



Full wwPDB EM Validation Report ⓘ

Aug 25, 2026 – 11:29 pm BST

PDB ID : 6YMX / pdb_00006ymx
EMDB ID : EMD-10847
Title : CIII2/CIV respiratory supercomplex from *Saccharomyces cerevisiae*
Authors : Berndtsson, J.; Rathore, S.; Ott, M.
Deposited on : 2020-04-10
Resolution : 3.17 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 : 1.8.4, 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

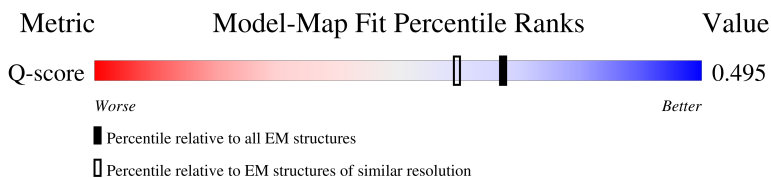
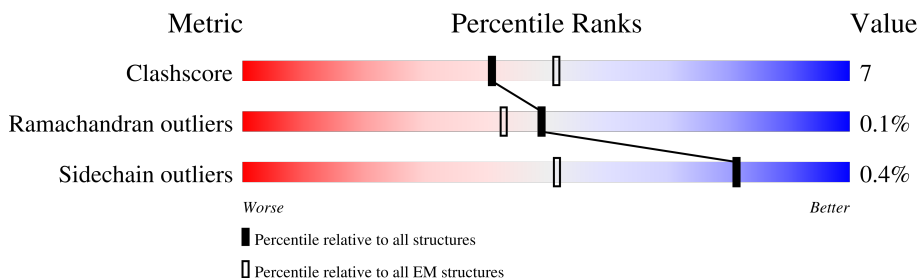
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.17 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.



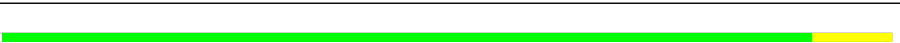
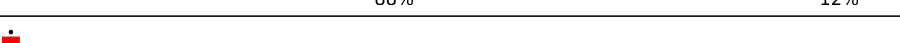
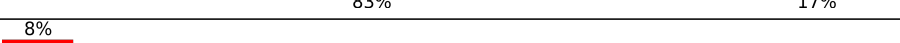
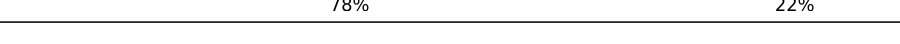
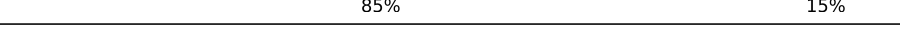
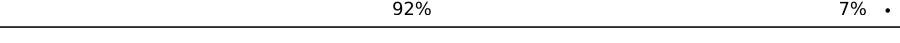
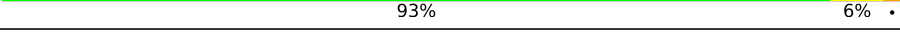
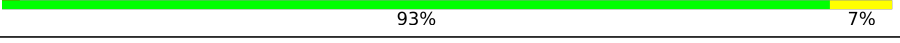
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14465 (2.67 - 3.67)

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	a	530	 82% 18%
2	b	236	 81% 19% 6%
3	c	268	 81% 19% 6%
4	d	117	 76% 24% 10%

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Mol	Chain	Length	Quality of chain
5	e	128	
6	f	99	
7	g	55	
8	h	51	
9	i	53	
10	j	78	
11	k	114	
12	m	38	
13	A	431	
13	L	431	
14	B	352	
14	M	352	
15	C	385	
15	N	385	
16	D	248	
16	O	248	
17	E	185	
17	P	185	
18	F	74	
19	G	126	
19	R	126	
20	H	93	
20	S	93	
21	I	54	
22	Q	75	

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Mol	Chain	Length	Quality of chain
23	T	54	 87% 13%
24	U	44	 93% 7%
25	V	51	 86% 14%

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
28	PTY	D	402	-	-	X	-
28	PTY	c	301	-	-	X	-
40	FES	P	301	-	-	X	-

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 47034 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	530	Total	C	N	O	S	0	0
			4126	2757	641	707	21		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	236	Total	C	N	O	S	0	0
			1888	1242	286	350	10		

- Molecule 3 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	c	268	Total	C	N	O	S	0	0
			2138	1425	343	356	14		

- Molecule 4 is a protein called Cytochrome c oxidase subunit 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	117	Total	C	N	O	S	0	0
			888	559	147	177	5		

- Molecule 5 is a protein called Cytochrome c oxidase subunit 5A, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	e	128	Total	C	N	O	S	0	0
			1008	639	175	190	4		

- Molecule 6 is a protein called Cytochrome c oxidase subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	99	Total	C	N	O	S	0	0
			828	533	134	160	1		

- Molecule 7 is a protein called Cytochrome c oxidase subunit 7, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	g	55	Total	C	N	O	0	0
			456	310	77	69		

- Molecule 8 is a protein called Cytochrome c oxidase subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	h	51	Total	C	N	O	S	0	0
			408	278	66	63	1		

- Molecule 9 is a protein called Cytochrome c oxidase subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	i	53	Total	C	N	O	S	0	0
			439	290	76	70	3		

- Molecule 10 is a protein called Cytochrome c oxidase subunit 12, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	j	78	Total	C	N	O	S	0	0
			649	414	111	119	5		

- Molecule 11 is a protein called Cytochrome c oxidase subunit 13, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	k	114	Total	C	N	O	S	0	0
			941	608	163	167	3		

- Molecule 12 is a protein called Cytochrome c oxidase subunit 26, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	m	38	Total	C	N	O	S	0	0
			308	207	49	51	1		

- Molecule 13 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	A	431	Total	C	N	O	S	0	0
			3344	2110	576	652	6		
13	L	431	Total	C	N	O	S	0	0
			3344	2110	576	652	6		

- Molecule 14 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	B	352	Total	C	N	O	S	0	0
			2735	1747	453	534	1		
14	M	352	Total	C	N	O	S	0	0
			2735	1747	453	534	1		

- Molecule 15 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	C	385	Total	C	N	O	S	0	0
			3090	2082	484	503	21		
15	N	385	Total	C	N	O	S	0	0
			3090	2082	484	503	21		

- Molecule 16 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	D	248	Total	C	N	O	S	0	0
			1961	1249	340	363	9		
16	O	248	Total	C	N	O	S	0	0
			1961	1249	340	363	9		

- Molecule 17 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	E	185	Total	C	N	O	S	0	0
			1411	893	242	266	10		
17	P	185	Total	C	N	O	S	0	0
			1411	893	242	266	10		

- Molecule 18 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	F	74	Total	C	N	O	S	0	0
			624	391	108	123	2		

- Molecule 19 is a protein called Cytochrome b-c1 complex subunit 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	G	126	Total	C	N	O	S	0	0
			1019	653	173	191	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
19	R	126	Total	C	N	O	S	0	0
			1019	653	173	191	2		

- Molecule 20 is a protein called Cytochrome b-c1 complex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	H	93	Total	C	N	O	S	0	0
			773	510	131	130	2		
20	S	93	Total	C	N	O	S	0	0
			773	510	131	130	2		

- Molecule 21 is a protein called Cytochrome b-c1 complex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	I	54	Total	C	N	O	0	0
			442	295	74	73		

- Molecule 22 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Q	75	Total	C	N	O	S	0	0
			633	396	109	126	2		

- Molecule 23 is a protein called Cytochrome b-c1 complex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	T	54	Total	C	N	O	0	0
			443	295	74	74		

- Molecule 24 is a protein called Cytochrome b-c1 complex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	U	44	Total	C	N	O	S	0	0
			347	230	58	57	2		

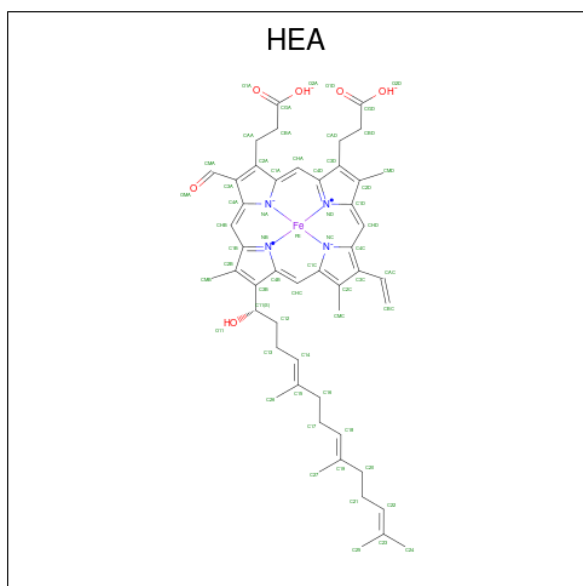
- Molecule 25 is a protein called Cytochrome b-c1 complex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	V	51	Total	C	N	O	S	0	0
			406	272	66	66	2		

- Molecule 26 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

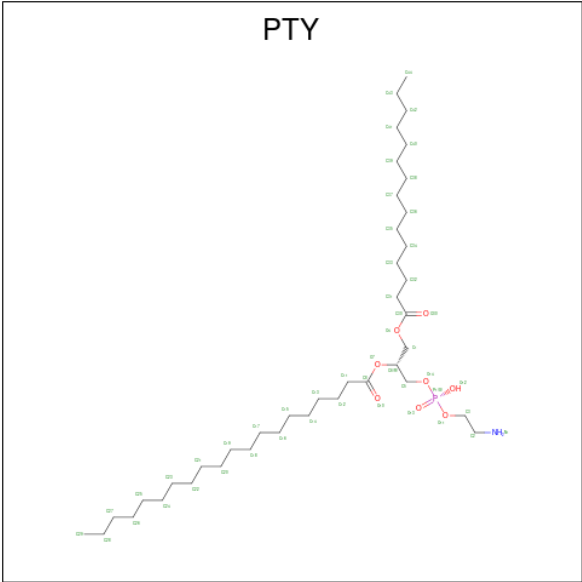
Mol	Chain	Residues	Atoms		AltConf
26	a	1	Total	Cu	0
			1	1	

- Molecule 27 is HEME-A (CCD ID: HEA) (formula: C₄₉H₅₆FeN₄O₆) (labeled as "Ligand of Interest" by depositor).



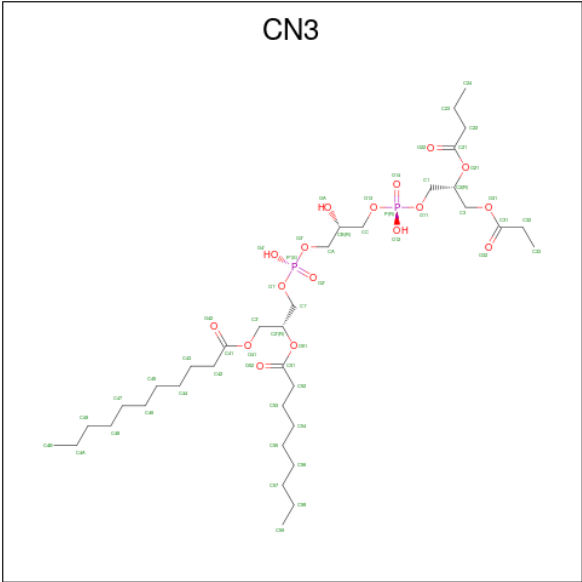
Mol	Chain	Residues	Atoms					AltConf
27	a	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
27	a	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

- Molecule 28 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: C₄₀H₈₀NO₈P) (labeled as "Ligand of Interest" by depositor).



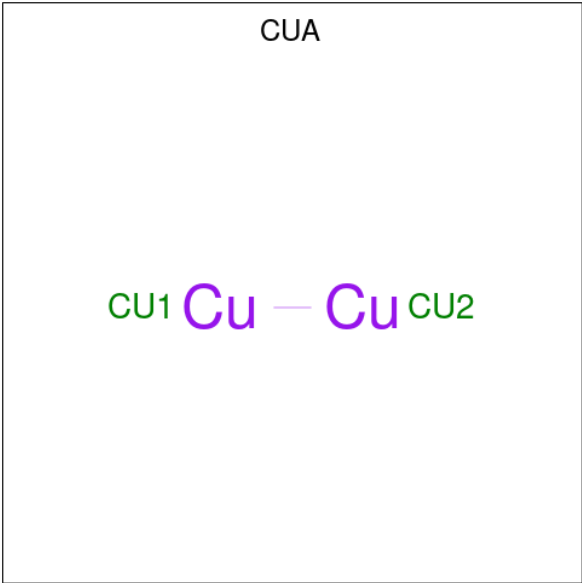
Mol	Chain	Residues	Atoms					AltConf
28	a	1	Total	C	N	O	P	0
			34	24	1	8	1	
28	b	1	Total	C	N	O	P	0
			35	25	1	8	1	
28	c	1	Total	C	N	O	P	0
			40	30	1	8	1	
28	i	1	Total	C	N	O	P	0
			40	30	1	8	1	
28	m	1	Total	C	N	O	P	0
			41	31	1	8	1	
28	m	1	Total	C	N	O	P	0
			30	20	1	8	1	
28	D	1	Total	C	N	O	P	0
			32	22	1	8	1	

- Molecule 29 is (2R,5S,11R,14R)-5,8,11-trihydroxy-2-(nonanoyloxy)-5,11-dioxido-16-oxo-14-[(propanoyloxy)methyl]-4,6,10,12,15-pentaoxa-5,11-diphosphanonadec-1-yl undecanoate (CCD ID: CN3) (formula: C₃₆H₆₈O₁₇P₂).



Mol	Chain	Residues	Atoms				AltConf
29	a	1	Total	C	O	P	0
			55	36	17	2	
29	N	1	Total	C	O	P	0
			55	36	17	2	

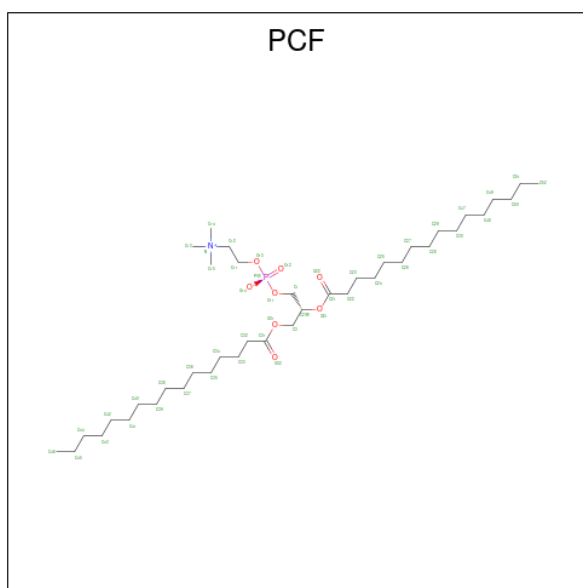
- Molecule 30 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).



Mol	Chain	Residues	Atoms		AltConf
30	b	1	Total	Cu	0
			2	2	

- Molecule 31 is 1,2-DIACYL-SN-GLYCERO-3-PHOSHOCHOLINE (CCD ID: PCF)

(formula: $C_{40}H_{80}NO_8P$) (labeled as "Ligand of Interest" by depositor).

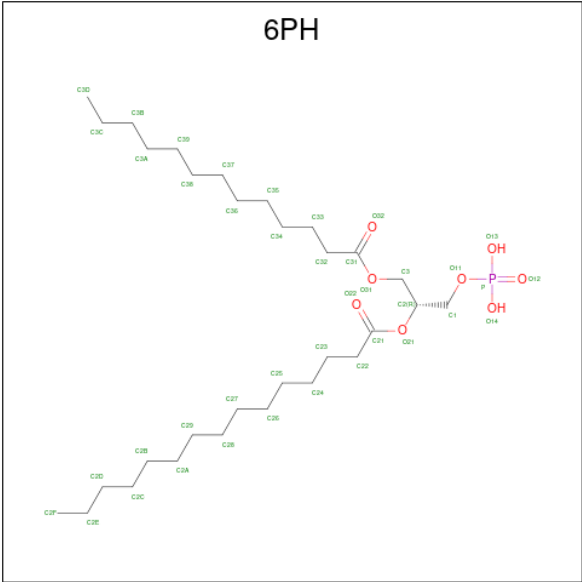


Mol	Chain	Residues	Atoms					AltConf
31	c	1	Total	C	N	O	P	0
			43	33	1	8	1	
31	e	1	Total	C	N	O	P	0
			36	26	1	8	1	
31	m	1	Total	C	N	O	P	0
			38	28	1	8	1	
31	I	1	Total	C	N	O	P	0
			35	25	1	8	1	
31	T	1	Total	C	N	O	P	0
			35	25	1	8	1	

- Molecule 32 is ZINC ION (CCD ID: ZN) (formula: Zn).

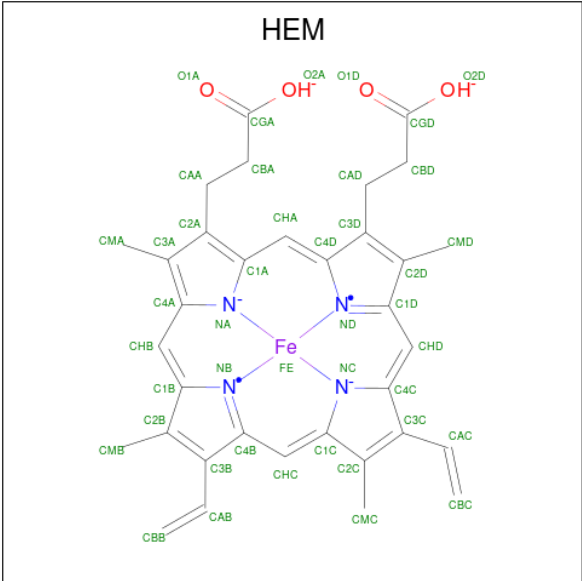
Mol	Chain	Residues	Atoms		AltConf
32	d	1	Total	Zn	0
			1	1	

- Molecule 33 is (1R)-2-(phosphonoxy)-1-[(tridecanoyloxy)methyl]ethyl pentadecanoate (CCD ID: 6PH) (formula: $C_{31}H_{61}O_8P$).



