C-C2C	-2.58	1.40	1.45
37	C1	501	HEA	CHB-C1B	2.57	1.45	1.39
37	c1	502	HEA	C4A-NA	2.56	1.44	1.39
37	c1	501	HEA	CHA-C4D	2.55	1.45	1.39
37	c1	502	HEA	CHD-C4C	2.54	1.45	1.39
37	c1	501	HEA	CHB-C4A	2.51	1.43	1.38
33	QD	301	HEC	CBB-CAB	-2.50	1.40	1.51
37	c1	502	HEA	O2D-CGD	-2.49	1.22	1.30
37	c1	501	HEA	C4D-ND	-2.48	1.33	1.38
31	Qc	401	HEM	C1D-ND	-2.48	1.33	1.38
37	C1	501	HEA	O2D-CGD	-2.47	1.22	1.30
37	C1	502	HEA	O2D-CGD	-2.47	1.22	1.30
37	C1	501	HEA	C4A-NA	2.46	1.44	1.39
33	Qd	301	HEC	CBB-CAB	-2.46	1.40	1.51
31	QC	402	HEM	FE-NB	2.45	2.02	1.94
37	c1	501	HEA	O2D-CGD	-2.44	1.22	1.30
37	C1	501	HEA	C1A-NA	2.44	1.44	1.39
37	C1	501	HEA	O2A-CGA	-2.44	1.22	1.30
37	C1	501	HEA	C4D-ND	-2.42	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	c1	502	HEA	O2A-CGA	-2.41	1.22	1.30
37	C1	501	HEA	CHB-C4A	2.39	1.43	1.38
35	QD	304	PX2	O5-C3	-2.38	1.39	1.45
37	C1	502	HEA	O2A-CGA	-2.38	1.22	1.30
31	Qc	401	HEM	FE-NB	2.38	2.02	1.94
37	c1	501	HEA	O2A-CGA	-2.37	1.22	1.30
37	C1	502	HEA	CHD-C4C	2.37	1.44	1.39
37	C1	502	HEA	C4D-ND	-2.36	1.33	1.38
37	c1	502	HEA	C1A-NA	2.36	1.44	1.39
31	QC	401	HEM	C3C-C4C	-2.36	1.41	1.46
31	QC	401	HEM	FE-NB	2.34	2.02	1.94
31	Qc	402	HEM	FE-NB	2.32	2.02	1.94
37	C1	502	HEA	C4A-NA	2.29	1.44	1.39
37	c1	501	HEA	CHB-C1B	2.27	1.44	1.39
35	4C	201	PX2	O5-C4	2.27	1.40	1.33
35	QJ	201	PX2	O5-C4	2.26	1.39	1.33
31	Qc	401	HEM	FE-ND	2.24	2.01	1.94
37	c1	501	HEA	C1A-NA	2.22	1.44	1.39
35	4C	201	PX2	O5-C3	-2.21	1.40	1.45
33	Qd	301	HEC	CAB-C3B	2.18	1.56	1.51
35	QJ	201	PX2	O5-C3	-2.17	1.40	1.45
31	Qc	402	HEM	C3C-C4C	-2.15	1.42	1.46
37	C1	501	HEA	C4B-C3B	2.14	1.48	1.44
31	Qc	401	HEM	C4B-NB	-2.13	1.34	1.38
33	QD	301	HEC	CAB-C3B	2.13	1.56	1.51
31	Qc	401	HEM	C3C-C4C	-2.12	1.42	1.46
31	QC	401	HEM	C4B-NB	-2.10	1.34	1.38
35	QD	304	PX2	O5-C4	2.10	1.39	1.33
31	QC	402	HEM	C3C-C4C	-2.08	1.42	1.46
31	QC	401	HEM	C1A-C2A	-2.04	1.40	1.44
31	QC	402	HEM	FE-ND	2.04	2.01	1.94
31	Qc	402	HEM	C4B-NB	-2.02	1.34	1.38
35	QD	304	PX2	O7-C16	2.02	1.40	1.34
33	Qd	301	HEC	FE-ND	2.00	2.01	1.94
35	4C	201	PX2	O7-C16	2.00	1.40	1.34

All (194) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	C1	501	HEA	CAD-CBD-CGD	-8.18	96.01	113.60
37	c1	501	HEA	CAD-CBD-CGD	-7.66	97.11	113.60
37	C1	501	HEA	CAA-CBA-CGA	-7.48	97.52	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	C1	502	HEA	CAD-CBD-CGD	-7.16	98.20	113.60
37	c1	501	HEA	CAA-CBA-CGA	-7.12	98.27	113.60
37	C1	501	HEA	C3C-C4C-NC	7.07	114.60	110.25
37	c1	502	HEA	C3C-C4C-NC	7.06	114.59	110.25
37	c1	502	HEA	CAD-CBD-CGD	-6.92	98.70	113.60
37	c1	502	HEA	CAA-CBA-CGA	-6.84	98.88	113.60
37	C1	502	HEA	C3C-C4C-NC	6.62	114.32	110.25
37	c1	501	HEA	C3C-C4C-NC	6.52	114.26	110.25
37	C1	502	HEA	CAA-CBA-CGA	-6.14	100.40	113.60
37	c1	501	HEA	C3D-C4D-ND	6.03	116.20	110.36
37	c1	502	HEA	C3C-C2C-C1C	-5.98	99.95	107.16
37	C1	502	HEA	C3C-C2C-C1C	-5.78	100.18	107.16
37	c1	501	HEA	C3C-C2C-C1C	-5.71	100.27	107.16
37	c1	501	HEA	C13-C12-C11	-5.64	105.88	114.35
37	C1	501	HEA	C3D-C4D-ND	5.60	115.78	110.36
31	QC	401	HEM	CHC-C4B-NB	5.36	130.24	124.42
37	C1	502	HEA	C3D-C4D-ND	5.32	115.51	110.36
37	C1	502	HEA	C13-C12-C11	-5.25	106.46	114.35
37	C1	501	HEA	C3C-C2C-C1C	-5.18	100.91	107.16
37	c1	502	HEA	C13-C12-C11	-5.16	106.59	114.35
37	c1	501	HEA	CHB-C1B-C2B	-5.05	117.08	124.98
37	C1	501	HEA	C13-C12-C11	-5.03	106.80	114.35
37	c1	502	HEA	C3D-C4D-ND	5.02	115.22	110.36
37	C1	502	HEA	C2D-C1D-ND	5.02	115.78	109.84
37	C1	501	HEA	C2B-C1B-NB	4.99	115.86	109.88
31	Qc	402	HEM	CHC-C4B-NB	4.96	129.81	124.42
37	C1	502	HEA	C1D-C2D-C3D	-4.94	101.76	106.96
37	C1	501	HEA	C2D-C1D-ND	4.94	115.69	109.84
31	Qc	401	HEM	CHC-C4B-NB	4.90	129.74	124.42
37	C1	502	HEA	C2B-C1B-NB	4.87	115.71	109.88
37	C1	501	HEA	CHB-C1B-C2B	-4.84	117.42	124.98
42	4F	102	S12	OG-CB-CA	4.81	112.25	108.06
37	c1	501	HEA	C2B-C1B-NB	4.76	115.58	109.88
37	c1	502	HEA	C2B-C1B-NB	4.68	115.48	109.88
37	C1	501	HEA	C1D-C2D-C3D	-4.60	102.12	106.96
31	Qc	401	HEM	CHD-C4C-NC	4.60	129.41	124.44
31	QC	402	HEM	CHC-C4B-NB	4.59	129.40	124.42
37	c1	502	HEA	C1D-C2D-C3D	-4.55	102.18	106.96
31	QC	401	HEM	CHD-C4C-NC	4.54	129.35	124.44
37	c1	501	HEA	C3B-C4B-NB	4.53	115.21	109.84
37	c1	502	HEA	C3B-C4B-NB	4.50	115.17	109.84
37	c1	502	HEA	C2D-C1D-ND	4.49	115.16	109.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	C1	502	HEA	CHB-C1B-C2B	-4.45	118.03	124.98
35	QJ	201	PX2	O7-C16-C17	4.42	121.03	111.50
31	QC	402	HEM	CHD-C4C-NC	4.37	129.16	124.44
31	Qc	402	HEM	CHD-C4C-NC	4.31	129.10	124.44
37	c1	501	HEA	C2C-C1C-NC	4.30	116.62	110.08
37	c1	501	HEA	C2D-C1D-ND	4.29	114.93	109.84
37	c1	502	HEA	C2C-C1C-NC	4.26	116.57	110.08
37	C1	502	HEA	C2C-C1C-NC	4.26	116.56	110.08
37	c1	502	HEA	CHB-C1B-C2B	-4.24	118.35	124.98
37	c1	501	HEA	C1D-C2D-C3D	-4.22	102.52	106.96
37	C1	502	HEA	C3B-C4B-NB	4.22	114.84	109.84
37	C1	501	HEA	C3B-C4B-NB	4.19	114.80	109.84
35	4C	201	PX2	O7-C16-C17	4.13	120.40	111.50
31	QC	402	HEM	CHB-C1B-NB	4.06	129.38	124.37
42	4d	203	S12	OG-CB-CA	4.01	111.55	108.06
31	Qc	402	HEM	CHB-C1B-NB	3.95	129.24	124.37
31	Qc	401	HEM	C4D-ND-C1D	3.89	109.09	105.07
37	c1	501	HEA	C4B-C3B-C2B	-3.87	100.80	107.41
31	Qc	401	HEM	CHB-C1B-NB	3.85	129.12	124.37
35	QD	304	PX2	O7-C16-C17	3.80	119.68	111.50
37	C1	501	HEA	C2C-C1C-NC	3.73	115.76	110.08
37	c1	501	HEA	CHA-C4D-C3D	-3.69	119.42	124.84
37	C1	502	HEA	C4B-C3B-C2B	-3.65	101.17	107.41
37	c1	502	HEA	C4B-C3B-C2B	-3.65	101.18	107.41
31	QC	401	HEM	CHB-C1B-NB	3.60	128.81	124.37
37	C1	501	HEA	C4B-C3B-C2B	-3.59	101.27	107.41
31	QC	402	HEM	C4D-ND-C1D	3.51	108.69	105.07
37	C1	501	HEA	CHA-C4D-C3D	-3.46	119.75	124.84
37	c1	502	HEA	CHA-C4D-C3D	-3.42	119.81	124.84
31	Qc	401	HEM	CHA-C4D-ND	3.41	128.58	124.37
31	Qc	402	HEM	C4D-ND-C1D	3.38	108.56	105.07
31	QC	401	HEM	C1B-NB-C4B	3.33	108.52	105.07
31	QC	401	HEM	C4D-ND-C1D	3.29	108.47	105.07
31	Qc	402	HEM	CHA-C4D-ND	3.22	128.34	124.37
31	Qc	402	HEM	C1B-NB-C4B	3.19	108.37	105.07
31	QC	401	HEM	CHA-C4D-ND	3.18	128.30	124.37
31	Qc	401	HEM	C1B-NB-C4B	3.12	108.30	105.07
37	C1	502	HEA	CHA-C4D-C3D	-3.10	120.28	124.84
37	c1	501	HEA	C13-C14-C15	-3.09	120.21	127.66
31	QC	402	HEM	C1B-NB-C4B	2.96	108.13	105.07
31	QC	402	HEM	CHA-C4D-ND	2.95	128.01	124.37
31	Qc	402	HEM	CHA-C1A-NA	2.93	129.24	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	C1	501	HEA	OMA-CMA-C3A	-2.92	119.09	125.69
31	QC	402	HEM	CHA-C1A-NA	2.88	129.15	123.85
33	QD	301	HEC	O1D-CGD-CBD	-2.86	113.88	123.08
37	c1	501	HEA	C27-C19-C20	2.86	120.08	115.27
31	Qc	401	HEM	CAA-CBA-CGA	-2.86	107.46	113.60
31	Qc	402	HEM	CHD-C1D-ND	2.83	127.50	124.42
37	C1	501	HEA	CMB-C2B-C1B	-2.83	120.73	125.04
37	c1	502	HEA	CMB-C2B-C1B	-2.82	120.75	125.04
33	Qd	301	HEC	O1D-CGD-CBD	-2.80	114.08	123.08
31	QC	401	HEM	CHD-C1D-ND	2.80	127.46	124.42
35	QD	304	PX2	O5-C4-C5	2.80	120.69	111.91
37	C1	501	HEA	C13-C14-C15	-2.79	120.94	127.66
31	QC	401	HEM	CHA-C1A-NA	2.79	128.98	123.85
31	QC	402	HEM	C4C-NC-C1C	2.75	108.05	105.35
37	C1	502	HEA	CMB-C2B-C1B	-2.74	120.86	125.04
37	C1	501	HEA	C27-C19-C20	2.72	119.85	115.27
37	C1	501	HEA	C17-C18-C19	-2.71	121.13	127.66
37	C1	501	HEA	CHC-C4B-NB	-2.70	121.04	124.37
37	c1	501	HEA	C17-C18-C19	-2.69	121.17	127.66
37	c1	501	HEA	CHB-C1B-NB	2.69	127.34	124.42
31	Qc	401	HEM	C4C-NC-C1C	2.67	107.97	105.35
37	C1	502	HEA	CMB-C2B-C3B	2.67	135.43	130.34
31	Qc	402	HEM	CAD-CBD-CGD	-2.66	107.88	113.60
37	c1	502	HEA	CMB-C2B-C3B	2.65	135.40	130.34
31	QC	402	HEM	CHD-C1D-ND	2.64	127.28	124.42
31	QC	402	HEM	CAD-CBD-CGD	-2.63	107.94	113.60
37	c1	501	HEA	CMB-C2B-C1B	-2.62	121.06	125.04
37	C1	501	HEA	O1A-CGA-CBA	-2.59	114.77	123.08
37	C1	502	HEA	C1B-C2B-C3B	-2.59	103.71	106.80
37	c1	501	HEA	O1A-CGA-CBA	-2.58	114.78	123.08
31	Qc	401	HEM	CHD-C1D-ND	2.58	127.22	124.42
37	c1	501	HEA	C4D-C3D-C2D	-2.58	103.14	106.90
42	4d	203	S12	O4-P-O3	2.57	124.93	112.24
37	C1	501	HEA	CMB-C2B-C3B	2.56	135.22	130.34
31	Qc	401	HEM	C4A-NA-C1A	2.55	107.84	105.35
37	c1	501	HEA	C26-C15-C16	2.55	119.56	115.27
35	4C	201	PX2	O5-C4-C5	2.53	119.84	111.91
35	QJ	201	PX2	O5-C4-C5	2.53	119.84	111.91
42	4F	102	S12	O4-P-O3	2.51	124.62	112.24
31	Qc	401	HEM	CHA-C1A-NA	2.50	128.45	123.85
31	QC	402	HEM	CHB-C1B-C2B	-2.49	119.81	126.73
31	QC	401	HEM	CAA-CBA-CGA	-2.49	108.25	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	C1	502	HEA	C27-C19-C18	-2.48	117.31	123.68
37	c1	502	HEA	OMA-CMA-C3A	-2.48	120.08	125.69
37	c1	502	HEA	C1B-C2B-C3B	-2.47	103.85	106.80
37	C1	501	HEA	C27-C19-C18	-2.47	117.35	123.68
37	C1	501	HEA	C4D-C3D-C2D	-2.46	103.32	106.90
31	QC	401	HEM	C4A-NA-C1A	2.46	107.75	105.35
37	C1	502	HEA	O1A-CGA-CBA	-2.45	115.20	123.08
37	c1	501	HEA	C27-C19-C18	-2.45	117.39	123.68
37	c1	502	HEA	O1A-CGA-CBA	-2.45	115.22	123.08
31	Qc	401	HEM	C1C-CHC-C4B	-2.44	120.80	126.06
33	QD	301	HEC	C1D-ND-C4D	2.42	107.57	105.07
33	Qd	301	HEC	O1A-CGA-CBA	-2.41	115.34	123.08
33	QD	301	HEC	O1A-CGA-CBA	-2.38	115.42	123.08
31	QC	401	HEM	C1C-CHC-C4B	-2.38	120.93	126.06
37	C1	502	HEA	C13-C14-C15	-2.37	121.94	127.66
37	c1	502	HEA	C27-C19-C18	-2.37	117.60	123.68
31	QC	402	HEM	C4A-CHB-C1B	-2.36	120.73	126.34
33	Qd	301	HEC	O2A-CGA-O1A	2.35	129.16	123.30
31	Qc	402	HEM	C4C-NC-C1C	2.35	107.65	105.35
37	c1	502	HEA	CMC-C2C-C3C	2.33	132.24	126.59
31	QC	401	HEM	C4C-NC-C1C	2.33	107.63	105.35
31	QC	401	HEM	CAD-CBD-CGD	-2.32	108.61	113.60
37	c1	501	HEA	CHC-C1C-C2C	-2.32	120.69	127.24
37	c1	501	HEA	CMB-C2B-C3B	2.32	134.76	130.34
31	QC	402	HEM	C4A-NA-C1A	2.32	107.62	105.35
37	c1	502	HEA	C17-C18-C19	-2.31	122.10	127.66
37	c1	501	HEA	OMA-CMA-C3A	-2.31	120.47	125.69
37	C1	501	HEA	C1B-C2B-C3B	-2.30	104.05	106.80
37	c1	502	HEA	C13-C14-C15	-2.28	122.16	127.66
33	QD	301	HEC	O2A-CGA-O1A	2.27	128.96	123.30
31	Qc	402	HEM	CHB-C1B-C2B	-2.27	120.43	126.73
31	Qc	402	HEM	C4A-NA-C1A	2.24	107.54	105.35
37	c1	501	HEA	CAD-C3D-C2D	2.23	132.03	127.88
37	c1	501	HEA	O1D-CGD-CBD	-2.23	115.93	123.08
37	C1	502	HEA	OMA-CMA-C3A	-2.22	120.67	125.69
42	4d	203	S12	O52-C5-O51	-2.22	117.99	123.59
37	C1	501	HEA	O1D-CGD-CBD	-2.21	115.98	123.08
37	c1	502	HEA	C4D-C3D-C2D	-2.21	103.68	106.90
31	Qc	402	HEM	C4A-CHB-C1B	-2.20	121.12	126.34
37	C1	502	HEA	C17-C18-C19	-2.19	122.38	127.66
37	c1	501	HEA	C1B-C2B-C3B	-2.19	104.19	106.80
31	Qc	401	HEM	CHB-C1B-C2B	-2.18	120.66	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	c1	501	HEA	CMC-C2C-C1C	2.18	128.69	125.37
31	QC	402	HEM	C2A-C1A-NA	-2.17	107.72	110.15
37	C1	502	HEA	C25-C23-C22	-2.14	116.46	122.65
31	Qc	401	HEM	C2A-C1A-NA	-2.13	107.76	110.15
31	QC	402	HEM	C1C-CHC-C4B	-2.13	121.46	126.06
37	C1	502	HEA	O1D-CGD-CBD	-2.12	116.27	123.08
37	C1	502	HEA	C27-C19-C20	2.12	118.83	115.27
37	C1	501	HEA	CHB-C1B-NB	2.11	126.71	124.42
31	Qc	402	HEM	C1C-CHC-C4B	-2.11	121.51	126.06
37	C1	502	HEA	C1D-ND-C4D	-2.10	102.91	105.07
37	c1	502	HEA	C26-C15-C14	-2.09	118.31	123.68
33	Qd	301	HEC	C1D-ND-C4D	2.09	107.23	105.07
37	C1	501	HEA	CHD-C1D-C2D	-2.08	120.94	126.73
37	c1	501	HEA	CMD-C2D-C1D	2.08	128.21	125.04
37	C1	502	HEA	CHD-C1D-C2D	-2.08	120.96	126.73
34	DC	201	PC1	O21-C2-C1	2.08	115.92	108.40
37	c1	502	HEA	O1D-CGD-CBD	-2.07	116.44	123.08
37	C1	502	HEA	CMC-C2C-C3C	2.03	131.50	126.59
31	QC	401	HEM	CHB-C1B-C2B	-2.03	121.09	126.73
33	QD	301	HEC	C3D-C4D-ND	-2.02	108.40	110.36
31	Qc	401	HEM	O2A-CGA-CBA	2.02	120.51	114.03
33	QD	301	HEC	C4B-NB-C1B	2.00	107.14	105.07
37	C1	502	HEA	CHC-C4B-NB	-2.00	121.90	124.37

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
33	QD	301	HEC	NA
33	Qd	301	HEC	NA

All (887) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
31	QC	401	HEM	C2C-C3C-CAC-CBC
31	QC	401	HEM	C4C-C3C-CAC-CBC
31	QC	402	HEM	C2C-C3C-CAC-CBC
31	QC	402	HEM	C4C-C3C-CAC-CBC
32	QC	403	CDL	CA2-OA2-PA1-OA3
32	QC	403	CDL	CB3-OB5-PB2-OB3
32	QD	302	CDL	CB3-OB5-PB2-OB3
32	QD	302	CDL	CB3-OB5-PB2-OB4
32	QH	101	CDL	CA2-OA2-PA1-OA3

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Mol	Chain	Res	Type	Atoms
32	QH	101	CDL	CA2-OA2-PA1-OA4
32	QH	101	CDL	CA2-OA2-PA1-OA5
32	QJ	202	CDL	CB2-OB2-PB2-OB4
32	QJ	202	CDL	CB2-OB2-PB2-OB5
32	Qc	404	CDL	CA3-OA5-PA1-OA4
32	Qd	302	CDL	CA2-OA2-PA1-OA3
32	Qd	302	CDL	CA3-OA5-PA1-OA2
32	Qd	302	CDL	CA3-OA5-PA1-OA3
32	Qd	302	CDL	CA3-OA5-PA1-OA4
32	Qd	302	CDL	CB2-OB2-PB2-OB3
32	Qh	102	CDL	CA2-OA2-PA1-OA4
32	Qh	102	CDL	CB2-OB2-PB2-OB3
32	Qj	202	CDL	CA2-OA2-PA1-OA4
32	Qj	202	CDL	CB2-OB2-PB2-OB3
32	Qj	202	CDL	CB3-OB5-PB2-OB4
32	4c	201	CDL	CA2-OA2-PA1-OA3
32	4c	201	CDL	CA2-OA2-PA1-OA4
32	4c	201	CDL	CA3-OA5-PA1-OA4
32	4c	201	CDL	CA4-CA3-OA5-PA1
32	4c	201	CDL	CB2-OB2-PB2-OB3
32	4c	201	CDL	CB2-OB2-PB2-OB4
32	4c	201	CDL	CB2-OB2-PB2-OB5
32	4c	201	CDL	OB5-CB3-CB4-OB6
32	4e	202	CDL	CA2-OA2-PA1-OA4
32	4e	202	CDL	CB3-OB5-PB2-OB4
32	7c	201	CDL	CA2-OA2-PA1-OA3
32	7c	201	CDL	CA2-OA2-PA1-OA4
32	7c	201	CDL	CA2-OA2-PA1-OA5
32	7c	201	CDL	CB3-OB5-PB2-OB4
32	4E	202	CDL	CA2-OA2-PA1-OA3
32	4E	202	CDL	CA2-OA2-PA1-OA4
32	4E	202	CDL	CB3-OB5-PB2-OB3
32	QE	302	CDL	CA2-OA2-PA1-OA3
32	QE	302	CDL	CA2-OA2-PA1-OA4
32	QE	302	CDL	CA2-OA2-PA1-OA5
32	QE	302	CDL	CB2-OB2-PB2-OB3
32	QE	302	CDL	CB2-OB2-PB2-OB5
32	QE	302	CDL	CB3-OB5-PB2-OB3
34	QD	303	PC1	C1-O11-P-O14
34	QD	303	PC1	C1-O11-P-O13
34	Qc	403	PC1	C11-O13-P-O12
34	Qc	403	PC1	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
34	Qc	403	PC1	C11-O13-P-O11
34	Qd	303	PC1	C1-O11-P-O12
34	Qd	303	PC1	C1-O11-P-O14
34	Qj	201	PC1	C1-O11-P-O12
34	Qj	201	PC1	C1-O11-P-O14
34	Qj	201	PC1	C1-O11-P-O13
34	4a	301	PC1	C11-O13-P-O12
34	4a	301	PC1	C1-O11-P-O14
34	7c	202	PC1	C11-O13-P-O12
34	7c	202	PC1	C11-O13-P-O14
34	7c	202	PC1	C1-O11-P-O13
34	c1	505	PC1	C11-O13-P-O12
34	c1	505	PC1	C11-O13-P-O14
34	c1	505	PC1	C1-O11-P-O14
34	c1	505	PC1	O21-C2-C3-O31
34	c1	508	PC1	C11-O13-P-O12
34	c3	201	PC1	C11-O13-P-O14
34	c3	201	PC1	C1-O11-P-O13
34	4A	301	PC1	C11-O13-P-O12
34	4A	301	PC1	C1-O11-P-O14
34	4A	302	PC1	O21-C2-C3-O31
34	C1	505	PC1	C1-O11-P-O12
34	C1	509	PC1	C11-O13-P-O12
34	C3	201	PC1	C11-O13-P-O14
34	DC	201	PC1	C11-O13-P-O14
34	DC	201	PC1	C1-O11-P-O12
34	DC	201	PC1	O13-C11-C12-N
34	QE	303	PC1	C11-O13-P-O14
34	QE	303	PC1	C1-O11-P-O12
34	Qe	301	PC1	C11-O13-P-O11
34	Qe	302	PC1	C11-O13-P-O12
34	Qg	301	PC1	C1-O11-P-O12
34	Qg	301	PC1	C1-O11-P-O14
35	QD	304	PX2	C1-O4-P1-O1
35	QD	304	PX2	C1-O4-P1-O2
35	QD	304	PX2	C1-O4-P1-O3
35	QJ	201	PX2	C1-O4-P1-O1
35	QJ	201	PX2	C1-O4-P1-O2
35	QJ	201	PX2	C1-O4-P1-O3
35	4C	201	PX2	C1-O4-P1-O1
35	4C	201	PX2	C1-O4-P1-O2
36	4a	302	3PE	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
36	4a	302	3PE	C1-O11-P-O14
36	4a	302	3PE	C11-O13-P-O12
36	4a	302	3PE	O13-C11-C12-N
36	c1	506	3PE	O13-C11-C12-N
36	c1	507	3PE	C1-O11-P-O13
36	c1	507	3PE	C11-O13-P-O12
36	c1	507	3PE	C11-O13-P-O14
36	C1	507	3PE	C1-O11-P-O13
36	C1	507	3PE	C2-C1-O11-P
36	C1	507	3PE	C12-C11-O13-P
36	C1	507	3PE	O13-C11-C12-N
36	C1	508	3PE	C1-O11-P-O14
36	C1	508	3PE	C11-O13-P-O14
36	4D	201	3PE	C11-O13-P-O14
36	4F	101	3PE	O13-C11-C12-N
36	4d	201	3PE	C11-O13-P-O14
36	4d	202	3PE	O13-C11-C12-N
36	7A	201	3PE	C1-O11-P-O12
36	7A	201	3PE	C11-O13-P-O12
36	7A	201	3PE	O13-C11-C12-N
37	c1	501	HEA	C1A-C2A-CAA-CBA
37	c1	501	HEA	C3A-C2A-CAA-CBA
37	c1	501	HEA	C2A-C3A-CMA-OMA
37	c1	501	HEA	C4A-C3A-CMA-OMA
37	c1	501	HEA	C17-C18-C19-C27
37	c1	501	HEA	C19-C20-C21-C22
37	c1	502	HEA	C2A-C3A-CMA-OMA
37	c1	502	HEA	C4A-C3A-CMA-OMA
37	c1	502	HEA	C3B-C11-C12-C13
37	c1	502	HEA	O11-C11-C12-C13
37	c1	502	HEA	C13-C14-C15-C16
37	c1	502	HEA	C13-C14-C15-C26
37	c1	502	HEA	C17-C18-C19-C27
37	c1	502	HEA	C27-C19-C20-C21
37	C1	501	HEA	C2A-C3A-CMA-OMA
37	C1	501	HEA	C4A-C3A-CMA-OMA
37	C1	501	HEA	C17-C18-C19-C27
37	C1	502	HEA	C1A-C2A-CAA-CBA
37	C1	502	HEA	C2A-C3A-CMA-OMA
37	C1	502	HEA	C4A-C3A-CMA-OMA
37	C1	502	HEA	C3B-C11-C12-C13
37	C1	502	HEA	O11-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
37	C1	502	HEA	C13-C14-C15-C16
37	C1	502	HEA	C13-C14-C15-C26
37	C1	502	HEA	C15-C16-C17-C18
37	C1	502	HEA	C17-C18-C19-C20
37	C1	502	HEA	C19-C20-C21-C22
42	4F	102	S12	O-C-CA-CB
42	4F	102	S12	OXT-C-CA-CB
42	4F	102	S12	O11-C3-C4-O52
42	4d	203	S12	C2-O2-P-OG
42	4d	203	S12	C2-O2-P-O3
42	4d	203	S12	C2-O2-P-O4
42	4d	203	S12	CA-CB-OG-P
42	4d	203	S12	O11-C3-C4-O52
42	4d	203	S12	N-CA-CB-OG
37	c1	502	HEA	C21-C22-C23-C24
37	c1	502	HEA	C3A-C2A-CAA-CBA
37	C1	502	HEA	C3A-C2A-CAA-CBA
37	c1	502	HEA	C1A-C2A-CAA-CBA
37	C1	502	HEA	C17-C18-C19-C27
42	4F	102	S12	OXT-C-CA-N
42	4d	203	S12	OXT-C-CA-N
37	c1	501	HEA	C17-C18-C19-C20
37	C1	501	HEA	C17-C18-C19-C20
32	7c	201	CDL	O1-C1-CA2-OA2
35	QD	304	PX2	C16-C17-C18-C19
37	c1	502	HEA	C21-C22-C23-C25
36	4a	302	3PE	C37-C38-C39-C3A
36	4F	101	3PE	C39-C3A-C3B-C3C
32	QE	302	CDL	C1-CB2-OB2-PB2
37	c1	502	HEA	C15-C16-C17-C18
37	c1	502	HEA	C19-C20-C21-C22
36	4F	101	3PE	C28-C29-C2A-C2B
32	C1	506	CDL	C13-C14-C15-C16
34	7c	202	PC1	C33-C34-C35-C36
32	QD	302	CDL	OA6-CA4-CA6-OA8
34	7c	202	PC1	C39-C3A-C3B-C3C
35	QJ	201	PX2	C5-C4-O5-C3
34	c3	201	PC1	C31-C32-C33-C34
42	4F	102	S12	C5-C6-C7-C8
32	QC	403	CDL	CA5-C11-C12-C13
35	QJ	201	PX2	C4-C5-C6-C7
34	DC	201	PC1	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
34	4a	301	PC1	C11-C12-N-C13
34	4A	302	PC1	C11-C12-N-C14
32	7c	201	CDL	CB5-C51-C52-C53
34	c1	505	PC1	C24-C25-C26-C27
37	C1	501	HEA	C19-C20-C21-C22
32	QD	302	CDL	CA2-OA2-PA1-OA5
32	QD	302	CDL	CA3-OA5-PA1-OA2
32	QD	302	CDL	CB3-OB5-PB2-OB2
32	Qd	302	CDL	CA2-OA2-PA1-OA5
32	Qd	302	CDL	CB2-OB2-PB2-OB5
32	Qh	101	CDL	CA3-OA5-PA1-OA2
32	Qh	101	CDL	CB3-OB5-PB2-OB2
32	Qh	102	CDL	CA2-OA2-PA1-OA5
32	Qj	202	CDL	CB3-OB5-PB2-OB2
32	4c	201	CDL	CA2-OA2-PA1-OA5
32	4c	201	CDL	CA3-OA5-PA1-OA2
32	4e	202	CDL	CA2-OA2-PA1-OA5
32	4e	202	CDL	CB3-OB5-PB2-OB2
32	7c	201	CDL	CB3-OB5-PB2-OB2
32	4E	202	CDL	CA2-OA2-PA1-OA5
32	4E	202	CDL	CB2-OB2-PB2-OB5
32	4E	202	CDL	CB3-OB5-PB2-OB2
32	QE	302	CDL	CB3-OB5-PB2-OB2
34	QD	303	PC1	C11-O13-P-O11
34	Qc	403	PC1	C1-O11-P-O13
34	Qd	303	PC1	C1-O11-P-O13
34	4a	301	PC1	C11-O13-P-O11
34	4a	301	PC1	C1-O11-P-O13
34	4e	201	PC1	C1-O11-P-O13
34	7c	202	PC1	C11-O13-P-O11
34	c1	505	PC1	C11-O13-P-O11
34	c1	508	PC1	C11-O13-P-O11
34	C1	505	PC1	C11-O13-P-O11
34	C1	505	PC1	C1-O11-P-O13
34	C1	509	PC1	C11-O13-P-O11
34	C3	201	PC1	C11-O13-P-O11
34	DC	201	PC1	C1-O11-P-O13
34	Qe	301	PC1	C1-O11-P-O13
34	Qe	302	PC1	C11-O13-P-O11
34	Qe	304	PC1	C1-O11-P-O13
34	Qg	301	PC1	C1-O11-P-O13
36	4a	302	3PE	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
36	4a	302	3PE	C11-O13-P-O11
36	c1	506	3PE	C11-O13-P-O11
36	c1	507	3PE	C11-O13-P-O11
36	C1	507	3PE	C11-O13-P-O11
36	4D	201	3PE	C11-O13-P-O11
36	7a	201	3PE	C11-O13-P-O11
36	4d	202	3PE	C11-O13-P-O11
36	7A	201	3PE	C11-O13-P-O11
42	4F	102	S12	C2-O2-P-OG
32	C1	506	CDL	CA7-C31-C32-C33
34	Qc	403	PC1	C11-C12-N-C14
34	Qc	403	PC1	C11-C12-N-C15
34	DC	201	PC1	C11-C12-N-C13
34	DC	201	PC1	C11-C12-N-C15
34	Qe	301	PC1	C11-C12-N-C13
34	Qe	301	PC1	C11-C12-N-C14
34	Qe	301	PC1	C11-C12-N-C15
34	DC	201	PC1	C35-C36-C37-C38
34	DC	201	PC1	C2D-C2E-C2F-C2G
35	QD	304	PX2	C18-C19-C20-C21
35	QJ	201	PX2	C6-C7-C8-C9
36	4F	101	3PE	C2E-C2F-C2G-C2H
36	4d	202	3PE	C32-C33-C34-C35
36	4d	202	3PE	C28-C29-C2A-C2B
42	4d	203	S12	C11-C10-C9-C8
42	4d	203	S12	C15-C16-C17-C18
32	Qd	302	CDL	C22-C23-C24-C25
35	QJ	201	PX2	C17-C18-C19-C20
36	4a	302	3PE	C33-C34-C35-C36
36	4a	302	3PE	C34-C35-C36-C37
36	4a	302	3PE	C39-C3A-C3B-C3C
36	4d	202	3PE	C27-C28-C29-C2A
35	QD	304	PX2	C11-C12-C13-C14
34	Qc	403	PC1	C2-C1-O11-P
35	QJ	201	PX2	O6-C4-O5-C3
34	C3	201	PC1	C33-C34-C35-C36
42	4F	102	S12	C15-C16-C17-C18
32	QH	101	CDL	O1-C1-CB2-OB2
35	4C	201	PX2	C22-C23-C24-C25
32	QE	302	CDL	C51-C52-C53-C54
34	7c	202	PC1	C34-C35-C36-C37
36	4a	302	3PE	C28-C29-C2A-C2B