Mol	Chain	Residues	Atoms				AltConf
33	C	1	Total	C	O	P	0
			40	31	8	1	
33	O	1	Total	C	O	P	0
			40	31	8	1	

- Molecule 34 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



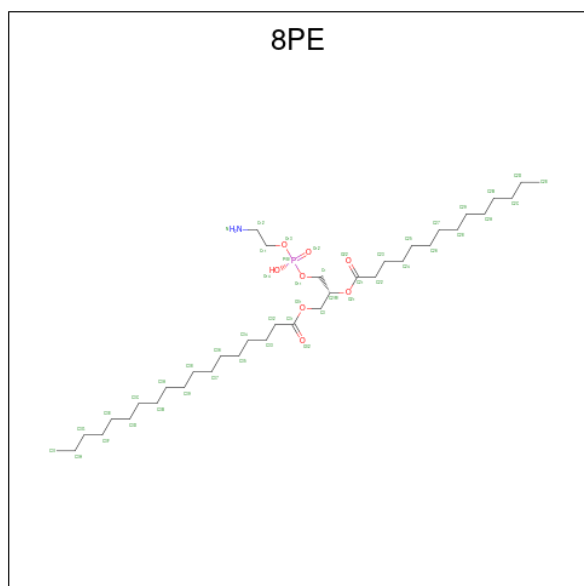
Mol	Chain	Residues	Atoms					AltConf
34	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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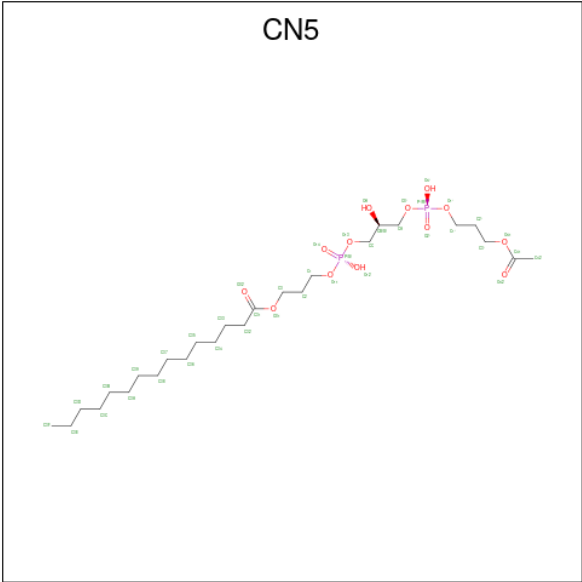
Mol	Chain	Residues	Atoms					AltConf
34	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
34	D	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
34	N	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
34	N	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
34	O	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 35 is (2R)-3-{[(S)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-2-(tetradecanoyloxy)propyl octadecanoate (CCD ID: 8PE) (formula: C₃₇H₇₄NO₈P).



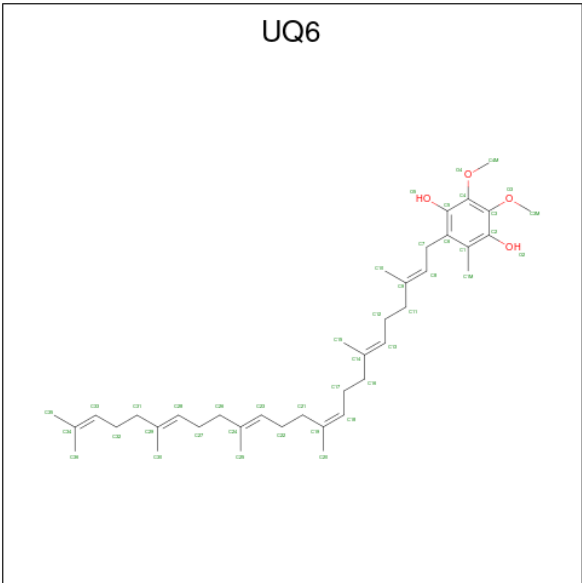
Mol	Chain	Residues	Atoms					AltConf
35	C	1	Total	C	N	O	P	0
			47	37	1	8	1	
35	N	1	Total	C	N	O	P	0
			47	37	1	8	1	

- Molecule 36 is (5S,11R)-5,8,11-trihydroxy-5,11-dioxido-17-oxo-4,6,10,12,16-pentaoxa-5,11-di phosphaoctadec-1-yl pentadecanoate (CCD ID: CN5) (formula: C₂₆H₅₂O₁₃P₂).



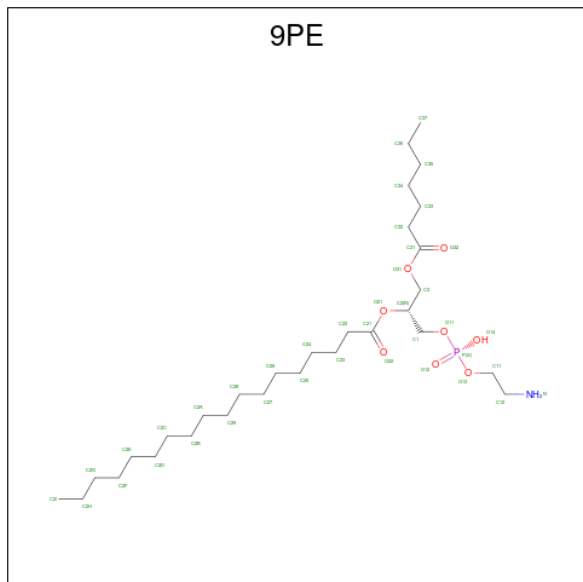
Mol	Chain	Residues	Atoms				AltConf
36	C	1	Total	C	O	P	0
			41	26	13	2	

- Molecule 37 is 5-(3,7,11,15,19,23-HEXAMETHYL-TETRACOSA-2,6,10,14,18,22-HEXA ENYL)-2,3-DIMETHOXY-6-METHYL-BENZENE-1,4-DIOL (CCD ID: UQ6) (formula: C₃₉H₆₀O₄).



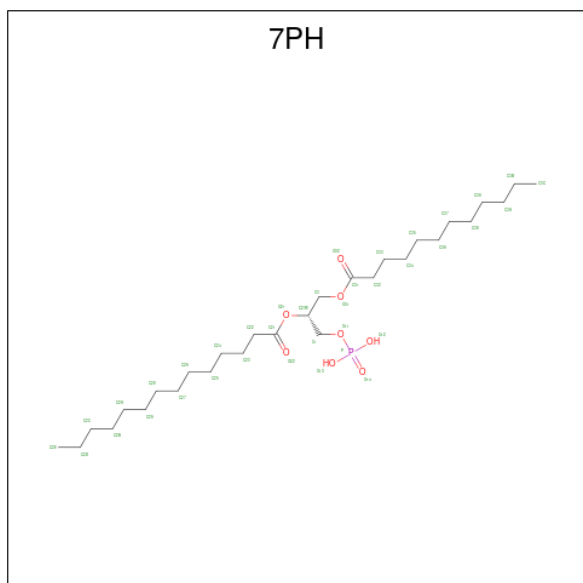
Mol	Chain	Residues	Atoms				AltConf
37	C	1	Total	C	O		0
			43	39	4		
37	N	1	Total	C	O		0
			43	39	4		

- Molecule 38 is (1R)-2-{[(S)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-1-[(heptanoyloxy)methyl]ethyl octadecanoate (CCD ID: 9PE) (formula: $C_{30}H_{60}NO_8P$).



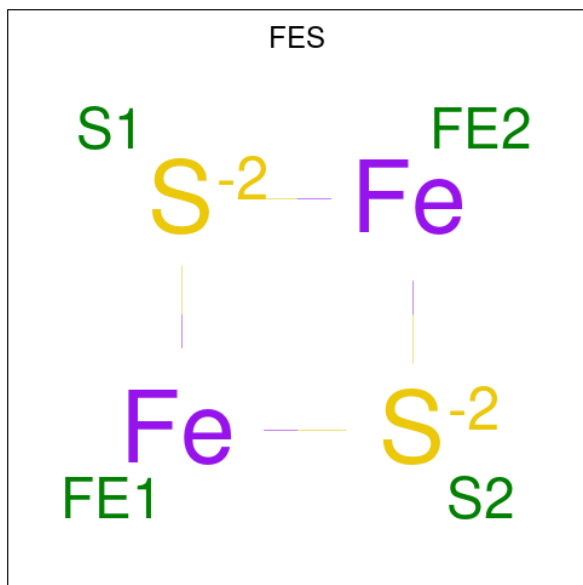
Mol	Chain	Residues	Atoms					AltConf
38	C	1	Total	C	N	O	P	0
			40	30	1	8	1	
38	N	1	Total	C	N	O	P	0
			40	30	1	8	1	

- Molecule 39 is (1R)-2-(dodecanoyloxy)-1-[(phosphonoxy)methyl]ethyl tetradecanoate (CCD ID: 7PH) (formula: $C_{29}H_{57}O_8P$).



Mol	Chain	Residues	Atoms				AltConf
39	E	1	Total	C	O	P	0
			38	29	8	1	
39	O	1	Total	C	O	P	0
			38	29	8	1	

- Molecule 40 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).

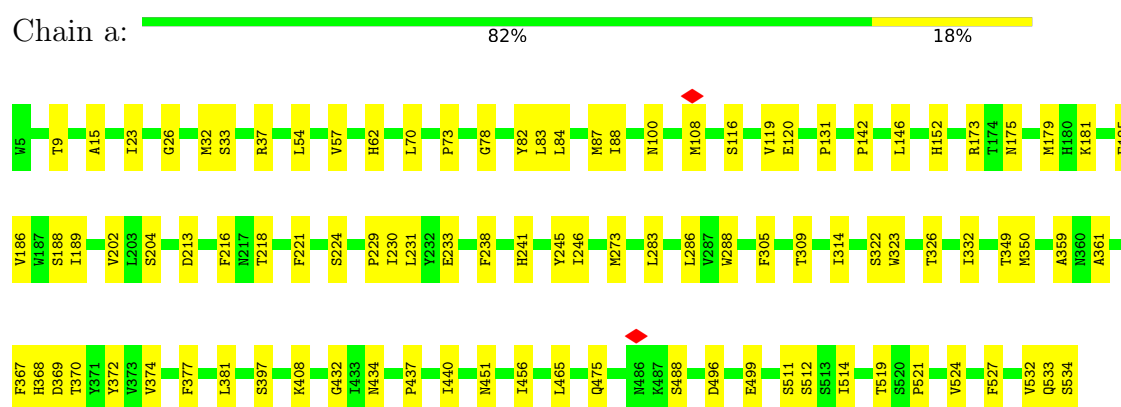


Mol	Chain	Residues	Atoms			AltConf
40	E	1	Total	Fe	S	0
			4	2	2	
40	P	1	Total	Fe	S	0
			4	2	2	

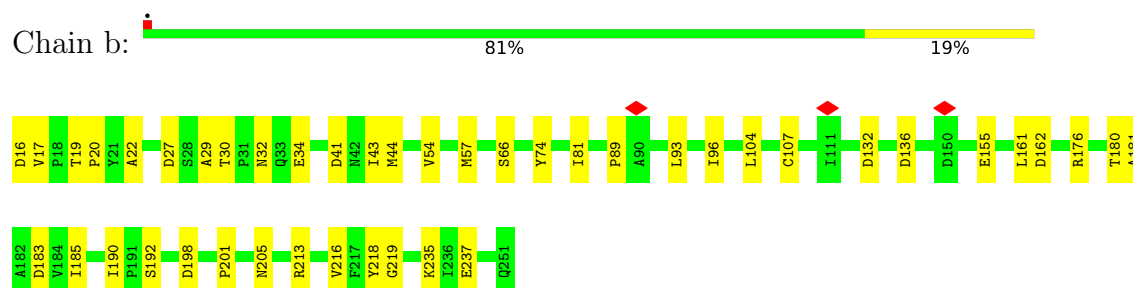
3 Residue-property plots [i](#)

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.

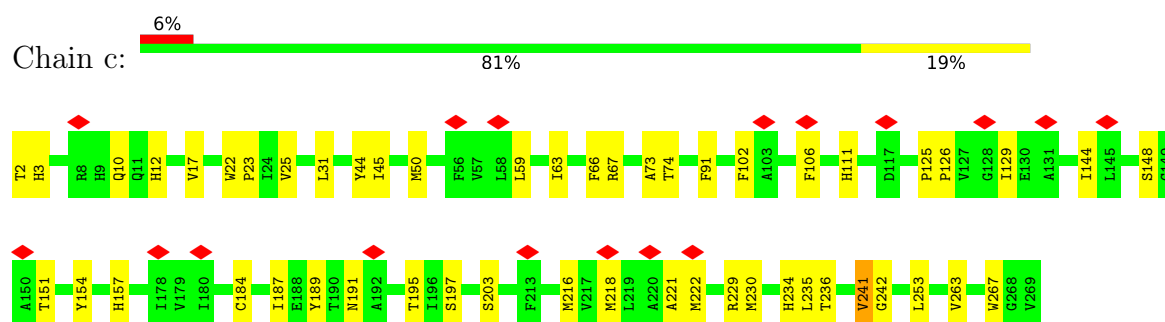
• Molecule 1: Cytochrome c oxidase subunit 1



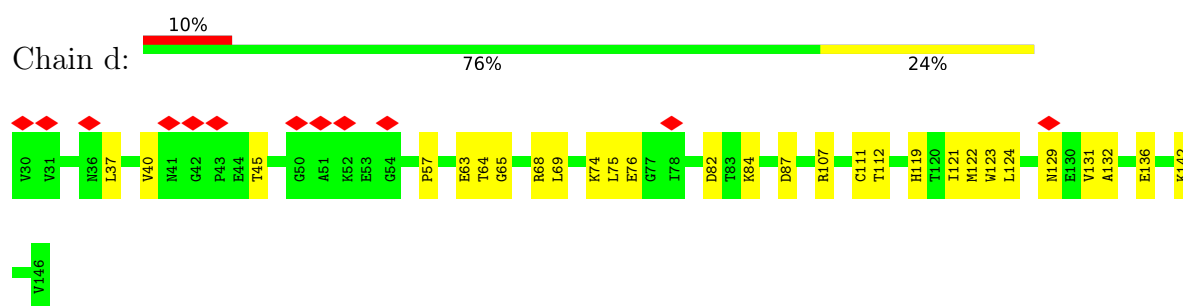
• Molecule 2: Cytochrome c oxidase subunit 2



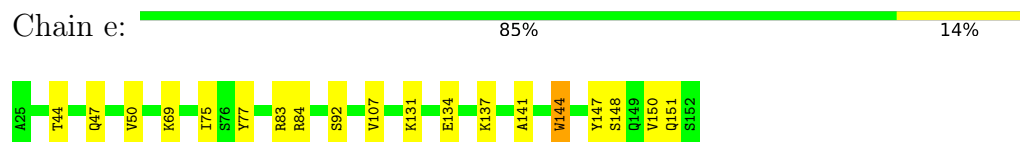
• Molecule 3: Cytochrome c oxidase subunit 3



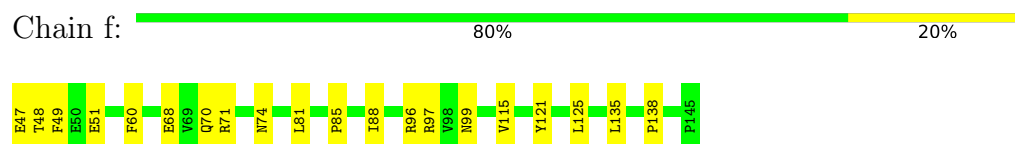
• Molecule 4: Cytochrome c oxidase subunit 4, mitochondrial



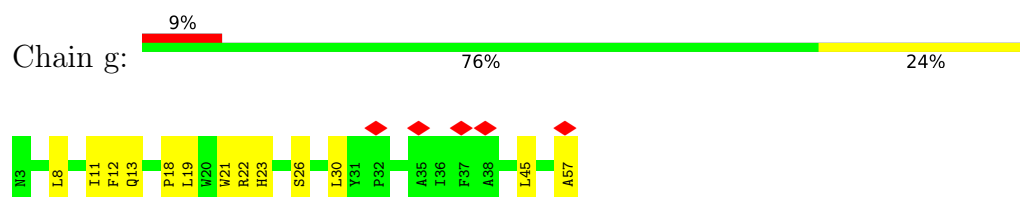
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



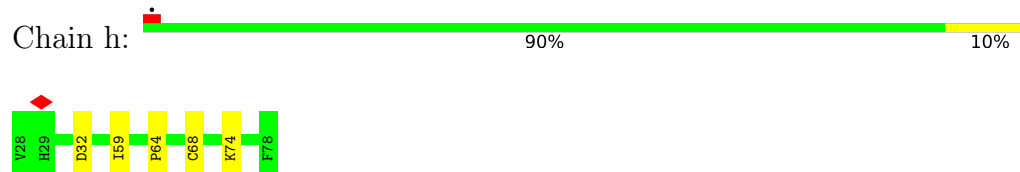
- Molecule 6: Cytochrome c oxidase subunit 6, mitochondrial



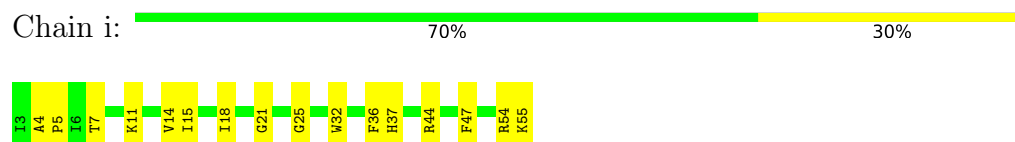
- Molecule 7: Cytochrome c oxidase subunit 7, mitochondrial



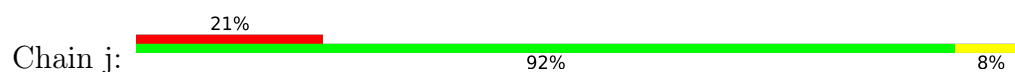
- Molecule 8: Cytochrome c oxidase subunit 8, mitochondrial



- Molecule 9: Cytochrome c oxidase subunit 9, mitochondrial

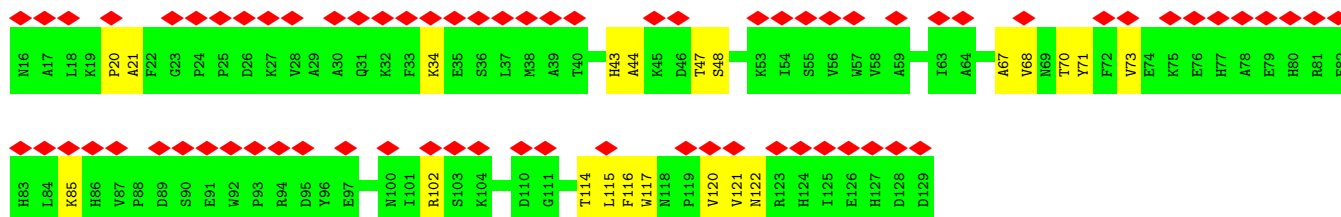
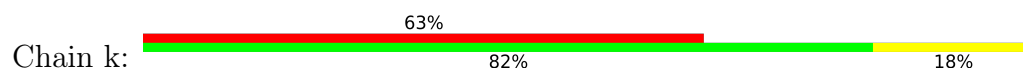


- Molecule 10: Cytochrome c oxidase subunit 12, mitochondrial





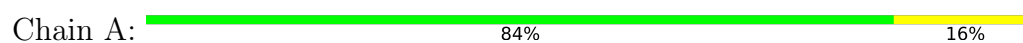
- Molecule 11: Cytochrome c oxidase subunit 13, mitochondrial



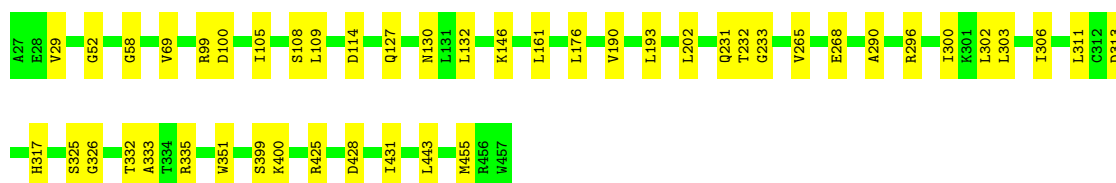
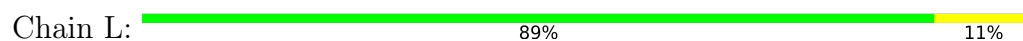
- Molecule 12: Cytochrome c oxidase subunit 26, mitochondrial