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Mol	Chain	Res	Type	Atoms
37	c1	501	HEA	C27-C19-C20-C21
32	Qd	302	CDL	C17-C18-C19-C20
32	4e	202	CDL	C56-C57-C58-C59
34	7c	202	PC1	C35-C36-C37-C38
35	4C	201	PX2	C16-C17-C18-C19
32	4E	202	CDL	C56-C57-C58-C59
34	DC	201	PC1	C3B-C3C-C3D-C3E
32	Qd	302	CDL	C76-C77-C78-C79
36	c1	506	3PE	C33-C34-C35-C36
32	Qd	302	CDL	C21-C22-C23-C24
34	C1	505	PC1	C22-C23-C24-C25
34	DC	201	PC1	C2E-C2F-C2G-C2H
35	QJ	201	PX2	C9-C10-C11-C12
42	4F	102	S12	C10-C11-C12-C13
34	4E	201	PC1	C31-C32-C33-C34
34	C1	505	PC1	C21-C22-C23-C24
34	Qe	302	PC1	C2A-C2B-C2C-C2D
35	4C	201	PX2	C10-C11-C12-C13
34	Qc	403	PC1	C11-C12-N-C13
34	4a	301	PC1	C11-C12-N-C15
34	4A	302	PC1	C11-C12-N-C15
34	DC	201	PC1	C11-C12-N-C14
37	c1	501	HEA	C15-C16-C17-C18
34	4a	301	PC1	C28-C29-C2A-C2B
36	4a	302	3PE	C27-C28-C29-C2A
32	Qd	302	CDL	C58-C59-C60-C61
36	4F	101	3PE	C21-C22-C23-C24
36	4d	202	3PE	C31-C32-C33-C34
34	C1	505	PC1	C37-C38-C39-C3A
36	4F	101	3PE	C2B-C2C-C2D-C2E
36	4F	101	3PE	C2C-C2D-C2E-C2F
32	4E	202	CDL	C31-C32-C33-C34
35	QJ	201	PX2	C18-C19-C20-C21
36	C1	507	3PE	C33-C34-C35-C36
32	Qh	101	CDL	C52-C53-C54-C55
35	4C	201	PX2	C19-C20-C21-C22
32	4e	202	CDL	C31-C32-C33-C34
32	7c	201	CDL	C43-C44-C45-C46
34	c1	508	PC1	C23-C24-C25-C26
34	Qj	201	PC1	C1-C2-C3-O31
35	QD	304	PX2	C9-C10-C11-C12
37	C1	501	HEA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
36	4d	202	3PE	C24-C25-C26-C27
34	c1	505	PC1	C26-C27-C28-C29
34	DC	201	PC1	C23-C24-C25-C26
32	7c	201	CDL	C12-C13-C14-C15
32	C1	506	CDL	O1-C1-CB2-OB2
32	7c	201	CDL	CB2-C1-CA2-OA2
36	4d	202	3PE	C33-C34-C35-C36
32	4c	201	CDL	C36-C37-C38-C39
34	C1	505	PC1	C3B-C3C-C3D-C3E
34	Qe	301	PC1	C3D-C3E-C3F-C3G
34	7c	202	PC1	C11-C12-N-C13
34	4A	302	PC1	C11-C12-N-C13
34	Qe	302	PC1	C11-C12-N-C14
34	Qe	304	PC1	C11-C12-N-C15
32	QH	101	CDL	CB7-C71-C72-C73
32	C1	506	CDL	C34-C35-C36-C37
34	7c	202	PC1	C3D-C3E-C3F-C3G
32	7c	201	CDL	C39-C40-C41-C42
42	4d	203	S12	C6-C5-O52-C4
36	c1	506	3PE	C35-C36-C37-C38
34	4A	301	PC1	C27-C28-C29-C2A
34	DC	201	PC1	C26-C27-C28-C29
34	c1	505	PC1	C3C-C3D-C3E-C3F
34	DC	201	PC1	C27-C28-C29-C2A
36	4F	101	3PE	C33-C34-C35-C36
36	4d	202	3PE	C39-C3A-C3B-C3C
31	Qc	402	HEM	C2C-C3C-CAC-CBC
42	4d	203	S12	C-CA-CB-OG
34	Qe	301	PC1	C33-C34-C35-C36
32	QH	101	CDL	CA5-C11-C12-C13
32	Qc	404	CDL	C53-C54-C55-C56
31	Qc	402	HEM	C4C-C3C-CAC-CBC
42	4F	102	S12	C7-C8-C9-C10
36	4F	101	3PE	O21-C2-C3-O31
36	c1	506	3PE	C25-C26-C27-C28
36	4d	202	3PE	C2D-C2E-C2F-C2G
42	4d	203	S12	C7-C8-C9-C10
34	4a	301	PC1	C11-C12-N-C14
32	Qc	404	CDL	C11-C12-C13-C14
34	4a	301	PC1	C25-C26-C27-C28
34	C3	201	PC1	C3D-C3E-C3F-C3G
35	QD	304	PX2	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
36	4F	101	3PE	C24-C25-C26-C27
32	QC	403	CDL	CA2-OA2-PA1-OA5
32	QJ	202	CDL	CA2-OA2-PA1-OA5
32	4e	202	CDL	CB2-OB2-PB2-OB5
34	c1	505	PC1	C1-O11-P-O13
34	c3	201	PC1	C11-O13-P-O11
36	C1	508	3PE	C1-O11-P-O13
36	4d	201	3PE	C11-O13-P-O11
36	4a	302	3PE	C23-C24-C25-C26
36	7a	201	3PE	C3A-C3B-C3C-C3D
32	QH	101	CDL	OB5-CB3-CB4-CB6
32	4c	201	CDL	OA5-CA3-CA4-CA6
32	4c	201	CDL	OB5-CB3-CB4-CB6
35	4C	201	PX2	C11-C12-C13-C14
31	QC	401	HEM	C2A-CAA-CBA-CGA
42	4F	102	S12	C11-C10-C9-C8
36	4a	302	3PE	C25-C26-C27-C28
42	4F	102	S12	C9-C10-C11-C12
34	QE	303	PC1	C32-C33-C34-C35
42	4d	203	S12	O51-C5-O52-C4
32	Qh	101	CDL	CA3-CA4-CA6-OA8
34	c1	505	PC1	C1-C2-C3-O31
34	Qe	301	PC1	C1-C2-C3-O31
36	4a	302	3PE	C1-C2-C3-O31
34	4E	201	PC1	C24-C25-C26-C27
35	QJ	201	PX2	C24-C25-C26-C27
34	C3	201	PC1	C22-C23-C24-C25
36	c1	506	3PE	O31-C31-C32-C33
36	c1	507	3PE	C31-C32-C33-C34
35	4C	201	PX2	C17-C18-C19-C20
37	C1	501	HEA	C3A-C2A-CAA-CBA
34	DC	201	PC1	C1-C2-O21-C21
34	C1	505	PC1	O11-C1-C2-O21
34	C1	509	PC1	O11-C1-C2-O21
36	c1	506	3PE	O11-C1-C2-O21
36	4F	101	3PE	O11-C1-C2-O21
34	C1	505	PC1	C28-C29-C2A-C2B
42	4d	203	S12	C18-C19-C20-C21
42	4F	102	S12	C19-C20-C21-C22
36	C1	507	3PE	C3A-C3B-C3C-C3D
32	4c	201	CDL	C72-C71-CB7-OB8
37	C1	501	HEA	C27-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
34	c3	201	PC1	C26-C27-C28-C29
42	4d	203	S12	C16-C17-C18-C19
37	c1	501	HEA	C18-C19-C20-C21
34	C3	201	PC1	C3A-C3B-C3C-C3D
36	4d	202	3PE	C2C-C2D-C2E-C2F
35	4C	201	PX2	C5-C4-O5-C3
34	7c	202	PC1	C23-C24-C25-C26
42	4d	203	S12	O2-C2-C3-C4
32	4E	202	CDL	C62-C63-C64-C65
36	C1	507	3PE	C26-C27-C28-C29
36	C1	507	3PE	C32-C33-C34-C35
34	7c	202	PC1	C11-C12-N-C15
34	Qe	302	PC1	C11-C12-N-C15
34	Qe	304	PC1	C11-C12-N-C13
32	QH	101	CDL	OA5-CA3-CA4-CA6
32	Qh	102	CDL	OB5-CB3-CB4-CB6
36	4F	101	3PE	O11-C1-C2-C3
37	C1	501	HEA	C15-C16-C17-C18
34	7c	202	PC1	C3A-C3B-C3C-C3D
34	DC	201	PC1	C2F-C2G-C2H-C2I
36	C1	507	3PE	C31-C32-C33-C34
42	4F	102	S12	C16-C17-C18-C19
32	QJ	202	CDL	CA4-CA3-OA5-PA1
32	C1	506	CDL	CA4-CA3-OA5-PA1
42	4d	203	S12	C11-C12-C13-C14
36	4a	302	3PE	C24-C25-C26-C27
34	c3	201	PC1	C27-C28-C29-C2A
31	Qc	401	HEM	C2A-CAA-CBA-CGA
34	DC	201	PC1	C39-C3A-C3B-C3C
32	QD	302	CDL	CA3-CA4-CA6-OA8
32	Qh	101	CDL	CB3-CB4-CB6-OB8
32	Qh	102	CDL	CB3-CB4-CB6-OB8
32	4e	202	CDL	CB3-CB4-CB6-OB8
32	4E	202	CDL	CB3-CB4-CB6-OB8
32	QE	302	CDL	CA3-CA4-CA6-OA8
36	c1	506	3PE	C1-C2-C3-O31
32	C1	506	CDL	C39-C40-C41-C42
34	c3	201	PC1	C24-C25-C26-C27
36	4F	101	3PE	C3A-C3B-C3C-C3D
42	4d	203	S12	C2-C3-C4-O52
36	7a	201	3PE	C31-C32-C33-C34
32	C1	506	CDL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
34	4A	302	PC1	C27-C28-C29-C2A
36	7a	201	3PE	C33-C34-C35-C36
34	7c	202	PC1	C2F-C2G-C2H-C2I
32	Qc	404	CDL	CA3-OA5-PA1-OA2
32	Qh	102	CDL	CA3-OA5-PA1-OA2
32	QE	302	CDL	CA3-OA5-PA1-OA2
34	Qj	201	PC1	C11-O13-P-O11
34	4A	301	PC1	C1-O11-P-O13
36	C1	508	3PE	C11-O13-P-O11
37	C1	502	HEA	C21-C22-C23-C24
32	QH	101	CDL	OB5-CB3-CB4-OB6
32	4c	201	CDL	OA5-CA3-CA4-OA6
36	C1	507	3PE	O11-C1-C2-O21
35	4C	201	PX2	O6-C4-O5-C3
36	c1	506	3PE	C3A-C3B-C3C-C3D
32	Qh	101	CDL	OA6-CA4-CA6-OA8
32	4e	202	CDL	OA6-CA4-CA6-OA8
32	4E	202	CDL	OB6-CB4-CB6-OB8
32	QE	302	CDL	OB6-CB4-CB6-OB8
36	4a	302	3PE	O21-C2-C3-O31
32	QE	302	CDL	CA2-C1-CB2-OB2
42	4F	102	S12	O-C-CA-N
42	4d	203	S12	O-C-CA-N
32	Qc	404	CDL	CA4-CA3-OA5-PA1
34	QD	303	PC1	C2-C1-O11-P
36	7a	201	3PE	C2-C1-O11-P
36	4d	202	3PE	C2B-C2C-C2D-C2E
36	c1	507	3PE	C2B-C2C-C2D-C2E
32	4E	202	CDL	C33-C34-C35-C36
35	QJ	201	PX2	O4-C1-C2-C3
36	c1	507	3PE	O11-C1-C2-C3
36	C1	507	3PE	O11-C1-C2-C3
32	QJ	202	CDL	C32-C33-C34-C35
32	4e	202	CDL	C64-C65-C66-C67
36	4d	202	3PE	C3D-C3E-C3F-C3G
36	4F	101	3PE	C3D-C3E-C3F-C3G
34	DC	201	PC1	C37-C38-C39-C3A
36	4F	101	3PE	C35-C36-C37-C38
34	7c	202	PC1	C27-C28-C29-C2A
31	Qc	401	HEM	C2C-C3C-CAC-CBC
36	c1	506	3PE	C3-C2-O21-C21
32	4e	202	CDL	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
32	4e	202	CDL	C62-C63-C64-C65
32	Qh	102	CDL	C1-CB2-OB2-PB2
32	QE	302	CDL	CB3-CB4-CB6-OB8
34	4A	302	PC1	C1-C2-C3-O31
34	Qe	301	PC1	C2-C1-O11-P
36	c1	506	3PE	C2-C1-O11-P
35	4C	201	PX2	C18-C19-C20-C21
32	QC	403	CDL	OB5-CB3-CB4-OB6
32	QD	302	CDL	OB5-CB3-CB4-OB6
32	Qh	102	CDL	OB5-CB3-CB4-OB6
35	QJ	201	PX2	O4-C1-C2-O7
36	4d	202	3PE	C3E-C3F-C3G-C3H
32	Qc	404	CDL	OA6-CA4-CA6-OA8
32	Qh	101	CDL	OB6-CB4-CB6-OB8
32	Qh	102	CDL	OB6-CB4-CB6-OB8
32	4e	202	CDL	OB6-CB4-CB6-OB8
32	QE	302	CDL	OA6-CA4-CA6-OA8
34	Qe	301	PC1	O21-C2-C3-O31
36	4D	201	3PE	O21-C2-C3-O31
36	4F	101	3PE	C2D-C2E-C2F-C2G
34	7c	202	PC1	C2C-C2D-C2E-C2F
32	4e	202	CDL	C51-C52-C53-C54
32	4E	202	CDL	C64-C65-C66-C67
32	QJ	202	CDL	CA3-OA5-PA1-OA2
32	Qd	302	CDL	CB3-OB5-PB2-OB2
32	Qj	202	CDL	CB2-OB2-PB2-OB5
34	C3	201	PC1	C1-O11-P-O13
34	QE	303	PC1	C1-O11-P-O13
36	4F	101	3PE	C1-O11-P-O13
34	7c	202	PC1	C38-C39-C3A-C3B
34	DC	201	PC1	C24-C25-C26-C27
32	Qh	102	CDL	C1-CA2-OA2-PA1
32	4c	201	CDL	C1-CB2-OB2-PB2
32	4e	202	CDL	CA4-CA3-OA5-PA1
32	4E	202	CDL	C1-CB2-OB2-PB2
34	c1	505	PC1	C2-C1-O11-P
32	4E	202	CDL	C71-C72-C73-C74
32	QC	403	CDL	CA2-OA2-PA1-OA4
32	QD	302	CDL	CA2-OA2-PA1-OA3
32	QD	302	CDL	CA2-OA2-PA1-OA4
32	QD	302	CDL	CA3-OA5-PA1-OA3
32	QJ	202	CDL	CB2-OB2-PB2-OB3

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Mol	Chain	Res	Type	Atoms
32	Qc	404	CDL	CA3-OA5-PA1-OA3
32	Qd	302	CDL	CA2-OA2-PA1-OA4
32	Qd	302	CDL	CB2-OB2-PB2-OB4
32	Qh	101	CDL	CA3-OA5-PA1-OA3
32	Qh	101	CDL	CB3-OB5-PB2-OB3
32	Qj	202	CDL	CA2-OA2-PA1-OA3
32	Qj	202	CDL	CB2-OB2-PB2-OB4
32	4e	202	CDL	CA2-OA2-PA1-OA3
32	4e	202	CDL	CB2-OB2-PB2-OB3
32	4e	202	CDL	CB2-OB2-PB2-OB4
32	4E	202	CDL	CB2-OB2-PB2-OB3
32	4E	202	CDL	CB2-OB2-PB2-OB4
32	4E	202	CDL	CB3-OB5-PB2-OB4
34	QD	303	PC1	C11-O13-P-O12
34	QD	303	PC1	C11-O13-P-O14
34	Qc	403	PC1	C1-O11-P-O14
34	4e	201	PC1	C1-O11-P-O14
34	7c	202	PC1	C1-O11-P-O12
34	c1	505	PC1	C1-O11-P-O12
34	c3	201	PC1	C11-O13-P-O12
34	c3	201	PC1	C1-O11-P-O12
34	C1	505	PC1	C11-O13-P-O12
34	C1	505	PC1	C11-O13-P-O14
34	C3	201	PC1	C11-O13-P-O12
34	QE	303	PC1	C1-O11-P-O14
34	Qe	301	PC1	C11-O13-P-O12
34	Qe	301	PC1	C1-O11-P-O14
34	Qe	304	PC1	C1-O11-P-O12
34	Qe	304	PC1	C11-C12-N-C14
36	c1	506	3PE	C11-O13-P-O14
36	c1	507	3PE	C1-O11-P-O12
36	C1	507	3PE	C1-O11-P-O12
36	C1	507	3PE	C11-O13-P-O14
36	C1	508	3PE	C1-O11-P-O12
36	4D	201	3PE	C11-O13-P-O12
36	7a	201	3PE	C11-O13-P-O12
36	7a	201	3PE	C11-O13-P-O14
36	4d	201	3PE	C11-O13-P-O12
36	4d	202	3PE	C11-O13-P-O14
36	7A	201	3PE	C11-O13-P-O14
42	4F	102	S12	C2-O2-P-O3
34	c3	201	PC1	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
32	QD	302	CDL	OB5-CB3-CB4-CB6
34	C1	505	PC1	O11-C1-C2-C3
36	4F	101	3PE	C25-C26-C27-C28
42	4F	102	S12	C2-C3-C4-O52
34	7c	202	PC1	C12-C11-O13-P
34	c1	508	PC1	C12-C11-O13-P
36	c1	506	3PE	C12-C11-O13-P
36	c1	507	3PE	C12-C11-O13-P
36	7a	201	3PE	C12-C11-O13-P
36	4d	201	3PE	C23-C24-C25-C26
34	7c	202	PC1	C2B-C2C-C2D-C2E
32	QH	101	CDL	OA5-CA3-CA4-OA6
32	QJ	202	CDL	OA5-CA3-CA4-OA6
32	QJ	202	CDL	OB5-CB3-CB4-OB6
34	QD	303	PC1	O11-C1-C2-O21
34	Qg	301	PC1	O11-C1-C2-O21
36	c1	507	3PE	O11-C1-C2-O21
34	QD	303	PC1	C22-C23-C24-C25
34	Qj	201	PC1	C21-C22-C23-C24
34	Qe	301	PC1	C31-C32-C33-C34
32	Qh	101	CDL	O1-C1-CA2-OA2
32	QD	302	CDL	C52-C53-C54-C55
36	4a	302	3PE	C38-C39-C3A-C3B
34	7c	202	PC1	C11-C12-N-C14
34	C3	201	PC1	C11-C12-N-C15
34	QE	303	PC1	C31-C32-C33-C34
32	Qc	404	CDL	CA3-CA4-CA6-OA8
34	QD	303	PC1	O13-C11-C12-N
34	4a	301	PC1	O13-C11-C12-N
34	7c	202	PC1	O13-C11-C12-N
34	c1	508	PC1	O13-C11-C12-N
34	4A	301	PC1	O13-C11-C12-N
34	4A	302	PC1	O13-C11-C12-N
34	C1	509	PC1	O13-C11-C12-N
34	Qe	301	PC1	O13-C11-C12-N
34	Qe	302	PC1	O13-C11-C12-N
36	4F	101	3PE	C1-C2-C3-O31
34	Qj	201	PC1	O21-C2-C3-O31
36	c1	506	3PE	O21-C2-C3-O31
36	7A	201	3PE	C3C-C3D-C3E-C3F
34	c1	505	PC1	C25-C26-C27-C28
36	C1	507	3PE	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
32	QC	403	CDL	CB4-CB3-OB5-PB2
34	4a	301	PC1	C26-C27-C28-C29
37	C1	501	HEA	C18-C19-C20-C21
36	4a	302	3PE	C2E-C2F-C2G-C2H
34	c3	201	PC1	C3E-C3F-C3G-C3H
34	Qe	302	PC1	C11-C12-N-C13
34	DC	201	PC1	C25-C26-C27-C28
32	QD	302	CDL	CB6-CB4-OB6-CB5
32	4c	201	CDL	CB6-CB4-OB6-CB5
34	c3	201	PC1	C1-C2-O21-C21
34	C3	201	PC1	C3-C2-O21-C21
32	QJ	202	CDL	OA5-CA3-CA4-CA6
32	QJ	202	CDL	OB5-CB3-CB4-CB6
37	C1	501	HEA	C11-C12-C13-C14
32	4e	202	CDL	C71-C72-C73-C74
32	Qd	302	CDL	C40-C41-C42-C43
34	Qe	304	PC1	C21-C22-C23-C24
32	Qj	202	CDL	C1-CA2-OA2-PA1
35	QD	304	PX2	C21-C22-C23-C24
36	4F	101	3PE	C37-C38-C39-C3A
31	Qc	401	HEM	C3D-CAD-CBD-CGD
35	QJ	201	PX2	C23-C24-C25-C26
32	4E	202	CDL	OA6-CA4-CA6-OA8
34	7c	202	PC1	O21-C2-C3-O31
32	QC	403	CDL	CB3-OB5-PB2-OB2
32	Qh	102	CDL	CB2-OB2-PB2-OB5
32	Qj	202	CDL	CA2-OA2-PA1-OA5
32	Qj	202	CDL	CA3-OA5-PA1-OA2
34	4A	302	PC1	C11-O13-P-O11
34	DC	201	PC1	C11-O13-P-O11
36	c1	506	3PE	C1-O11-P-O13
32	C1	506	CDL	C12-C13-C14-C15
35	QJ	201	PX2	C10-C11-C12-C13
34	4E	201	PC1	C1-C2-C3-O31
34	Qe	304	PC1	C31-C32-C33-C34
34	QD	303	PC1	C32-C33-C34-C35
32	Qd	302	CDL	C13-C14-C15-C16
32	QH	101	CDL	CA4-CA3-OA5-PA1
32	Qd	302	CDL	CA4-CA3-OA5-PA1
32	Qh	101	CDL	CA4-CA3-OA5-PA1
32	QE	302	CDL	C1-CA2-OA2-PA1
32	Qd	302	CDL	C42-C43-C44-C45

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Mol	Chain	Res	Type	Atoms
33	Qd	301	HEC	CAD-CBD-CGD-O1D
32	QD	302	CDL	CB4-CB6-OB8-CB7
32	QC	403	CDL	OB5-CB3-CB4-CB6
34	QD	303	PC1	C33-C34-C35-C36
34	DC	201	PC1	C22-C23-C24-C25
31	Qc	401	HEM	C4C-C3C-CAC-CBC
42	4F	102	S12	C14-C15-C16-C17
36	7A	201	3PE	C3A-C3B-C3C-C3D
36	c1	507	3PE	C32-C33-C34-C35
34	4E	201	PC1	O21-C2-C3-O31
36	4d	201	3PE	O21-C2-C3-O31
34	DC	201	PC1	C3F-C3G-C3H-C3I
36	4D	201	3PE	C23-C24-C25-C26
32	4e	202	CDL	C1-CB2-OB2-PB2
34	7c	202	PC1	C2-C1-O11-P
34	4A	301	PC1	C28-C29-C2A-C2B
34	Qe	302	PC1	C29-C2A-C2B-C2C
31	QC	401	HEM	CAD-CBD-CGD-O1D
32	7c	201	CDL	C72-C71-CB7-OB8
34	Qj	201	PC1	C2-C3-O31-C31
42	4F	102	S12	C6-C5-O52-C4
42	4d	203	S12	O-C-CA-CB
42	4d	203	S12	OXT-C-CA-CB
34	4A	301	PC1	C21-C22-C23-C24
36	4a	302	3PE	C32-C31-O31-C3
34	4A	302	PC1	C39-C3A-C3B-C3C
35	4C	201	PX2	C9-C10-C11-C12
32	Qh	101	CDL	CB2-C1-CA2-OA2
34	QE	303	PC1	C1-C2-C3-O31
35	QD	304	PX2	C1-C2-C3-O5
36	c1	506	3PE	O32-C31-C32-C33
31	Qc	401	HEM	CAD-CBD-CGD-O2D
34	DC	201	PC1	C29-C2A-C2B-C2C
32	7c	201	CDL	C53-C54-C55-C56
31	Qc	402	HEM	CAD-CBD-CGD-O1D
32	QC	403	CDL	CB6-CB4-OB6-CB5
32	QH	101	CDL	CB3-CB4-OB6-CB5
32	QJ	202	CDL	CB6-CB4-OB6-CB5
32	Qh	101	CDL	CB3-CB4-OB6-CB5
32	4c	201	CDL	CA3-CA4-OA6-CA5
32	7c	201	CDL	CA6-CA4-OA6-CA5
32	C1	506	CDL	CA6-CA4-OA6-CA5

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Mol	Chain	Res	Type	Atoms
32	C1	506	CDL	CB3-CB4-OB6-CB5
32	C1	506	CDL	CB6-CB4-OB6-CB5
34	QD	303	PC1	C1-C2-O21-C21
34	Qc	403	PC1	C3-C2-O21-C21
34	Qd	303	PC1	C1-C2-O21-C21
34	Qe	302	PC1	C1-C2-O21-C21
34	Qe	302	PC1	C3-C2-O21-C21
36	C1	507	3PE	C3-C2-O21-C21
34	C3	201	PC1	C11-C12-N-C13
31	Qc	401	HEM	CAD-CBD-CGD-O1D
31	QC	402	HEM	CAD-CBD-CGD-O1D
31	QC	402	HEM	CAD-CBD-CGD-O2D
31	Qc	402	HEM	CAD-CBD-CGD-O2D
37	C1	501	HEA	CAD-CBD-CGD-O1D
34	Qe	302	PC1	C33-C34-C35-C36
34	C1	509	PC1	O11-C1-C2-C3
36	c1	506	3PE	O11-C1-C2-C3
36	4a	302	3PE	C2D-C2E-C2F-C2G
37	c1	501	HEA	CAD-CBD-CGD-O1D
32	QD	302	CDL	C33-C34-C35-C36
34	QE	303	PC1	C21-C22-C23-C24
42	4d	203	S12	O2-C2-C3-O11
34	4A	302	PC1	C25-C26-C27-C28
32	4c	201	CDL	C18-C19-C20-C21
42	4F	102	S12	O51-C5-O52-C4
34	C3	201	PC1	C11-C12-N-C14
33	Qd	301	HEC	CAD-CBD-CGD-O2D
34	C3	201	PC1	O21-C2-C3-O31
35	QD	304	PX2	O7-C2-C3-O5
32	4e	202	CDL	CA5-C11-C12-C13
32	7c	201	CDL	C32-C31-CA7-OA8
36	C1	507	3PE	O31-C31-C32-C33
32	QD	302	CDL	C36-C37-C38-C39
34	Qe	302	PC1	C3B-C3C-C3D-C3E
32	7c	201	CDL	C1-CA2-OA2-PA1
32	4E	202	CDL	CA4-CA3-OA5-PA1
34	C1	505	PC1	C33-C34-C35-C36
32	4c	201	CDL	C72-C71-CB7-OB9
34	c1	505	PC1	O21-C21-C22-C23
36	4d	202	3PE	C25-C26-C27-C28
32	QJ	202	CDL	C32-C31-CA7-OA8
31	QC	401	HEM	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
37	c1	501	HEA	CAD-CBD-CGD-O2D
32	Qd	302	CDL	C62-C63-C64-C65
34	QD	303	PC1	O11-C1-C2-C3
36	4d	202	3PE	C2A-C2B-C2C-C2D
34	C3	201	PC1	O31-C31-C32-C33
32	QH	101	CDL	OA6-CA4-CA6-OA8
32	C1	506	CDL	OA6-CA4-CA6-OA8
34	QD	303	PC1	O21-C2-C3-O31
34	4a	301	PC1	O21-C21-C22-C23
32	C1	506	CDL	C60-C61-C62-C63
33	QD	301	HEC	CAD-CBD-CGD-O1D
35	4C	201	PX2	C1-O4-P1-O3
32	Qc	404	CDL	C72-C71-CB7-OB8
34	Qe	302	PC1	C38-C39-C3A-C3B
31	QC	402	HEM	CAA-CBA-CGA-O2A
32	4e	202	CDL	C72-C73-C74-C75
34	C1	509	PC1	C31-C32-C33-C34
36	4a	302	3PE	C2A-C2B-C2C-C2D
32	Qh	102	CDL	C12-C11-CA5-OA6
32	Qh	102	CDL	C32-C31-CA7-OA8
34	C1	509	PC1	O21-C21-C22-C23
36	C1	508	3PE	O21-C21-C22-C23
32	QC	403	CDL	CB3-CB4-OB6-CB5
32	7c	201	CDL	CA3-CA4-OA6-CA5
34	Qc	403	PC1	C1-C2-O21-C21
34	Qe	301	PC1	C1-C2-O21-C21
37	C1	501	HEA	CAA-CBA-CGA-O2A
32	QD	302	CDL	C52-C51-CB5-OB6
32	QE	302	CDL	C32-C31-CA7-OA8
36	c1	507	3PE	O21-C21-C22-C23
34	Qe	301	PC1	C38-C39-C3A-C3B
31	Qc	402	HEM	CAA-CBA-CGA-O2A
34	Qc	403	PC1	C24-C25-C26-C27
32	Qd	302	CDL	OA5-CA3-CA4-OA6
35	QD	304	PX2	O4-C1-C2-O7
35	4C	201	PX2	O4-C1-C2-O7
34	Qd	303	PC1	O31-C31-C32-C33
34	c3	201	PC1	C32-C33-C34-C35
31	Qc	402	HEM	CAA-CBA-CGA-O1A
34	c3	201	PC1	C37-C38-C39-C3A
32	4E	202	CDL	C72-C73-C74-C75
32	C1	506	CDL	C12-C11-CA5-OA6

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Mol	Chain	Res	Type	Atoms
31	QC	402	HEM	CAA-CBA-CGA-O1A
37	C1	501	HEA	CAD-CBD-CGD-O2D
32	Qd	302	CDL	C52-C51-CB5-OB6
32	Qd	302	CDL	C77-C78-C79-C80
35	4C	201	PX2	O4-C1-C2-C3
35	QJ	201	PX2	C22-C23-C24-C25
32	4c	201	CDL	C52-C51-CB5-OB6
34	4A	302	PC1	O21-C21-C22-C23
32	QC	403	CDL	OB6-CB4-CB6-OB8
32	QD	302	CDL	OB6-CB4-CB6-OB8
32	7c	201	CDL	OA6-CA4-CA6-OA8
34	QE	303	PC1	O21-C2-C3-O31
34	DC	201	PC1	C28-C29-C2A-C2B
32	Qc	404	CDL	C32-C31-CA7-OA8
32	Qd	302	CDL	C72-C71-CB7-OB8
32	QE	302	CDL	C12-C11-CA5-OA6
34	Qe	302	PC1	O31-C31-C32-C33
32	4e	202	CDL	C60-C61-C62-C63
36	4F	101	3PE	C32-C33-C34-C35
34	4A	302	PC1	C23-C24-C25-C26
34	c1	505	PC1	C33-C34-C35-C36
32	QH	101	CDL	C12-C11-CA5-OA6
34	DC	201	PC1	O31-C31-C32-C33
42	4d	203	S12	C19-C20-C21-C22
34	4A	301	PC1	C36-C37-C38-C39
34	4A	301	PC1	O21-C21-C22-C23
33	QD	301	HEC	CAD-CBD-CGD-O2D
34	4a	301	PC1	O22-C21-C22-C23
36	4D	201	3PE	C24-C25-C26-C27
32	Qh	101	CDL	C32-C31-CA7-OA8
35	QJ	201	PX2	O5-C4-C5-C6
37	c1	502	HEA	C12-C13-C14-C15
34	4A	301	PC1	C2A-C2B-C2C-C2D
32	Qh	102	CDL	C12-C11-CA5-OA7
32	Qc	404	CDL	C32-C31-CA7-OA9
32	Qc	404	CDL	C72-C71-CB7-OB9
32	QE	302	CDL	C32-C31-CA7-OA9
32	QH	101	CDL	CA2-C1-CB2-OB2
34	7c	202	PC1	C3E-C3F-C3G-C3H
36	c1	506	3PE	C37-C38-C39-C3A
37	c1	501	HEA	CAA-CBA-CGA-O2A
32	4E	202	CDL	C61-C62-C63-C64

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Mol	Chain	Res	Type	Atoms
36	4d	202	3PE	C3F-C3G-C3H-C3I
32	Qd	302	CDL	C52-C51-CB5-OB7
34	QD	303	PC1	C1-C2-C3-O31
34	4e	201	PC1	C1-C2-C3-O31
34	QE	303	PC1	C11-O13-P-O11
34	Qd	303	PC1	O32-C31-C32-C33
36	c1	507	3PE	O22-C21-C22-C23
32	4c	201	CDL	C12-C13-C14-C15
32	QD	302	CDL	C12-C11-CA5-OA6
34	c3	201	PC1	O31-C31-C32-C33
32	C1	506	CDL	C38-C39-C40-C41
34	C3	201	PC1	O32-C31-C32-C33
32	QJ	202	CDL	CA2-OA2-PA1-OA3
32	Qh	101	CDL	CA2-OA2-PA1-OA3
32	Qj	202	CDL	CA3-OA5-PA1-OA3
32	C1	506	CDL	CB2-OB2-PB2-OB3
32	QE	302	CDL	CB3-OB5-PB2-OB4
34	4A	301	PC1	C11-O13-P-O14
34	4A	302	PC1	C11-O13-P-O14
34	C1	509	PC1	C1-O11-P-O14
34	Qe	304	PC1	C11-O13-P-O14
34	Qg	301	PC1	C11-O13-P-O14
36	c1	506	3PE	C1-O11-P-O14
36	7A	201	3PE	C1-O11-P-O14
35	QJ	201	PX2	O6-C4-C5-C6
32	C1	506	CDL	CA5-C11-C12-C13
32	C1	506	CDL	C12-C11-CA5-OA7
34	Qe	302	PC1	O32-C31-C32-C33
32	QJ	202	CDL	C72-C71-CB7-OB8
36	c1	507	3PE	C29-C2A-C2B-C2C
35	QD	304	PX2	O7-C16-C17-C18
32	QD	302	CDL	C52-C51-CB5-OB7
32	QH	101	CDL	C12-C11-CA5-OA7
32	4E	202	CDL	C51-C52-C53-C54
32	QH	101	CDL	CB6-CB4-OB6-CB5
32	QJ	202	CDL	CB3-CB4-OB6-CB5
32	Qh	101	CDL	CB6-CB4-OB6-CB5
32	4c	201	CDL	CA6-CA4-OA6-CA5
32	C1	506	CDL	CA3-CA4-OA6-CA5
34	4a	301	PC1	C12-C11-O13-P
34	4A	302	PC1	C12-C11-O13-P
34	C3	201	PC1	C1-C2-O21-C21

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Mol	Chain	Res	Type	Atoms
34	DC	201	PC1	C12-C11-O13-P
34	Qe	301	PC1	C3-C2-O21-C21
37	C1	501	HEA	C3B-C11-C12-C13
36	4a	302	3PE	O32-C31-O31-C3
32	Qd	302	CDL	C72-C71-CB7-OB9
32	Qh	102	CDL	C32-C31-CA7-OA9
42	4d	203	S12	C17-C18-C19-C20
34	c1	508	PC1	O21-C21-C22-C23
32	Qd	302	CDL	C63-C64-C65-C66
35	QD	304	PX2	C12-C13-C14-C15
34	4A	301	PC1	O22-C21-C22-C23
36	4d	202	3PE	O31-C31-C32-C33
34	QD	303	PC1	C21-C22-C23-C24
42	4F	102	S12	C17-C18-C19-C20
36	7a	201	3PE	C39-C3A-C3B-C3C
32	QE	302	CDL	C52-C51-CB5-OB6
34	QD	303	PC1	O21-C21-C22-C23
32	QC	403	CDL	OA5-CA3-CA4-OA6
32	4E	202	CDL	OB5-CB3-CB4-OB6
34	c3	201	PC1	O32-C31-C32-C33
32	Qh	101	CDL	C52-C51-CB5-OB6
32	4c	201	CDL	C12-C11-CA5-OA6
32	QD	302	CDL	C12-C11-CA5-OA7
32	Qh	101	CDL	C32-C31-CA7-OA9
34	7c	202	PC1	O21-C21-C22-C23
35	QD	304	PX2	C6-C7-C8-C9
34	c1	505	PC1	C21-C22-C23-C24
32	4c	201	CDL	C52-C51-CB5-OB7
32	QE	302	CDL	C12-C11-CA5-OA7
34	DC	201	PC1	O32-C31-C32-C33
32	QE	302	CDL	O1-C1-CB2-OB2
34	4E	201	PC1	O21-C21-C22-C23
32	QE	302	CDL	C52-C51-CB5-OB7
34	4A	302	PC1	O22-C21-C22-C23
33	Qd	301	HEC	CAA-CBA-CGA-O2A
32	Qd	302	CDL	C83-C84-C85-C86
32	QJ	202	CDL	C72-C71-CB7-OB9
35	4C	201	PX2	O7-C16-C17-C18

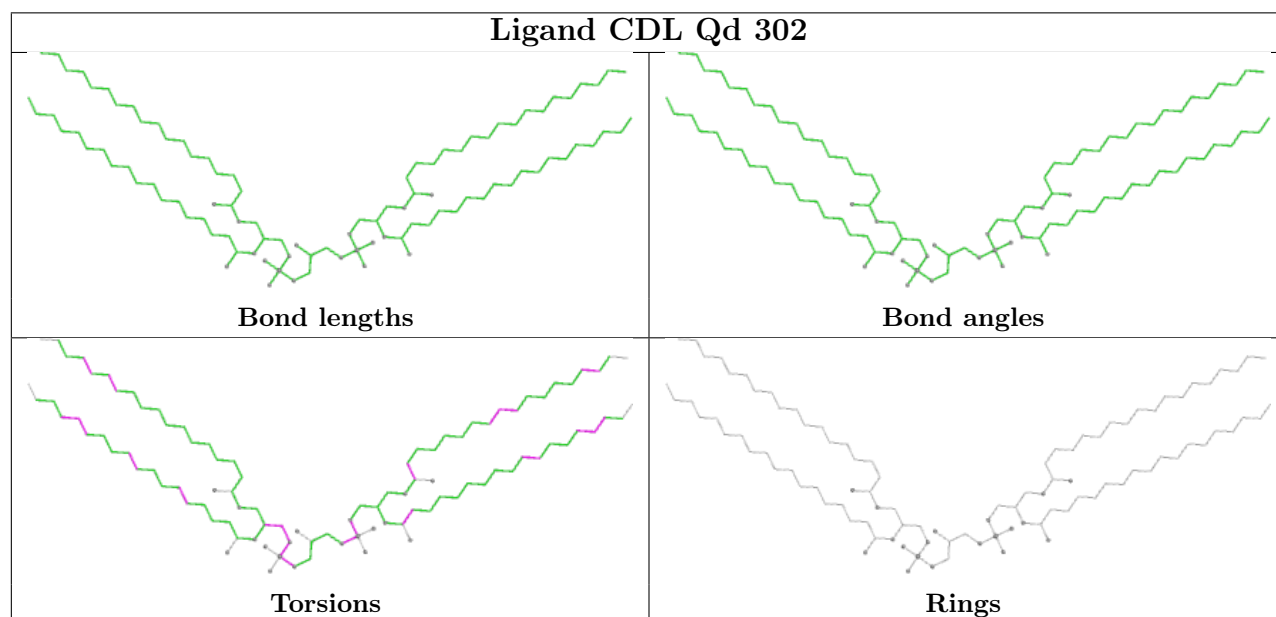
There are no ring outliers.

33 monomers are involved in 78 short contacts:

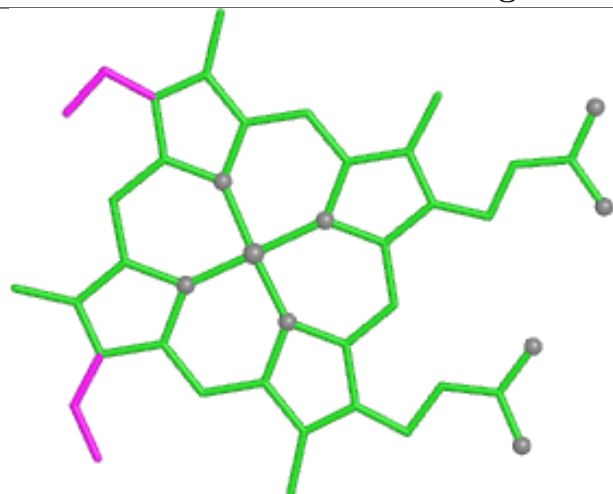
Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	Qd	302	CDL	2	0
33	QD	301	HEC	6	0
34	c1	508	PC1	1	0
34	QE	303	PC1	1	0
31	QC	402	HEM	3	0
34	Qe	301	PC1	1	0
36	C1	507	3PE	1	0
37	c1	501	HEA	14	0
31	Qc	402	HEM	3	0
36	c1	506	3PE	1	0
37	c1	502	HEA	4	0
34	Qe	302	PC1	2	0
34	4E	201	PC1	1	0
40	QE	301	FES	1	0
35	4C	201	PX2	4	0
37	C1	501	HEA	6	0
32	Qj	202	CDL	1	0
42	4F	102	S12	1	0
35	QJ	201	PX2	2	0
34	Qe	304	PC1	1	0
31	QC	401	HEM	1	0
34	C1	505	PC1	1	0
34	4e	201	PC1	1	0
36	4F	101	3PE	1	0
37	C1	502	HEA	4	0
31	Qc	401	HEM	4	0
35	QD	304	PX2	3	0
32	Qc	404	CDL	2	0
32	QJ	202	CDL	1	0
32	QD	302	CDL	1	0
33	Qd	301	HEC	2	0
34	DC	201	PC1	1	0
32	QC	403	CDL	1	0

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

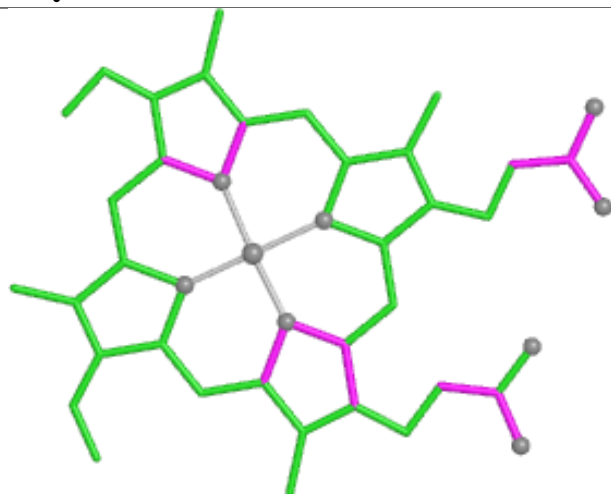
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



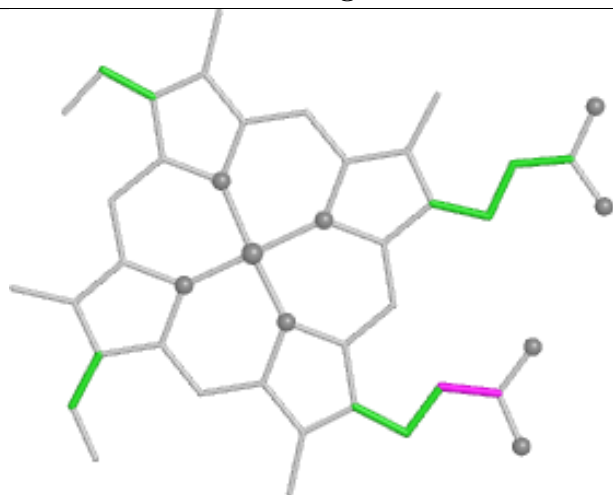
Ligand HEC QD 301



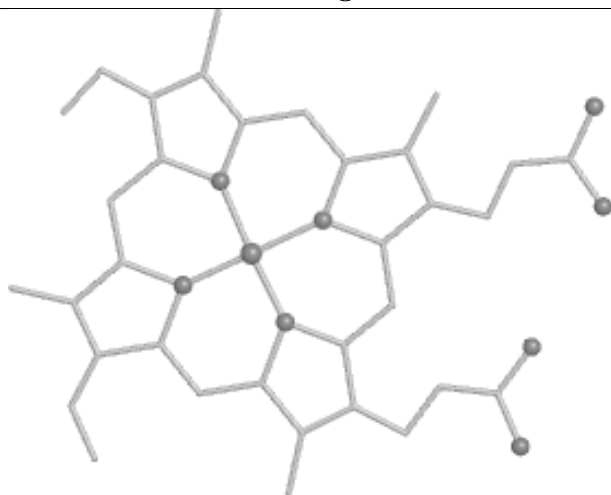
Bond lengths



Bond angles

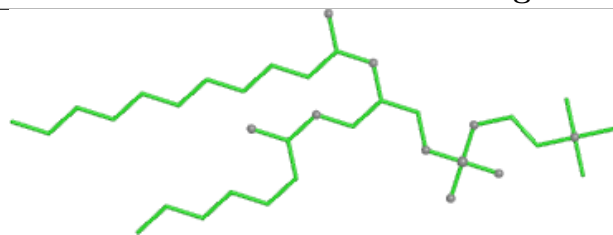


Torsions

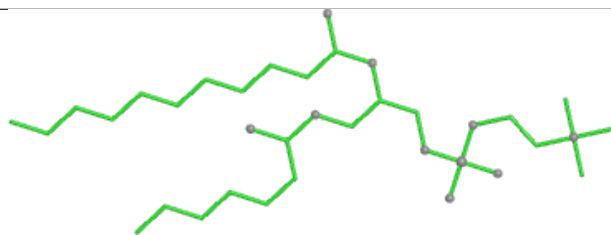


Rings

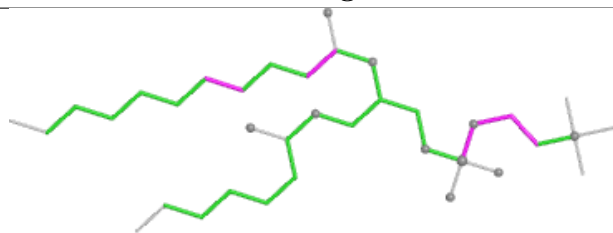
Ligand PC1 c1 508



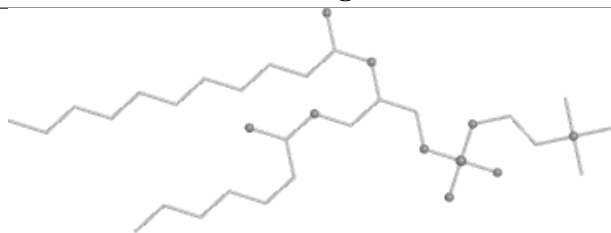
Bond lengths



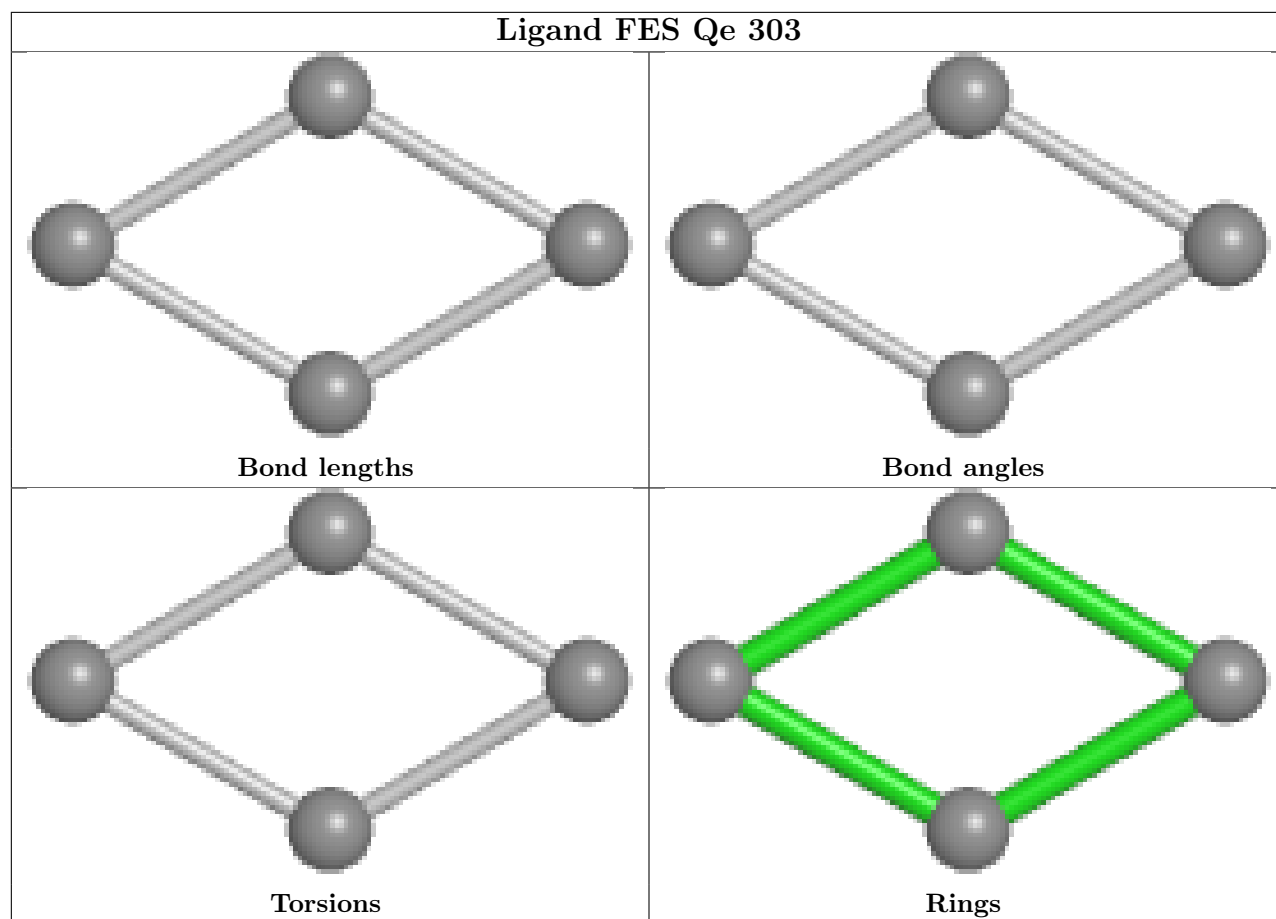
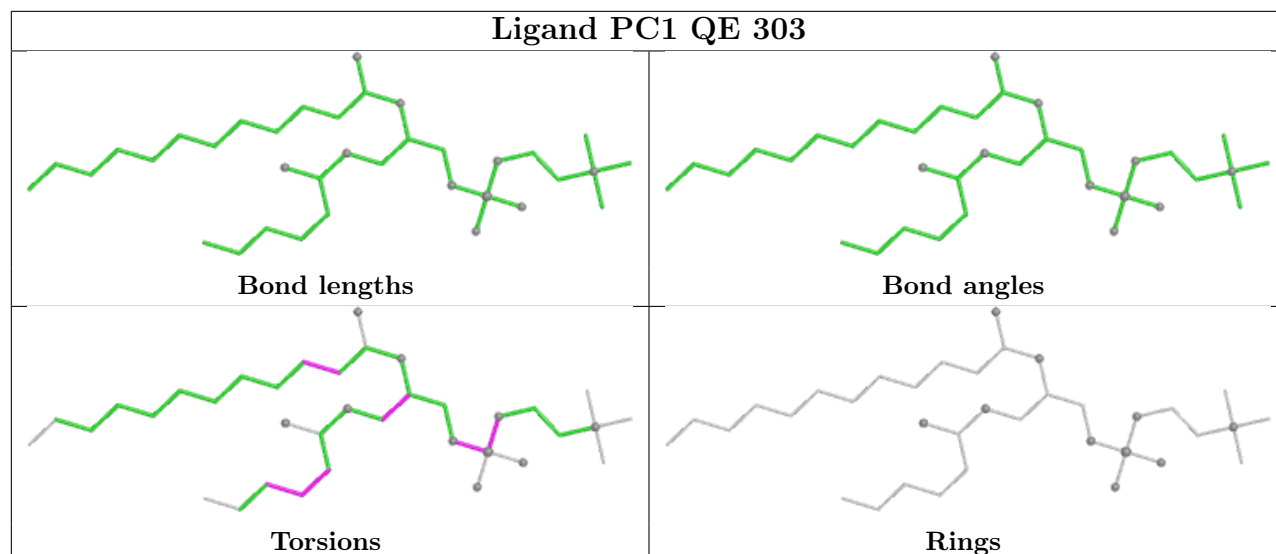
Bond angles



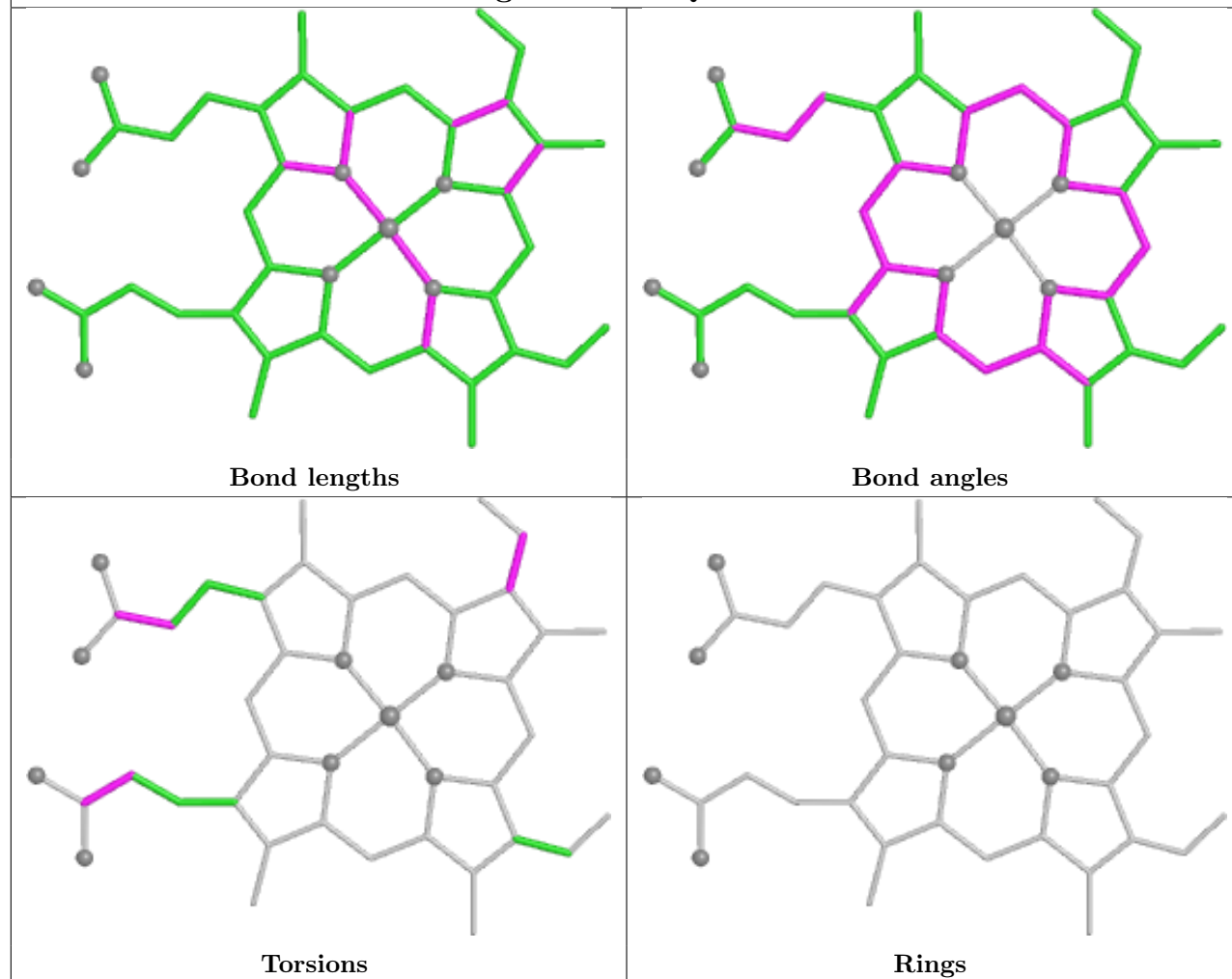
Torsions



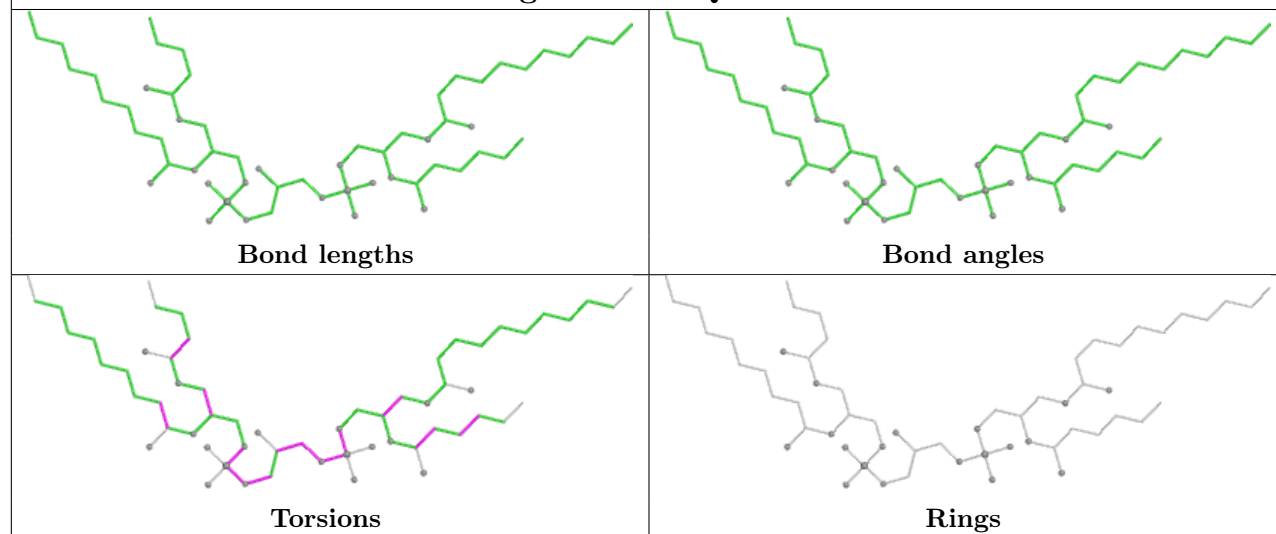
Rings

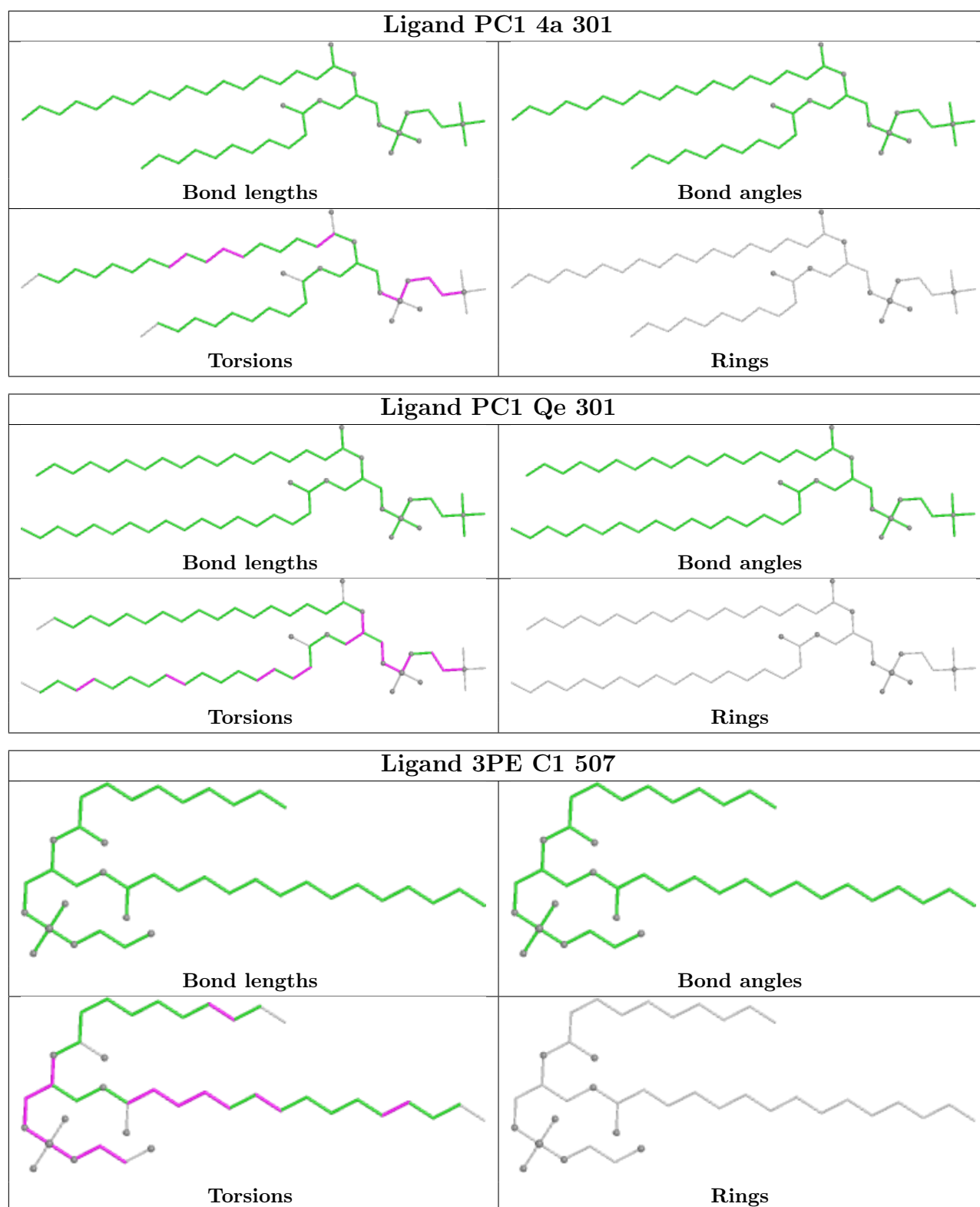


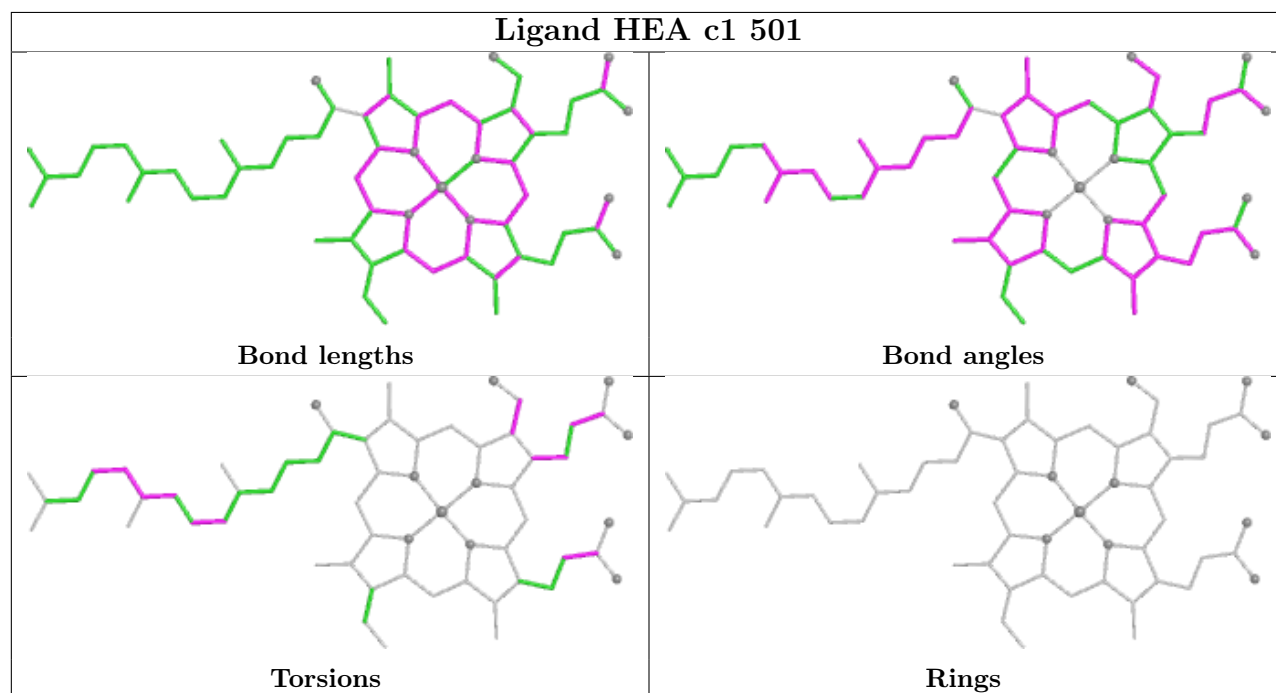
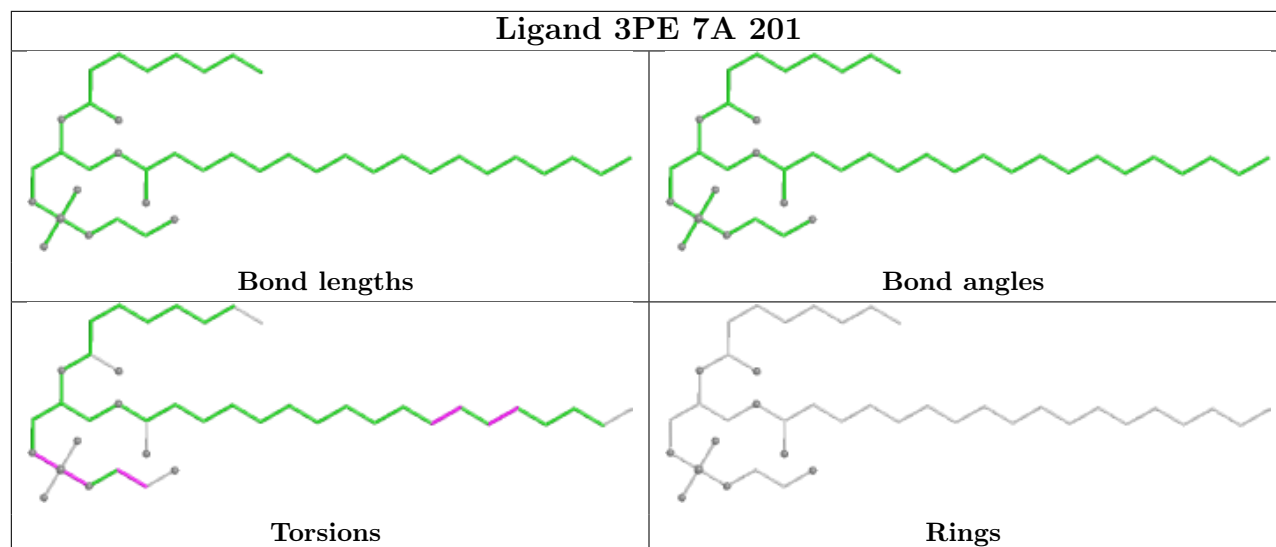
Ligand HEM QC 402