- Molecule 13: Cytochrome b-c1 complex subunit 1, mitochondrial

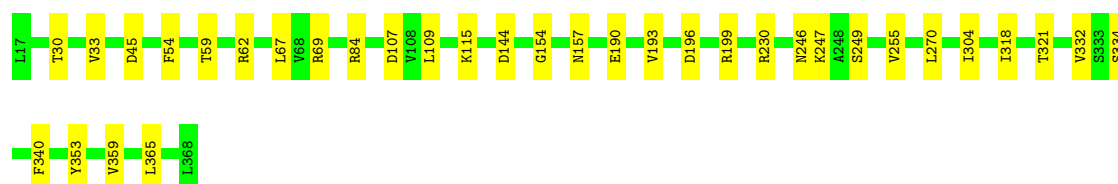


- Molecule 13: Cytochrome b-c1 complex subunit 1, mitochondrial



- Molecule 14: Cytochrome b-c1 complex subunit 2, mitochondrial





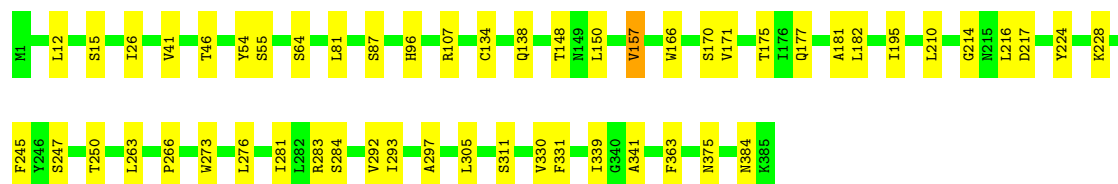
- Molecule 14: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain M: 91% 9%



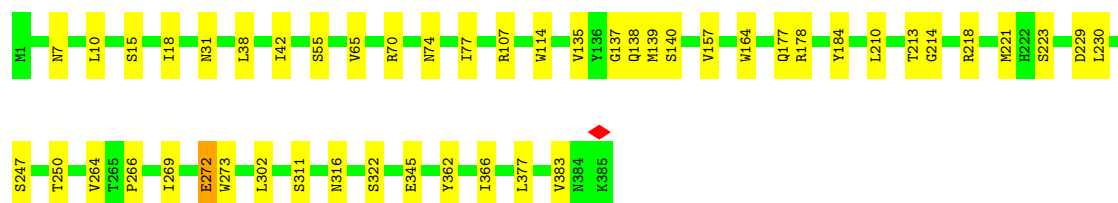
- Molecule 15: Cytochrome b

Chain C: 86% 14%



- Molecule 15: Cytochrome b

Chain N: 88% 12%



- Molecule 16: Cytochrome c1, heme protein, mitochondrial

Chain D: 89% 11%

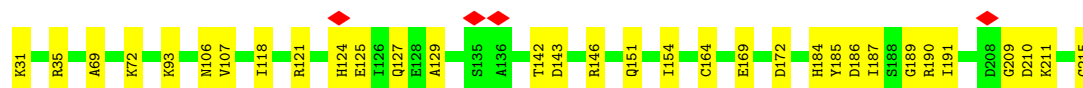
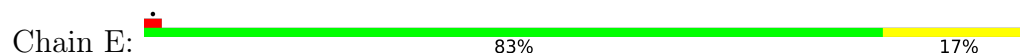


- Molecule 16: Cytochrome c1, heme protein, mitochondrial

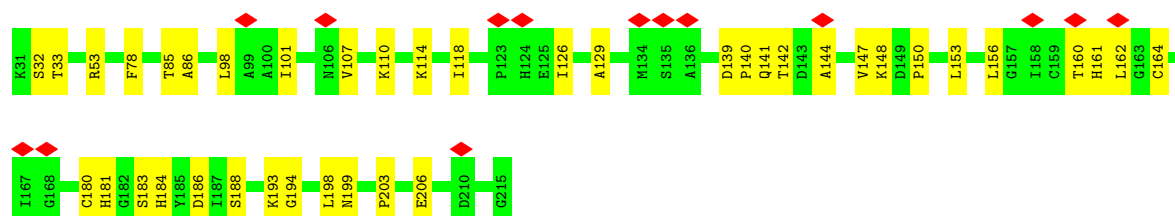
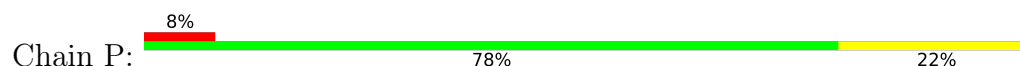
Chain O: 88% 12%



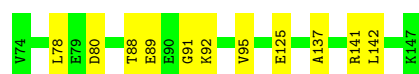
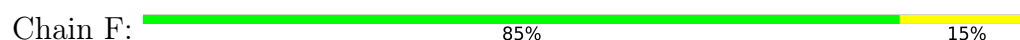
- Molecule 17: Cytochrome b-c1 complex subunit Rieske, mitochondrial



- Molecule 17: Cytochrome b-c1 complex subunit Rieske, mitochondrial



- Molecule 18: Cytochrome b-c1 complex subunit 6, mitochondrial



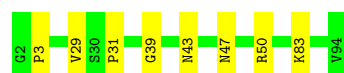
- Molecule 19: Cytochrome b-c1 complex subunit 7, mitochondrial



- Molecule 19: Cytochrome b-c1 complex subunit 7, mitochondrial



- Molecule 20: Cytochrome b-c1 complex subunit 8, mitochondrial



- Molecule 20: Cytochrome b-c1 complex subunit 8, mitochondrial

Chain S:  87% 11%

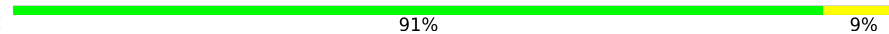


- Molecule 21: Cytochrome b-c1 complex subunit 9, mitochondrial

Chain I:  93% 7%



- Molecule 22: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain Q:  91% 9%

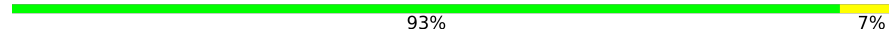


- Molecule 23: Cytochrome b-c1 complex subunit 9, mitochondrial

Chain T:  87% 13%



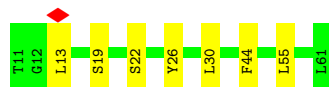
- Molecule 24: Cytochrome b-c1 complex subunit 10, mitochondrial

Chain U:  93% 7%



- Molecule 25: Cytochrome b-c1 complex subunit 10, mitochondrial

Chain V:  86% 14%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	201223	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	-1.4	Depositor
Maximum defocus (nm)	-3.0	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.373	Depositor
Minimum map value	-1.240	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.069	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	392.2, 392.2, 392.2	wwPDB
Map dimensions	370, 370, 370	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0600001, 1.0600001, 1.0600001	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, FES, HEA, 7PH, CN5, 9PE, CU, PTY, HEM, CUA, 6PH, CN3, PCF, UQ6, 8PE

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	a	0.30	0/4254	0.57	4/5811 (0.1%)
2	b	0.24	0/1940	0.51	0/2653
3	c	0.18	0/2210	0.47	1/3026 (0.0%)
4	d	0.25	0/905	0.63	0/1231
5	e	0.35	0/1032	0.63	1/1396 (0.1%)
6	f	0.25	0/845	0.57	2/1143 (0.2%)
7	g	0.21	0/472	0.52	0/645
8	h	0.22	0/423	0.52	0/569
9	i	0.20	0/451	0.42	0/605
10	j	0.19	0/671	0.48	0/910
11	k	0.22	0/974	0.58	0/1324
12	m	0.23	0/319	0.58	0/435
13	A	0.45	0/3405	0.54	1/4615 (0.0%)
13	L	0.43	0/3405	0.50	0/4615
14	B	0.43	0/2781	0.48	0/3764
14	M	0.41	0/2781	0.49	0/3764
15	C	0.48	0/3192	0.51	0/4354
15	N	0.52	0/3192	0.56	3/4354 (0.1%)
16	D	0.43	0/2022	0.47	0/2751
16	O	0.43	0/2022	0.46	0/2751
17	E	0.27	0/1444	0.47	0/1957
17	P	0.26	0/1444	0.45	0/1957
18	F	0.33	0/638	0.48	0/858
19	G	0.44	0/1040	0.54	0/1408
19	R	0.43	0/1040	0.55	0/1408
20	H	0.40	0/804	0.46	0/1088
20	S	0.42	0/804	0.48	0/1088
21	I	0.41	0/455	0.41	0/614
22	Q	0.31	0/647	0.42	0/870
23	T	0.39	0/456	0.42	0/615
24	U	0.32	0/358	0.48	0/483
25	V	0.35	0/419	0.65	0/567

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.38	0/46845	0.52	12/63629 (0.0%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	144	VAL	N-CA-C	-11.80	100.45	111.67
15	N	273	TRP	N-CA-C	8.46	121.56	111.33
1	a	246	ILE	N-CA-C	-8.34	105.79	113.71
15	N	18	ILE	N-CA-C	6.89	117.48	111.56
6	f	115	VAL	CA-C-N	6.03	133.05	121.54
6	f	115	VAL	C-N-CA	6.03	133.05	121.54
15	N	18	ILE	CB-CA-C	-5.82	105.91	111.44
5	e	144	TRP	N-CA-C	-5.80	99.73	109.07
1	a	23	ILE	N-CA-C	-5.52	107.44	112.96
1	a	216	PHE	CA-C-N	5.37	131.79	121.54
1	a	216	PHE	C-N-CA	5.37	131.79	121.54
3	c	241	VAL	N-CA-C	-5.35	107.57	111.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	4126	0	4149	94	0
2	b	1888	0	1867	42	0
3	c	2138	0	2125	65	0
4	d	888	0	883	36	0
5	e	1008	0	990	24	0
6	f	828	0	807	13	0
7	g	456	0	481	9	0
8	h	408	0	408	5	0
9	i	439	0	449	32	0
10	j	649	0	592	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	k	941	0	902	17	0
12	m	308	0	302	5	0
13	A	3344	0	3323	39	0
13	L	3344	0	3323	29	0
14	B	2735	0	2774	20	0
14	M	2735	0	2774	18	0
15	C	3090	0	3129	39	0
15	N	3090	0	3129	33	0
16	D	1961	0	1890	27	0
16	O	1961	0	1890	23	0
17	E	1411	0	1388	22	0
17	P	1411	0	1388	25	0
18	F	624	0	581	7	0
19	G	1019	0	1034	8	0
19	R	1019	0	1034	8	0
20	H	773	0	736	5	0
20	S	773	0	736	11	0
21	I	442	0	440	4	0
22	Q	633	0	587	5	0
23	T	443	0	440	7	0
24	U	347	0	345	3	0
25	V	406	0	414	5	0
26	a	1	0	0	0	0
27	a	120	0	108	7	0
28	D	32	0	37	39	0
28	a	34	0	41	11	0
28	b	35	0	39	2	0
28	c	40	0	51	40	0
28	i	40	0	53	18	0
28	m	71	0	88	29	0
29	N	55	0	66	2	0
29	a	55	0	66	1	0
30	b	2	0	0	0	0
31	I	35	0	44	1	0
31	T	35	0	44	2	0
31	c	43	0	60	1	0
31	e	36	0	46	8	0
31	m	38	0	50	1	0
32	d	1	0	0	0	0
33	C	40	0	59	0	0
33	O	40	0	59	4	0
34	C	86	0	60	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	D	43	0	30	3	0
34	N	86	0	60	1	0
34	O	43	0	30	3	0
35	C	47	0	73	2	0
35	N	47	0	73	2	0
36	C	41	0	50	2	0
37	C	43	0	58	2	0
37	N	43	0	58	0	0
38	C	40	0	59	0	0
38	N	40	0	59	0	0
39	E	38	0	55	2	0
39	O	38	0	55	4	0
40	E	4	0	0	1	0
40	P	4	0	0	2	0
All	All	47034	0	46941	651	0