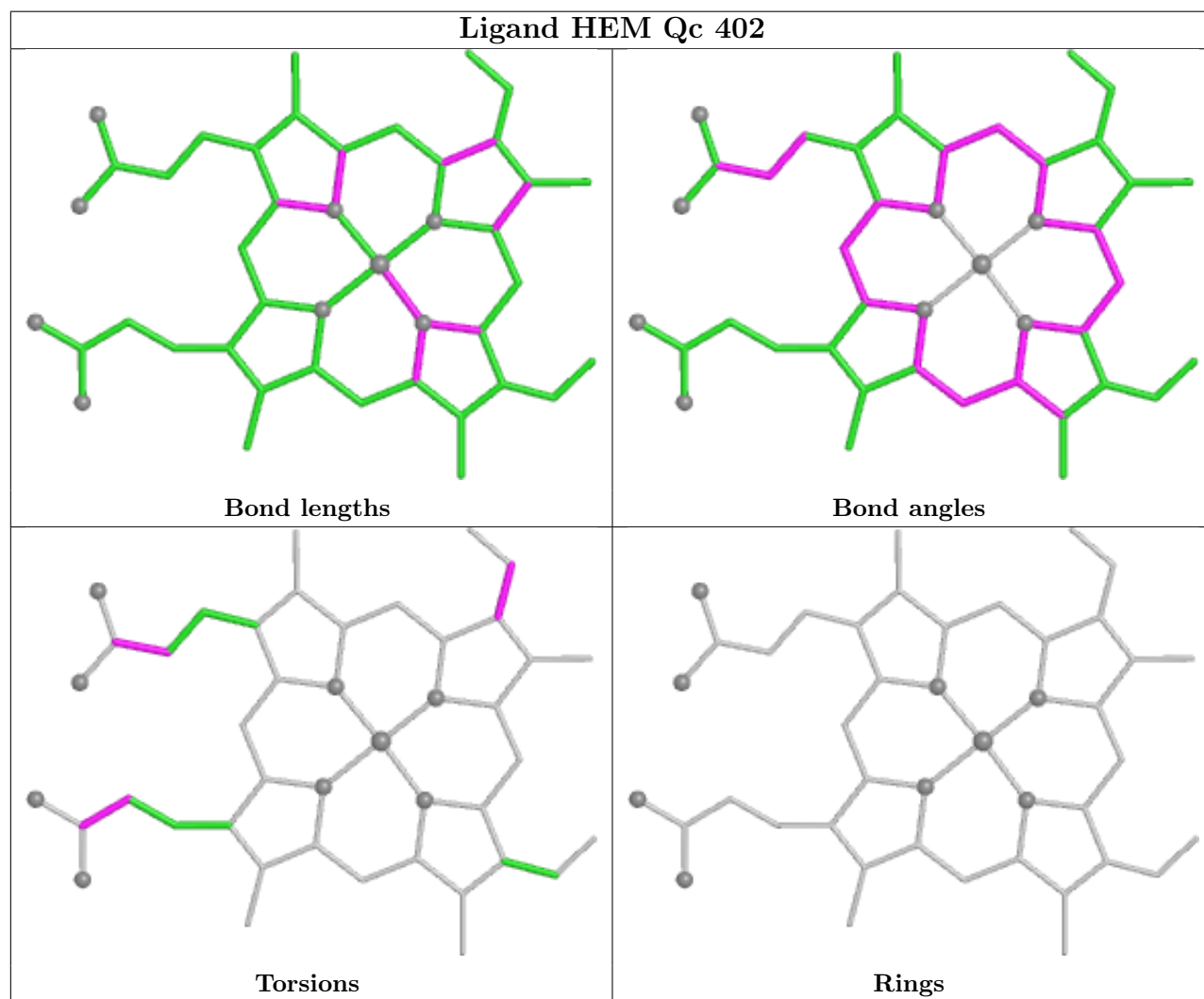
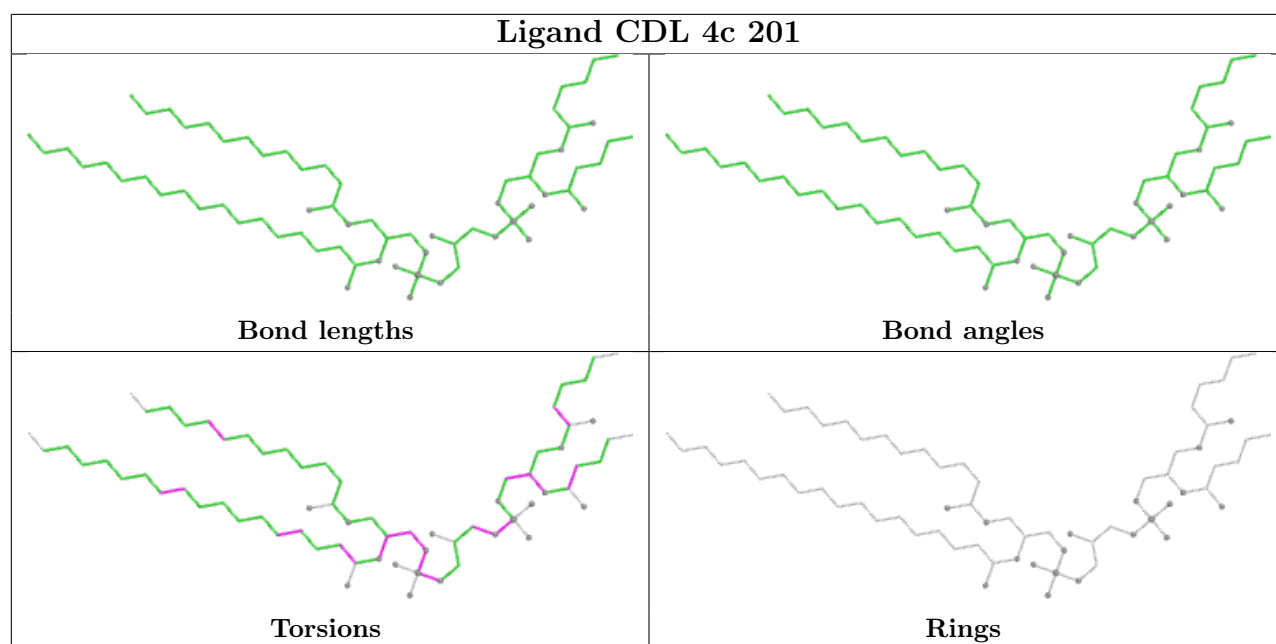


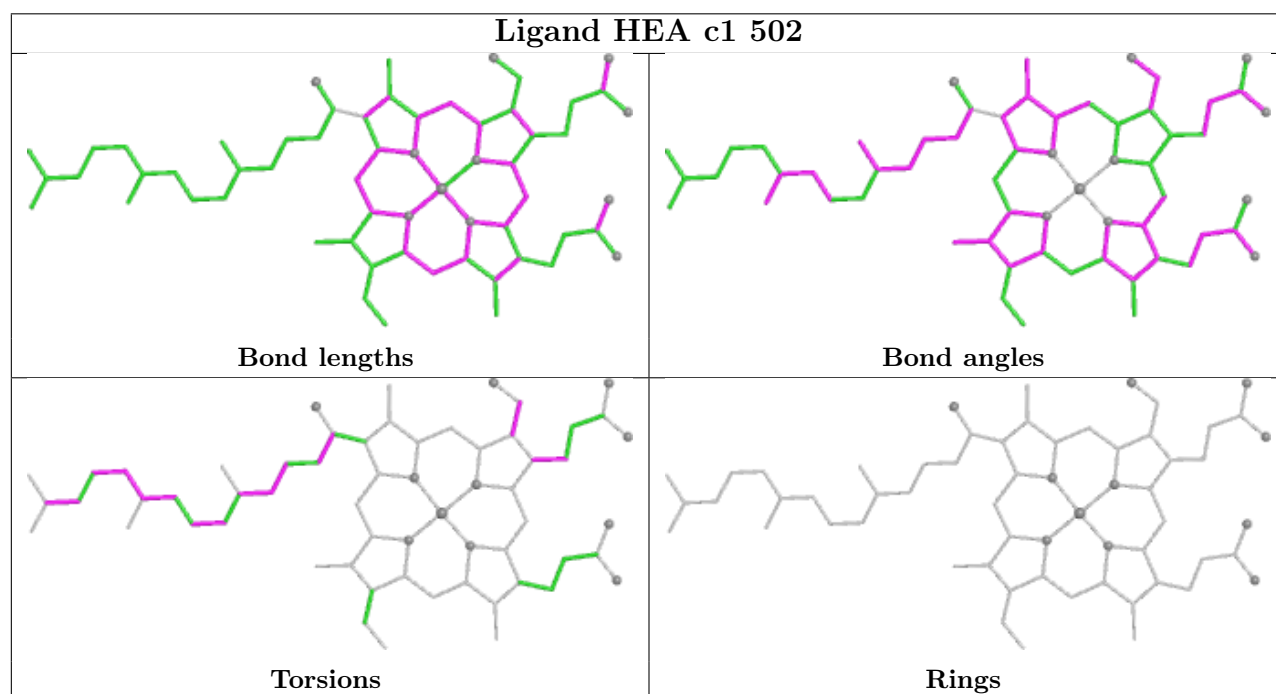
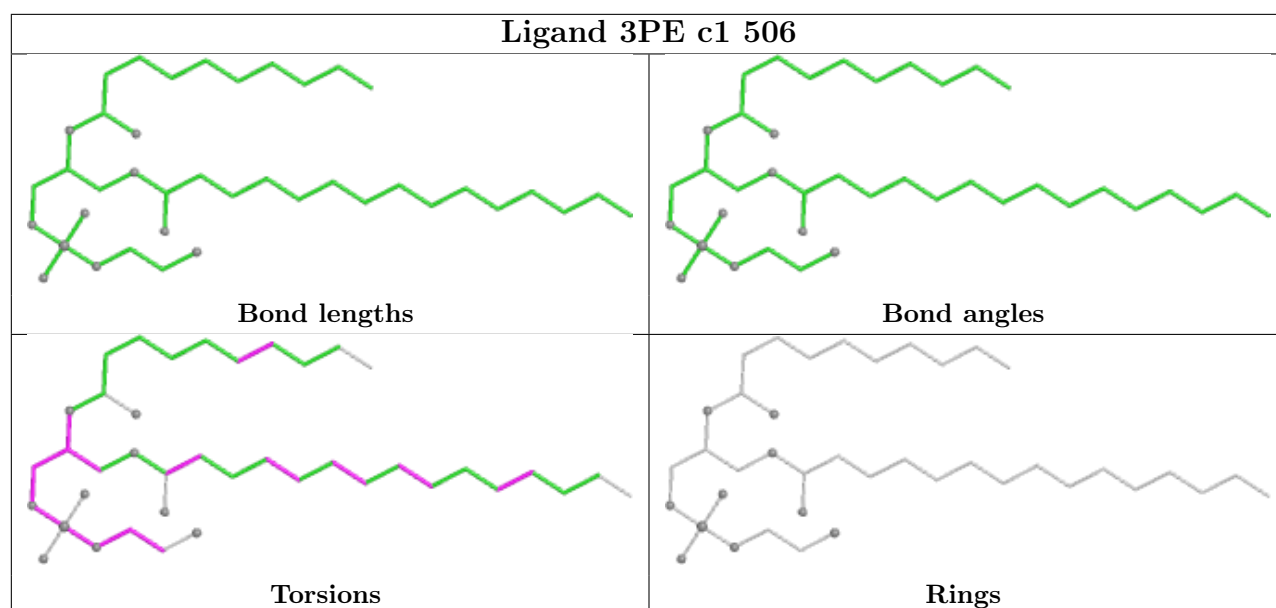
Ligand CDL QE 302

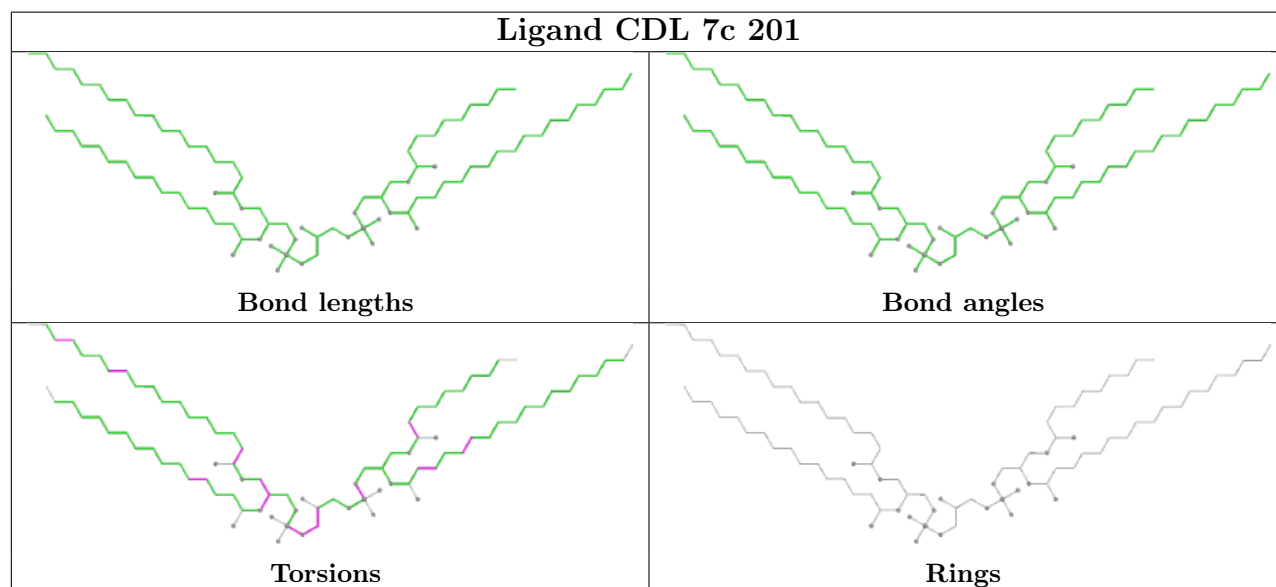
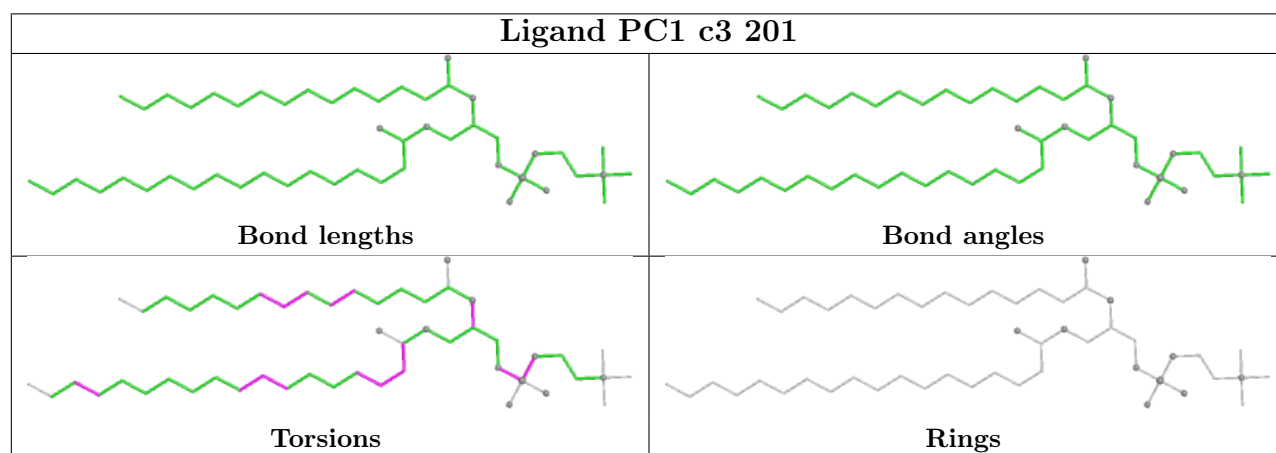
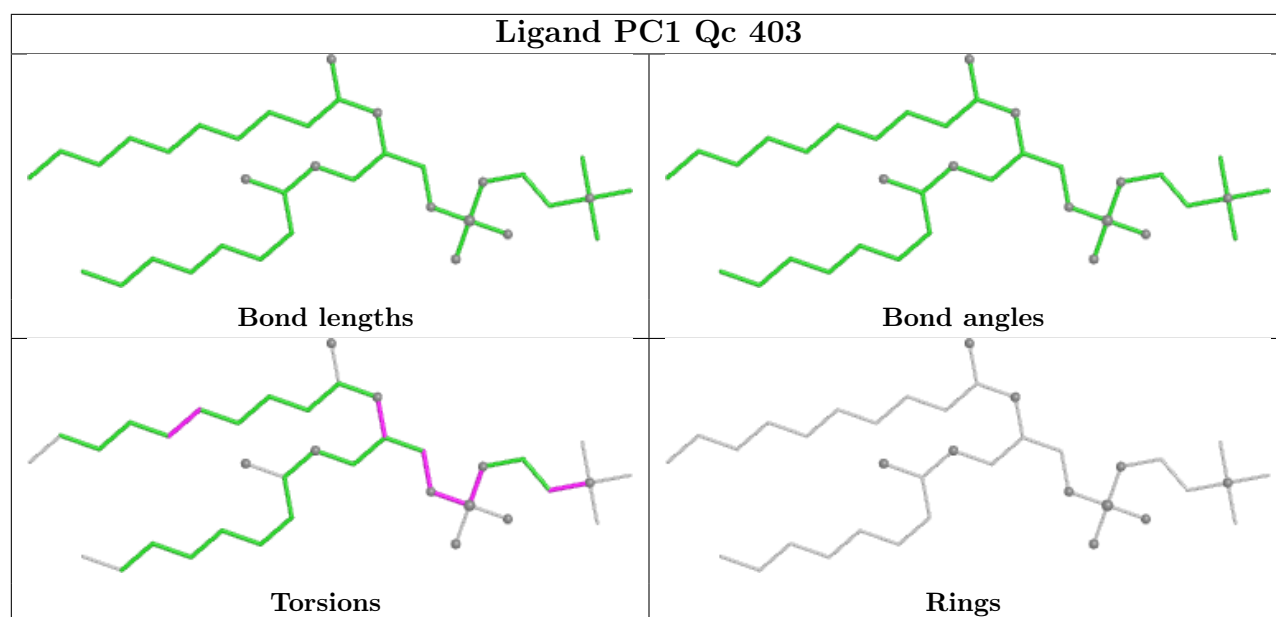


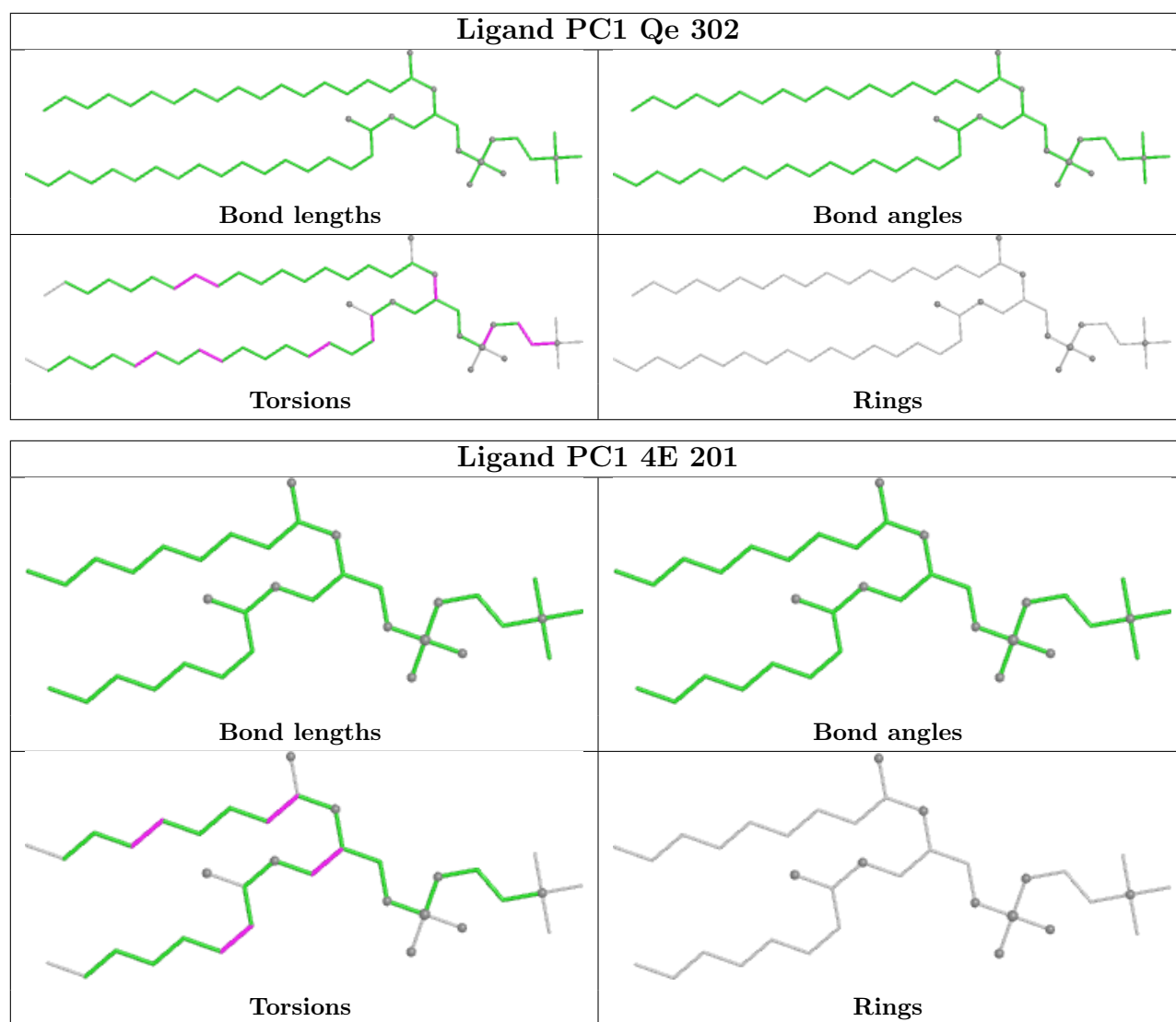


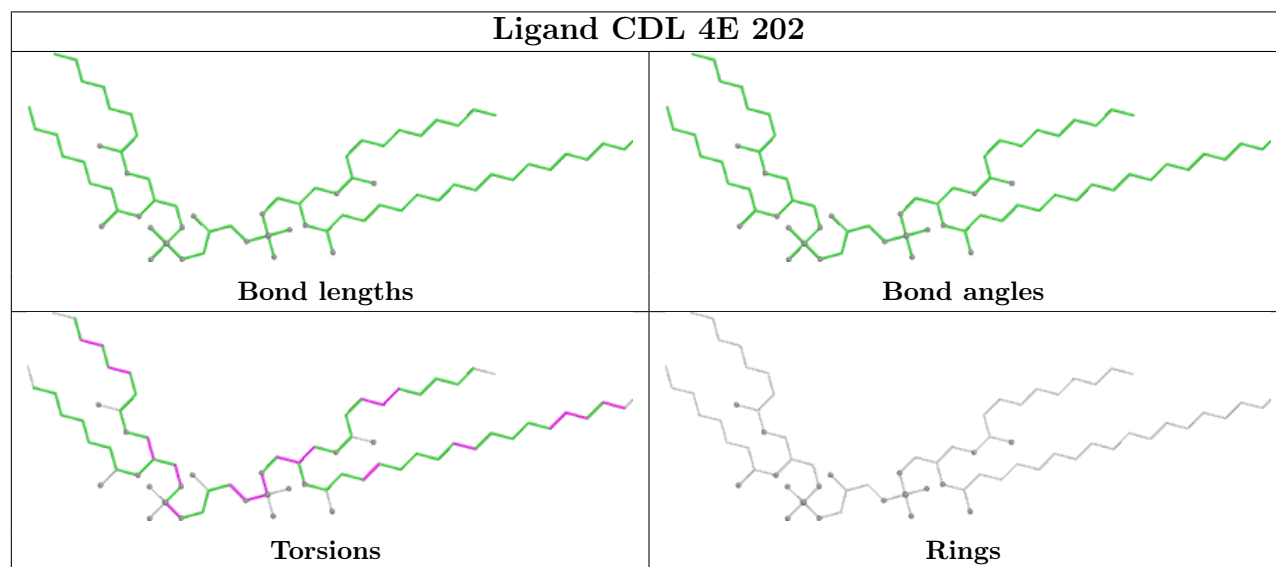
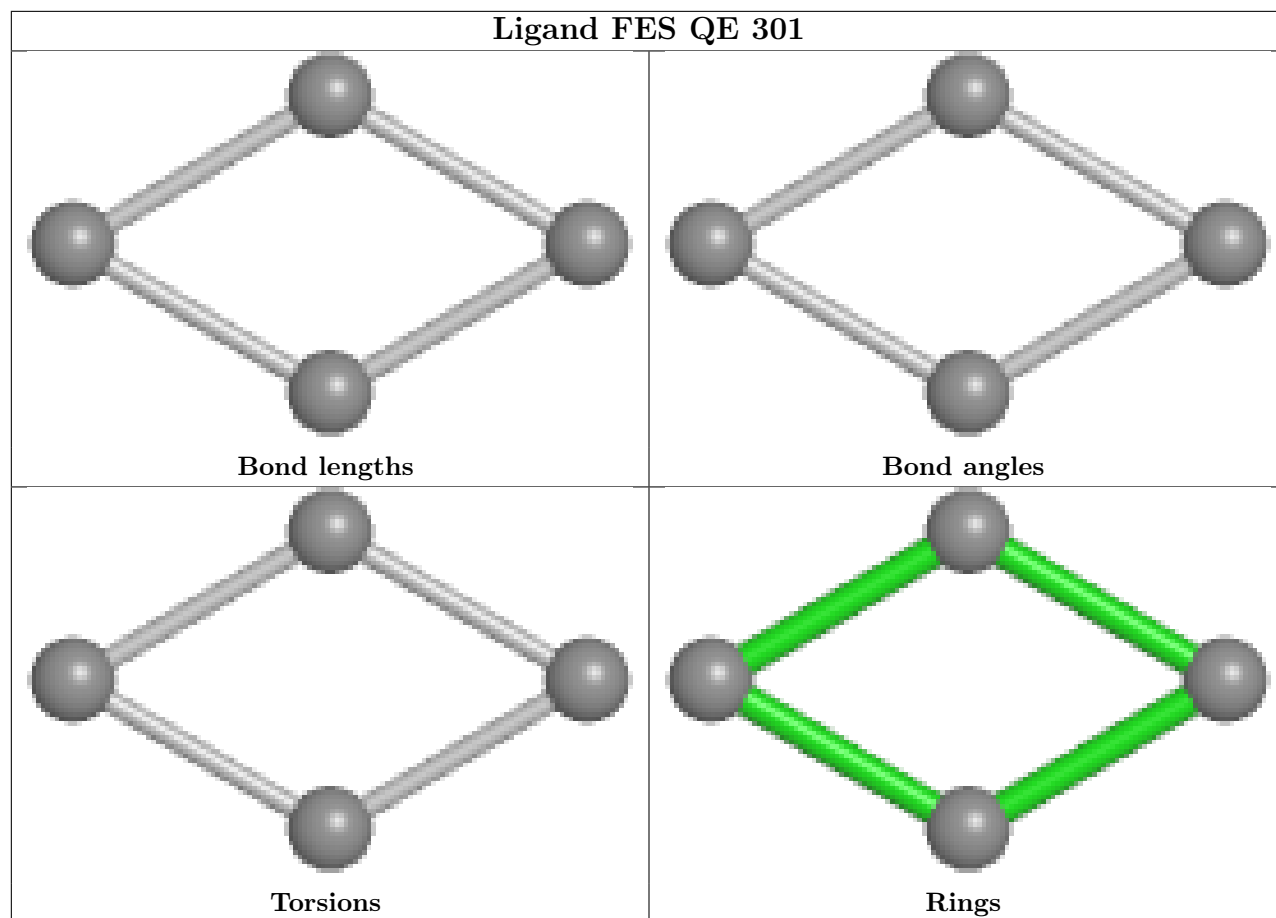


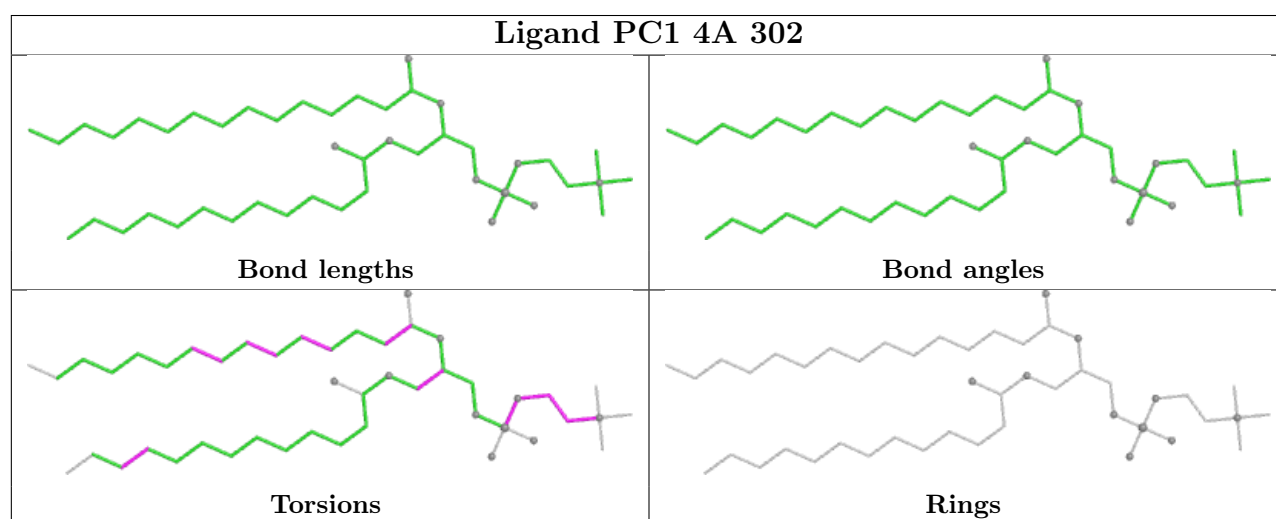
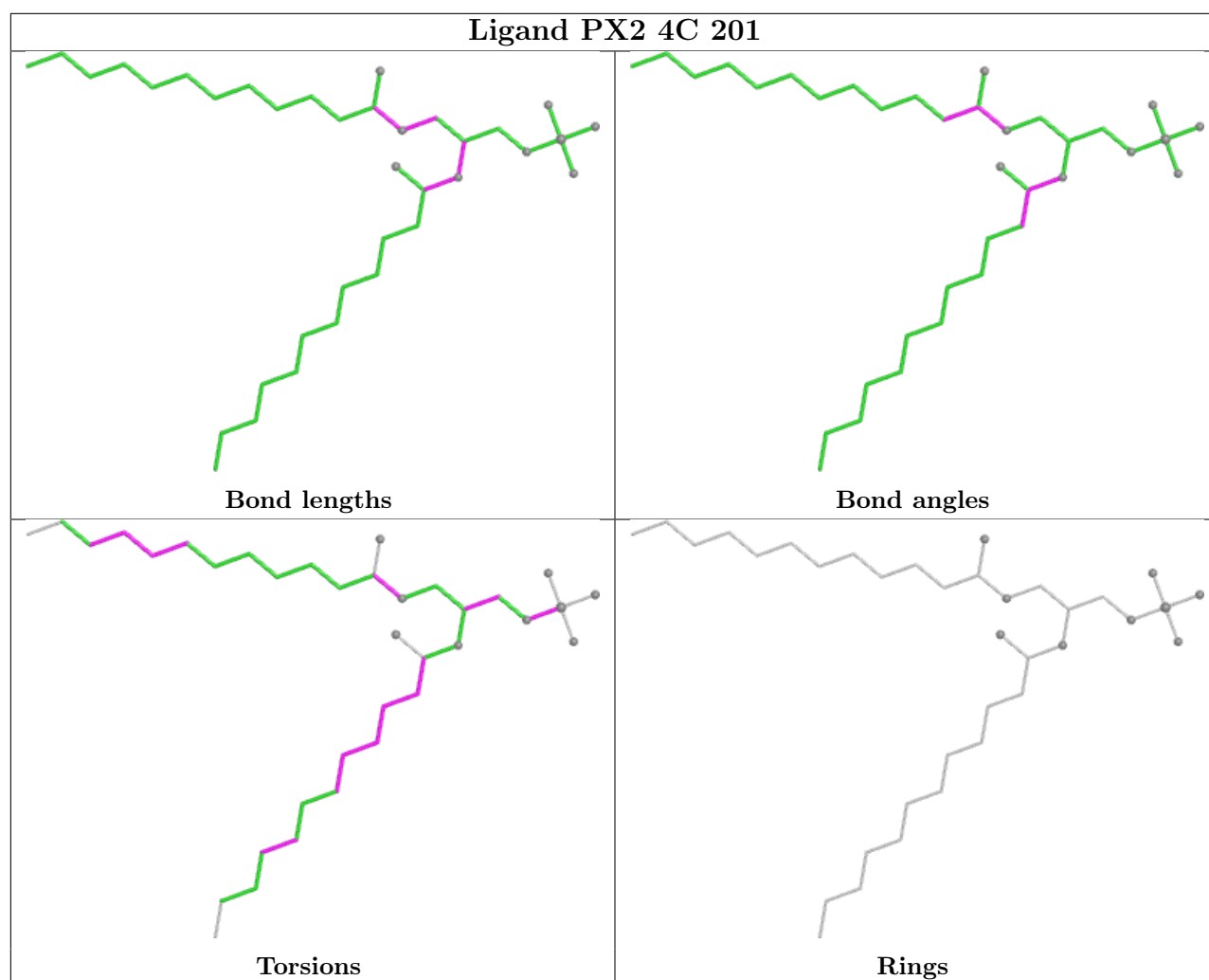


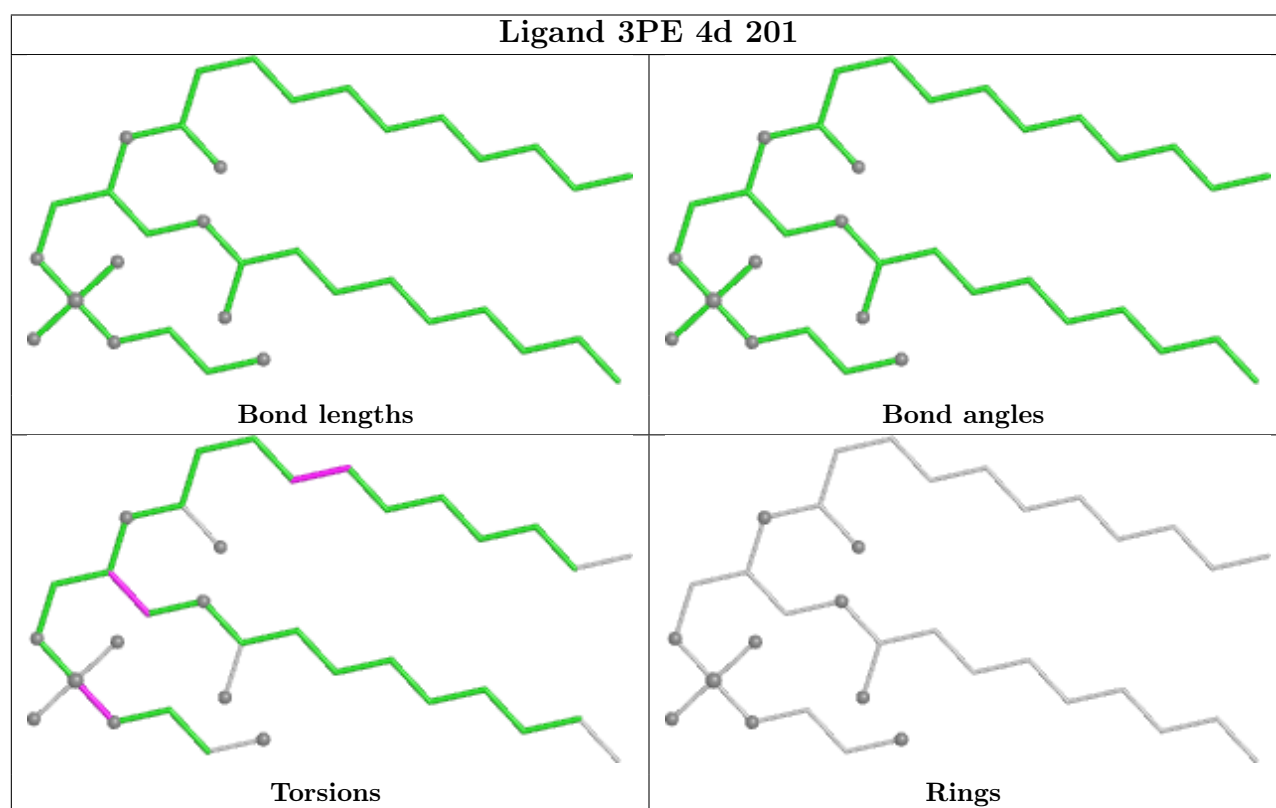
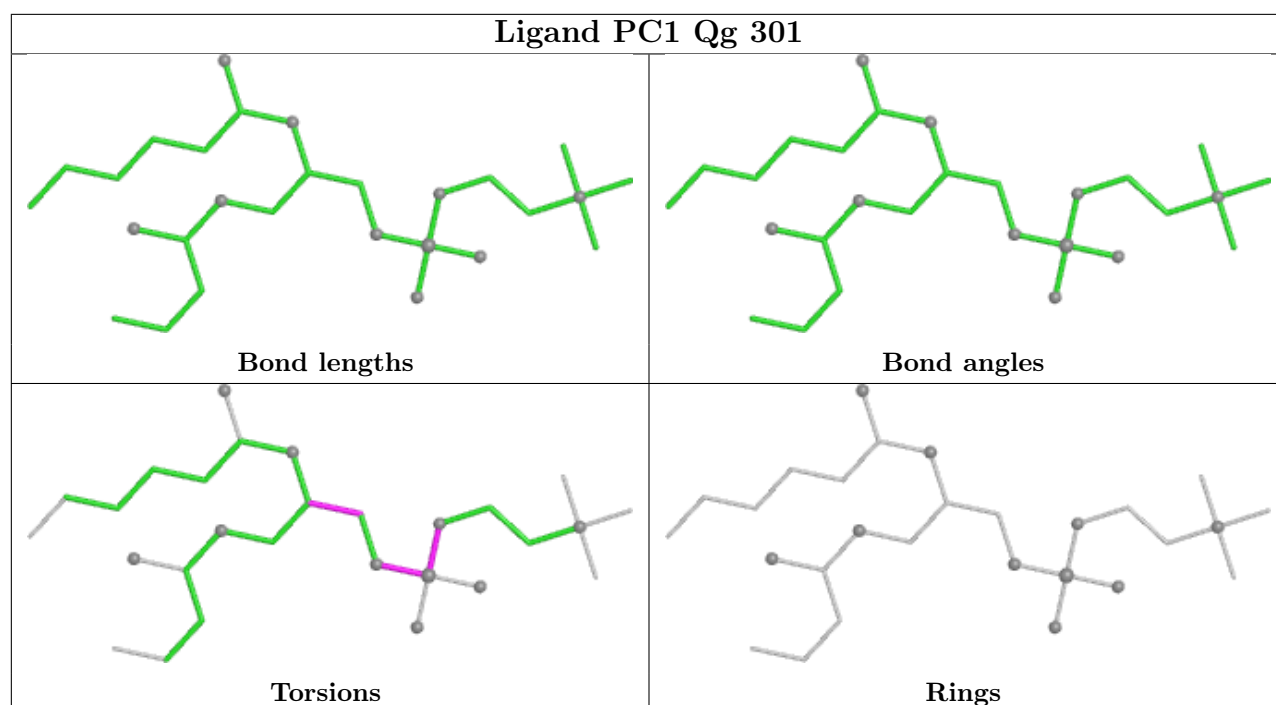


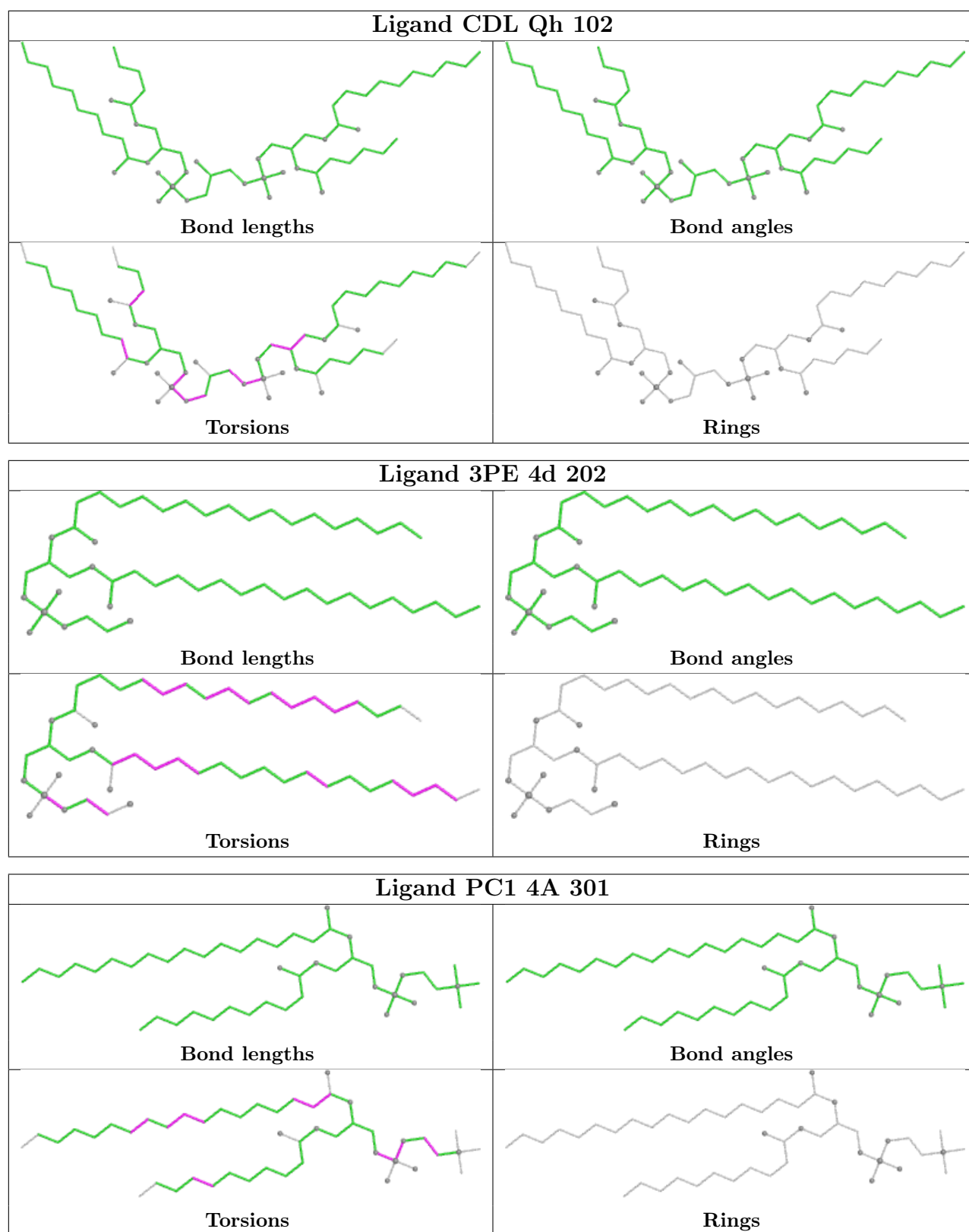


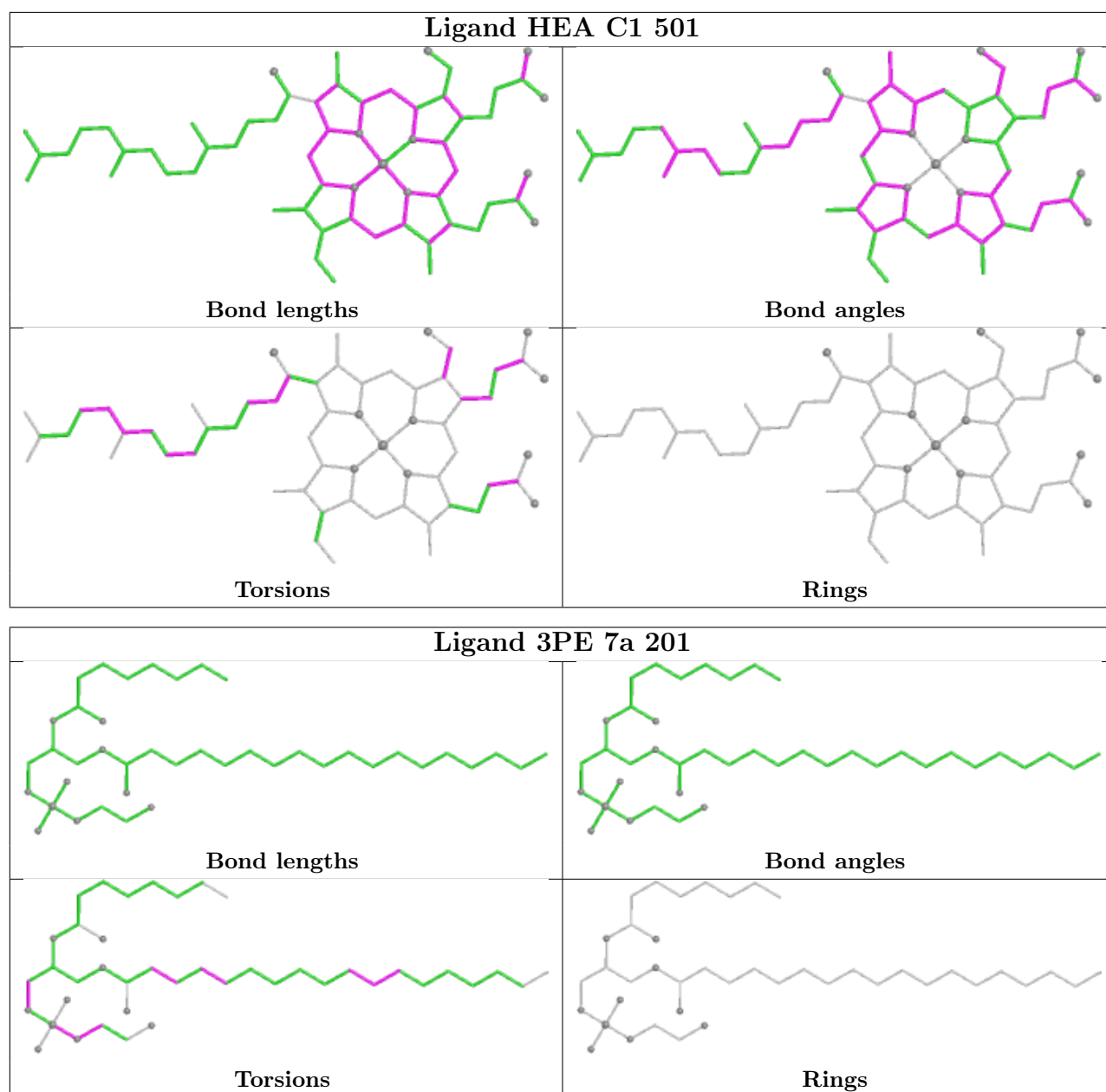


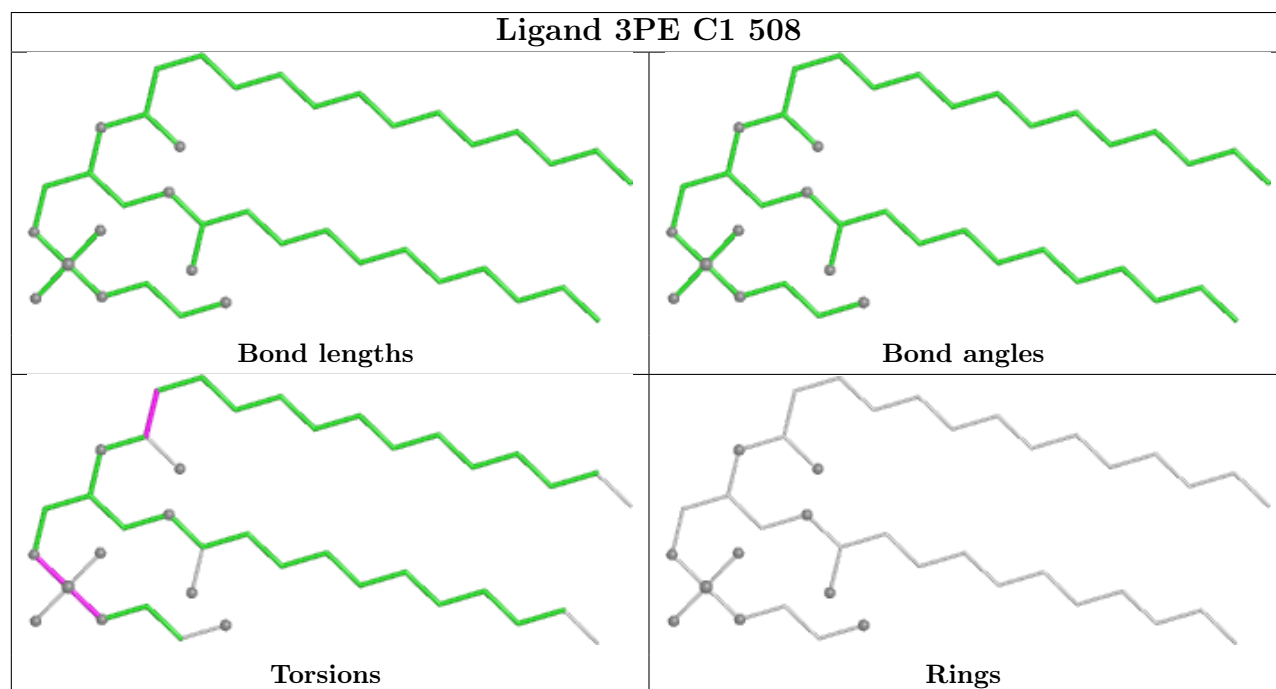
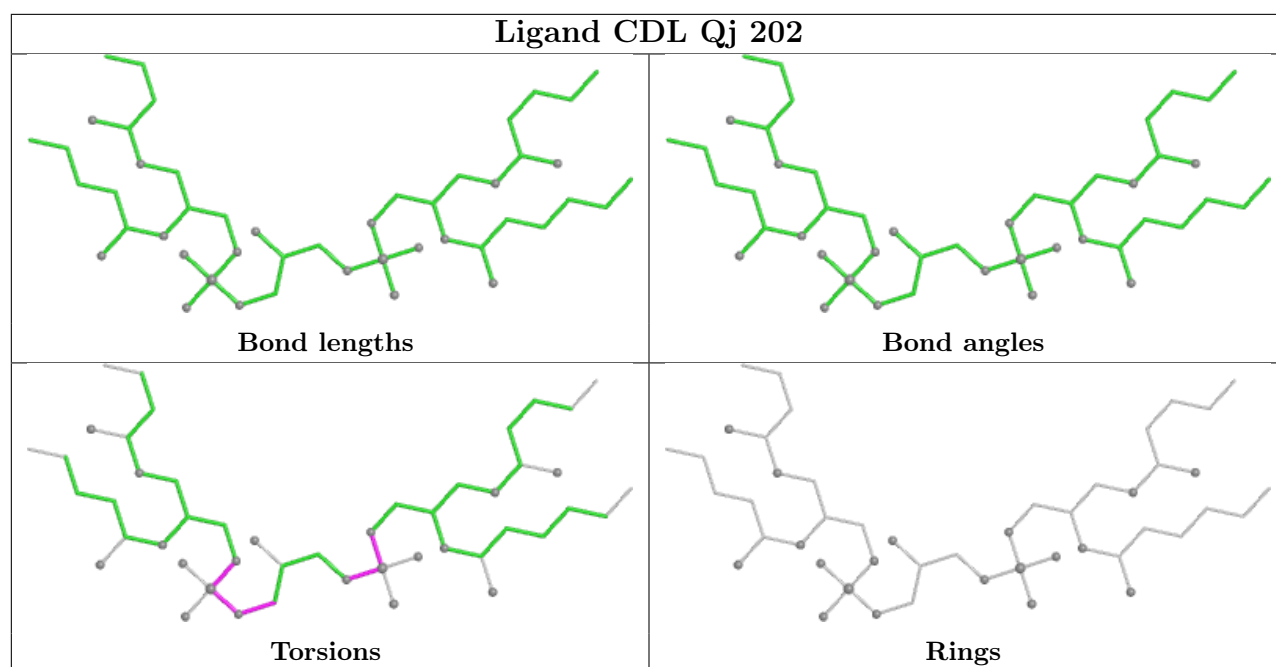


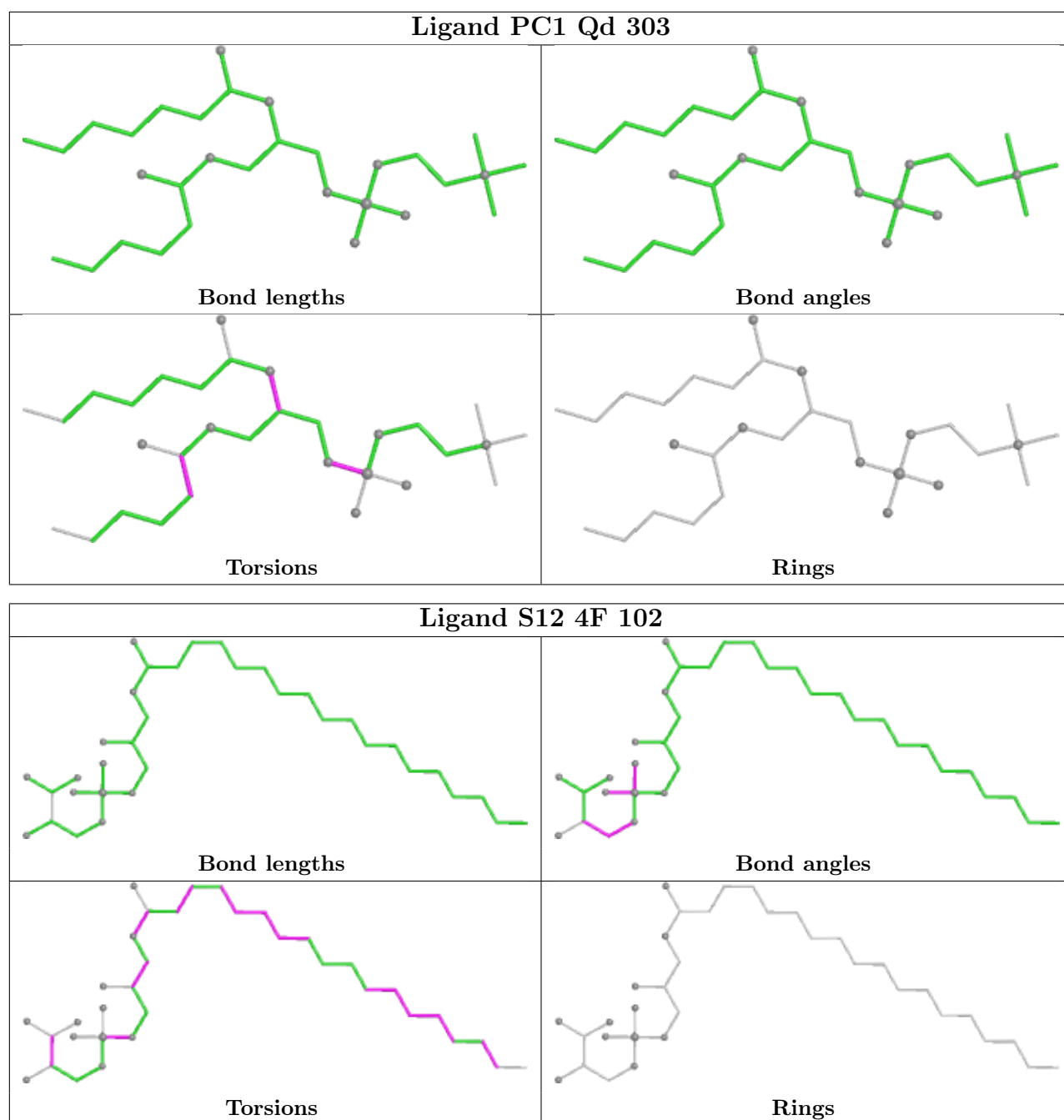


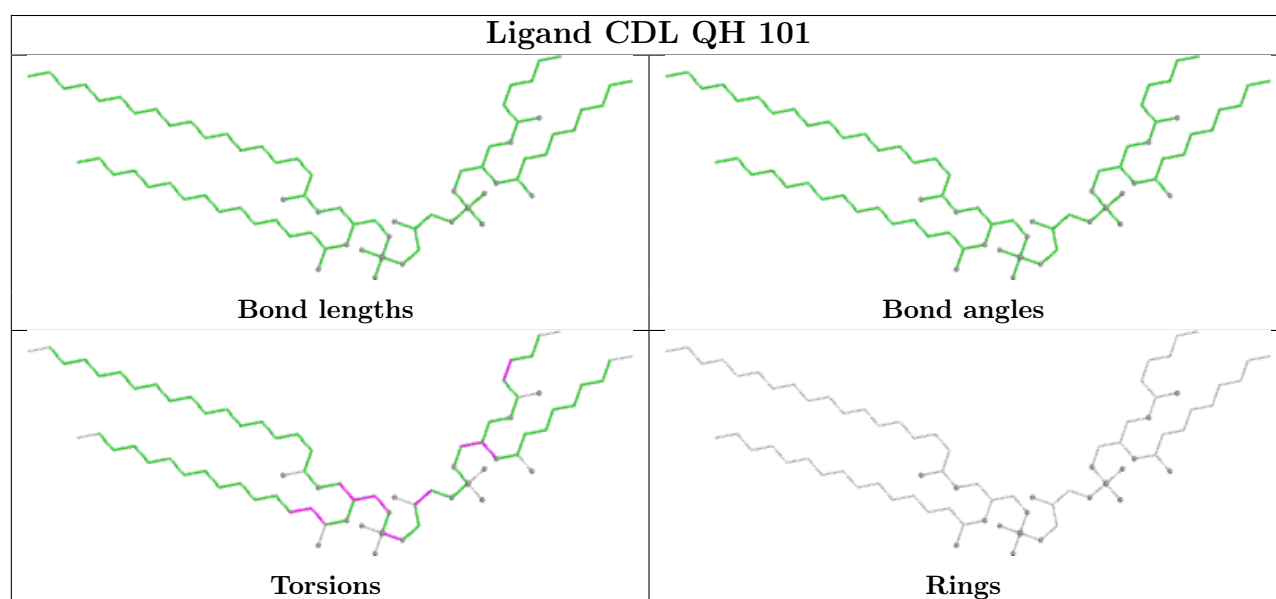
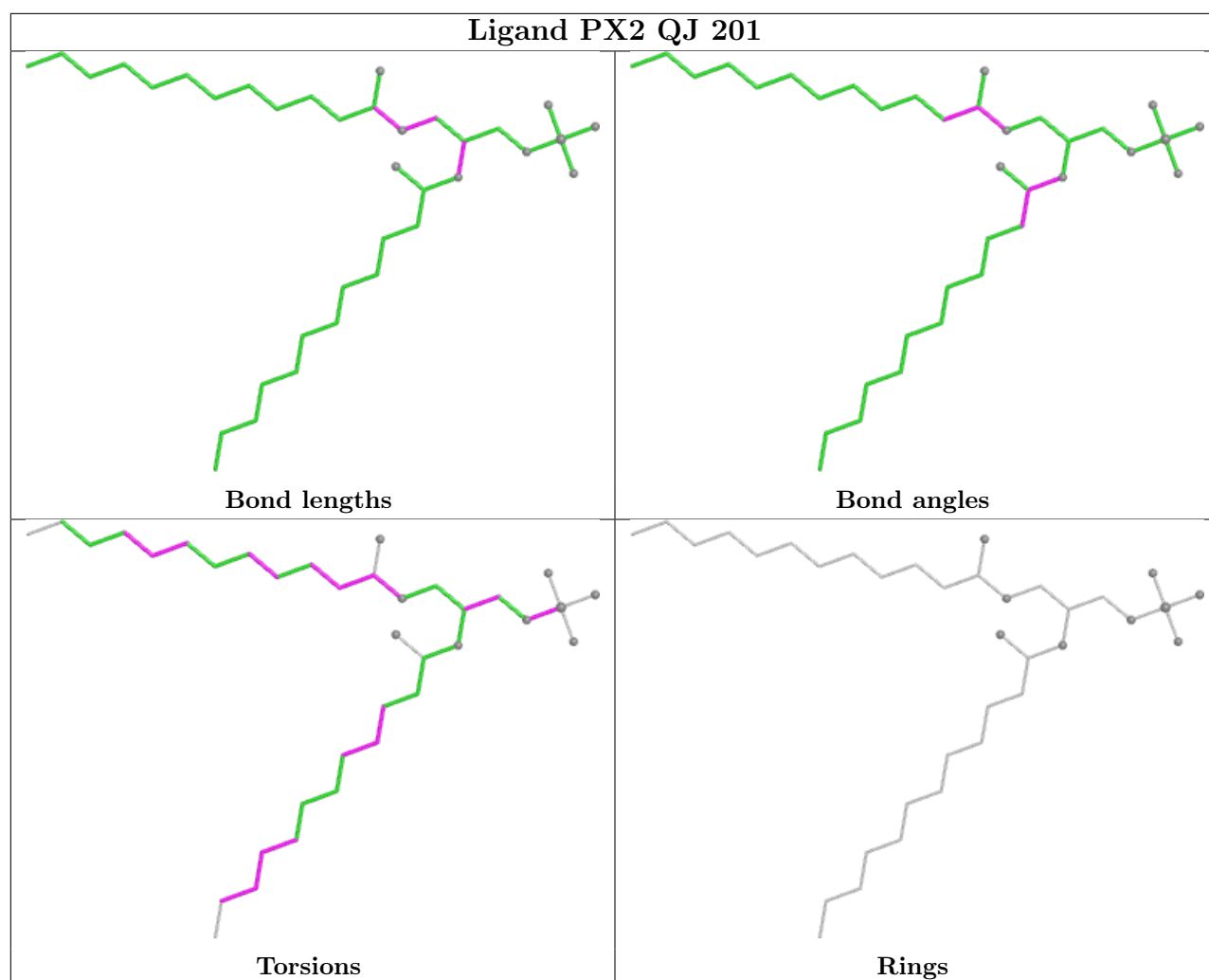


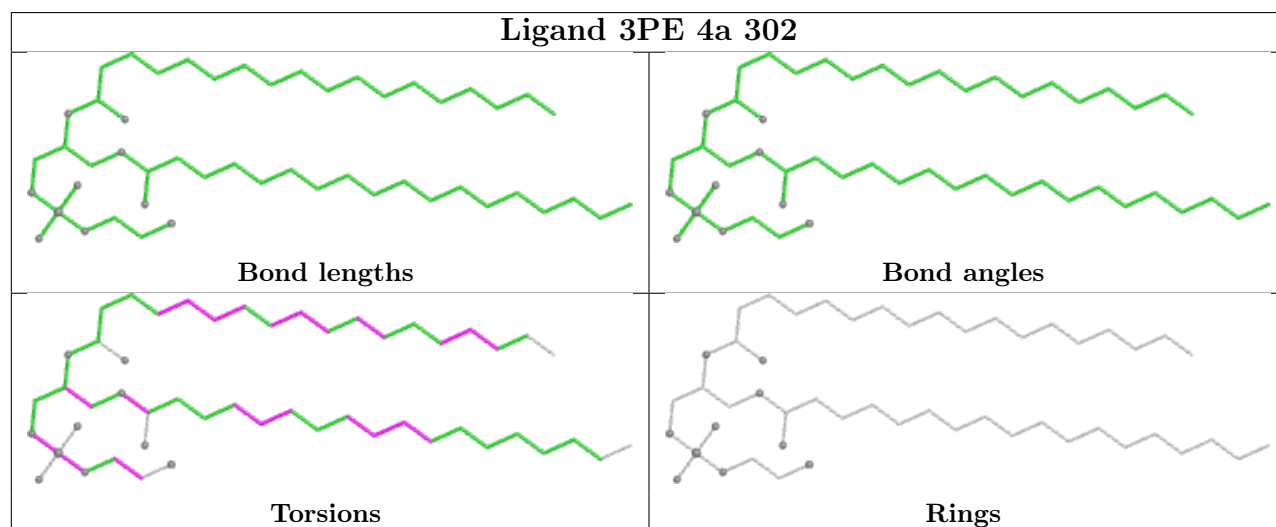
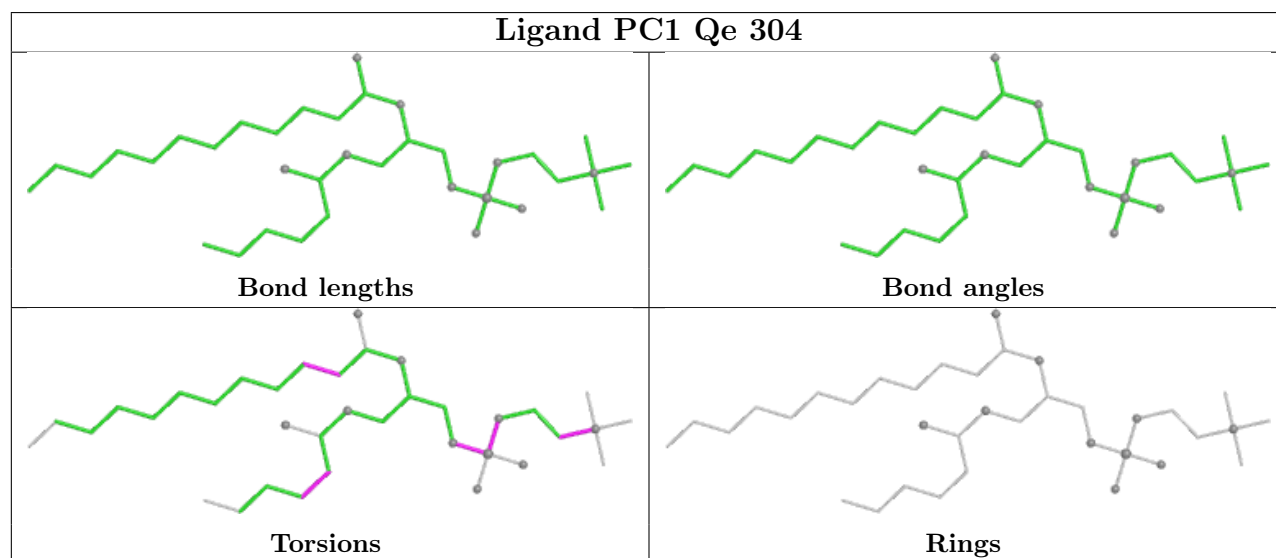
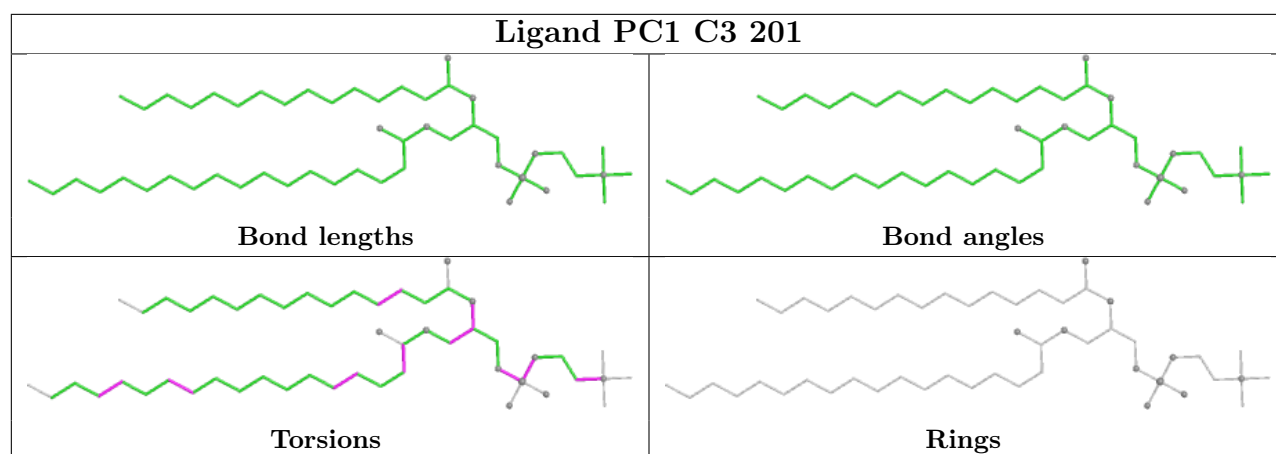