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

All (651) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:241:HIS:NE2	1:a:245:TYR:CE2	1.81	1.48
1:a:241:HIS:NE2	1:a:245:TYR:HE2	0.94	1.44
3:c:91:PHE:CE1	28:c:301:PTY:H151	1.59	1.35
1:a:241:HIS:CE1	1:a:245:TYR:CE2	2.15	1.33
1:a:534:SER:HB2	4:d:112:THR:CG2	1.65	1.23
20:S:36:PRO:O	20:S:37:LEU:HD12	1.36	1.23
9:i:36:PHE:CZ	28:m:101:PTY:H111	1.75	1.20
1:a:241:HIS:CE1	1:a:245:TYR:HE2	1.56	1.14
1:a:532:VAL:CG2	4:d:107:ARG:HH12	1.60	1.13
9:i:11:LYS:CE	28:i:101:PTY:O12	1.96	1.12
3:c:59:LEU:HD21	28:c:301:PTY:H401	1.14	1.11
28:m:102:PTY:H171	28:m:102:PTY:H132	1.14	1.09
2:b:161:LEU:HD11	2:b:218:TYR:HB3	1.16	1.09
1:a:534:SER:HB2	4:d:112:THR:HG23	1.13	1.08
9:i:15:ILE:HD11	28:i:101:PTY:H322	1.34	1.08
1:a:532:VAL:CG2	4:d:107:ARG:NH1	2.16	1.07
16:D:82:PHE:CZ	28:D:402:PTY:H201	1.92	1.04
3:c:59:LEU:HD21	28:c:301:PTY:C40	1.89	1.02
3:c:59:LEU:CD2	28:c:301:PTY:H401	1.91	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:m:101:PTY:C40	28:m:102:PTY:H312	1.93	0.98
20:S:36:PRO:O	20:S:37:LEU:CD1	2.12	0.97
9:i:11:LYS:HE2	28:i:101:PTY:O12	1.65	0.97
3:c:241:VAL:N	28:c:301:PTY:O13	1.98	0.96
3:c:91:PHE:CE1	28:c:301:PTY:C15	2.48	0.96
9:i:15:ILE:HD11	28:i:101:PTY:C32	1.96	0.95
16:D:82:PHE:CE1	28:D:402:PTY:H202	2.01	0.94
3:c:91:PHE:CZ	28:c:301:PTY:H151	2.03	0.93
28:a:604:PTY:H171	28:c:301:PTY:H182	1.50	0.92
1:a:534:SER:CB	4:d:112:THR:CG2	2.50	0.90
15:N:272:GLU:N	15:N:272:GLU:OE1	2.06	0.89
28:m:102:PTY:C33	28:m:102:PTY:H182	2.02	0.89
16:D:82:PHE:CE1	28:D:402:PTY:C20	2.57	0.88
28:D:402:PTY:H201	28:D:402:PTY:H161	1.55	0.88
28:D:402:PTY:HC6	28:D:402:PTY:H121	1.56	0.85
9:i:11:LYS:NZ	28:i:101:PTY:O12	2.10	0.85
9:i:36:PHE:CE1	28:m:101:PTY:H111	2.13	0.84
2:b:161:LEU:CD1	2:b:218:TYR:HB3	2.06	0.83
1:a:532:VAL:HG23	4:d:107:ARG:NH1	1.93	0.83
3:c:74:THR:OG1	28:c:301:PTY:HC22	1.78	0.83
2:b:81:ILE:HD12	28:i:101:PTY:H311	1.60	0.83
28:m:102:PTY:H132	28:m:102:PTY:C17	2.06	0.83
1:a:532:VAL:HG22	4:d:107:ARG:HH12	1.44	0.82
16:D:82:PHE:CZ	28:D:402:PTY:C20	2.62	0.82
3:c:229:ARG:HH22	28:c:301:PTY:HC51	1.46	0.81
9:i:15:ILE:CD1	28:i:101:PTY:H321	2.12	0.80
28:m:102:PTY:H171	28:m:102:PTY:C13	2.02	0.80
9:i:15:ILE:CD1	28:i:101:PTY:C32	2.60	0.80
1:a:241:HIS:HE2	1:a:245:TYR:HE2	0.81	0.79
1:a:534:SER:CB	4:d:112:THR:HG23	2.05	0.79
28:D:402:PTY:H162	28:D:402:PTY:H122	1.65	0.79
28:D:402:PTY:H162	28:D:402:PTY:C12	2.14	0.78
2:b:20:PRO:CB	5:e:151:GLN:OE1	2.32	0.78
1:a:532:VAL:HG23	4:d:107:ARG:CZ	2.13	0.78
3:c:91:PHE:CZ	28:c:301:PTY:C15	2.66	0.78
2:b:20:PRO:HB3	5:e:151:GLN:OE1	1.84	0.77
28:D:402:PTY:C20	28:D:402:PTY:H161	2.14	0.77
16:D:82:PHE:HE1	28:D:402:PTY:H202	1.48	0.77
3:c:59:LEU:HD11	28:c:301:PTY:C40	2.16	0.75
28:D:402:PTY:H321	28:D:402:PTY:H131	1.68	0.75
1:a:534:SER:HB2	4:d:112:THR:HG21	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:59:LEU:HD11	28:c:301:PTY:H402	1.67	0.74
1:a:532:VAL:HG21	4:d:107:ARG:HH12	1.52	0.73
1:a:532:VAL:HG22	4:d:107:ARG:NH1	2.01	0.73
28:D:402:PTY:H111	28:D:402:PTY:C17	2.19	0.73
5:e:151:GLN:O	5:e:151:GLN:HG3	1.88	0.72
1:a:181:LYS:HE3	1:a:533:GLN:HE22	1.56	0.71
28:m:102:PTY:H311	28:m:102:PTY:C18	2.19	0.71
3:c:66:PHE:CE1	28:c:301:PTY:H322	2.25	0.71
28:a:604:PTY:C17	28:c:301:PTY:H182	2.19	0.70
1:a:241:HIS:NE2	1:a:245:TYR:CD2	2.57	0.70
3:c:229:ARG:HH22	28:c:301:PTY:C5	2.05	0.70
1:a:273:MET:HE2	1:a:322:SER:HB2	1.74	0.69
28:a:604:PTY:H171	28:c:301:PTY:C18	2.23	0.69
2:b:57:MET:HE3	28:i:101:PTY:H192	1.75	0.69
28:m:101:PTY:C40	28:m:101:PTY:H362	2.23	0.68
9:i:36:PHE:CE1	28:m:101:PTY:C11	2.76	0.67
6:f:96:ARG:HH21	6:f:99:ASN:HD22	1.42	0.66
1:a:175:ASN:HD22	4:d:84:LYS:H	1.43	0.66
3:c:222:MET:HG3	28:c:301:PTY:H351	1.78	0.66
28:a:604:PTY:H111	28:c:301:PTY:C13	2.26	0.65
9:i:36:PHE:CZ	28:m:101:PTY:C11	2.68	0.65
28:D:402:PTY:H111	28:D:402:PTY:H171	1.79	0.65
28:b:302:PTY:O10	5:e:92:SER:OG	2.15	0.64
9:i:15:ILE:HD13	28:i:101:PTY:H321	1.77	0.64
2:b:20:PRO:HB2	5:e:151:GLN:OE1	1.98	0.64
28:D:402:PTY:H162	28:D:402:PTY:C11	2.27	0.64
16:D:82:PHE:CE1	28:D:402:PTY:H201	2.28	0.64
17:E:210:ASP:O	17:E:211:LYS:HD2	1.97	0.63
17:P:129:ALA:HB1	17:P:188:SER:HB3	1.80	0.63
17:P:126:ILE:HG12	17:P:150:PRO:HB2	1.80	0.63
15:C:41:VAL:HG22	37:C:406:UQ6:H18	1.81	0.63
28:D:402:PTY:H162	28:D:402:PTY:H111	1.80	0.63
14:M:30:THR:HG22	14:M:92:THR:HG22	1.81	0.62
14:M:40:ARG:HD3	14:M:85:GLU:HG2	1.81	0.62
28:m:102:PTY:H182	28:m:102:PTY:H311	1.81	0.62
3:c:66:PHE:CZ	28:c:301:PTY:H322	2.34	0.62
3:c:216:MET:HE1	3:c:253:LEU:HD11	1.81	0.62
28:m:102:PTY:H131	28:m:102:PTY:O7	2.00	0.62
2:b:161:LEU:HD12	2:b:161:LEU:O	2.00	0.61
28:D:402:PTY:H161	28:D:402:PTY:C21	2.29	0.61
16:O:181:VAL:HG21	16:O:256:ASN:HA	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:D:402:PTY:H111	28:D:402:PTY:C16	2.31	0.60
1:a:181:LYS:HE3	1:a:533:GLN:NE2	2.16	0.60
1:a:532:VAL:CG2	4:d:107:ARG:CZ	2.74	0.60
28:a:604:PTY:H111	28:c:301:PTY:H131	1.83	0.60
16:D:188:CYS:SG	16:D:256:ASN:ND2	2.75	0.60
1:a:37:ARG:NH2	27:a:602:HEA:OMA	2.34	0.60
13:A:443:LEU:HD13	13:A:447:ARG:HE	1.67	0.59
5:e:148:SER:O	5:e:150:VAL:HG23	2.02	0.59
1:a:241:HIS:CE1	1:a:245:TYR:CZ	2.88	0.59
28:D:402:PTY:H131	28:D:402:PTY:C32	2.31	0.59
2:b:161:LEU:HD11	2:b:218:TYR:CB	2.11	0.59
3:c:59:LEU:CG	28:c:301:PTY:H401	2.33	0.58
15:N:107:ARG:NH2	15:N:311:SER:O	2.36	0.58
16:O:77:SER:O	23:T:47:LYS:NZ	2.36	0.58
31:e:201:PCF:H242	28:D:402:PTY:O30	2.02	0.58
36:C:405:CN5:H3E	33:O:401:6PH:H2B	1.85	0.58
13:L:99:ARG:NH2	13:L:176:LEU:O	2.37	0.58
14:M:162:ASP:OD1	14:M:162:ASP:N	2.37	0.58
31:e:201:PCF:C23	28:D:402:PTY:O30	2.52	0.58
9:i:36:PHE:HZ	28:m:101:PTY:H111	1.56	0.58
28:D:402:PTY:H171	28:D:402:PTY:C11	2.34	0.58
6:f:60:PHE:O	6:f:97:ARG:NH1	2.37	0.57
16:D:224:ALA:HB3	34:D:401:HEM:HBD2	1.86	0.57
2:b:43:ILE:HA	2:b:96:ILE:HD11	1.85	0.57
28:D:402:PTY:HC31	28:D:402:PTY:C5	2.34	0.57
12:m:54:PRO:C	28:m:101:PTY:H312	2.29	0.57
13:L:313:ASP:OD2	13:L:335:ARG:NH2	2.37	0.57
15:C:55:SER:OG	15:N:177:GLN:NE2	2.37	0.57
13:A:70:SER:OG	13:A:102:GLN:NE2	2.38	0.57
7:g:23:HIS:HB3	7:g:26:SER:HB3	1.87	0.57
31:e:201:PCF:H262	28:D:402:PTY:H311	1.85	0.56
13:A:349:LYS:NZ	13:A:451:ASP:OD1	2.38	0.56
28:D:402:PTY:H321	28:D:402:PTY:C13	2.35	0.56
15:C:81:LEU:HD11	39:E:301:7PH:H28A	1.88	0.56
15:C:247:SER:HG	15:C:250:THR:HG1	1.50	0.56
18:F:88:THR:HG23	18:F:91:GLY:H	1.70	0.56
14:M:260:LEU:HD22	14:M:267:LEU:HD11	1.88	0.56
15:C:245:PHE:O	16:D:266:ARG:NH2	2.38	0.56
15:N:70:ARG:NH1	16:O:258:CYS:O	2.37	0.56
1:a:533:GLN:HB2	4:d:123:TRP:CH2	2.40	0.56
28:b:302:PTY:O10	28:b:302:PTY:HC52	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:i:32:TRP:HD1	28:m:102:PTY:H321	1.71	0.56
14:B:154:GLY:O	14:B:157:ASN:ND2	2.38	0.56
17:P:186:ASP:OD1	17:P:186:ASP:N	2.39	0.56
1:a:175:ASN:ND2	4:d:82:ASP:OD2	2.39	0.56
12:m:52:GLY:HA3	28:m:102:PTY:H152	1.87	0.56
13:A:317:HIS:HE1	13:A:351:TRP:HE1	1.54	0.56
15:C:148:THR:OG1	15:C:166:TRP:NE1	2.35	0.56
2:b:32:ASN:ND2	2:b:107:CYS:SG	2.79	0.56
2:b:213:ARG:NH2	5:e:141:ALA:O	2.37	0.56
13:L:325:SER:OG	13:L:326:GLY:N	2.38	0.56
13:A:140:THR:O	13:A:144:VAL:HG23	2.05	0.55
31:e:201:PCF:C24	28:D:402:PTY:O30	2.55	0.55
31:e:201:PCF:H262	28:D:402:PTY:O30	2.06	0.55
15:N:65:VAL:HG21	15:N:135:VAL:HG23	1.87	0.55
13:L:202:LEU:HA	13:L:231:GLN:HB2	1.88	0.55
16:O:200:ASP:OD1	16:O:200:ASP:N	2.40	0.55
13:A:99:ARG:NH2	13:A:176:LEU:O	2.39	0.55
17:E:121:ARG:N	17:E:151:GLN:O	2.40	0.55
28:D:402:PTY:C21	28:D:402:PTY:H172	2.36	0.55
3:c:221:ALA:CB	28:c:301:PTY:C41	2.84	0.55
9:i:15:ILE:CD1	28:i:101:PTY:H352	2.37	0.55
13:A:252:ARG:NH1	13:A:254:ASP:OD1	2.36	0.55
2:b:29:ALA:HB2	2:b:213:ARG:HH11	1.72	0.55
5:e:77:TYR:OH	6:f:70:GLN:NE2	2.40	0.55
23:T:23:ALA:HB2	24:U:39:LEU:HD13	1.88	0.55
1:a:349:THR:HG21	2:b:54:VAL:HG11	1.89	0.54
1:a:173:ARG:NH1	1:a:179:MET:SD	2.79	0.54
13:A:144:VAL:O	13:A:147:GLN:N	2.40	0.54
1:a:218:THR:O	3:c:203:SER:OG	2.25	0.54
16:D:230:PHE:H	16:D:233:MET:HE3	1.71	0.54
15:N:139:MET:HE1	15:N:269:ILE:HA	1.89	0.54
1:a:83:LEU:HB3	1:a:87:MET:HE2	1.89	0.54
28:D:402:PTY:C21	28:D:402:PTY:C16	2.86	0.54
28:D:402:PTY:C5	28:D:402:PTY:C3	2.85	0.54
2:b:155:GLU:HG2	5:e:131:LYS:HD2	1.90	0.54
3:c:218:MET:SD	28:c:301:PTY:H402	2.48	0.54
13:L:300:ILE:HG22	13:L:302:LEU:H	1.73	0.54
13:A:428:ASP:O	13:A:449:ARG:NH1	2.40	0.54
28:D:402:PTY:C17	28:D:402:PTY:C21	2.85	0.54
14:M:63:SER:OG	14:M:64:ALA:N	2.41	0.54
1:a:120:GLU:HG3	8:h:74:LYS:HZ3	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:m:101:PTY:HC51	28:m:102:PTY:HC32	1.90	0.54
13:A:252:ARG:HH12	13:A:440:GLU:HB2	1.72	0.54
14:B:84:ARG:NH2	14:B:144:ASP:OD1	2.40	0.54
15:C:177:GLN:NE2	15:N:55:SER:OG	2.41	0.54
17:E:186:ASP:OD2	17:E:190:ARG:NH2	2.40	0.54
13:L:303:LEU:HA	13:L:306:ILE:HG22	1.89	0.54
17:P:142:THR:HG23	17:P:144:ALA:H	1.72	0.54
1:a:314:ILE:HD13	2:b:89:PRO:HB2	1.90	0.54
28:a:604:PTY:H111	28:c:301:PTY:H132	1.90	0.54
6:f:68:GLU:HA	6:f:71:ARG:HG2	1.90	0.54
1:a:533:GLN:HG3	4:d:121:ILE:HD11	1.90	0.53
9:i:11:LYS:HE3	28:i:101:PTY:O12	2.01	0.53
13:A:325:SER:OG	13:A:326:GLY:N	2.41	0.53
1:a:456:ILE:HG21	31:m:103:PCF:H332	1.90	0.53
5:e:50:VAL:HG12	5:e:75:ILE:HD13	1.89	0.53
12:m:52:GLY:CA	28:m:102:PTY:H152	2.38	0.53
13:L:29:VAL:HG21	13:L:400:LYS:HB3	1.89	0.53
16:O:83:GLU:HA	23:T:44:ASN:HD21	1.72	0.53
1:a:116:SER:HB2	1:a:146:LEU:HB2	1.91	0.53
1:a:499:GLU:O	5:e:83:ARG:NH2	2.41	0.53
1:a:532:VAL:HG23	4:d:107:ARG:NH2	2.24	0.53
13:A:165:HIS:NE2	13:A:322:TYR:OH	2.37	0.53
13:A:306:ILE:HA	13:A:311:LEU:HD12	1.89	0.53
15:C:375:ASN:HD22	19:G:3:GLN:HG2	1.73	0.53
17:E:185:TYR:HE1	17:E:191:ILE:HG22	1.72	0.53
13:A:98:SER:OG	13:A:99:ARG:N	2.41	0.53
13:A:352:ASN:ND2	13:A:452:MET:O	2.42	0.53
13:L:100:ASP:OD1	13:L:100:ASP:N	2.37	0.53
2:b:176:ARG:NH2	10:j:12:VAL:O	2.41	0.53
3:c:184:CYS:HA	3:c:187:ILE:HD12	1.90	0.53
13:L:108:SER:OG	13:L:109:LEU:N	2.40	0.53
14:M:56:PHE:H	14:M:108:VAL:HG21	1.73	0.53
11:k:70:THR:HA	11:k:73:VAL:HG22	1.91	0.53
35:N:404:8PE:H1A	20:S:55:GLN:HG2	1.90	0.53
17:P:148:LYS:NZ	17:P:206:GLU:OE1	2.42	0.53
1:a:496:ASP:OD2	6:f:74:ASN:ND2	2.42	0.53
3:c:151:THR:HA	3:c:154:TYR:HB3	1.90	0.53
3:c:236:THR:HA	4:d:57:PRO:HG2	1.91	0.53
14:B:332:VAL:HG23	14:B:334:SER:H	1.73	0.53
13:L:265:VAL:HG12	13:L:431:ILE:HG22	1.91	0.53
16:O:224:ALA:HB3	34:O:402:HEM:HBD2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:119:VAL:HG21	1:a:142:PRO:HG2	1.91	0.53
1:a:434:ASN:HD21	2:b:22:ALA:HB3	1.73	0.53
15:C:87:SER:OG	15:C:273:TRP:NE1	2.35	0.53
16:D:273:THR:HG23	39:E:301:7PH:H32	1.91	0.53
28:D:402:PTY:C11	28:D:402:PTY:C16	2.85	0.53
13:L:132:LEU:HD22	13:L:190:VAL:HG13	1.91	0.53
1:a:381:LEU:HD13	27:a:602:HEA:HAC	1.90	0.52
4:d:64:THR:O	7:g:13:GLN:NE2	2.43	0.52
14:M:231:VAL:HB	14:M:356:VAL:HG22	1.91	0.52
31:e:201:PCF:H232	28:D:402:PTY:O30	2.09	0.52
13:A:247:SER:OG	13:A:248:GLU:N	2.43	0.52
15:N:316:ASN:ND2	15:N:322:SER:O	2.43	0.52
3:c:242:GLY:HA3	28:c:301:PTY:HC52	1.92	0.52
9:i:15:ILE:HD12	28:i:101:PTY:H352	1.90	0.52
14:M:35:VAL:HG12	14:M:185:LEU:HB3	1.92	0.52
2:b:22:ALA:HA	28:m:101:PTY:O13	2.08	0.52
2:b:132:ASP:OD2	2:b:132:ASP:N	2.41	0.52
5:e:69:LYS:HD3	6:f:138:PRO:HG3	1.92	0.52
11:k:85:LYS:HB3	11:k:120:VAL:HG12	1.91	0.52
15:N:272:GLU:H	15:N:272:GLU:CD	2.16	0.52
15:N:137:GLY:H	15:N:140:SER:HB3	1.75	0.52
5:e:134:GLU:HA	5:e:137:LYS:HB3	1.92	0.52
1:a:397:SER:OG	1:a:475:GLN:NE2	2.36	0.51
28:m:102:PTY:H311	28:m:102:PTY:H181	1.92	0.51
17:E:124:HIS:O	17:E:127:GLN:NE2	2.42	0.51
16:O:273:THR:HG23	39:O:403:7PH:H32	1.93	0.51
2:b:198:ASP:OD2	2:b:205:ASN:ND2	2.44	0.51
14:B:196:ASP:OD1	14:B:199:ARG:NH2	2.40	0.51
3:c:91:PHE:CZ	28:c:301:PTY:H152	2.44	0.51
15:C:15:SER:HB3	20:S:3:PRO:HG3	1.93	0.51
3:c:63:ILE:HA	3:c:66:PHE:HB2	1.92	0.51
14:B:45:ASP:OD2	14:M:232:ARG:NH1	2.40	0.51
16:D:293:ALA:HB3	20:H:31:PRO:HB3	1.92	0.51
16:O:265:GLU:OE2	16:O:268:ARG:NH2	2.39	0.51
13:A:290:ALA:O	13:A:296:ARG:NH2	2.44	0.51
19:R:53:ASN:OD1	19:R:53:ASN:N	2.44	0.51
1:a:465:LEU:HD13	27:a:602:HEA:H261	1.92	0.51
14:M:249:SER:O	14:M:249:SER:OG	2.28	0.51
4:d:111:CYS:O	4:d:119:HIS:NE2	2.39	0.51
4:d:124:LEU:HD22	4:d:132:ALA:HB1	1.93	0.51
28:m:101:PTY:O10	28:m:101:PTY:HC52	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:86:ASP:HB3	16:O:89:SER:HB3	1.92	0.51
1:a:229:PRO:HB2	2:b:185:ILE:HD11	1.93	0.51
14:B:230:ARG:NH1	14:B:359:VAL:O	2.45	0.51
17:E:121:ARG:HD2	17:E:187:ILE:HG13	1.93	0.51
2:b:136:ASP:OD1	2:b:136:ASP:N	2.44	0.50
15:C:217:ASP:OD1	16:D:298:ARG:NH1	2.43	0.50
15:N:218:ARG:NH2	20:S:10:MET:SD	2.83	0.50
7:g:19:LEU:HD12	7:g:22:ARG:HD2	1.93	0.50
16:O:188:CYS:SG	16:O:256:ASN:ND2	2.84	0.50
2:b:162:ASP:OD1	2:b:235:LYS:NZ	2.44	0.50
15:C:330:VAL:HG13	35:C:404:8PE:H3CA	1.92	0.50
2:b:180:THR:OG1	2:b:181:ALA:N	2.45	0.50
12:m:54:PRO:O	28:m:101:PTY:H312	2.11	0.50
14:B:30:THR:HB	14:B:190:GLU:HB3	1.92	0.50
18:F:137:ALA:O	18:F:141:ARG:NH1	2.43	0.50
15:N:31:ASN:ND2	15:N:229:ASP:OD1	2.44	0.50
15:N:247:SER:OG	15:N:250:THR:OG1	2.27	0.50
15:C:107:ARG:NH1	15:C:311:SER:O	2.36	0.50
17:E:69:ALA:HA	21:I:29:GLN:HE21	1.76	0.50
18:F:92:LYS:HA	18:F:95:VAL:HG12	1.94	0.50
16:D:166:ARG:NH2	16:D:171:GLY:O	2.44	0.50
19:G:53:ASN:OD1	19:G:53:ASN:N	2.35	0.50
16:O:181:VAL:HG12	16:O:191:ILE:HG13	1.94	0.50
17:P:183:SER:HA	17:P:194:GLY:HA3	1.94	0.50
13:A:53:VAL:HG12	13:A:208:VAL:HG22	1.94	0.49
13:L:428:ASP:O	17:P:53:ARG:NH2	2.45	0.49
2:b:93:LEU:HA	2:b:96:ILE:HG22	1.94	0.49
7:g:8:LEU:HD23	7:g:11:ILE:HD12	1.94	0.49
35:N:404:8PE:H22	20:S:59:VAL:HG21	1.95	0.49
29:N:406:CN3:H2'	29:N:406:CN3:H55	1.93	0.49
28:m:101:PTY:C40	28:m:102:PTY:C31	2.80	0.49
3:c:229:ARG:NH2	28:c:301:PTY:HC51	2.23	0.49
13:L:268:GLU:OE2	13:L:425:ARG:NE	2.43	0.49
1:a:87:MET:HE1	1:a:185:PHE:HB3	1.95	0.49
16:D:194:LEU:HD12	16:D:215:ASN:HD21	1.77	0.49
13:L:317:HIS:HE1	13:L:351:TRP:HE1	1.59	0.49
2:b:216:VAL:HA	2:b:237:GLU:HA	1.93	0.49
6:f:48:THR:HG23	6:f:51:GLU:H	1.77	0.49
15:C:210:LEU:HD21	19:G:82:GLU:HG3	1.94	0.49
19:R:122:ASN:HB3	25:V:13:LEU:HB3	1.94	0.49
17:E:125:GLU:HB3	17:E:187:ILE:HG21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:107:VAL:HB	17:P:118:ILE:HB	1.94	0.49
2:b:74:TYR:OH	4:d:136:GLU:OE2	2.28	0.49
11:k:114:THR:OG1	11:k:115:LEU:N	2.46	0.49
16:D:147:ARG:NH1	16:D:153:ASP:OD2	2.46	0.49
17:P:184:HIS:N	17:P:193:LYS:O	2.43	0.49
20:S:36:PRO:O	20:S:37:LEU:CG	2.61	0.49
6:f:81:LEU:HB3	9:i:7:THR:HG23	1.95	0.49
5:e:144:TRP:CZ2	9:i:44:ARG:HG3	2.48	0.48
13:A:313:ASP:OD2	13:A:335:ARG:NH2	2.46	0.48
15:C:170:SER:OG	15:C:171:VAL:N	2.46	0.48
13:L:114:ASP:N	13:L:114:ASP:OD1	2.45	0.48
31:c:302:PCF:H151	11:k:122:ASN:HD21	1.78	0.48
13:A:127:GLN:OE1	13:A:130:ASN:ND2	2.46	0.48
14:B:255:VAL:HG22	14:B:321:THR:HG21	1.95	0.48
13:L:127:GLN:OE1	13:L:130:ASN:ND2	2.47	0.48
17:P:183:SER:OG	40:P:301:FES:S1	2.65	0.48
9:i:21:GLY:O	9:i:25:GLY:N	2.47	0.48
15:C:166:TRP:O	15:C:175:THR:OG1	2.28	0.48
15:N:138:GLN:HG3	15:N:266:PRO:HG3	1.94	0.48
15:N:383:VAL:HG22	19:R:101:PRO:HG3	1.94	0.48
17:P:32:SER:OG	17:P:33:THR:N	2.45	0.48
9:i:14:VAL:HG21	28:i:101:PTY:H131	1.95	0.48
20:H:47:ASN:OD1	20:H:50:ARG:NH1	2.45	0.48
1:a:533:GLN:HB2	4:d:123:TRP:HH2	1.77	0.48
3:c:187:ILE:O	3:c:191:ASN:N	2.46	0.48
13:A:72:LEU:HD23	13:A:193:LEU:HD21	1.96	0.48
17:E:172:ASP:OD1	17:E:184:HIS:NE2	2.47	0.48
1:a:532:VAL:CG2	4:d:107:ARG:NH2	2.77	0.48
3:c:157:HIS:HB3	11:k:44:ALA:HA	1.96	0.48
28:D:402:PTY:C20	28:D:402:PTY:C16	2.85	0.48
28:a:604:PTY:H372	28:c:301:PTY:H211	1.96	0.47
4:d:65:GLY:O	4:d:69:LEU:N	2.46	0.47
17:E:186:ASP:OD1	17:E:190:ARG:N	2.48	0.47
4:d:37:LEU:HD22	4:d:76:GLU:HG3	1.96	0.47
7:g:8:LEU:HD13	7:g:12:PHE:HE2	1.79	0.47