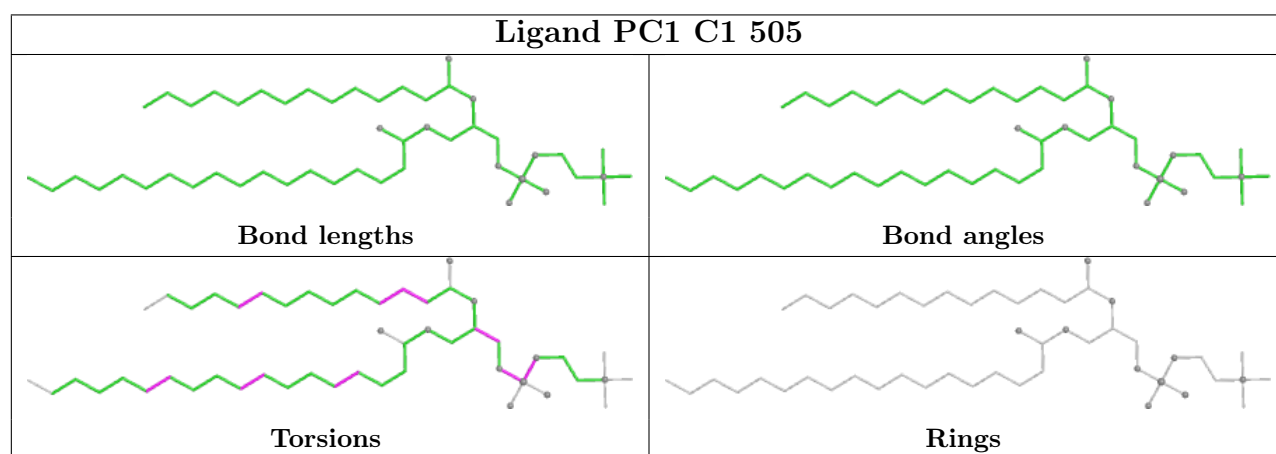
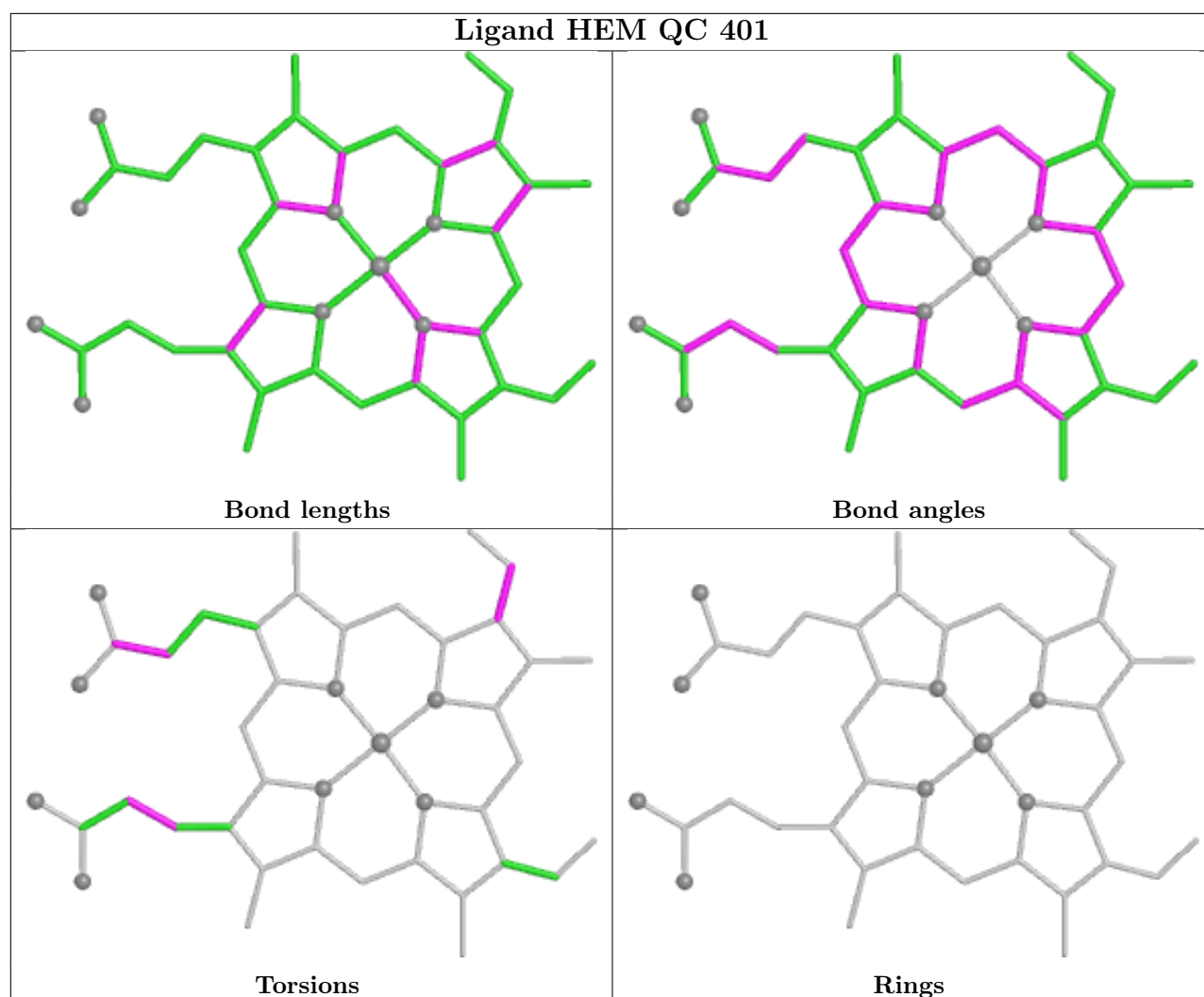


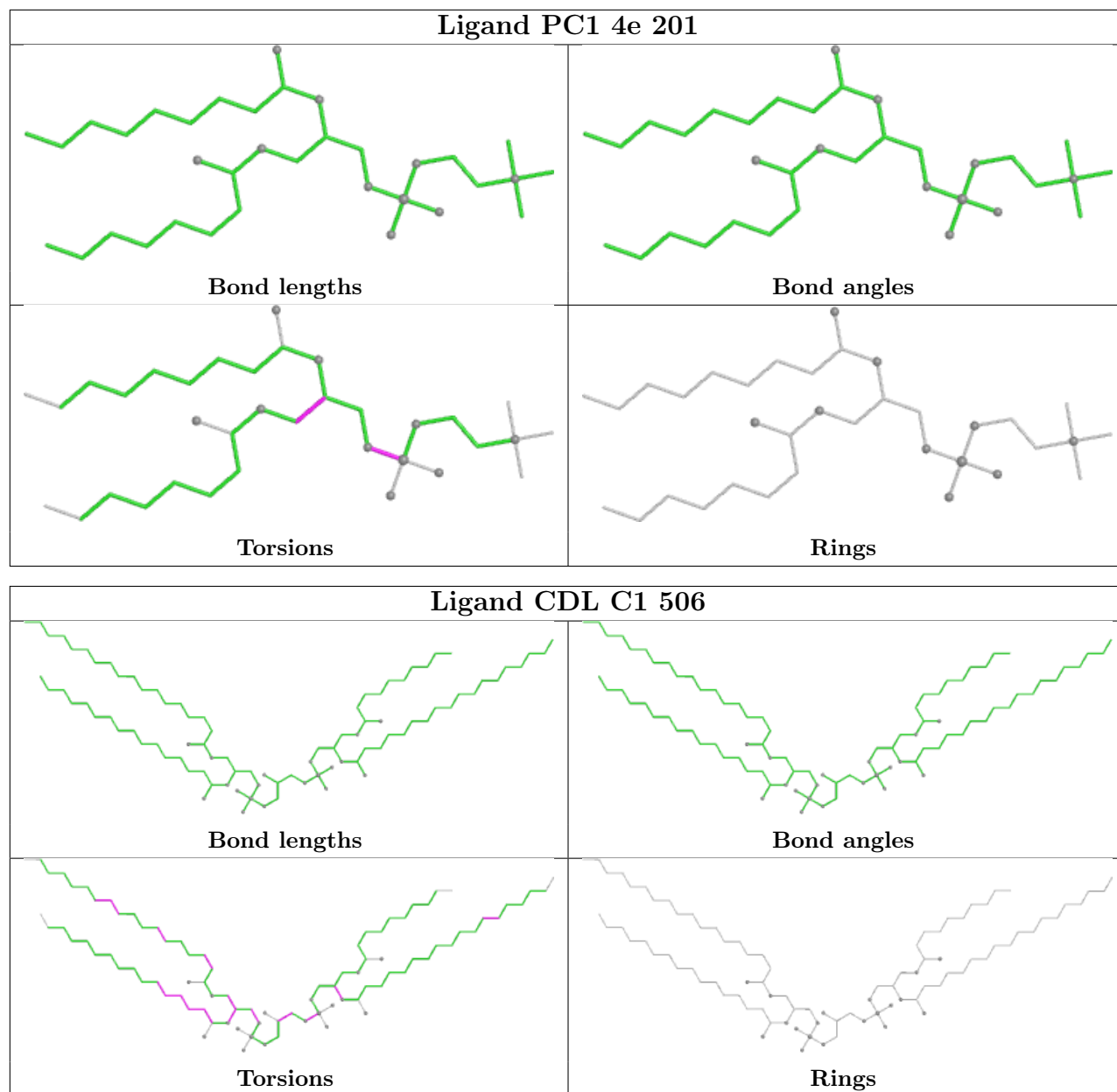


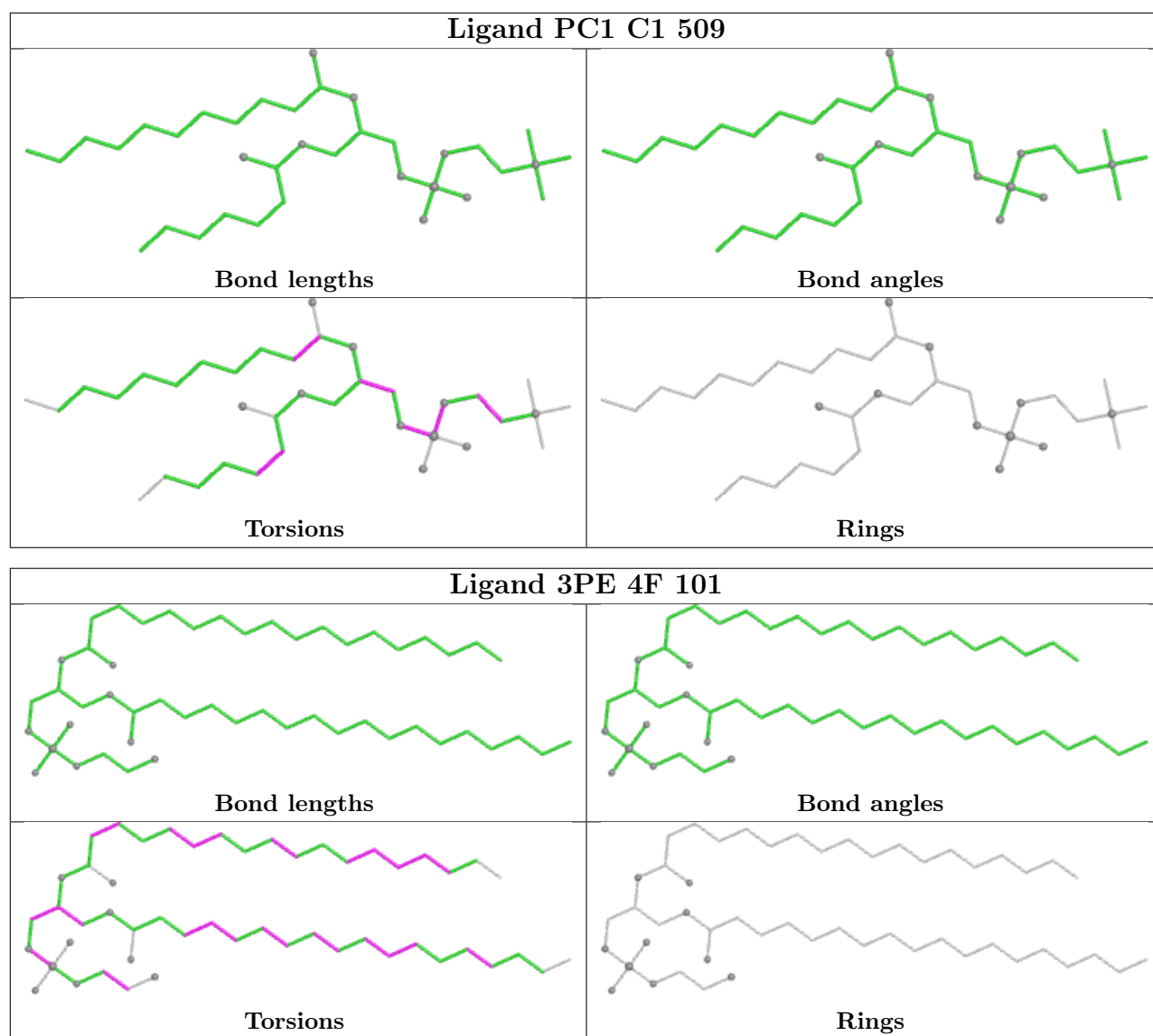




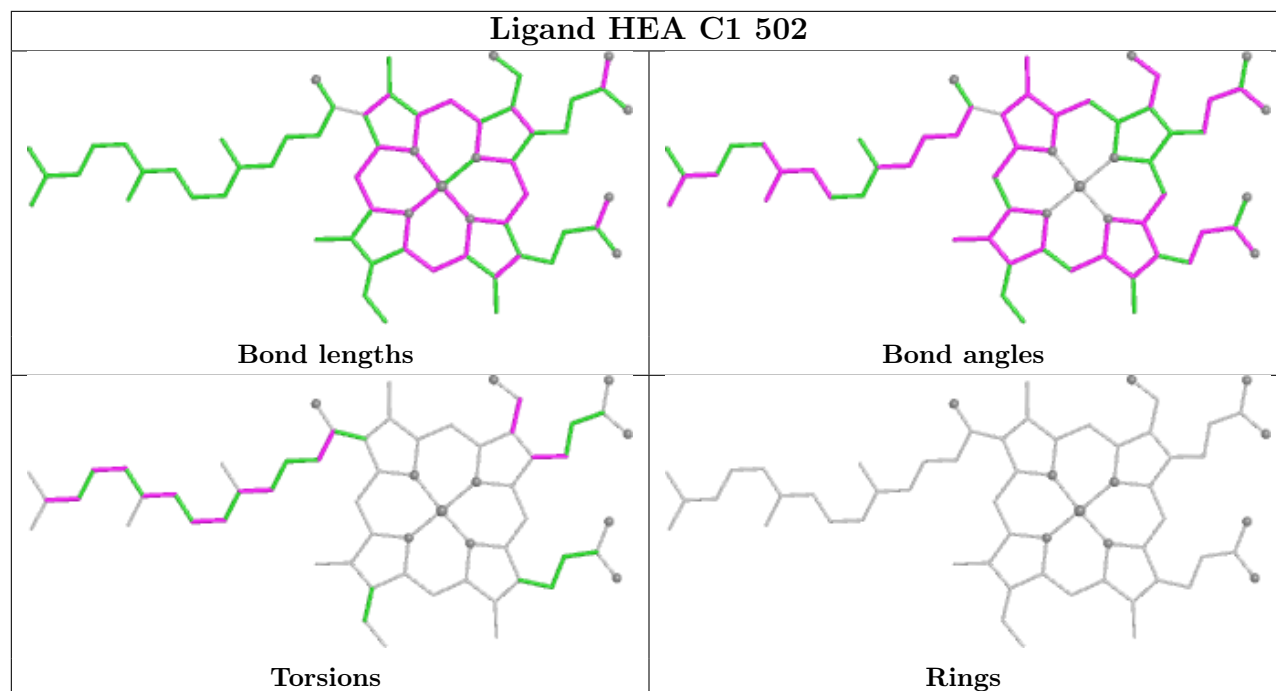




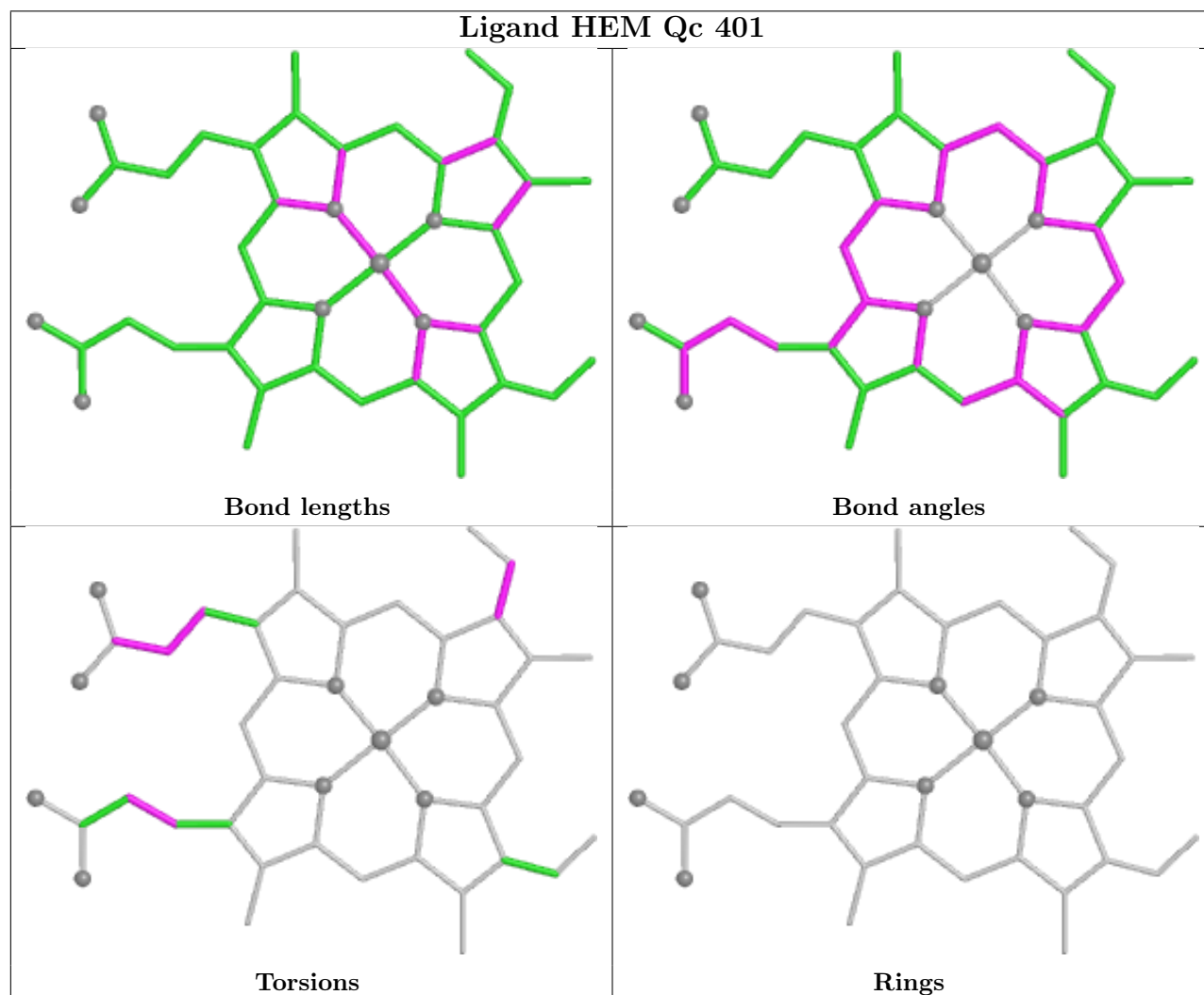


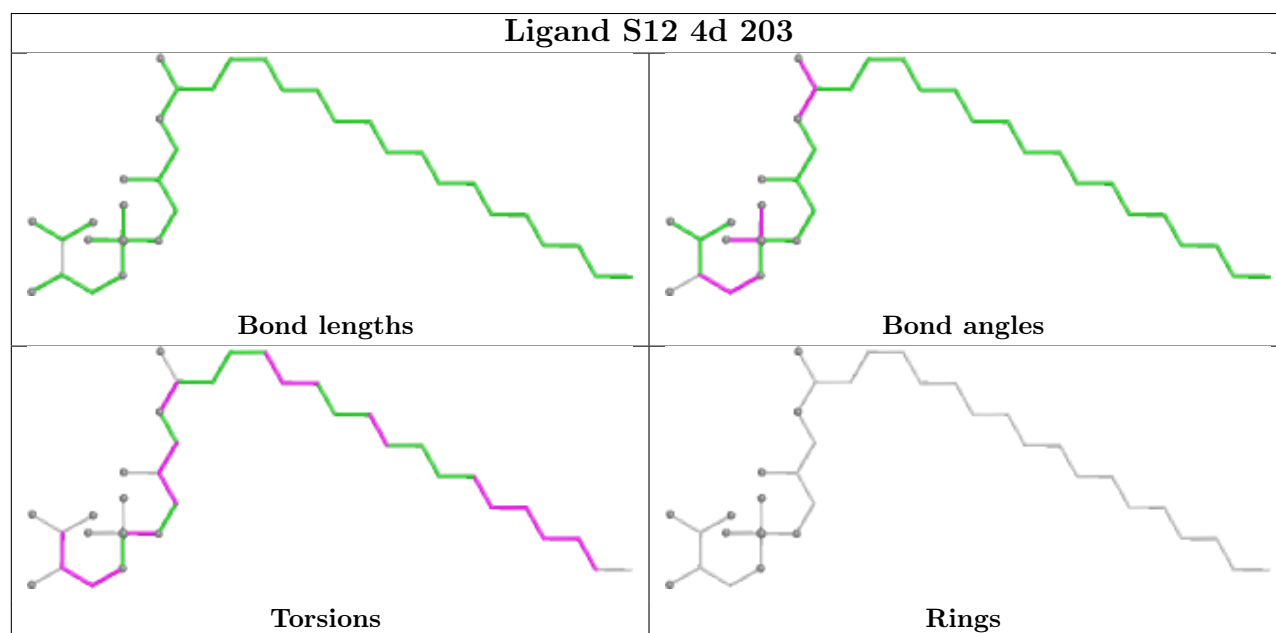
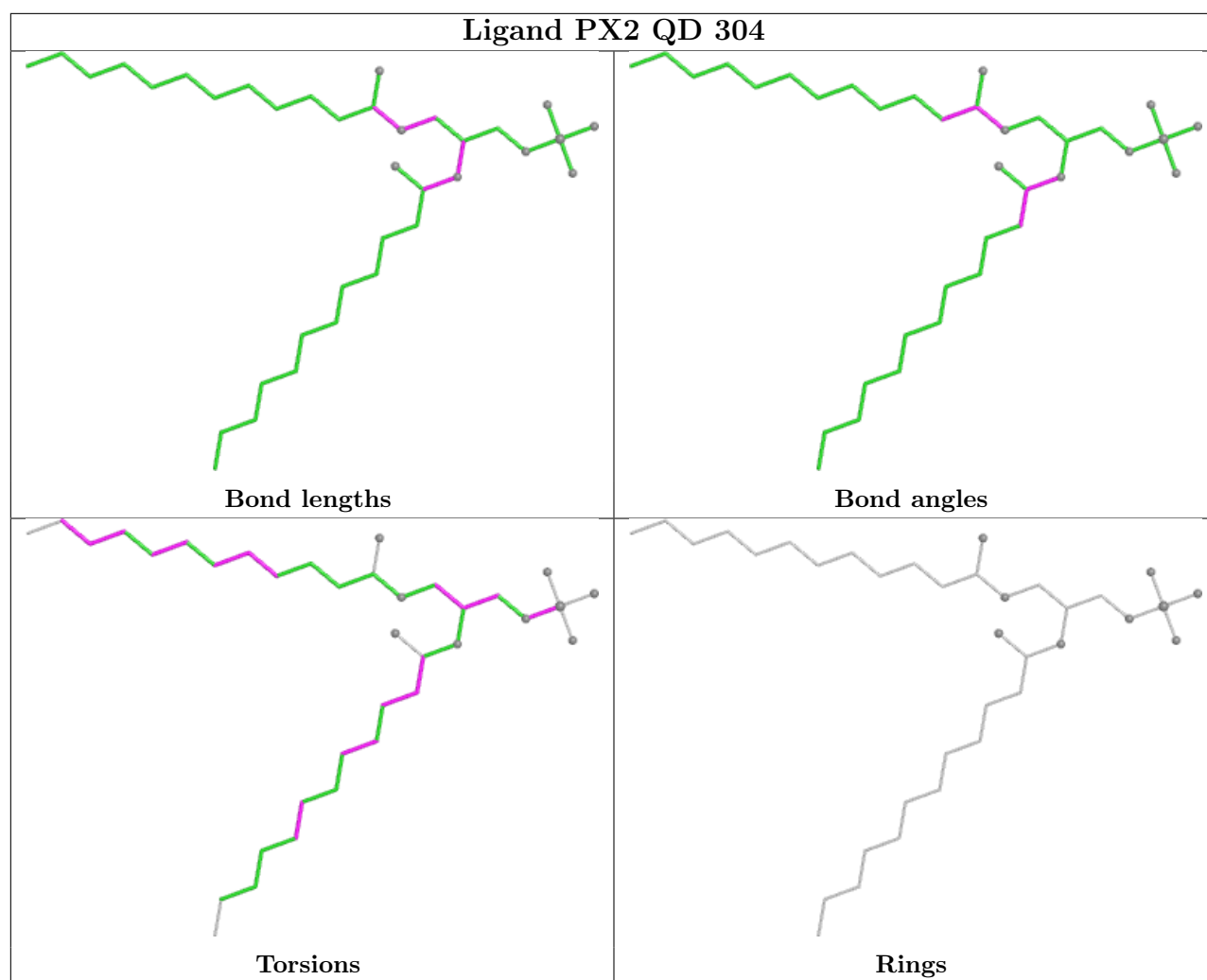


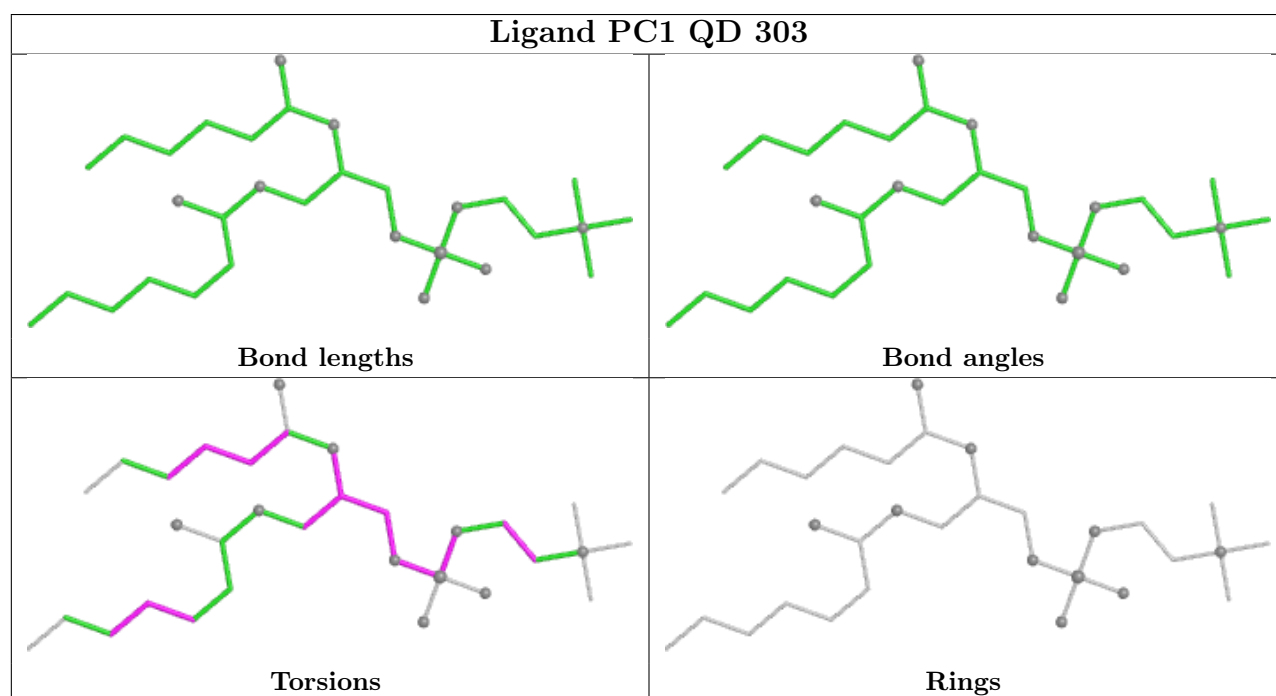
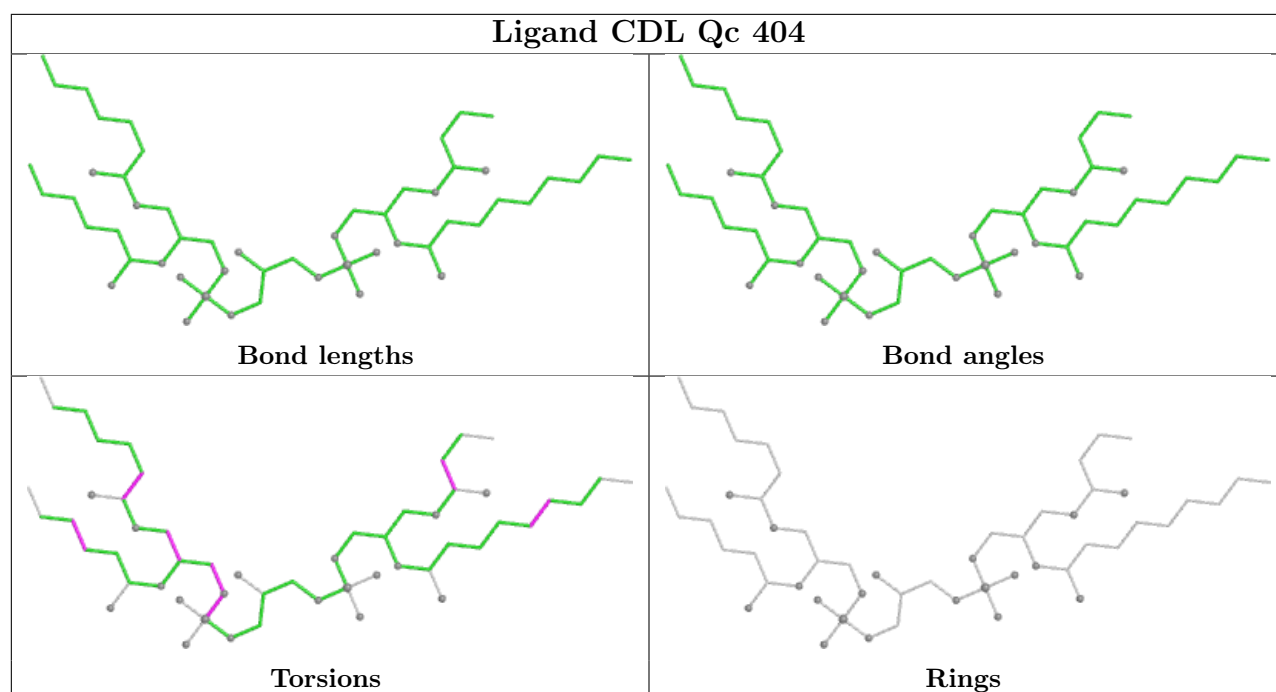
Ligand HEA C1 502