17:E:31:LYS:NZ	17:E:35:ARG:O	2.47	0.47
17:E:121:ARG:NH2	17:E:143:ASP:OD1	2.43	0.47
15:N:74:ASN:HB3	15:N:77:ILE:HD12	1.96	0.47
3:c:235:LEU:CD2	28:c:301:PTY:O12	2.62	0.47
13:A:289:ASN:O	13:A:295:SER:OG	2.32	0.47
16:D:147:ARG:HH22	16:D:150:LYS:HG2	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:84:THR:OG1	16:O:264:ASP:OD1	2.32	0.47
28:m:102:PTY:C33	28:m:102:PTY:C18	2.86	0.47
10:j:36:LYS:NZ	10:j:79:ASP:O	2.44	0.47
1:a:231:LEU:HD13	3:c:111:HIS:CG	2.50	0.47
13:A:232:THR:OG1	13:A:233:GLY:N	2.48	0.47
1:a:84:LEU:HD11	1:a:186:VAL:HA	1.97	0.47
2:b:185:ILE:HG12	2:b:201:PRO:HD3	1.97	0.47
3:c:263:VAL:HA	3:c:267:TRP:HB3	1.96	0.47
13:A:41:GLU:HB3	13:A:211:THR:HG23	1.95	0.47
22:Q:78:LEU:HD13	22:Q:142:LEU:HD22	1.96	0.47
28:D:402:PTY:C12	28:D:402:PTY:C16	2.90	0.47
17:P:101:ILE:HD12	17:P:107:VAL:HG21	1.95	0.46
5:e:151:GLN:O	5:e:151:GLN:CG	2.59	0.46
14:B:249:SER:O	14:B:249:SER:OG	2.28	0.46
16:D:292:TRP:HZ3	19:G:83:LEU:HD11	1.79	0.46
3:c:230:MET:HG3	3:c:235:LEU:HD12	1.96	0.46
34:D:401:HEM:HBC2	34:D:401:HEM:HHD	1.96	0.46
14:M:252:GLN:HE21	14:M:346:PHE:HD1	1.63	0.46
3:c:157:HIS:HB2	11:k:48:SER:HB2	1.97	0.46
18:F:125:GLU:HB2	20:H:83:LYS:HD3	1.98	0.46
13:L:58:GLY:N	13:L:100:ASP:O	2.48	0.46
16:O:92:ARG:NH2	16:O:250:ASP:OD2	2.48	0.46
6:f:48:THR:OG1	6:f:49:PHE:N	2.49	0.46
9:i:54:ARG:O	9:i:55:LYS:NZ	2.43	0.46
11:k:120:VAL:HG23	11:k:121:VAL:HG13	1.98	0.46
28:m:101:PTY:C40	28:m:101:PTY:C36	2.85	0.46
13:A:41:GLU:OE2	13:A:400:LYS:NZ	2.43	0.46
17:P:147:VAL:HG21	17:P:153:LEU:HD12	1.98	0.46
23:T:4:SER:OG	23:T:5:SER:N	2.46	0.46
3:c:242:GLY:CA	28:c:301:PTY:HC52	2.45	0.46
1:a:288:TRP:H	1:a:305:PHE:HE1	1.64	0.46
1:a:496:ASP:O	5:e:83:ARG:NH2	2.48	0.46
4:d:122:MET:HE3	4:d:122:MET:HB2	1.74	0.46
15:C:195:ILE:HG23	36:C:405:CN5:H3'	1.98	0.46
16:D:84:THR:OG1	16:D:264:ASP:OD1	2.33	0.46
1:a:241:HIS:CD2	1:a:245:TYR:CE2	2.87	0.46
1:a:309:THR:HG23	1:a:359:ALA:HB1	1.97	0.46
17:P:160:THR:HG21	17:P:198:LEU:HB2	1.97	0.46
23:T:5:SER:O	23:T:5:SER:OG	2.31	0.46
1:a:152:HIS:HE1	1:a:204:SER:HA	1.81	0.46
15:C:46:THR:HG21	15:C:81:LEU:HD23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:D:105:HIS:NE2	34:D:401:HEM:NC	2.63	0.46
20:S:71:LYS:HA	20:S:71:LYS:HD3	1.73	0.46
15:C:96:HIS:NE2	34:C:403:HEM:ND	2.63	0.46
16:D:84:THR:OG1	16:D:85:PHE:N	2.49	0.46
16:O:183:ALA:O	16:O:184:ARG:NH2	2.42	0.46
1:a:377:PHE:HD2	1:a:381:LEU:HD12	1.82	0.45
4:d:87:ASP:OD1	4:d:87:ASP:N	2.49	0.45
28:m:102:PTY:C20	28:m:102:PTY:C16	2.94	0.45
16:D:83:GLU:OE1	21:I:47:LYS:NZ	2.44	0.45
15:N:230:LEU:HD13	33:O:401:6PH:H26A	1.98	0.45
31:I:101:PCF:H332	31:I:101:PCF:H361	1.80	0.45
1:a:37:ARG:HH12	1:a:451:ASN:HD22	1.64	0.45
2:b:30:THR:HG22	2:b:32:ASN:H	1.80	0.45
15:C:283:ARG:NH1	15:C:339:ILE:O	2.44	0.45
14:M:83:ASP:HB2	14:M:86:TYR:H	1.81	0.45
2:b:183:ASP:OD1	2:b:183:ASP:N	2.48	0.45
5:e:147:TYR:O	5:e:147:TYR:CD2	2.70	0.45
4:d:40:VAL:O	4:d:45:THR:OG1	2.27	0.45
13:A:144:VAL:O	13:A:145:LEU:C	2.57	0.45
14:M:28:ILE:O	14:M:191:ASN:ND2	2.37	0.45
1:a:73:PRO:O	1:a:78:GLY:N	2.48	0.45
14:B:33:VAL:HG11	14:B:109:LEU:HD11	1.99	0.45
17:P:85:THR:OG1	17:P:86:ALA:N	2.50	0.45
27:a:603:HEA:HHA	27:a:603:HEA:HAD1	1.74	0.45
15:C:311:SER:HA	15:C:375:ASN:HD21	1.80	0.45
17:P:156:LEU:HB2	17:P:203:PRO:HD3	1.99	0.45
25:V:26:TYR:O	25:V:30:LEU:N	2.50	0.45
1:a:54:LEU:HA	1:a:57:VAL:HB	1.98	0.45
3:c:44:TYR:H	7:g:57:ALA:H	1.63	0.45
4:d:75:LEU:HA	11:k:34:LYS:HD2	1.98	0.45
1:a:332:ILE:HB	2:b:66:SER:HA	1.99	0.45
15:C:276:LEU:HD21	15:C:341:ALA:HB2	1.98	0.45
15:N:214:GLY:HA2	19:R:79:HIS:HE1	1.81	0.45
3:c:45:ILE:HD13	3:c:50:MET:HG3	1.97	0.45
3:c:144:ILE:O	3:c:148:SER:OG	2.30	0.45
3:c:229:ARG:HB3	3:c:234:HIS:HB2	1.99	0.45
16:D:272:LYS:HG3	21:I:36:ILE:HG21	1.99	0.45
2:b:19:THR:HB	2:b:22:ALA:HB2	1.99	0.44
15:C:305:LEU:HD13	15:C:363:PHE:HD1	1.81	0.44
28:D:402:PTY:C17	28:D:402:PTY:C11	2.92	0.44
1:a:100:ASN:HB3	3:c:23:PRO:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:202:VAL:HG11	1:a:238:PHE:HD2	1.81	0.44
12:m:61:SER:O	12:m:61:SER:OG	2.34	0.44
17:E:72:LYS:HG3	25:V:44:PHE:HA	1.98	0.44
1:a:524:VAL:HG13	8:h:32:ASP:HB3	1.99	0.44
3:c:242:GLY:N	28:c:301:PTY:HC52	2.31	0.44
5:e:144:TRP:HZ3	9:i:47:PHE:CD2	2.36	0.44
37:C:406:UQ6:H251	37:C:406:UQ6:H302	1.99	0.44
18:F:78:LEU:HD13	18:F:142:LEU:HD22	1.98	0.44
13:L:146:LYS:HD2	13:L:146:LYS:HA	1.75	0.44
20:S:80:LEU:HD13	20:S:89:LEU:HD13	1.99	0.44
9:i:55:LYS:HA	9:i:55:LYS:HD3	1.84	0.44
28:D:402:PTY:O10	28:D:402:PTY:HC52	2.16	0.44
31:T:101:PCF:H143	31:T:101:PCF:H111	1.81	0.44
28:a:604:PTY:H122	3:c:91:PHE:HD1	1.82	0.44
9:i:32:TRP:CD1	28:m:102:PTY:H321	2.51	0.44
14:M:109:LEU:HD12	14:M:206:LEU:HD11	1.99	0.44
15:N:164:TRP:O	15:N:178:ARG:NH2	2.49	0.44
16:O:84:THR:OG1	16:O:85:PHE:N	2.51	0.44
2:b:27:ASP:O	2:b:192:SER:OG	2.31	0.44
3:c:63:ILE:O	3:c:67:ARG:N	2.49	0.44
3:c:242:GLY:H	28:c:301:PTY:HC52	1.83	0.44
4:d:74:LYS:O	11:k:34:LYS:NZ	2.39	0.44
19:G:88:LEU:O	19:G:93:TRP:NE1	2.49	0.44
15:C:216:LEU:HD13	19:G:75:ILE:HG21	2.00	0.44
25:V:22:SER:O	25:V:22:SER:OG	2.35	0.44
27:a:602:HEA:H202	27:a:602:HEA:H172	1.69	0.44
5:e:144:TRP:CD1	5:e:144:TRP:O	2.70	0.44
11:k:117:TRP:HB2	11:k:122:ASN:HD22	1.83	0.44
17:E:142:THR:OG1	17:E:143:ASP:N	2.50	0.44
15:N:247:SER:HG	15:N:250:THR:HG1	1.59	0.44
19:R:5:PHE:HA	19:R:8:ILE:HG12	1.99	0.44
23:T:14:ASN:HB2	31:T:101:PCF:H153	1.99	0.44
10:j:31:TYR:OH	10:j:68:ASP:OD1	2.34	0.44
15:C:281:ILE:O	15:C:284:SER:OG	2.35	0.44
3:c:74:THR:HG1	28:c:301:PTY:HC22	1.79	0.43
3:c:189:TYR:HB3	11:k:116:PHE:HE2	1.82	0.43
17:E:129:ALA:O	17:E:190:ARG:NH2	2.50	0.43
1:a:131:PRO:HG2	1:a:229:PRO:HB3	1.99	0.43
6:f:47:GLU:N	6:f:51:GLU:OE1	2.50	0.43
15:C:12:LEU:HA	15:C:12:LEU:HD23	1.84	0.43
15:C:150:LEU:HB3	15:C:292:VAL:HG22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:283:LEU:HD12	1:a:286:LEU:HD12	1.99	0.43
14:B:318:ILE:HD11	14:B:340:PHE:HB3	2.01	0.43
13:L:317:HIS:CE1	13:L:351:TRP:HE1	2.34	0.43
17:P:161:HIS:HB3	17:P:162:LEU:HD12	2.00	0.43
1:a:224:SER:O	1:a:224:SER:OG	2.32	0.43
1:a:437:PRO:HG2	1:a:440:ILE:HD13	2.00	0.43
3:c:22:TRP:HH2	7:g:30:LEU:HD11	1.83	0.43
1:a:408:LYS:NZ	29:a:605:CN3:OA	2.44	0.43
15:C:64:SER:O	15:C:64:SER:OG	2.35	0.43
17:E:93:LYS:NZ	17:E:215:GLY:O	2.51	0.43
13:L:232:THR:OG1	13:L:233:GLY:N	2.52	0.43
13:L:306:ILE:HA	13:L:311:LEU:HD12	2.00	0.43
1:a:374:VAL:HG11	27:a:602:HEA:HBA2	2.01	0.43
3:c:73:ALA:O	28:c:301:PTY:HC21	2.18	0.43
16:D:309:LYS:HD3	16:D:309:LYS:HA	1.81	0.43
28:D:402:PTY:H121	28:D:402:PTY:C6	2.39	0.43
9:i:14:VAL:HG11	28:i:101:PTY:H312	1.99	0.43
13:A:317:HIS:CE1	13:A:351:TRP:HE1	2.36	0.43
15:C:181:ALA:O	15:N:184:TYR:OH	2.35	0.43
16:D:191:ILE:HB	16:D:252:THR:HG23	1.99	0.43
15:N:114:TRP:NE1	15:N:302:LEU:O	2.38	0.43
16:O:190:TYR:OH	34:O:402:HEM:O2A	2.32	0.43
2:b:34:GLU:OE2	9:i:44:ARG:NH1	2.52	0.43
14:M:115:LYS:HD3	14:M:115:LYS:HA	1.87	0.43
1:a:88:ILE:HD11	1:a:186:VAL:HG11	2.00	0.43
1:a:361:ALA:HB3	2:b:104:LEU:HD11	2.01	0.43
1:a:367:PHE:O	1:a:370:THR:OG1	2.32	0.43
1:a:519:THR:OG1	1:a:521:PRO:O	2.34	0.43
5:e:144:TRP:CZ3	9:i:47:PHE:CD2	3.07	0.43
13:A:428:ASP:OD1	13:A:449:ARG:NH1	2.51	0.43
17:E:106:ASN:HD21	17:E:169:GLU:HG3	1.83	0.43
17:E:118:ILE:HG23	17:E:154:ILE:HG12	2.01	0.43
1:a:15:ALA:HB3	1:a:82:TYR:HD1	1.84	0.42
1:a:241:HIS:CD2	1:a:245:TYR:CD2	3.07	0.42
3:c:125:PRO:HA	3:c:126:PRO:HD3	1.88	0.42
5:e:44:THR:HA	5:e:47:GLN:HE21	1.83	0.42
6:f:85:PRO:HA	6:f:88:ILE:HG22	2.01	0.42
11:k:67:ALA:O	11:k:71:TYR:N	2.52	0.42
16:O:277:LEU:HD11	39:O:403:7PH:H34	2.00	0.42
3:c:3:HIS:NE2	11:k:21:ALA:O	2.53	0.42
3:c:22:TRP:HA	3:c:25:VAL:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:C:331:PHE:HE1	35:C:404:8PE:H2AA	1.83	0.42
17:E:164:CYS:HB2	40:E:302:FES:S2	2.59	0.42
29:N:406:CN3:H44	29:N:406:CN3:H47A	1.90	0.42
6:f:96:ARG:HB2	6:f:135:LEU:HD21	2.00	0.42
6:f:121:TYR:O	6:f:125:LEU:N	2.52	0.42
15:C:224:TYR:O	16:D:292:TRP:NE1	2.45	0.42
13:L:290:ALA:O	13:L:296:ARG:NH2	2.52	0.42
15:N:38:LEU:HB2	33:O:401:6PH:H2C	2.01	0.42
16:O:225:MET:HB2	34:O:402:HEM:C1D	2.55	0.42
1:a:368:HIS:CD2	1:a:369:ASP:HB2	2.55	0.42
28:a:604:PTY:H171	28:c:301:PTY:C19	2.49	0.42
3:c:10:GLN:HE21	3:c:12:HIS:CD2	2.37	0.42
3:c:241:VAL:HG12	28:c:301:PTY:C11	2.50	0.42
14:M:233:PHE:HB3	14:M:357:GLY:HA2	2.01	0.42
2:b:16:ASP:HB3	2:b:17:VAL:H	1.69	0.42
2:b:57:MET:HE1	9:i:18:ILE:HA	2.01	0.42
5:e:107:VAL:HG11	31:e:201:PCF:H272	2.01	0.42
13:A:76:ILE:HA	13:A:79:SER:HB3	1.99	0.42
18:F:88:THR:OG1	18:F:89:GLU:N	2.52	0.42
16:O:272:LYS:HG2	23:T:36:ILE:HG21	2.01	0.42
1:a:9:THR:HG21	3:c:17:VAL:HG13	2.01	0.42
28:a:604:PTY:H322	28:a:604:PTY:H352	1.87	0.42
3:c:218:MET:SD	28:c:301:PTY:C40	3.07	0.42
3:c:241:VAL:HG12	28:c:301:PTY:C8	2.49	0.42
11:k:102:ARG:HD3	11:k:102:ARG:HA	1.85	0.42
15:C:138:GLN:HG3	15:C:266:PRO:HG3	2.01	0.42
19:G:125:VAL:HG21	14:M:73:LEU:HD22	2.01	0.42
15:N:42:ILE:HG12	39:O:403:7PH:H2BA	2.00	0.42
17:P:141:GLN:OE1	17:P:199:ASN:ND2	2.40	0.42
4:d:63:GLU:HB3	4:d:68:ARG:HB2	2.02	0.42
10:j:53:LYS:HE2	10:j:53:LYS:HB3	1.78	0.42
16:D:139:ASP:N	16:D:139:ASP:OD1	2.50	0.42
34:N:401:HEM:HBC2	34:N:401:HEM:HHD	2.00	0.42
22:Q:144:ASP:OD2	22:Q:144:ASP:N	2.51	0.42
1:a:108:MET:N	1:a:108:MET:SD	2.92	0.42
2:b:190:ILE:HD13	2:b:219:GLY:HA3	2.00	0.42
11:k:43:HIS:O	11:k:47:THR:OG1	2.28	0.42
11:k:68:VAL:HA	11:k:71:TYR:HB2	2.01	0.42
13:A:339:MET:HE2	13:A:339:MET:HB3	1.84	0.42
17:E:146:ARG:HH11	17:E:189:GLY:HA3	1.85	0.42
15:N:7:ASN:HB3	15:N:10:LEU:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:345:GLU:OE2	16:O:62:MET:N	2.52	0.42
16:O:194:LEU:HD12	16:O:215:ASN:HD21	1.83	0.42
17:P:164:CYS:HB3	17:P:180:CYS:HB2	1.88	0.42
1:a:188:SER:OG	1:a:189:ILE:N	2.53	0.42
1:a:534:SER:CB	4:d:112:THR:HG21	2.38	0.42
17:P:181:HIS:HB2	40:P:301:FES:S1	2.59	0.42
1:a:532:VAL:HG21	4:d:107:ARG:HH22	1.84	0.42
2:b:44:MET:HE3	2:b:44:MET:HB2	1.97	0.42
28:i:101:PTY:H201	28:i:101:PTY:H172	1.78	0.42
13:A:32:LEU:HD12	13:A:220:VAL:HG11	2.01	0.42
13:A:166:SER:HA	13:A:175:SER:HB2	2.00	0.42
13:A:332:THR:OG1	13:A:333:ALA:N	2.52	0.42
15:C:54:TYR:OH	15:C:134:CYS:O	2.24	0.42
1:a:350:MET:HE2	1:a:350:MET:HB3	1.90	0.41
3:c:3:HIS:CE1	11:k:20:PRO:HD2	2.55	0.41
22:Q:122:ASP:OD1	22:Q:122:ASP:N	2.44	0.41
3:c:102:PHE:O	3:c:106:PHE:N	2.43	0.41
9:i:11:LYS:HG2	28:i:101:PTY:HC12	2.02	0.41
20:H:39:GLY:O	20:H:43:ASN:ND2	2.53	0.41
16:O:283:LEU:HD23	16:O:283:LEU:HA	1.92	0.41
17:P:139:ASP:HA	17:P:140:PRO:HD3	1.95	0.41
1:a:511:SER:OG	1:a:512:SER:N	2.53	0.41
3:c:195:THR:HG23	3:c:197:SER:H	1.86	0.41
4:d:131:VAL:HG12	4:d:142:LYS:HG2	2.03	0.41
14:B:59:THR:HG21	14:B:107:ASP:HB3	2.02	0.41
14:B:353:TYR:HB3	14:B:365:LEU:HD13	2.01	0.41
13:L:161:LEU:HA	13:L:161:LEU:HD12	1.88	0.41
13:L:69:VAL:HG23	13:L:193:LEU:HD22	2.01	0.41
13:L:443:LEU:HD12	13:L:443:LEU:HA	1.85	0.41
13:L:455:MET:HE1	33:O:401:6PH:H1	2.01	0.41
15:N:362:TYR:HA	15:N:366:ILE:HB	2.01	0.41
20:S:7:LYS:HE2	20:S:7:LYS:HB2	1.87	0.41
3:c:2:THR:OG1	3:c:3:HIS:N	2.54	0.41
3:c:126:PRO:HD2	3:c:129:ILE:HD12	2.01	0.41
8:h:59:ILE:HD13	8:h:59:ILE:HA	1.93	0.41
15:C:293:ILE:O	15:C:297:ALA:N	2.49	0.41
1:a:33:SER:HB2	1:a:62:HIS:CE1	2.55	0.41
1:a:488:SER:O	5:e:84:ARG:NH2	2.53	0.41
15:C:214:GLY:HA2	19:G:79:HIS:HE1	1.86	0.41
15:C:263:LEU:HD21	17:P:110:LYS:HD3	2.02	0.41
20:H:3:PRO:HG3	15:N:15:SER:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:I:45:LYS:HB2	21:I:45:LYS:HE3	1.88	0.41
1:a:54:LEU:HD21	8:h:68:CYS:HA	2.02	0.41
1:a:70:LEU:HD11	27:a:602:HEA:H201	2.02	0.41
13:A:378:TYR:HD2	13:A:403:LEU:HD13	1.85	0.41
1:a:514:ILE:HG21	1:a:527:PHE:HZ	1.86	0.41
3:c:229:ARG:NH1	28:c:301:PTY:O12	2.53	0.41
7:g:18:PRO:HG2	7:g:21:TRP:HB2	2.01	0.41
28:m:102:PTY:H112	28:m:102:PTY:H141	1.86	0.41
13:A:114:ASP:OD1	13:A:114:ASP:N	2.41	0.41
13:A:163:HIS:CG	13:A:251:LEU:HD11	2.55	0.41
13:A:431:ILE:O	13:A:445:TYR:OH	2.31	0.41
14:B:247:LYS:HE2	14:B:247:LYS:HB3	1.86	0.41
15:C:182:LEU:HD23	15:C:182:LEU:HA	1.90	0.41
14:M:267:LEU:HD13	14:M:304:ILE:HD12	2.03	0.41
17:P:98:LEU:HD23	17:P:98:LEU:HA	1.89	0.41
24:U:53:ASP:OD1	24:U:53:ASP:N	2.53	0.41
25:V:19:SER:HB2	25:V:22:SER:HB3	2.03	0.41
2:b:57:MET:CE	28:i:101:PTY:H192	2.48	0.41
3:c:148:SER:HA	3:c:151:THR:HG22	2.03	0.41
14:B:62:ARG:HD2	14:B:67:LEU:HD13	2.03	0.41
14:B:115:LYS:HA	14:B:115:LYS:HD3	1.87	0.41
14:B:193:VAL:HG13	14:B:196:ASP:HB2	2.02	0.41
18:F:80:ASP:OD1	18:F:80:ASP:N	2.48	0.41
13:L:332:THR:OG1	13:L:333:ALA:N	2.54	0.41
13:L:399:SER:OG	13:L:400:LYS:N	2.54	0.41
1:a:323:TRP:HA	1:a:326:THR:HG22	2.03	0.40
5:e:144:TRP:O	5:e:144:TRP:CG	2.74	0.40
9:i:4:ALA:HA	9:i:5:PRO:HD3	1.95	0.40
14:B:69:ARG:NH2	19:R:121:ASP:OD1	2.52	0.40
17:E:107:VAL:HB	17:E:118:ILE:HB	2.03	0.40
13:L:52:GLY:HA3	13:L:105:ILE:HD13	2.02	0.40
15:N:210:LEU:HD12	19:R:79:HIS:HD2	1.85	0.40
15:N:223:SER:O	15:N:223:SER:OG	2.33	0.40
15:N:377:LEU:HD23	15:N:377:LEU:HA	1.94	0.40
1:a:32:MET:HG3	8:h:64:PRO:HB3	2.03	0.40
1:a:372:TYR:N	1:a:432:GLY:HA3	2.37	0.40
3:c:31:LEU:HD21	7:g:45:LEU:HD21	2.03	0.40
13:A:169:PHE:O	13:A:175:SER:HB3	2.21	0.40
15:C:26:ILE:O	15:C:228:LYS:NZ	2.54	0.40
28:D:402:PTY:HC31	28:D:402:PTY:HC52	2.02	0.40
15:N:213:THR:N	19:R:51:GLU:OE2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:241:PRO:HB3	22:Q:74:VAL:HG11	2.03	0.40
39:O:403:7PH:H2EA	17:P:78:PHE:HE2	1.86	0.40
1:a:230:ILE:HA	1:a:233:GLU:HG2	2.02	0.40
14:B:270:LEU:HB2	14:B:304:ILE:HD11	2.02	0.40
15:C:157:VAL:HG13	24:U:48:TRP:HH2	1.86	0.40
17:E:209:GLY:O	17:E:210:ASP:HB3	2.21	0.40
17:P:114:LYS:HE2	17:P:114:LYS:HB2	1.92	0.40
20:S:42:HIS:ND1	20:S:42:HIS:O	2.54	0.40
1:a:26:GLY:HA2	1:a:70:LEU:HD12	2.04	0.40
1:a:213:ASP:OD2	1:a:221:PHE:N	2.39	0.40
28:a:604:PTY:H141	28:a:604:PTY:H112	1.86	0.40
15:N:221:MET:HE2	15:N:221:MET:HB2	1.98	0.40
2:b:41:ASP:OD2	9:i:37:HIS:ND1	2.48	0.40
31:e:201:PCF:H142	31:e:201:PCF:H112	1.95	0.40
13:A:367:LYS:NZ	13:A:413:ILE:O	2.44	0.40
14:B:246:ASN:OD1	14:B:246:ASN:N	2.48	0.40
22:Q:106:LYS:HA	22:Q:109:GLN:HG2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	528/530 (100%)	485 (92%)	43 (8%)	0	100	100
2	b	234/236 (99%)	213 (91%)	21 (9%)	0	100	100
3	c	266/268 (99%)	252 (95%)	14 (5%)	0	100	100
4	d	115/117 (98%)	94 (82%)	20 (17%)	1 (1%)	14	45
5	e	126/128 (98%)	113 (90%)	13 (10%)	0	100	100
6	f	97/99 (98%)	91 (94%)	6 (6%)	0	100	100
7	g	53/55 (96%)	50 (94%)	3 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	h	49/51 (96%)	44 (90%)	5 (10%)	0	100	100
9	i	51/53 (96%)	50 (98%)	1 (2%)	0	100	100
10	j	76/78 (97%)	71 (93%)	5 (7%)	0	100	100
11	k	112/114 (98%)	93 (83%)	19 (17%)	0	100	100
12	m	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
13	A	429/431 (100%)	403 (94%)	26 (6%)	0	100	100
13	L	429/431 (100%)	400 (93%)	29 (7%)	0	100	100
14	B	350/352 (99%)	333 (95%)	17 (5%)	0	100	100
14	M	350/352 (99%)	330 (94%)	20 (6%)	0	100	100
15	C	383/385 (100%)	371 (97%)	12 (3%)	0	100	100
15	N	383/385 (100%)	370 (97%)	13 (3%)	0	100	100
16	D	246/248 (99%)	238 (97%)	8 (3%)	0	100	100
16	O	246/248 (99%)	237 (96%)	9 (4%)	0	100	100
17	E	183/185 (99%)	172 (94%)	11 (6%)	0	100	100
17	P	183/185 (99%)	175 (96%)	8 (4%)	0	100	100
18	F	72/74 (97%)	70 (97%)	2 (3%)	0	100	100
19	G	124/126 (98%)	119 (96%)	4 (3%)	1 (1%)	16	47
19	R	124/126 (98%)	120 (97%)	3 (2%)	1 (1%)	16	47
20	H	91/93 (98%)	83 (91%)	8 (9%)	0	100	100
20	S	91/93 (98%)	84 (92%)	7 (8%)	0	100	100
21	I	52/54 (96%)	49 (94%)	3 (6%)	0	100	100
22	Q	73/75 (97%)	70 (96%)	3 (4%)	0	100	100
23	T	52/54 (96%)	51 (98%)	1 (2%)	0	100	100
24	U	42/44 (96%)	39 (93%)	3 (7%)	0	100	100
25	V	49/51 (96%)	43 (88%)	6 (12%)	0	100	100
All	All	5695/5759 (99%)	5347 (94%)	345 (6%)	3 (0%)	49	77