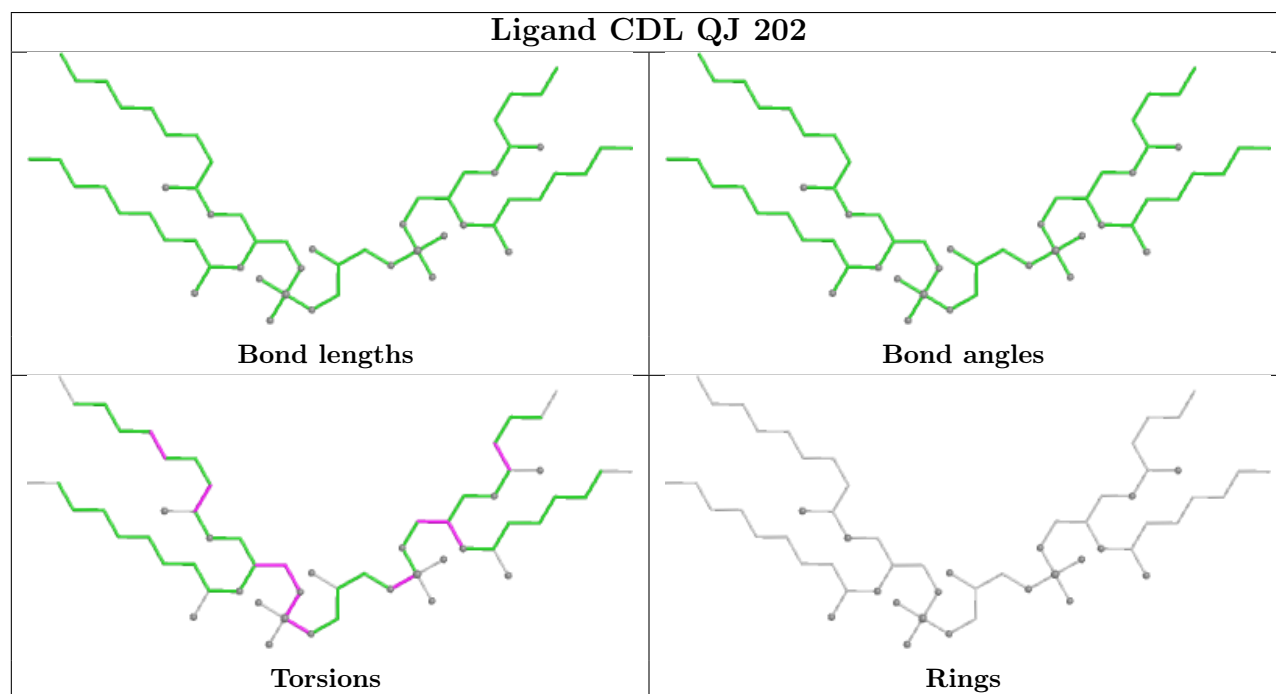
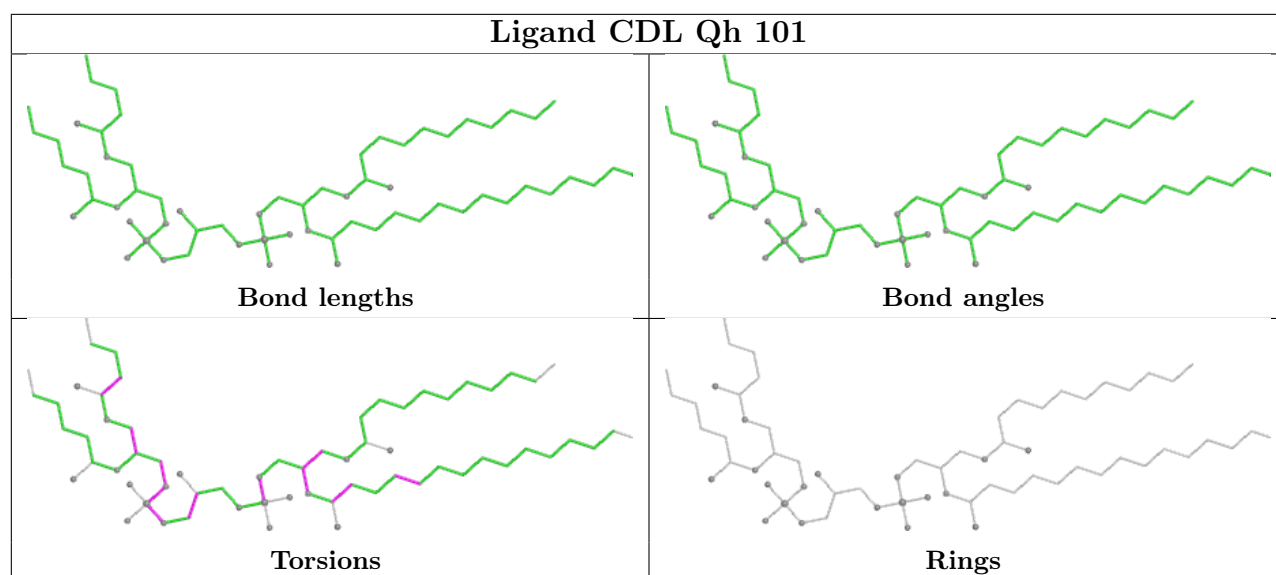


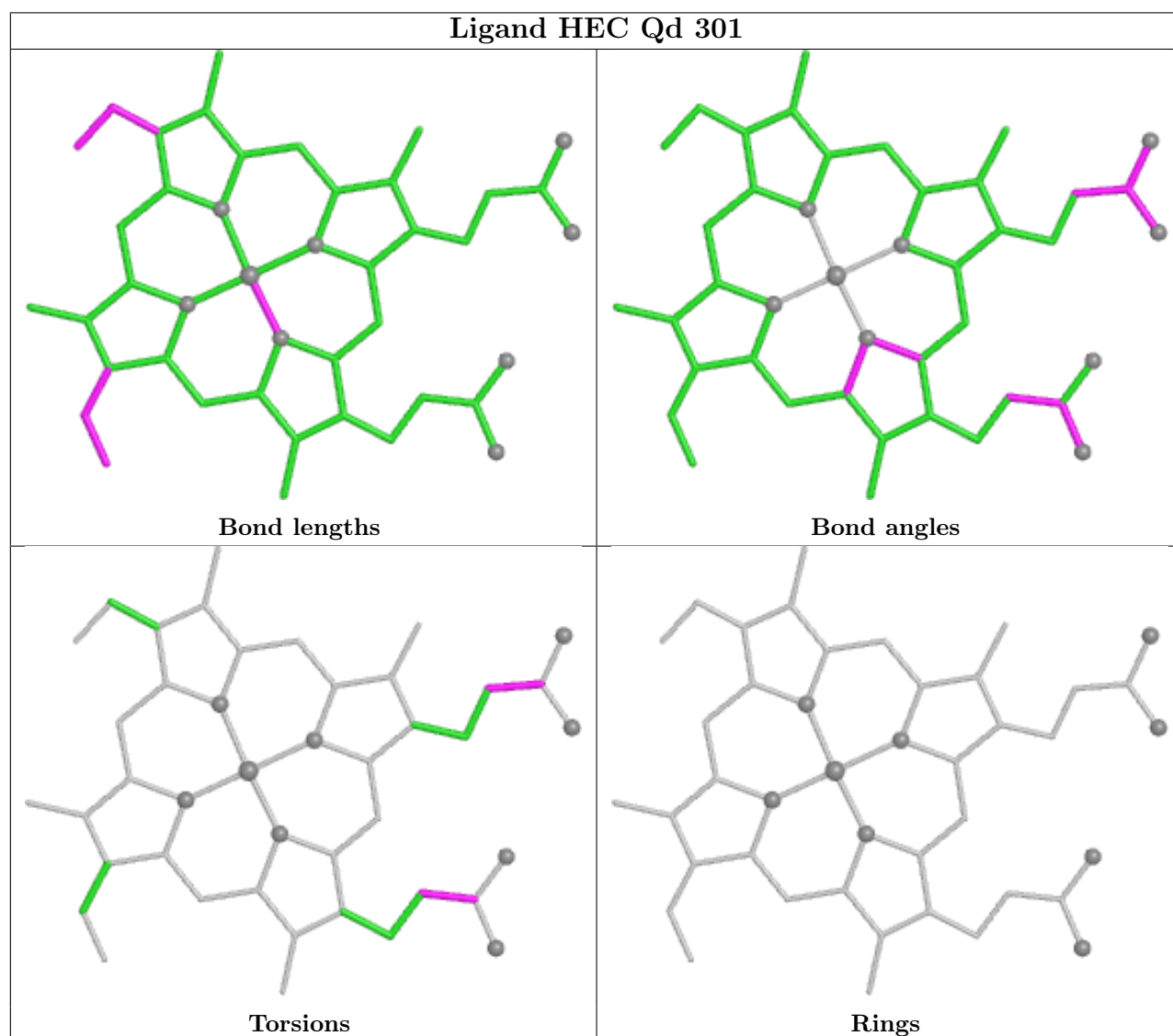
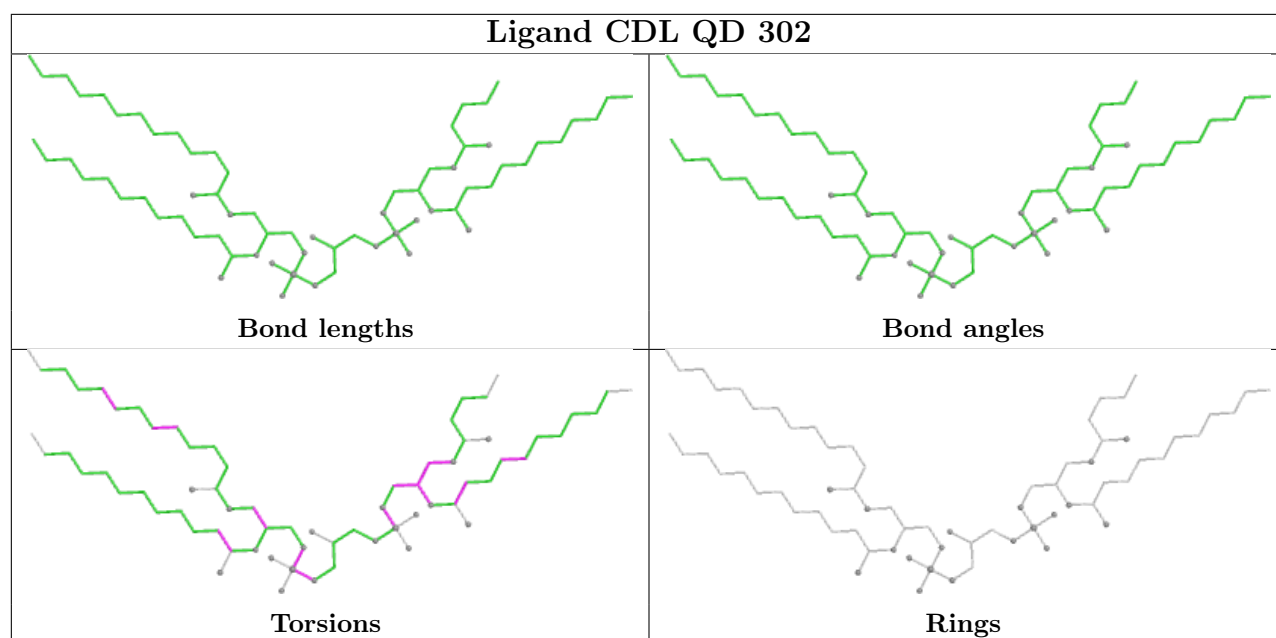
Ligand HEM Qc 401

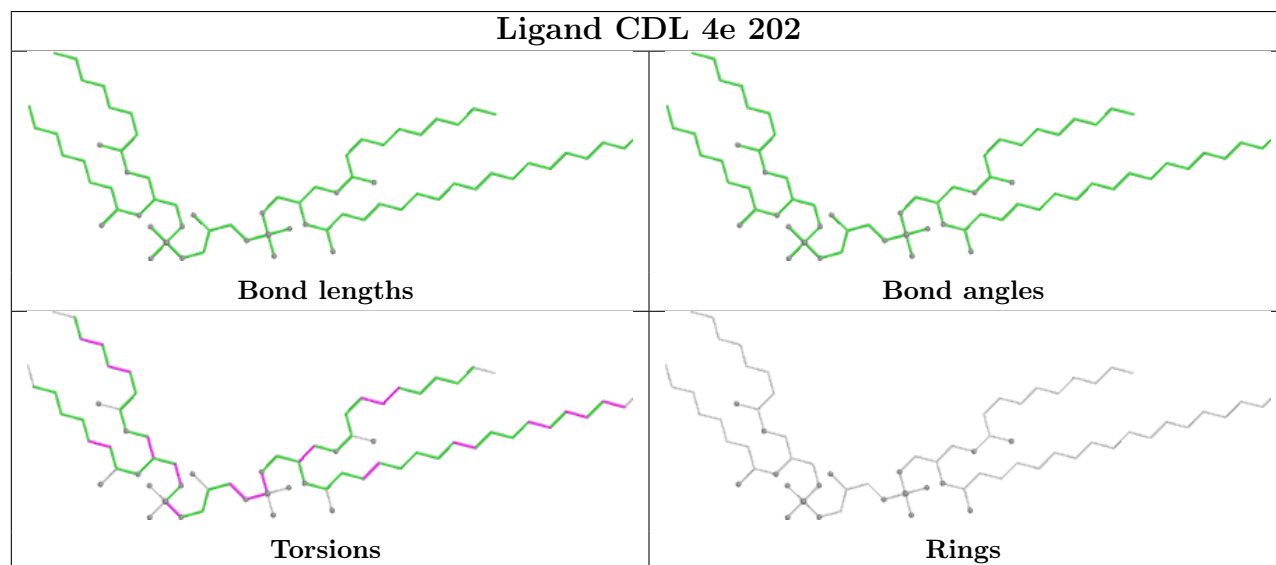
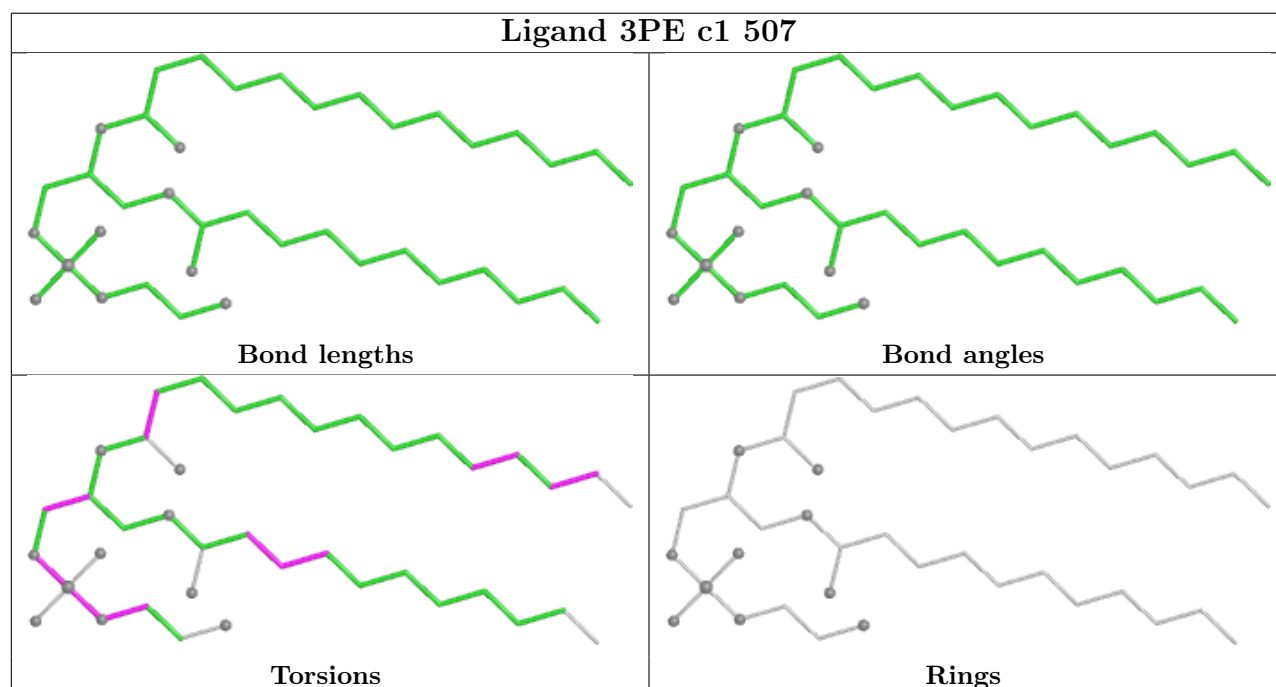
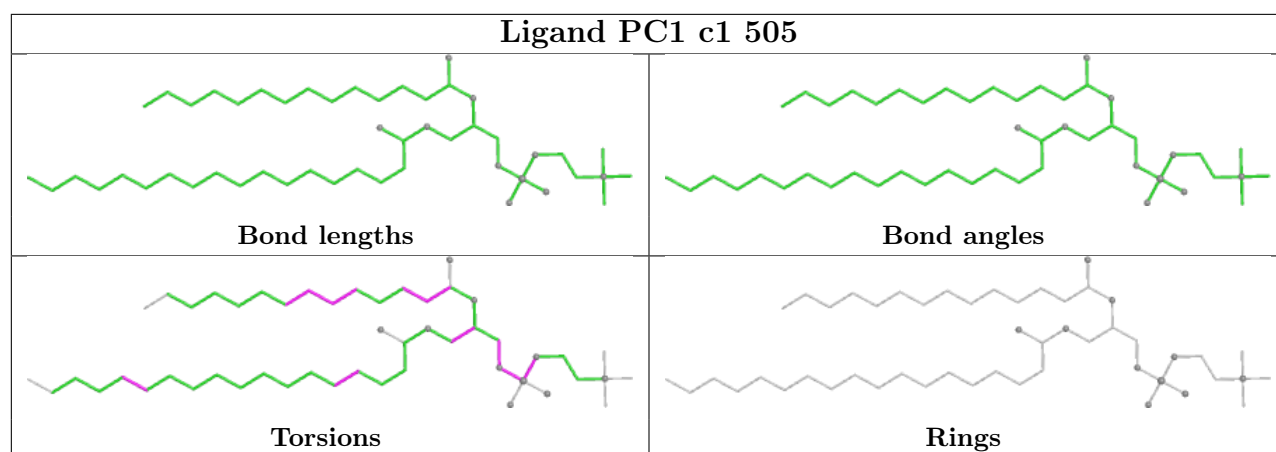


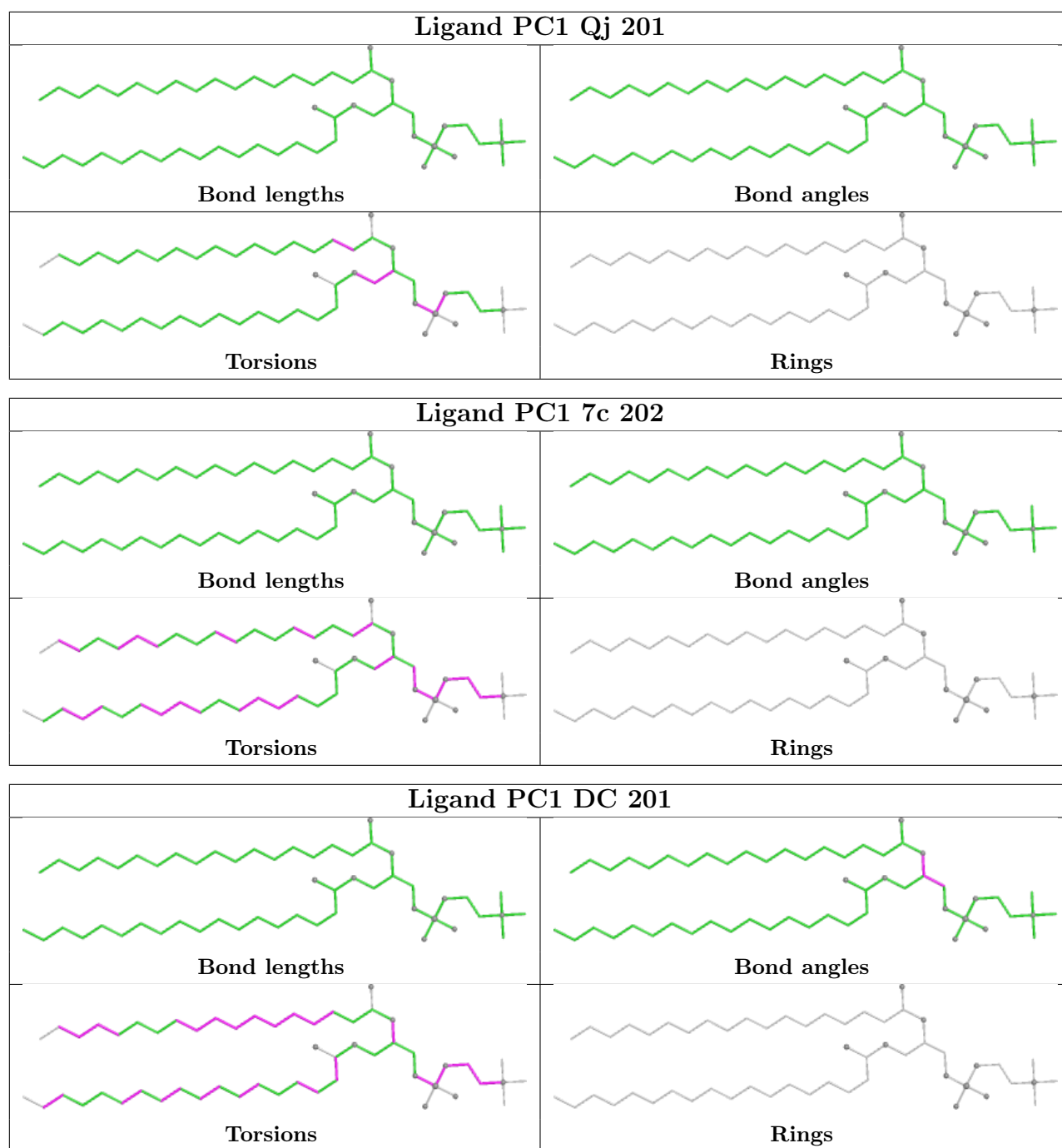


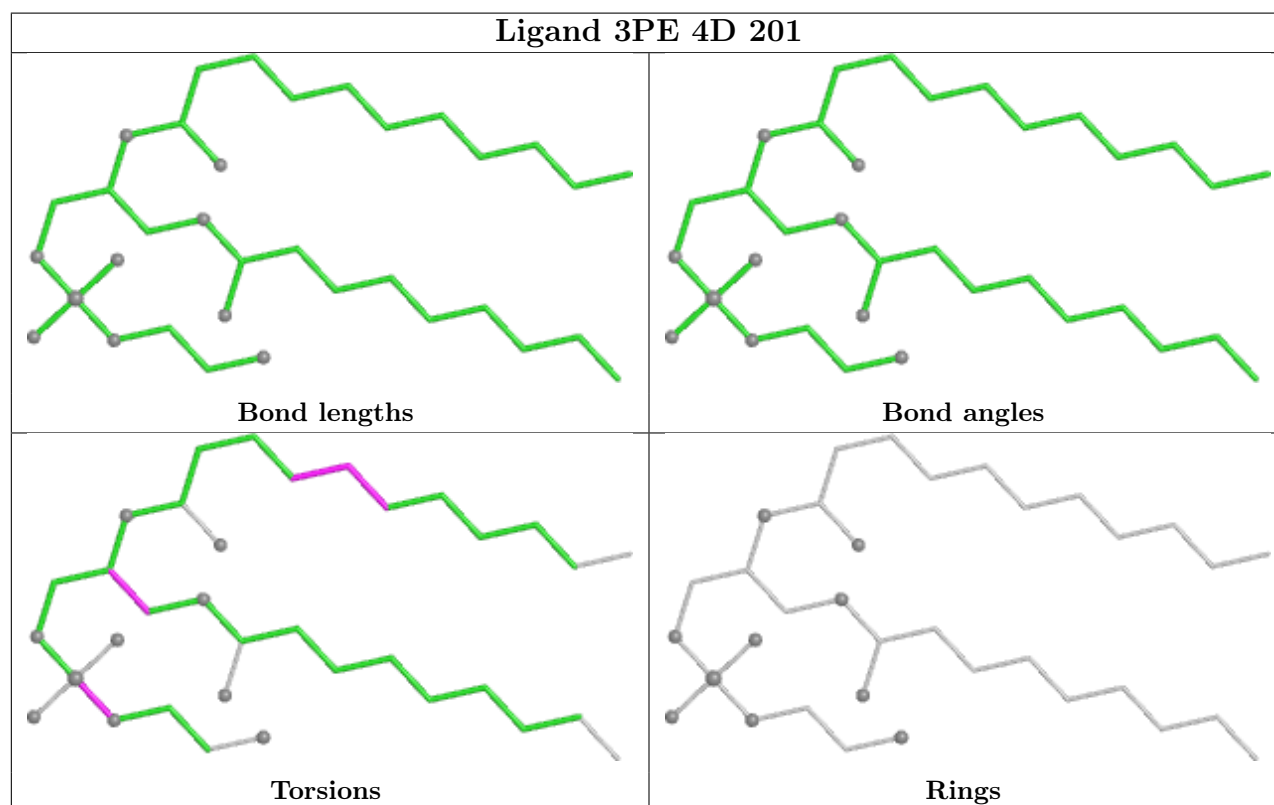
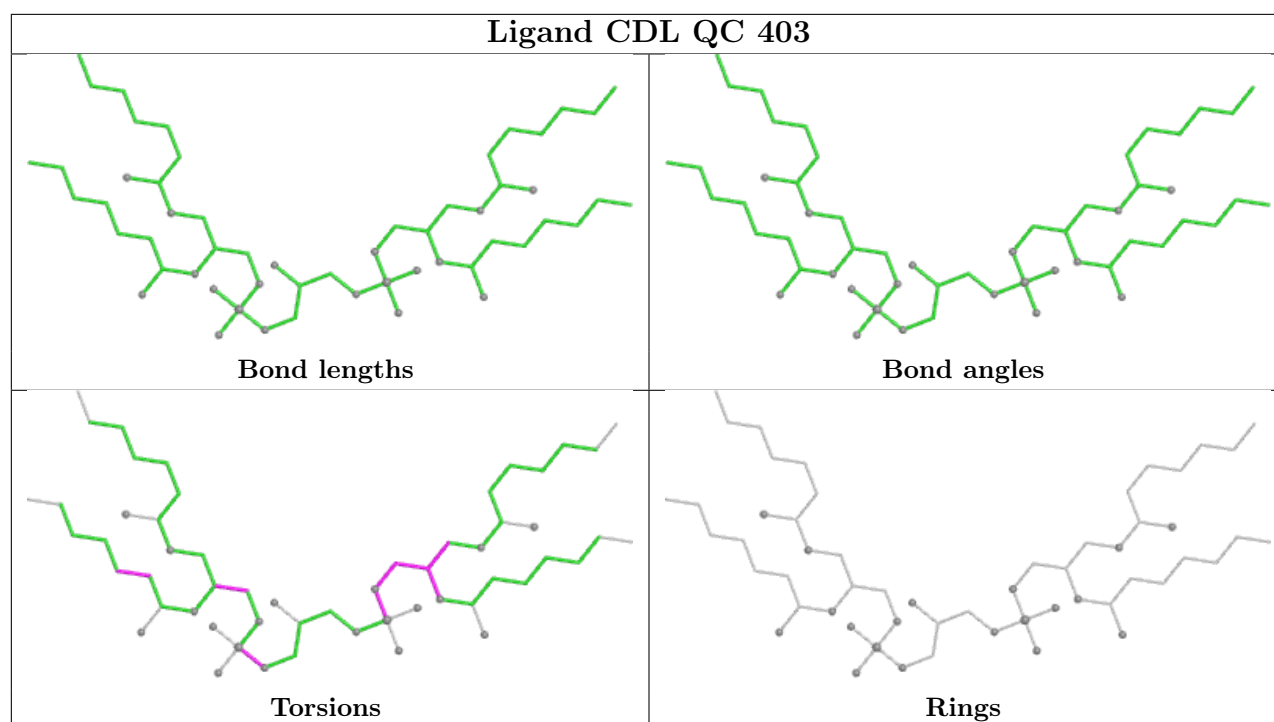












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

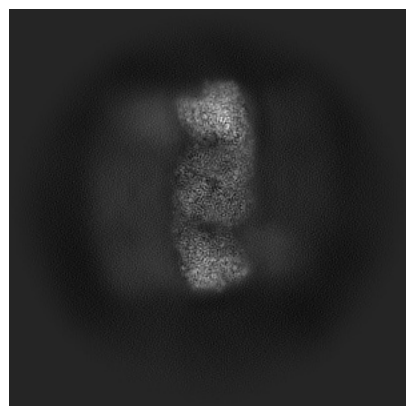
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35723. These allow visual inspection of the internal detail of the map and identification of artifacts.

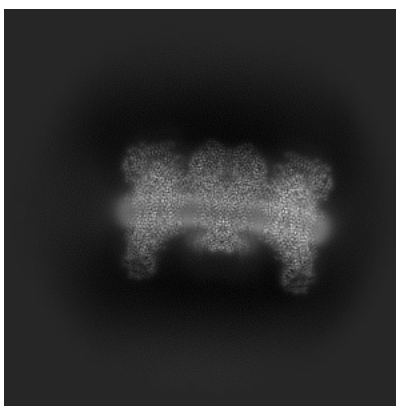
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

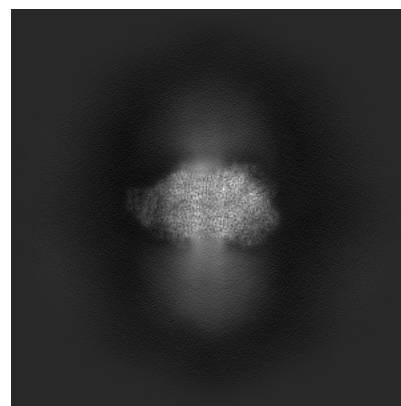
6.1.1 Primary map



X

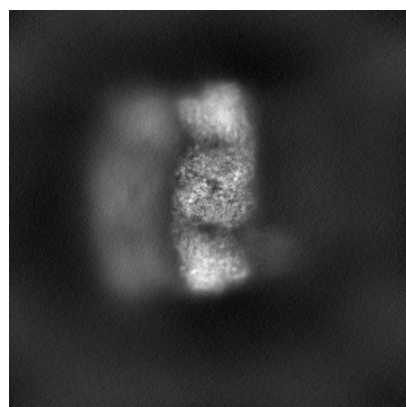


Y

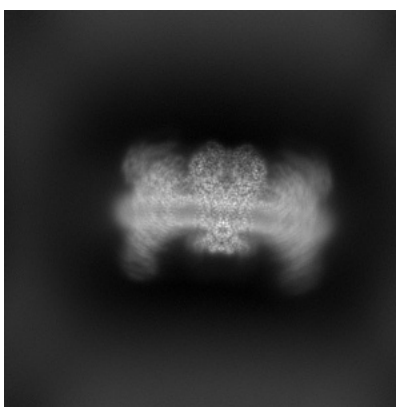


Z

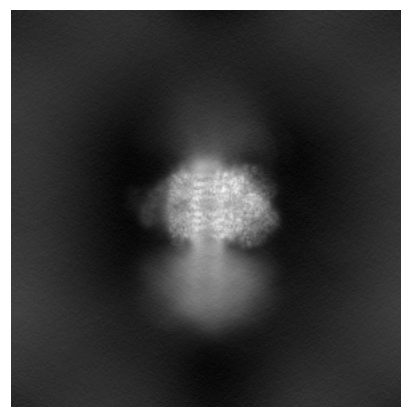
6.1.2 Raw map



X



Y

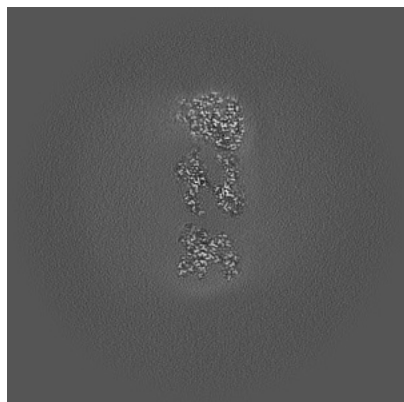


Z

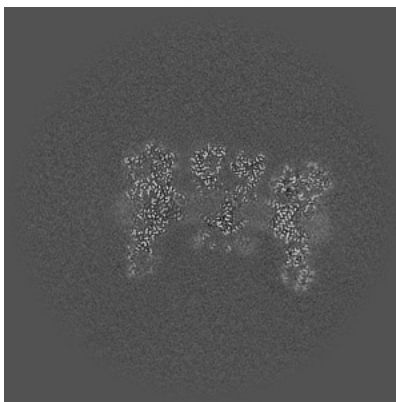
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

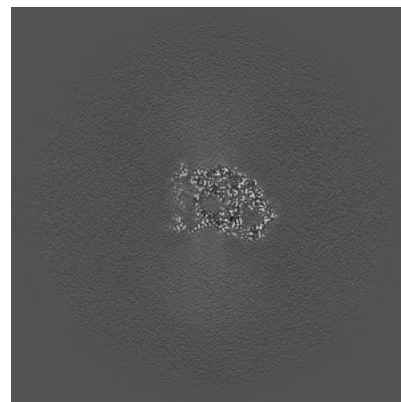
6.2.1 Primary map



X Index: 224

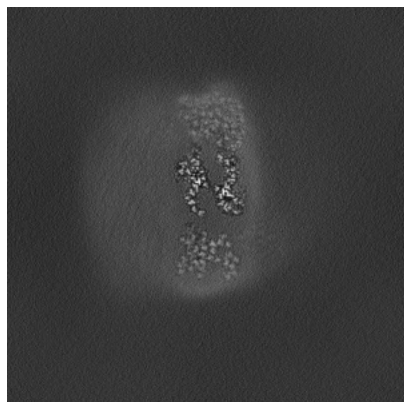


Y Index: 224

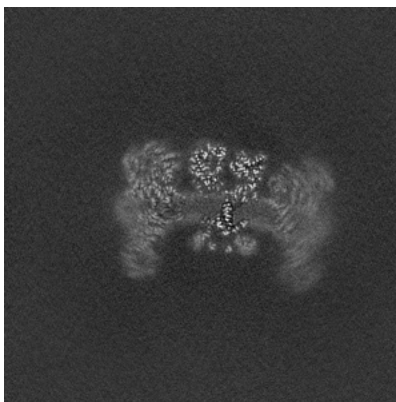


Z Index: 224

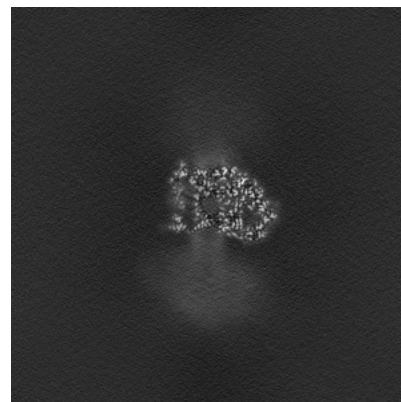
6.2.2 Raw map



X Index: 224



Y Index: 224

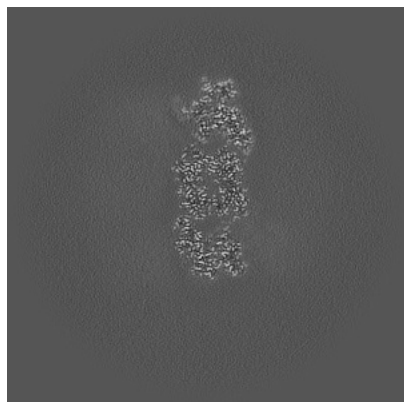


Z Index: 224

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

6.3 Largest variance slices [i](#)

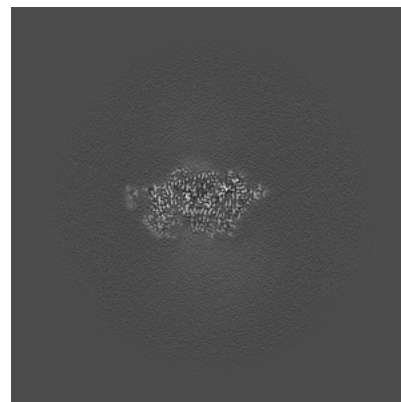
6.3.1 Primary map



X Index: 248

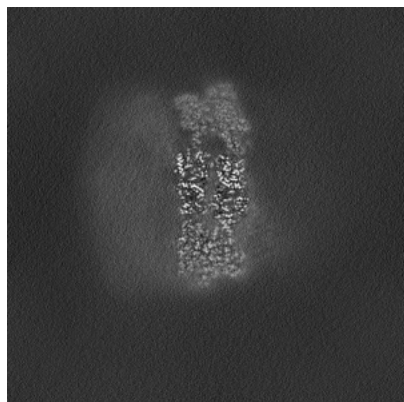


Y Index: 240

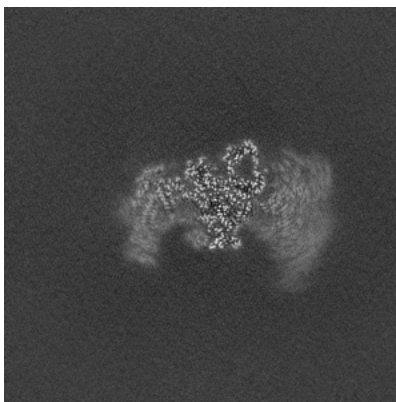


Z Index: 326

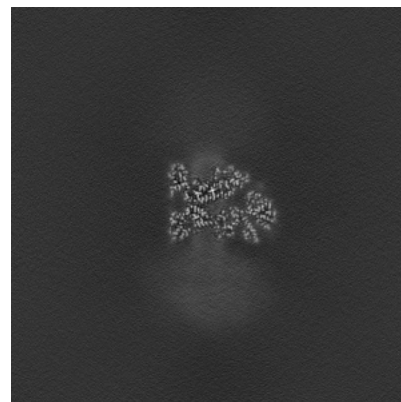
6.3.2 Raw map



X Index: 237



Y Index: 245

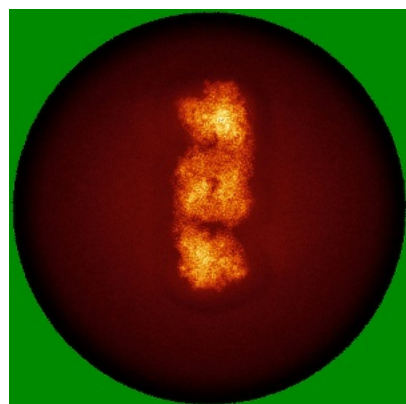


Z Index: 242

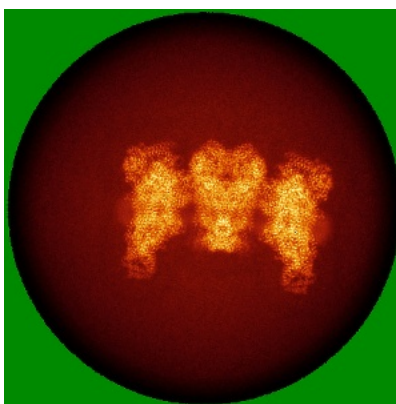
The images above show the largest variance slices of the map in three orthogonal directions.