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
19	R	5	PHE
19	G	5	PHE
4	d	129	ASN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a	443/443 (100%)	443 (100%)	0	100	100
2	b	209/209 (100%)	209 (100%)	0	100	100
3	c	227/227 (100%)	227 (100%)	0	100	100
4	d	99/99 (100%)	99 (100%)	0	100	100
5	e	106/106 (100%)	106 (100%)	0	100	100
6	f	88/88 (100%)	88 (100%)	0	100	100
7	g	48/48 (100%)	48 (100%)	0	100	100
8	h	41/41 (100%)	41 (100%)	0	100	100
9	i	44/44 (100%)	44 (100%)	0	100	100
10	j	70/70 (100%)	70 (100%)	0	100	100
11	k	100/100 (100%)	100 (100%)	0	100	100
12	m	32/32 (100%)	32 (100%)	0	100	100
13	A	370/370 (100%)	367 (99%)	3 (1%)	73	80
13	L	370/370 (100%)	370 (100%)	0	100	100
14	B	301/301 (100%)	300 (100%)	1 (0%)	86	86
14	M	301/301 (100%)	299 (99%)	2 (1%)	76	81
15	C	338/338 (100%)	336 (99%)	2 (1%)	78	82
15	N	338/338 (100%)	335 (99%)	3 (1%)	70	79
16	D	206/206 (100%)	206 (100%)	0	100	100
16	O	206/206 (100%)	206 (100%)	0	100	100
17	E	151/151 (100%)	151 (100%)	0	100	100
17	P	151/151 (100%)	151 (100%)	0	100	100
18	F	67/67 (100%)	67 (100%)	0	100	100
19	G	110/110 (100%)	109 (99%)	1 (1%)	70	79
19	R	110/110 (100%)	108 (98%)	2 (2%)	51	71
20	H	77/77 (100%)	76 (99%)	1 (1%)	61	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	S	77/77 (100%)	74 (96%)	3 (4%)	28	58
21	I	44/44 (100%)	44 (100%)	0	100	100
22	Q	68/68 (100%)	68 (100%)	0	100	100
23	T	45/45 (100%)	45 (100%)	0	100	100
24	U	35/35 (100%)	35 (100%)	0	100	100
25	V	42/42 (100%)	41 (98%)	1 (2%)	43	67
All	All	4914/4914 (100%)	4895 (100%)	19 (0%)	81	85

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	A	29	VAL
13	A	189	VAL
13	A	414	THR
14	B	54	PHE
15	C	157	VAL
15	C	384	ASN
19	G	53	ASN
20	H	29	VAL
14	M	238	VAL
14	M	255	VAL
15	N	157	VAL
15	N	264	VAL
15	N	272	GLU
19	R	51	GLU
19	R	83	LEU
20	S	25	THR
20	S	37	LEU
20	S	59	VAL
25	V	55	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (102) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	49	HIS
1	a	53	GLN
1	a	81	ASN
1	a	152	HIS
1	a	215	ASN

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Mol	Chain	Res	Type
1	a	399	GLN
1	a	434	ASN
1	a	451	ASN
1	a	481	ASN
1	a	528	ASN
1	a	533	GLN
2	b	26	GLN
2	b	32	ASN
2	b	33	GLN
2	b	123	GLN
2	b	135	ASN
2	b	206	GLN
3	c	10	GLN
3	c	12	HIS
3	c	79	HIS
3	c	111	HIS
3	c	163	ASN
4	d	36	ASN
5	e	57	GLN
5	e	63	GLN
6	f	70	GLN
6	f	99	ASN
7	g	7	GLN
7	g	50	ASN
10	j	23	GLN
11	k	31	GLN
11	k	100	ASN
11	k	122	ASN
13	A	47	HIS
13	A	102	GLN
13	A	126	GLN
13	A	154	ASN
13	A	199	ASN
13	A	227	ASN
13	A	274	ASN
13	A	317	HIS
13	A	350	GLN
13	A	352	ASN
13	A	388	ASN
14	B	57	GLN
14	B	58	ASN
14	B	136	GLN

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Mol	Chain	Res	Type
15	C	215	ASN
15	C	316	ASN
15	C	375	ASN
16	D	79	ASN
16	D	127	ASN
16	D	169	ASN
16	D	215	ASN
16	D	256	ASN
16	D	303	ASN
17	E	161	HIS
19	G	30	ASN
20	H	34	GLN
20	H	77	ASN
21	I	29	GLN
21	I	43	HIS
21	I	44	ASN
13	L	31	GLN
13	L	126	GLN
13	L	130	ASN
13	L	171	ASN
13	L	199	ASN
13	L	227	ASN
13	L	231	GLN
13	L	274	ASN
13	L	317	HIS
13	L	352	ASN
13	L	385	ASN
13	L	388	ASN
14	M	36	HIS
14	M	55	ASN
14	M	170	GLN
14	M	252	GLN
15	N	14	ASN
15	N	31	ASN
15	N	159	ASN
15	N	177	GLN
15	N	215	ASN
15	N	222	HIS
15	N	249	ASN
16	O	87	HIS
16	O	127	ASN
16	O	143	ASN

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Mol	Chain	Res	Type
16	O	169	ASN
16	O	215	ASN
16	O	246	GLN
16	O	256	ASN
17	P	161	HIS
22	Q	87	ASN
22	Q	108	GLN
22	Q	110	GLN
22	Q	119	HIS
19	R	79	HIS
20	S	21	GLN
20	S	55	GLN
23	T	44	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 38 ligands modelled in this entry, 2 are monoatomic - leaving 36 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	$\# Z > 2$
33	6PH	O	401	-	39,39,39	0.49	0	43,44,44	1.16	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	PTY	m	101	-	40,40,49	1.04	2 (5%)	43,45,54	1.20	4 (9%)
28	PTY	m	102	-	29,29,49	1.16	2 (6%)	32,34,54	1.24	4 (12%)
28	PTY	a	604	-	33,33,49	1.06	4 (12%)	36,38,54	1.10	2 (5%)
34	HEM	C	402	15	50,50,50	1.49	6 (12%)	66,82,82	1.68	12 (18%)
28	PTY	b	302	2	32,32,49	1.08	2 (6%)	35,37,54	1.07	2 (5%)
36	CN5	C	405	-	40,40,40	1.04	2 (5%)	44,48,48	0.96	2 (4%)
31	PCF	e	201	-	35,35,49	0.69	0	41,43,57	0.56	0
29	CN3	a	605	-	54,54,54	0.51	0	60,66,66	1.14	4 (6%)
33	6PH	C	401	-	39,39,39	0.49	0	43,44,44	1.19	2 (4%)
31	PCF	m	103	-	37,37,49	0.66	0	43,45,57	0.60	0
38	9PE	C	407	-	39,39,39	0.43	0	42,44,44	1.14	2 (4%)
39	7PH	O	403	-	37,37,37	0.52	0	41,42,42	1.14	2 (4%)
28	PTY	c	301	3	39,39,49	1.02	3 (7%)	42,44,54	1.25	4 (9%)
34	HEM	O	402	16	50,50,50	1.28	5 (10%)	66,82,82	1.37	6 (9%)
29	CN3	N	406	-	54,54,54	0.51	0	60,66,66	1.30	4 (6%)
34	HEM	D	401	16	50,50,50	1.32	6 (12%)	66,82,82	1.28	7 (10%)
40	FES	P	301	-	0,4,4	-	-	-	-	-
38	9PE	N	405	-	39,39,39	0.44	0	42,44,44	1.13	2 (4%)
35	8PE	N	404	-	46,46,46	0.42	0	49,51,51	1.15	2 (4%)
31	PCF	T	101	-	34,34,49	0.62	0	40,42,57	0.67	0
34	HEM	N	401	15	50,50,50	1.37	6 (12%)	66,82,82	1.20	6 (9%)
34	HEM	N	402	15	50,50,50	1.30	5 (10%)	66,82,82	1.17	4 (6%)
27	HEA	a	603	-	66,67,67	1.25	10 (15%)	78,103,103	1.52	16 (20%)
40	FES	E	302	-	0,4,4	-	-	-	-	-
37	UQ6	C	406	-	43,43,43	0.46	0	51,55,55	1.59	13 (25%)
39	7PH	E	301	-	37,37,37	0.52	0	41,42,42	1.15	2 (4%)
30	CUA	b	301	2	0,1,1	-	-	-	-	-
27	HEA	a	602	1	66,67,67	1.23	7 (10%)	78,103,103	1.55	17 (21%)
37	UQ6	N	403	-	43,43,43	0.51	0	51,55,55	1.59	12 (23%)
28	PTY	D	402	-	31,31,49	1.08	2 (6%)	34,36,54	1.21	3 (8%)
34	HEM	C	403	15	50,50,50	1.28	4 (8%)	66,82,82	1.15	4 (6%)
35	8PE	C	404	-	46,46,46	0.44	0	49,51,51	1.15	2 (4%)
28	PTY	i	101	-	39,39,49	0.99	2 (5%)	42,44,54	1.08	3 (7%)
31	PCF	I	101	-	34,34,49	0.63	0	40,42,57	0.61	0
31	PCF	c	302	-	42,42,49	0.64	0	48,50,57	0.61	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
33	6PH	O	401	-	-	9/41/41/41	-
28	PTY	m	101	-	-	18/44/44/53	-
28	PTY	m	102	-	-	16/33/33/53	-
28	PTY	a	604	-	-	15/37/37/53	-
34	HEM	C	402	15	-	6/14/54/54	-
28	PTY	b	302	2	-	9/36/36/53	-
36	CN5	C	405	-	-	18/44/44/44	-
31	PCF	e	201	-	-	11/39/39/53	-
29	CN3	a	605	-	-	25/65/65/65	-
33	6PH	C	401	-	-	13/41/41/41	-
31	PCF	m	103	-	-	17/41/41/53	-
38	9PE	C	407	-	-	14/43/43/43	-
39	7PH	O	403	-	-	14/39/39/39	-
28	PTY	c	301	3	-	18/43/43/53	-
34	HEM	O	402	16	-	0/14/54/54	-
29	CN3	N	406	-	-	34/65/65/65	-
34	HEM	D	401	16	-	1/14/54/54	-
40	FES	P	301	-	-	-	0/1/1/1
38	9PE	N	405	-	-	19/43/43/43	-
35	8PE	N	404	-	-	23/50/50/50	-
31	PCF	T	101	-	-	14/38/38/53	-
34	HEM	N	401	15	-	3/14/54/54	-
34	HEM	N	402	15	-	2/14/54/54	-
27	HEA	a	603	-	-	12/36/76/76	-
40	FES	E	302	-	-	-	0/1/1/1
37	UQ6	C	406	-	-	13/39/39/39	0/1/1/1
39	7PH	E	301	-	-	12/39/39/39	-
27	HEA	a	602	1	-	15/36/76/76	-
37	UQ6	N	403	-	-	7/39/39/39	0/1/1/1
28	PTY	D	402	-	-	11/35/35/53	-
34	HEM	C	403	15	-	4/14/54/54	-
35	8PE	C	404	-	-	22/50/50/50	-
28	PTY	i	101	-	-	14/43/43/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	PCF	I	101	-	-	12/38/38/53	-
31	PCF	c	302	-	-	15/46/46/53	-

All (68) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	C	402	HEM	FE-ND	5.00	2.10	1.94
27	a	602	HEA	CMA-C3A	-4.43	1.35	1.45
27	a	603	HEA	CMA-C3A	-4.36	1.36	1.45
28	m	101	PTY	O4-C30	4.34	1.46	1.33
28	c	301	PTY	O4-C30	4.30	1.45	1.33
28	m	101	PTY	O7-C8	4.14	1.46	1.34
28	m	102	PTY	O4-C30	4.09	1.45	1.33
28	i	101	PTY	O4-C30	4.09	1.45	1.33
28	b	302	PTY	O4-C30	3.91	1.44	1.33
28	D	402	PTY	O4-C30	3.89	1.44	1.33
28	m	102	PTY	O7-C8	3.80	1.45	1.34
28	i	101	PTY	O7-C8	3.76	1.44	1.34
28	b	302	PTY	O7-C8	3.71	1.44	1.34
28	D	402	PTY	O7-C8	3.63	1.44	1.34
28	c	301	PTY	O7-C8	3.52	1.44	1.34
34	N	401	HEM	FE-NC	3.27	2.06	1.95
34	N	401	HEM	C3C-C2C	-3.24	1.30	1.37
36	C	405	CN5	P'-O1'	3.15	1.72	1.59
34	O	402	HEM	CAB-C3B	2.93	1.55	1.47
36	C	405	CN5	P-O11	2.84	1.70	1.59
34	D	401	HEM	CAB-C3B	2.84	1.55	1.47
34	O	402	HEM	C3C-C2C	-2.81	1.31	1.37
34	N	402	HEM	CAB-C3B	2.77	1.55	1.47
34	N	402	HEM	CAC-C3C	2.77	1.55	1.47
34	D	401	HEM	C3C-C2C	-2.72	1.31	1.37
34	C	403	HEM	CAB-C3B	2.72	1.54	1.47
34	D	401	HEM	FE-NC	2.70	2.04	1.95
34	C	402	HEM	C2A-C3A	-2.68	1.31	1.38
34	N	401	HEM	CAB-C3B	2.66	1.54	1.47
34	C	402	HEM	CAB-C3B	2.64	1.54	1.47
34	C	403	HEM	CAC-C3C	2.63	1.54	1.47
27	a	602	HEA	C4C-NC	-2.58	1.34	1.39
34	O	402	HEM	C2A-C3A	-2.53	1.32	1.38
28	a	604	PTY	O7-C6	-2.52	1.40	1.46
27	a	603	HEA	C1D-C2D	2.51	1.49	1.44
34	N	401	HEM	C2A-C3A	-2.50	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	C	402	HEM	CAC-C3C	2.50	1.54	1.47
34	N	401	HEM	FE-ND	2.48	2.02	1.94
34	D	401	HEM	CAC-C3C	2.46	1.54	1.47
27	a	603	HEA	CHC-C1C	-2.43	1.33	1.39
28	a	604	PTY	O4-C30	2.42	1.40	1.33
34	O	402	HEM	CAC-C3C	2.40	1.54	1.47
27	a	603	HEA	C3C-C4C	2.39	1.48	1.42
34	O	402	HEM	FE-NB	2.38	2.02	1.94
34	D	401	HEM	C2A-C3A	-2.38	1.32	1.38
34	C	403	HEM	C2A-C3A	-2.37	1.32	1.38
34	N	401	HEM	CAC-C3C	2.34	1.53	1.47
27	a	602	HEA	CHC-C1C	-2.33	1.34	1.39
34	N	402	HEM	C2A-C3A	-2.31	1.32	1.38
34	C	402	HEM	C3D-C2D	-2.29	1.31	1.36
27	a	602	HEA	C4B-C3B	2.29	1.48	1.44
27	a	602	HEA	FE-NC	2.27	2.02	1.95
27	a	603	HEA	FE-NC	2.23	2.02	1.95
28	a	604	PTY	O4-C1	-2.22	1.40	1.45
27	a	603	HEA	C4C-NC	-2.20	1.35	1.39
34	D	401	HEM	FE-NB	2.19	2.01	1.94
27	a	602	HEA	C1D-ND	-2.19	1.36	1.40
27	a	603	HEA	C4B-C3B	2.17	1.48	1.44
28	a	604	PTY	O7-C8	2.17	1.40	1.34
34	C	403	HEM	FE-ND	2.16	2.01	1.94
27	a	603	HEA	CMD-C2D	2.15	1.55	1.50
28	c	301	PTY	O7-C6	-2.15	1.41	1.46
34	C	402	HEM	C3C-C4C	-2.10	1.42	1.46
34	N	402	HEM	C3D-C2D	-2.10	1.32	1.36
34	N	402	HEM	FE-ND	2.09	2.01	1.94
27	a	602	HEA	C1D-C2D	2.08	1.48	1.44
27	a	603	HEA	C3C-C2C	-2.08	1.34	1.41
27	a	603	HEA	C1D-ND	-2.06	1.36	1.40

All (145) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	C	402	HEM	CAD-C3D-C4D	6.18	135.46	124.66
34	C	402	HEM	CAD-C3D-C2D	-5.41	117.80	127.88
37	N	403	UQ6	C7-C8-C9	-5.19	119.18	127.24
37	C	406	UQ6	C7-C8-C9	-4.93	119.59	127.24
29	N	406	CN3	O51-C51-C52	4.57	121.36	111.50
28	m	101	PTY	O7-C8-C11	4.56	121.33	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	602	HEA	C3C-C4C-NC	4.22	112.84	110.25
29	N	406	CN3	O21-C21-C22	4.17	120.49	111.50
35	C	404	8PE	O21-C21-C22	4.16	120.46	111.50
28	D	402	PTY	C6-O7-C8	-4.13	107.63	117.79
34	O	402	HEM	CAA-CBA-CGA	-4.12	104.73	113.60
33	C	401	6PH	O21-C21-C22	4.01	120.13	111.50
35	N	404	8PE	O21-C21-C22	4.00	120.12	111.50
28	c	301	PTY	O7-C8-C11	4.00	120.12	111.50
28	a	604	PTY	O7-C8-C11	3.96	120.04	111.50
29	a	605	CN3	O51-C51-C52	3.92	119.94	111.50
38	N	405	9PE	O21-C21-C22	3.81	119.72	111.50
34	O	402	HEM	CMB-C2B-C1B	-3.79	119.26	125.04
28	b	302	PTY	O7-C8-C11	3.74	119.56	111.50
28	i	101	PTY	O7-C8-C11	3.74	119.55	111.50
29	a	605	CN3	O21-C21-C22	3.69	119.45	111.50
39	E	301	7PH	O21-C21-C22	3.68	119.42	111.50
39	O	403	7PH	O21-C21-C22	3.67	119.42	111.50
34	C	403	HEM	CAD-CBD-CGD	-3.65	105.75	113.60
38	C	407	9PE	O21-C21-C22	3.61	119.27	111.50
34	N	402	HEM	CAD-CBD-CGD	-3.56	105.94	113.60
27	a	602	HEA	OMA-CMA-C3A	-3.55	117.67	125.69
33	O	401	6PH	O21-C21-C22	3.54	119.12	111.50
29	N	406	CN3	O31-C31-C32	3.50	120.57	111.38
37	C	406	UQ6	C20-C19-C21	3.46	121.10	115.27
34	D	401	HEM	CAA-CBA-CGA	-3.41	106.26	113.60
27	a	602	HEA	CMD-C2D-C1D	3.38	130.18	125.04
28	D	402	PTY	O7-C8-C11	3.24	118.48	111.50
29	a	605	CN3	O31-C31-C32	3.23	119.86	111.38
27	a	603	HEA	CHB-C4A-NA	-3.23	120.95	124.44
28	m	102	PTY	O4-C30-C31	3.20	121.96	111.91
34	C	402	HEM	CAD-CBD-CGD	-3.18	106.76	113.60
37	N	403	UQ6	C30-C29-C31	3.14	120.56	115.27
34	N	401	HEM	CAC-C3C-C4C	3.11	132.41	124.90
27	a	602	HEA	CHB-C4A-NA	-3.06	121.13	124.44
34	N	402	HEM	CMB-C2B-C1B	-3.05	120.39	125.04
29	N	406	CN3	O41-C41-C42	3.01	121.37	111.91
34	D	401	HEM	CAD-CBD-CGD	-3.01	107.12	113.60
28	c	301	PTY	O4-C30-C31	3.00	121.32	111.91
35	C	404	8PE	O31-C31-C32	3.00	121.31	111.91
34	C	402	HEM	CAC-C3C-C4C	-2.97	117.73	124.90
27	a	603	HEA	C3D-C4D-ND	2.97	113.23	110.36
34	C	403	HEM	CMB-C2B-C1B	-2.96	120.54	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	N	405	9PE	O31-C31-C32	2.91	121.05	111.91
34	O	402	HEM	CAC-C3C-C4C	2.90	131.90	124.90
27	a	603	HEA	CBD-CAD-C3D	2.89	120.66	112.63
34	D	401	HEM	CAC-C3C-C4C	2.89	131.87	124.90
38	C	407	9PE	O31-C31-C32	2.87	120.93	111.91
34	C	402	HEM	CMB-C2B-C1B	-2.87	120.67	125.04
34	C	402	HEM	CHD-C4C-NC	2.85	127.52	124.44
27	a	603	HEA	OMA-CMA-C3A	-2.83	119.30	125.69
28	m	102	PTY	O7-C8-C11	2.82	117.59	111.50
28	m	101	PTY	O4-C30-C31	2.81	120.72	111.91
37	C	406	UQ6	C15-C14-C16	2.79	119.96	115.27
37	N	403	UQ6	C7-C6-C5	-2.76	117.19	120.82
33	O	401	6PH	O31-C31-C32	2.75	120.53	111.91
33	C	401	6PH	O31-C31-C32	2.74	120.50	111.91
28	a	604	PTY	O4-C30-C31	2.73	120.48	111.91
27	a	602	HEA	C26-C15-C14	-2.72	116.71	123.68
28	c	301	PTY	C6-O7-C8	-2.70	111.14	117.79
37	N	403	UQ6	C15-C14-C16	2.69	119.79	115.27
34	N	401	HEM	CAA-CBA-CGA	-2.69	107.82	113.60
27	a	603	HEA	CAD-C3D-C2D	2.67	132.86	127.88
29	a	605	CN3	O41-C41-C42	2.67	120.29	111.91
34	D	401	HEM	CMB-C2B-C1B	-2.67	120.97	125.04
34	N	402	HEM	CAA-CBA-CGA	-2.66	107.87	113.60
34	C	402	HEM	CHA-C4D-ND	-2.64	121.11	124.37
37	N	403	UQ6	C30-C29-C28	-2.64	116.91	123.68
39	E	301	7PH	O31-C31-C32	2.63	120.17	111.91
37	N	403	UQ6	C12-C13-C14	-2.63	121.32	127.66
34	C	402	HEM	CHA-C4D-C3D	2.61	130.23	125.33
37	C	406	UQ6	C25-C24-C26	2.61	119.66	115.27
34	N	401	HEM	CAC-C3C-C2C	-2.61	120.02	128.60
27	a	603	HEA	CHA-C4D-C3D	-2.60	121.01	124.84
34	D	401	HEM	CHC-C1C-NC	2.60	127.25	124.44
34	C	402	HEM	CBA-CAA-C2A	-2.57	105.48	112.63
27	a	602	HEA	C13-C14-C15	-2.57	121.48	127.66
28	b	302	PTY	O4-C30-C31	2.54	119.87	111.91
37	N	403	UQ6	C22-C23-C24	-2.53	121.56	127.66
27	a	603	HEA	C1D-C2D-C3D	-2.53	104.30	106.96
37	C	406	UQ6	C22-C23-C24	-2.52	121.59	127.66
35	N	404	8PE	O31-C31-C32	2.52	119.81	111.91
27	a	603	HEA	CAD-C3D-C4D	-2.50	120.29	124.66
37	N	403	UQ6	C17-C18-C19	-2.49	121.66	127.66
39	O	403	7PH	O31-C31-C32	2.49	119.71	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	C	406	UQ6	C20-C19-C18	-2.48	117.33	123.68
37	C	406	UQ6	C30-C29-C31	2.47	119.43	115.27
34	O	402	HEM	CAC-C3C-C2C	-2.47	120.47	128.60
28	m	102	PTY	O4-C30-O30	-2.46	117.39	123.59
27	a	602	HEA	CMB-C2B-C3B	-2.45	125.67	130.34
34	O	402	HEM	C3B-C2B-C1B	2.42	108.28	106.49
37	N	403	UQ6	C4M-O4-C4	-2.39	108.24	114.78
27	a	603	HEA	C20-C19-C18	-2.38	116.30	121.12
27	a	603	HEA	CMB-C2B-C3B	-2.38	125.80	130.34
27	a	603	HEA	CMD-C2D-C1D	2.38	128.66	125.04
27	a	602	HEA	C2A-C1A-NA	2.38	112.64	110.32
34	D	401	HEM	CAC-C3C-C2C	-2.37	120.79	128.60
34	C	403	HEM	CAA-CBA-CGA	-2.36	108.52	113.60
27	a	603	HEA	C2A-C1A-NA	2.36	112.62	110.32
34	C	402	HEM	CBD-CAD-C3D	2.36	119.17	112.63
37	C	406	UQ6	C7-C6-C5	-2.34	117.74	120.82
37	C	406	UQ6	C12-C13-C14	-2.31	122.09	127.66
34	N	401	HEM	CAD-CBD-CGD	-2.31	108.63	113.60
27	a	602	HEA	C3D-C4D-ND	2.30	112.58	110.36
27	a	602	HEA	O1D-CGD-CBD	-2.30	115.71	123.08
28	D	402	PTY	O4-C30-C31	2.29	119.10	111.91
34	N	401	HEM	CMB-C2B-C1B	-2.29	121.56	125.04
27	a	603	HEA	C3C-C4C-NC	2.29	111.65	110.25
34	O	402	HEM	CAD-CBD-CGD	-2.28	108.69	113.60
27	a	602	HEA	C1D-C2D-C3D	-2.28	104.56	106.96
37	C	406	UQ6	C4M-O4-C4	-2.25	108.62	114.78
34	C	403	HEM	CAC-C3C-C4C	-2.24	119.48	124.90
28	i	101	PTY	C6-O7-C8	-2.24	112.28	117.79
36	C	405	CN5	O4'-P'-O2'	2.23	123.26	112.24
37	C	406	UQ6	C10-C9-C11	2.22	119.01	115.27
28	c	301	PTY	O4-C1-C6	2.22	114.89	108.43
27	a	602	HEA	C2B-C1B-NB	2.21	112.53	109.88
34	C	402	HEM	CHD-C1D-ND	2.20	126.81	124.42
27	a	602	HEA	C4C-NC-C1C	-2.19	103.20	105.35
37	C	406	UQ6	C27-C28-C29	-2.19	122.40	127.66
36	C	405	CN5	O12-P-O14	2.15	122.89	112.24
34	N	402	HEM	CMC-C2C-C1C	-2.15	120.92	124.71
27	a	602	HEA	CHA-C4D-C3D	-2.15	121.68	124.84
37	C	406	UQ6	C36-C34-C35	2.15	119.34	114.60
28	m	101	PTY	C5-C6-C1	-2.14	106.72	111.79
27	a	603	HEA	O1D-CGD-CBD	-2.14	116.21	123.08
27	a	603	HEA	C2B-C1B-NB	2.13	112.43	109.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	N	403	UQ6	C25-C24-C26	2.12	118.84	115.27
27	a	602	HEA	CMC-C2C-C3C	2.09	131.66	126.59
28	i	101	PTY	O4-C30-C31	2.09	118.46	111.91
27	a	602	HEA	CMC-C2C-C1C	-2.08	122.19	125.37
27	a	603	HEA	C26-C15-C14	-2.08	118.33	123.68
27	a	602	HEA	C20-C19-C18	-2.08	116.90	121.12
34	C	402	HEM	CHD-C4C-C3C	-2.08	121.70	125.26
34	N	401	HEM	CMC-C2C-C3C	-2.07	123.24	128.30
37	N	403	UQ6	C36-C34-C35	2.04	119.10	114.60
37	N	403	UQ6	C20-C19-C21	2.03	118.69	115.27
28	m	102	PTY	C6-O7-C8	-2.02	112.81	117.79
34	D	401	HEM	C4A-NA-C1A	2.02	107.33	105.35
28	m	101	PTY	O4-C30-O30	-2.00	118.54	123.59

There are no chirality outliers.