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

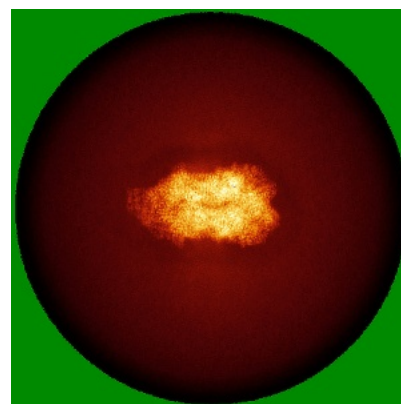
6.4.1 Primary map



X

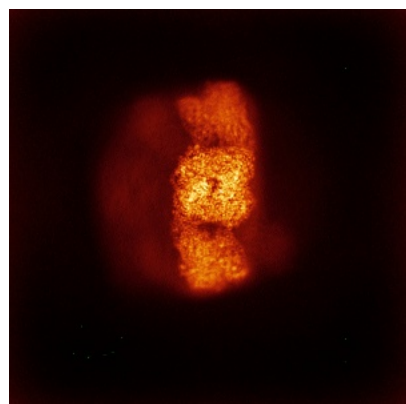


Y

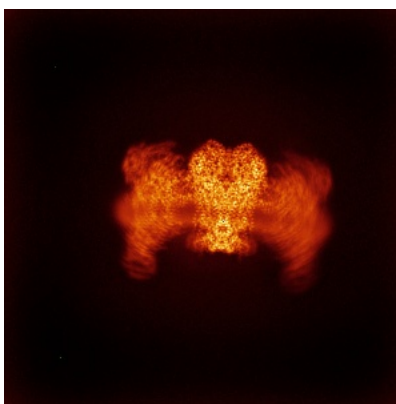


Z

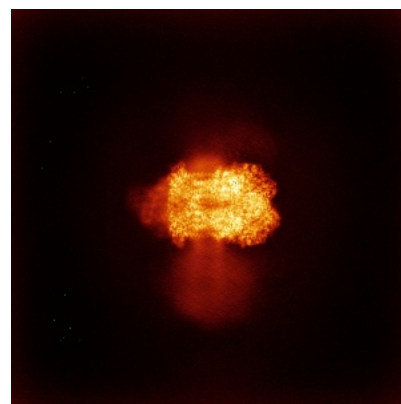
6.4.2 Raw map



X



Y



Z

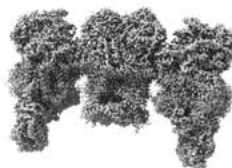
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



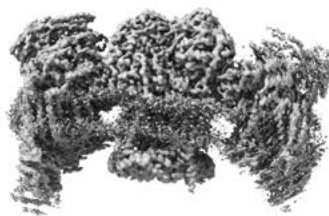
Z

The images above show the 3D surface view of the map at the recommended contour level 4.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

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

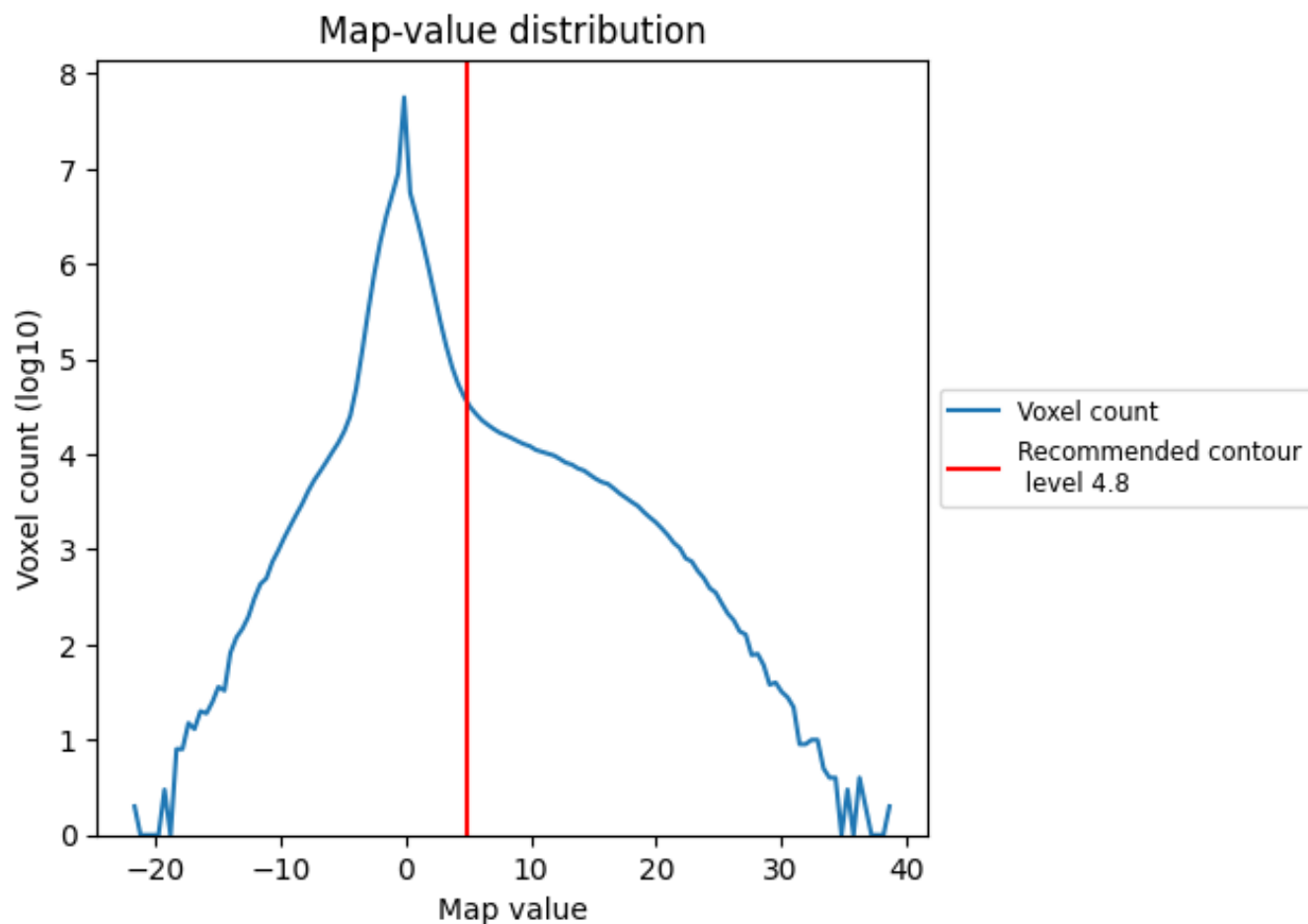
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

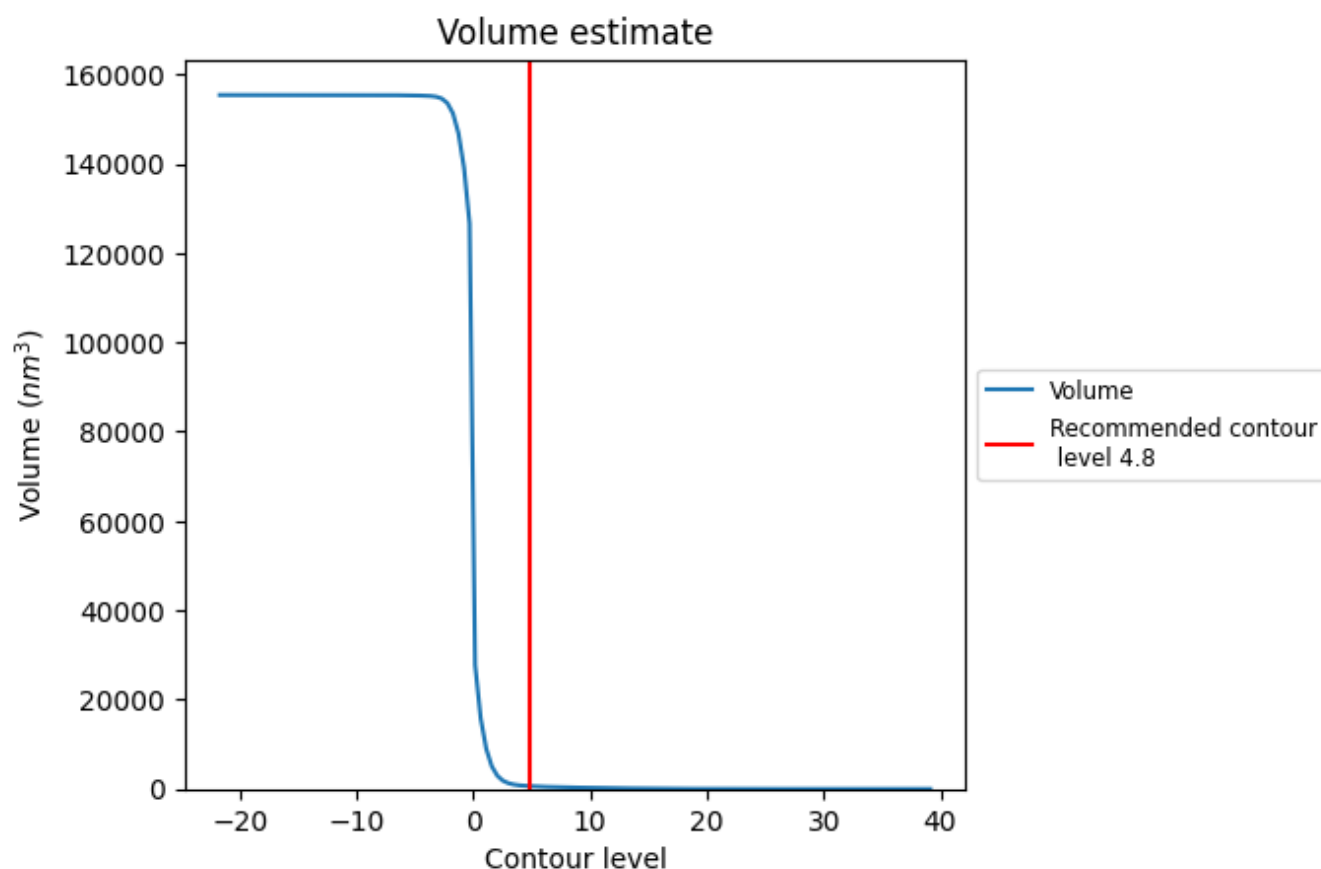
This section contains the results of statistical analysis of the map.

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.

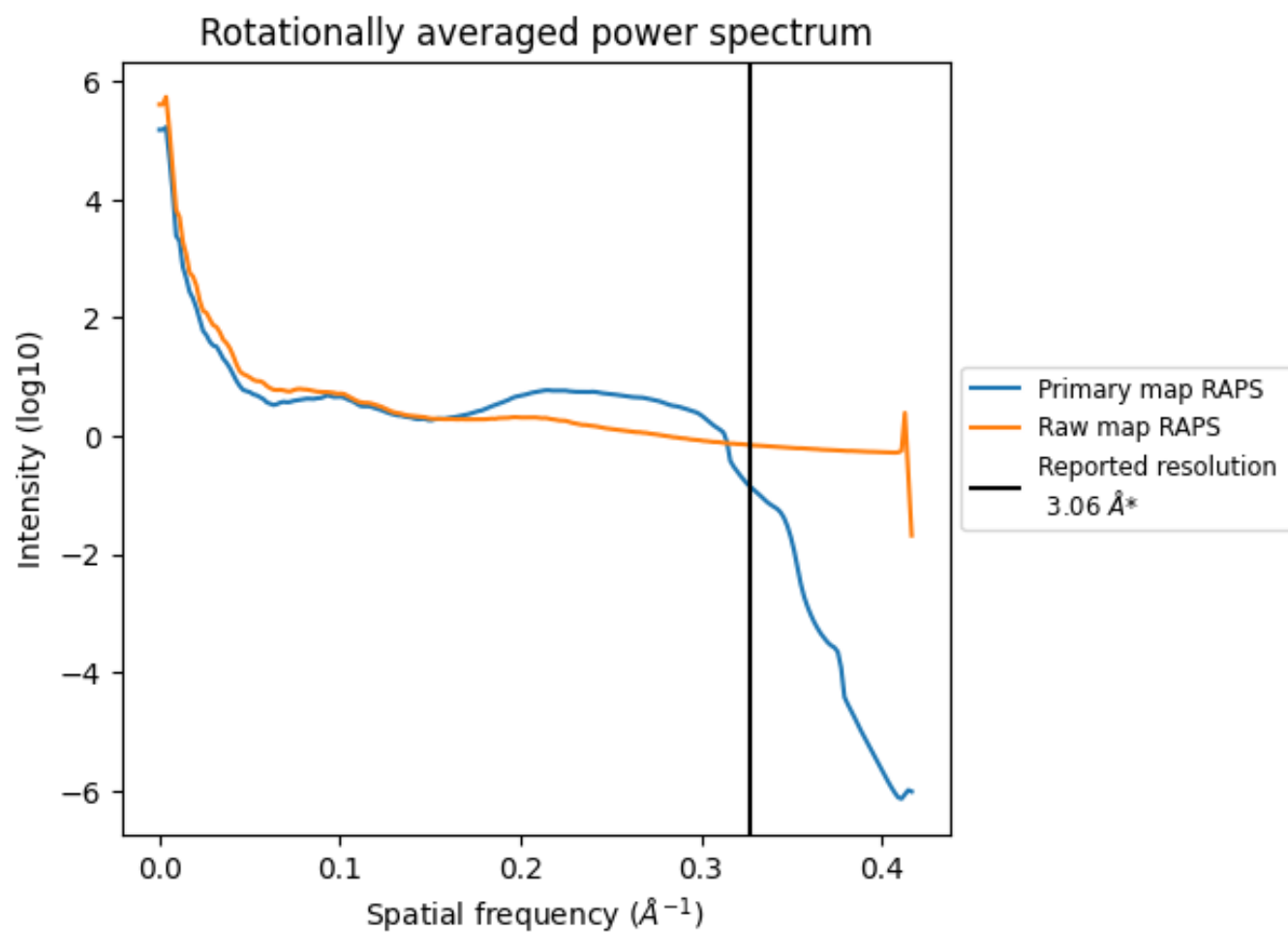
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 638 nm³; this corresponds to an approximate mass of 577 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 ⓘ

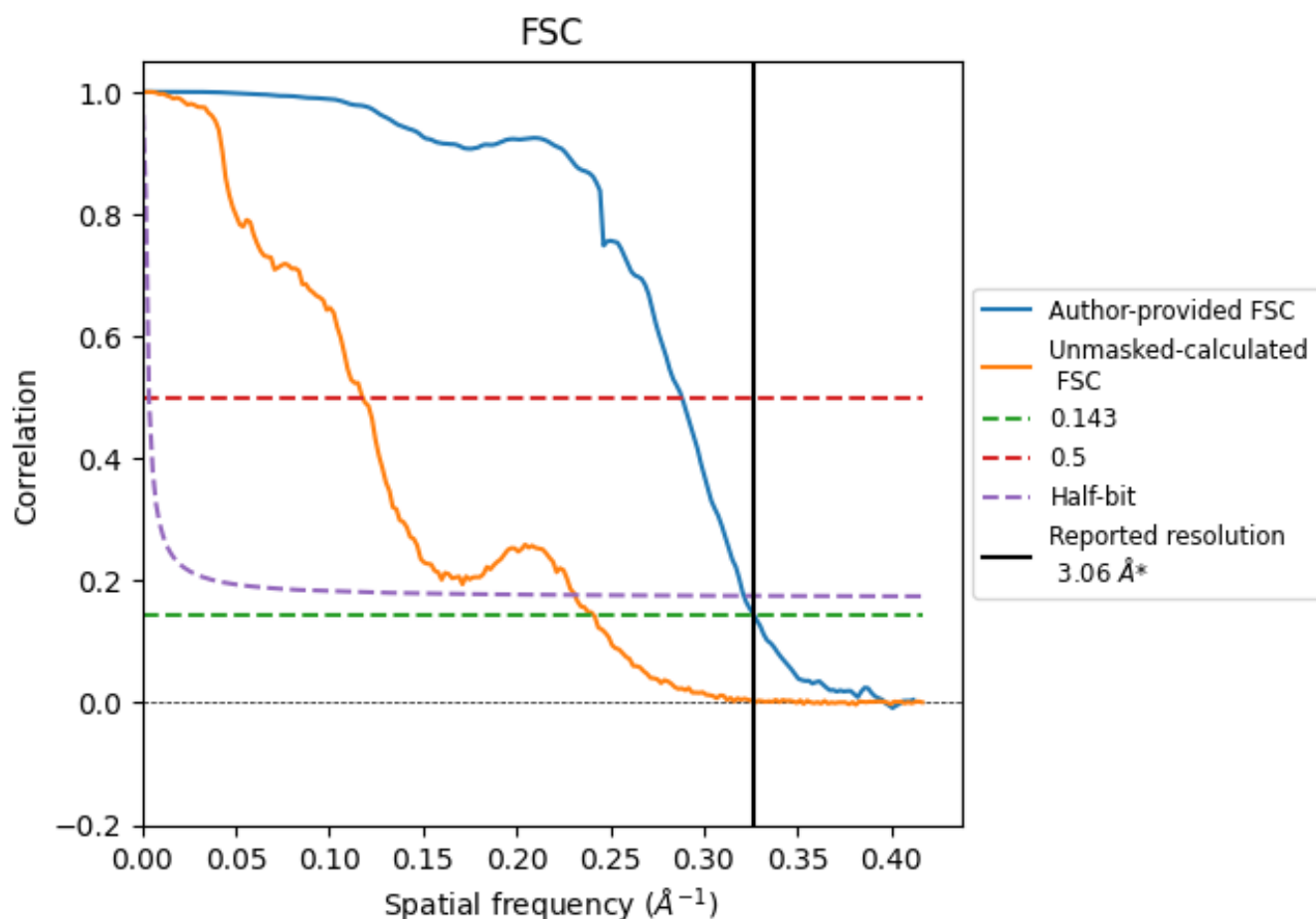


*Reported resolution corresponds to spatial frequency of 0.327 $\text{\AA}^{-1}$

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 0.327 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

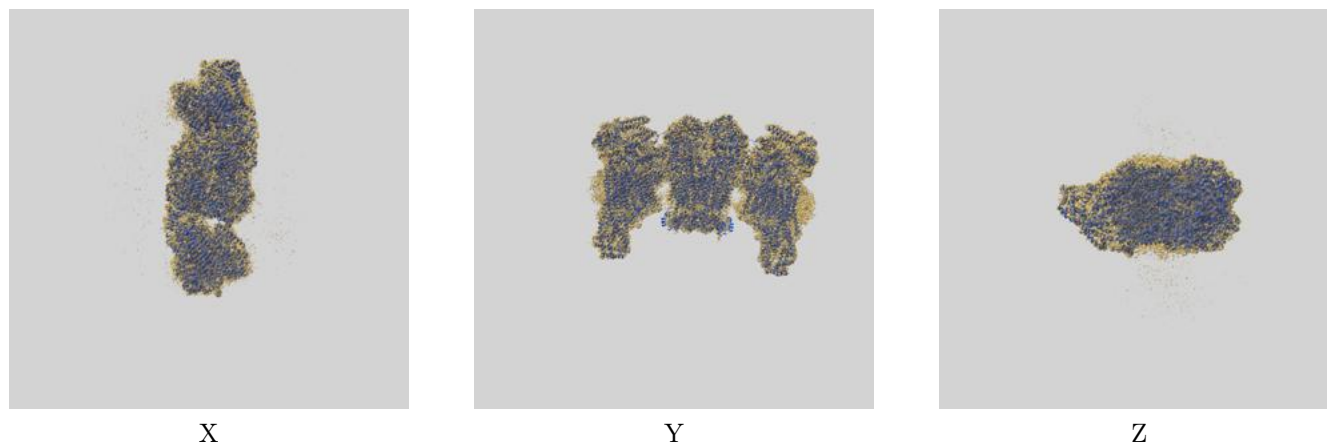
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.06	-	-
Author-provided FSC curve	3.06	3.47	3.11
Unmasked-calculated*	4.14	8.49	4.33

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.14 differs from the reported value 3.06 by more than 10 %

9 Map-model fit [i](#)

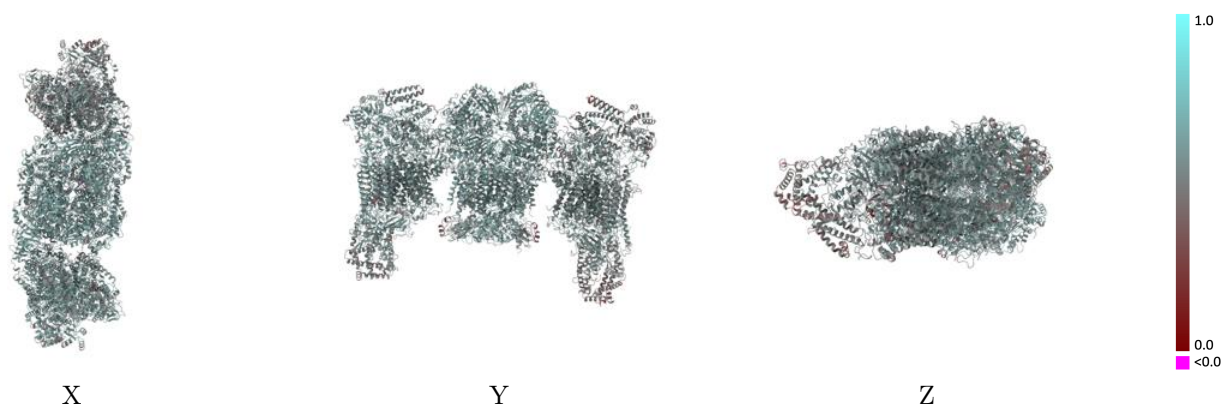
This section contains information regarding the fit between EMDB map EMD-35723 and PDB model 8IUJ. Per-residue inclusion information can be found in section 3 on page 21.

9.1 Map-model overlay [i](#)



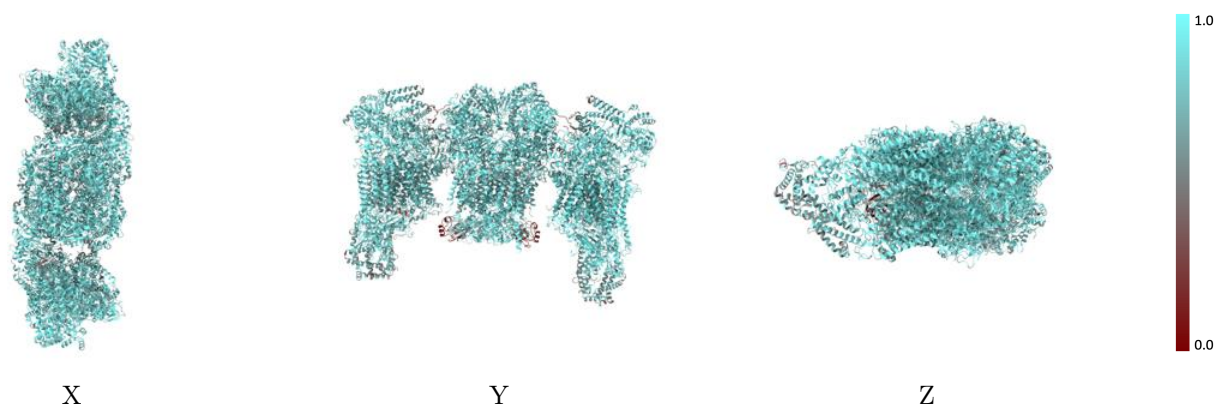
The images above show the 3D surface view of the map at the recommended contour level 4.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



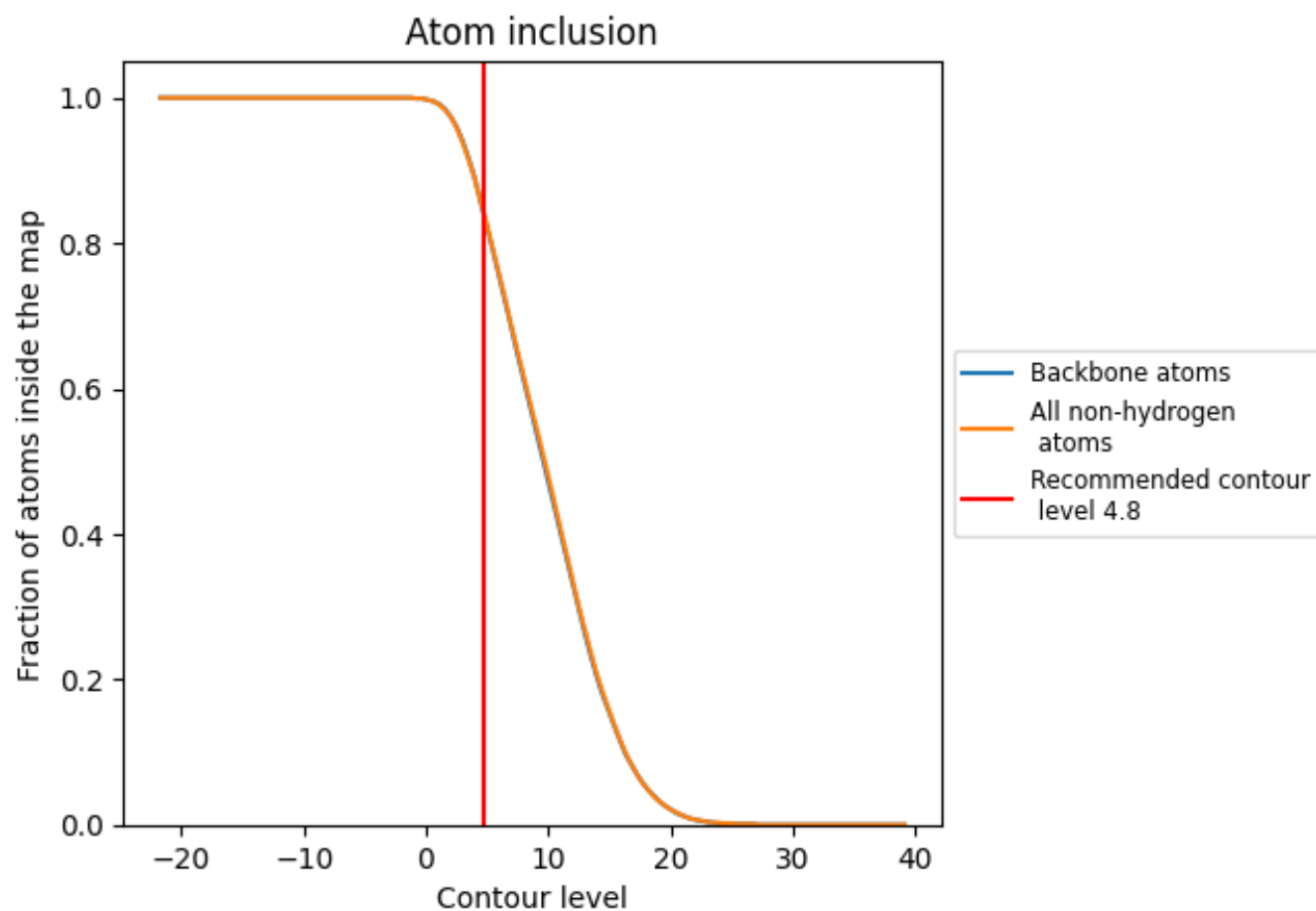
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4.8).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 84% 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 (4.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8380	 0.5610
4A	 0.7670	 0.5460
4C	 0.8170	 0.5460
4D	 0.8530	 0.5730
4E	 0.7640	 0.5250
4F	 0.8490	 0.5620
4G	 0.8070	 0.5490
4H	 0.8430	 0.5600
4I	 0.8950	 0.5910
4J	 0.8580	 0.5850
4a	 0.7740	 0.5010
4c	 0.8140	 0.4910
4d	 0.8570	 0.5230
4e	 0.7520	 0.4770
4f	 0.8630	 0.5130
4g	 0.8230	 0.5000
4h	 0.8320	 0.5110
4i	 0.9140	 0.5550
4j	 0.8530	 0.5390
5B	 0.9050	 0.5900
5C	 0.8750	 0.5800
5b	 0.9110	 0.5490
5c	 0.8900	 0.5410
6A	 0.7400	 0.5430
6B	 0.8050	 0.5460
6a	 0.8190	 0.4980
6b	 0.8040	 0.5050
7A	 0.8550	 0.5710
7C	 0.8630	 0.5810
7a	 0.8520	 0.5210
7c	 0.8730	 0.5500
C1	 0.8940	 0.5840
C2	 0.9060	 0.5890
C3	 0.8630	 0.5670
DC	 0.8480	 0.5830



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Chain	Atom inclusion	Q-score
QA	 0.8470	 0.5910
QB	 0.8490	 0.5930
QC	 0.8710	 0.5980
QD	 0.8720	 0.6000
QE	 0.5790	 0.5170
QF	 0.7130	 0.5470
QG	 0.8860	 0.6090
QH	 0.8410	 0.5910
QI	 0.8720	 0.5900
QJ	 0.7980	 0.5790
QK	 0.8320	 0.5860
Qa	 0.8590	 0.5900
Qb	 0.8300	 0.5760
Qc	 0.8740	 0.5930
Qd	 0.8690	 0.5900
Qe	 0.5830	 0.5140
Qf	 0.7320	 0.5380
Qg	 0.8890	 0.5990
Qh	 0.8180	 0.5870
Qi	 0.8790	 0.5770
Qj	 0.7820	 0.5710
Qk	 0.8440	 0.5880
c1	 0.9060	 0.5520
c2	 0.9140	 0.5570
c3	 0.8680	 0.5290
dc	 0.8820	 0.5440