All (436) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	a	602	HEA	C2A-C3A-CMA-OMA
27	a	602	HEA	C4A-C3A-CMA-OMA
27	a	602	HEA	C13-C14-C15-C26
27	a	602	HEA	C21-C22-C23-C25
27	a	603	HEA	C2A-C3A-CMA-OMA
27	a	603	HEA	C4A-C3A-CMA-OMA
28	a	604	PTY	C11-C8-O7-C6
28	c	301	PTY	O4-C1-C6-O7
28	c	301	PTY	C3-O11-P1-O13
28	c	301	PTY	C5-O14-P1-O11
28	c	301	PTY	C5-O14-P1-O12
28	c	301	PTY	C5-O14-P1-O13
28	i	101	PTY	N1-C2-C3-O11
28	i	101	PTY	C5-O14-P1-O11
28	m	101	PTY	C3-O11-P1-O13
28	m	101	PTY	C5-O14-P1-O11
28	m	101	PTY	C5-O14-P1-O13
28	m	102	PTY	C11-C8-O7-C6
28	m	102	PTY	C3-O11-P1-O12
28	m	102	PTY	C3-O11-P1-O13
28	m	102	PTY	C5-O14-P1-O12
28	m	102	PTY	C5-O14-P1-O13
28	D	402	PTY	C11-C8-O7-C6
28	D	402	PTY	C3-O11-P1-O12

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Mol	Chain	Res	Type	Atoms
28	D	402	PTY	C3-O11-P1-O13
28	D	402	PTY	C3-O11-P1-O14
29	a	605	CN3	C1-O11-P-O12
29	a	605	CN3	C1-O11-P-O14
29	a	605	CN3	CC-O13-P-O11
29	a	605	CN3	C1'-O1'-P'-O4'
29	a	605	CN3	C52-C51-O51-C2'
29	a	605	CN3	O3'-CA-CB-CC
29	N	406	CN3	CC-O13-P-O12
29	N	406	CN3	CC-O13-P-O14
29	N	406	CN3	C1'-O1'-P'-O2'
29	N	406	CN3	C1'-O1'-P'-O4'
29	N	406	CN3	CA-O3'-P'-O1'
29	N	406	CN3	CA-O3'-P'-O2'
29	N	406	CN3	CA-O3'-P'-O4'
29	N	406	CN3	O52-C51-O51-C2'
29	N	406	CN3	C52-C51-O51-C2'
29	N	406	CN3	O3'-CA-CB-CC
31	c	302	PCF	C1-O11-P-O12
31	c	302	PCF	C1-O11-P-O13
31	c	302	PCF	C1-O11-P-O14
31	c	302	PCF	C11-O13-P-O14
31	c	302	PCF	O13-C11-C12-N
31	c	302	PCF	C22-C21-O21-C2
31	e	201	PCF	C1-O11-P-O12
31	e	201	PCF	C1-O11-P-O14
31	m	103	PCF	C1-O11-P-O12
31	m	103	PCF	C1-O11-P-O14
31	m	103	PCF	C11-O13-P-O14
31	m	103	PCF	O13-C11-C12-N
31	I	101	PCF	C11-O13-P-O11
31	I	101	PCF	C11-O13-P-O12
31	I	101	PCF	O13-C11-C12-N
31	I	101	PCF	O21-C2-C3-O31
31	T	101	PCF	C11-O13-P-O14
31	T	101	PCF	O13-C11-C12-N
33	C	401	6PH	O21-C2-C3-O31
33	O	401	6PH	O21-C2-C3-O31
34	C	402	HEM	C2D-C3D-CAD-CBD
34	C	402	HEM	C4D-C3D-CAD-CBD
35	C	404	8PE	C11-O13-P-O11
35	C	404	8PE	C11-O13-P-O12

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Mol	Chain	Res	Type	Atoms
35	C	404	8PE	C11-O13-P-O14
35	N	404	8PE	C1-O11-P-O12
35	N	404	8PE	C1-O11-P-O14
36	C	405	CN5	C1-O11-P-O13
36	C	405	CN5	CC-O13-P-O14
36	C	405	CN5	CA-O3'-P'-O4'
37	C	406	UQ6	C9-C11-C12-C13
37	C	406	UQ6	C19-C21-C22-C23
37	C	406	UQ6	C23-C24-C26-C27
37	C	406	UQ6	C25-C24-C26-C27
37	N	403	UQ6	C9-C11-C12-C13
37	N	403	UQ6	C19-C21-C22-C23
37	N	403	UQ6	C28-C29-C31-C32
37	N	403	UQ6	C30-C29-C31-C32
38	C	407	9PE	C11-O13-P-O14
38	C	407	9PE	O13-C11-C12-N
38	N	405	9PE	C1-O11-P-O12
38	N	405	9PE	C1-O11-P-O13
38	N	405	9PE	C1-O11-P-O14
38	N	405	9PE	C11-O13-P-O11
38	N	405	9PE	C11-O13-P-O12
38	N	405	9PE	C11-O13-P-O14
38	N	405	9PE	O13-C11-C12-N
28	a	604	PTY	O10-C8-O7-C6
28	m	102	PTY	O10-C8-O7-C6
28	D	402	PTY	O10-C8-O7-C6
29	a	605	CN3	O52-C51-O51-C2'
31	c	302	PCF	O22-C21-O21-C2
37	C	406	UQ6	C12-C11-C9-C10
37	C	406	UQ6	C20-C19-C21-C22
37	C	406	UQ6	C12-C11-C9-C8
36	C	405	CN5	C32-C31-O31-C3
27	a	602	HEA	C13-C14-C15-C16
29	a	605	CN3	O3'-CA-CB-OA
29	N	406	CN3	C22-C21-O21-C2
28	c	301	PTY	C35-C36-C37-C38
36	C	405	CN5	O32-C31-O31-C3
27	a	602	HEA	C19-C20-C21-C22
37	C	406	UQ6	C24-C26-C27-C28
29	N	406	CN3	O22-C21-O21-C2
29	N	406	CN3	O3'-CA-CB-OA
29	N	406	CN3	OA-CB-CC-O13

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Mol	Chain	Res	Type	Atoms
29	a	605	CN3	O21-C2-C3-O31
31	T	101	PCF	O21-C2-C3-O31
37	C	406	UQ6	C18-C19-C21-C22
38	C	407	9PE	C21-C22-C23-C24
39	E	301	7PH	C31-C32-C33-C34
31	m	103	PCF	C21-C22-C23-C24
28	i	101	PTY	C8-C11-C12-C13
28	D	402	PTY	C8-C11-C12-C13
31	T	101	PCF	C31-C32-C33-C34
28	a	604	PTY	C30-C31-C32-C33
33	C	401	6PH	C31-C32-C33-C34
37	C	406	UQ6	C14-C16-C17-C18
28	m	101	PTY	C30-C31-C32-C33
36	C	405	CN5	O3'-CA-CB-OA
35	N	404	8PE	C32-C31-O31-C3
31	m	103	PCF	C22-C21-O21-C2
28	a	604	PTY	C3-O11-P1-O14
28	b	302	PTY	C3-O11-P1-O14
28	b	302	PTY	C5-O14-P1-O11
28	m	102	PTY	C3-O11-P1-O14
28	m	102	PTY	C5-O14-P1-O11
29	a	605	CN3	C1-O11-P-O13
29	a	605	CN3	C1'-O1'-P'-O3'
29	N	406	CN3	CC-O13-P-O11
29	N	406	CN3	C1'-O1'-P'-O3'
31	c	302	PCF	C11-O13-P-O11
31	e	201	PCF	C1-O11-P-O13
31	e	201	PCF	C11-O13-P-O11
31	m	103	PCF	C1-O11-P-O13
31	m	103	PCF	C11-O13-P-O11
31	T	101	PCF	C11-O13-P-O11
35	N	404	8PE	C1-O11-P-O13
36	C	405	CN5	CC-O13-P-O11
36	C	405	CN5	CA-O3'-P'-O1'
38	C	407	9PE	C11-O13-P-O11
27	a	602	HEA	C17-C18-C19-C20
33	O	401	6PH	C37-C38-C39-C3A
31	m	103	PCF	C26-C27-C28-C29
36	C	405	CN5	C39-C3A-C3B-C3C
31	m	103	PCF	O22-C21-O21-C2
35	N	404	8PE	C39-C3A-C3B-C3C
39	E	301	7PH	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
35	C	404	8PE	C39-C3A-C3B-C3C
36	C	405	CN5	C36-C37-C38-C39
38	C	407	9PE	C23-C24-C25-C26
38	N	405	9PE	C21-C22-C23-C24
28	m	101	PTY	C14-C15-C16-C17
31	c	302	PCF	C35-C36-C37-C38
38	C	407	9PE	C25-C26-C27-C28
39	O	403	7PH	C27-C28-C29-C2A
35	N	404	8PE	O32-C31-O31-C3
39	E	301	7PH	C22-C21-O21-C2
35	N	404	8PE	C3D-C3E-C3F-C3G
33	O	401	6PH	C2A-C2B-C2C-C2D
35	C	404	8PE	C38-C39-C3A-C3B
39	E	301	7PH	C26-C27-C28-C29
28	c	301	PTY	C11-C12-C13-C14
28	c	301	PTY	C17-C18-C19-C20
28	c	301	PTY	C33-C34-C35-C36
31	T	101	PCF	C32-C33-C34-C35
38	N	405	9PE	C2D-C2E-C2F-C2G
29	N	406	CN3	C53-C54-C55-C56
28	m	102	PTY	C30-C31-C32-C33
36	C	405	CN5	C3B-C3C-C3D-C3E
33	O	401	6PH	C31-C32-C33-C34
39	E	301	7PH	O22-C21-O21-C2
39	O	403	7PH	C26-C27-C28-C29
33	C	401	6PH	C37-C38-C39-C3A
28	D	402	PTY	C11-C12-C13-C14
28	c	301	PTY	C34-C35-C36-C37
27	a	602	HEA	C21-C22-C23-C24
28	m	101	PTY	O10-C8-O7-C6
33	C	401	6PH	C22-C23-C24-C25
39	O	403	7PH	C22-C23-C24-C25
38	N	405	9PE	C23-C24-C25-C26
39	O	403	7PH	C35-C36-C37-C38
28	m	101	PTY	C11-C8-O7-C6
35	N	404	8PE	C22-C21-O21-C2
31	c	302	PCF	O11-C1-C2-O21
31	m	103	PCF	C25-C26-C27-C28
35	N	404	8PE	O22-C21-O21-C2
39	O	403	7PH	C31-C32-C33-C34
28	b	302	PTY	C31-C32-C33-C34
31	e	201	PCF	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
28	b	302	PTY	C14-C15-C16-C17
38	N	405	9PE	C25-C26-C27-C28
28	m	101	PTY	C37-C38-C39-C40
29	a	605	CN3	CA-O3'-P'-O1'
28	i	101	PTY	C30-C31-C32-C33
33	C	401	6PH	C29-C2A-C2B-C2C
36	C	405	CN5	O3'-CA-CB-CC
28	c	301	PTY	O4-C1-C6-C5
28	i	101	PTY	O4-C1-C6-C5
31	m	103	PCF	C1-C2-C3-O31
31	T	101	PCF	C1-C2-C3-O31
33	C	401	6PH	C1-C2-C3-O31
33	O	401	6PH	C1-C2-C3-O31
27	a	603	HEA	C4D-C3D-CAD-CBD
38	N	405	9PE	C2B-C2C-C2D-C2E
38	C	407	9PE	O31-C31-C32-C33
27	a	602	HEA	C17-C18-C19-C27
28	c	301	PTY	C11-C8-O7-C6
31	m	103	PCF	C22-C23-C24-C25
27	a	603	HEA	C27-C19-C20-C21
35	C	404	8PE	C34-C35-C36-C37
29	a	605	CN3	C42-C41-O41-C3'
29	N	406	CN3	C42-C41-O41-C3'
28	b	302	PTY	C16-C17-C18-C19
35	C	404	8PE	C28-C29-C2A-C2B
28	i	101	PTY	O4-C1-C6-O7
31	e	201	PCF	O21-C2-C3-O31
33	C	401	6PH	C2A-C2B-C2C-C2D
29	a	605	CN3	C43-C44-C45-C46
39	O	403	7PH	C28-C29-C2A-C2B
28	D	402	PTY	C17-C18-C19-C20
39	O	403	7PH	C2B-C2C-C2D-C2E
28	m	102	PTY	O14-C5-C6-C1
29	a	605	CN3	O11-C1-C2-C3
31	c	302	PCF	O11-C1-C2-C3
36	C	405	CN5	O1'-C1'-C2'-C3'
29	N	406	CN3	C51-C52-C53-C54
33	C	401	6PH	C21-C22-C23-C24
39	O	403	7PH	C34-C35-C36-C37
28	D	402	PTY	C14-C15-C16-C17
35	C	404	8PE	C32-C31-O31-C3
39	O	403	7PH	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
31	I	101	PCF	C38-C39-C40-C41
35	C	404	8PE	C3D-C3E-C3F-C3G
28	m	102	PTY	O4-C1-C6-C5
29	a	605	CN3	C1-C2-C3-O31
29	a	605	CN3	C46-C47-C48-C49
35	N	404	8PE	C37-C38-C39-C3A
35	C	404	8PE	C37-C38-C39-C3A
31	m	103	PCF	C36-C37-C38-C39
31	I	101	PCF	C1-O11-P-O13
28	i	101	PTY	O14-C5-C6-O7
29	a	605	CN3	O11-C1-C2-O21
28	m	101	PTY	C11-C12-C13-C14
29	a	605	CN3	O42-C41-O41-C3'
28	m	101	PTY	C20-C21-C22-C23
35	C	404	8PE	C3A-C3B-C3C-C3D
28	c	301	PTY	O10-C8-O7-C6
29	N	406	CN3	C2-C1-O11-P
29	N	406	CN3	O42-C41-O41-C3'
35	C	404	8PE	C2B-C2C-C2D-C2E
35	C	404	8PE	C21-C22-C23-C24
27	a	602	HEA	C2A-CAA-CBA-CGA
38	N	405	9PE	C22-C21-O21-C2
28	m	101	PTY	C36-C37-C38-C39
29	N	406	CN3	C46-C47-C48-C49
33	O	401	6PH	C22-C23-C24-C25
39	E	301	7PH	C32-C31-O31-C3
35	N	404	8PE	C28-C29-C2A-C2B
27	a	603	HEA	C2D-C3D-CAD-CBD
28	i	101	PTY	C17-C18-C19-C20
38	N	405	9PE	C22-C23-C24-C25
28	a	604	PTY	O4-C1-C6-C5
29	N	406	CN3	C1'-C2'-C3'-O41
31	c	302	PCF	C1-C2-C3-O31
31	I	101	PCF	C1-C2-C3-O31
28	a	604	PTY	O14-C5-C6-O7
28	m	102	PTY	O14-C5-C6-O7
34	D	401	HEM	C4C-C3C-CAC-CBC
39	O	403	7PH	O32-C31-O31-C3
35	C	404	8PE	O32-C31-O31-C3
28	m	102	PTY	O4-C1-C6-O7
31	m	103	PCF	O21-C2-C3-O31
31	I	101	PCF	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
35	C	404	8PE	O22-C21-O21-C2
38	N	405	9PE	O22-C21-O21-C2
33	C	401	6PH	C39-C3A-C3B-C3C
35	N	404	8PE	C36-C37-C38-C39
39	O	403	7PH	O22-C21-O21-C2
29	a	605	CN3	C45-C46-C47-C48
28	c	301	PTY	C3-O11-P1-O14
28	i	101	PTY	C3-O11-P1-O14
35	N	404	8PE	C11-O13-P-O11
35	N	404	8PE	C3C-C3D-C3E-C3F
39	E	301	7PH	O32-C31-O31-C3
28	a	604	PTY	C3-O11-P1-O12
28	b	302	PTY	C3-O11-P1-O13
28	b	302	PTY	C5-O14-P1-O13
28	i	101	PTY	C5-O14-P1-O12
29	a	605	CN3	CC-O13-P-O12
29	a	605	CN3	C1'-O1'-P'-O2'
29	a	605	CN3	CA-O3'-P'-O4'
29	N	406	CN3	C1-O11-P-O12
31	e	201	PCF	C11-O13-P-O12
31	m	103	PCF	C11-O13-P-O12
35	C	404	8PE	C1-O11-P-O12
36	C	405	CN5	C1-O11-P-O14
36	C	405	CN5	CC-O13-P-O12
38	C	407	9PE	C11-O13-P-O12
33	C	401	6PH	C32-C31-O31-C3
28	a	604	PTY	O14-C5-C6-C1
28	i	101	PTY	O14-C5-C6-C1
35	C	404	8PE	O11-C1-C2-C3
35	N	404	8PE	O11-C1-C2-C3
33	O	401	6PH	C23-C24-C25-C26
28	i	101	PTY	C37-C38-C39-C40
27	a	603	HEA	C3B-C11-C12-C13
31	e	201	PCF	C12-C11-O13-P
35	C	404	8PE	O11-C1-C2-O21
35	N	404	8PE	O11-C1-C2-O21
35	C	404	8PE	C22-C21-O21-C2
39	O	403	7PH	C22-C21-O21-C2
31	e	201	PCF	O13-C11-C12-N
31	e	201	PCF	C1-C2-C3-O31
29	N	406	CN3	O51-C2'-C3'-O41
39	E	301	7PH	C27-C28-C29-C2A

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Mol	Chain	Res	Type	Atoms
38	N	405	9PE	C32-C33-C34-C35
37	N	403	UQ6	C15-C14-C16-C17
38	N	405	9PE	O31-C31-C32-C33
28	m	101	PTY	C32-C33-C34-C35
33	C	401	6PH	O32-C31-O31-C3
29	N	406	CN3	CA-CB-CC-O13
35	N	404	8PE	C23-C24-C25-C26
28	m	101	PTY	C18-C19-C20-C21
28	m	101	PTY	C3-O11-P1-O14
31	T	101	PCF	C1-O11-P-O13
36	C	405	CN5	C1'-O1'-P'-O3'
39	E	301	7PH	C28-C29-C2A-C2B
31	c	302	PCF	C26-C27-C28-C29
33	C	401	6PH	C36-C37-C38-C39
28	m	102	PTY	C12-C13-C14-C15
38	C	407	9PE	O32-C31-C32-C33
35	C	404	8PE	C3E-C3F-C3G-C3H
38	C	407	9PE	C32-C33-C34-C35
28	c	301	PTY	N1-C2-C3-O11
34	C	402	HEM	CAA-CBA-CGA-O1A
37	C	406	UQ6	C15-C14-C16-C17
36	C	405	CN5	O11-C1-C2-C3
28	i	101	PTY	C38-C39-C40-C41
27	a	602	HEA	CAA-CBA-CGA-O1A
38	C	407	9PE	C22-C23-C24-C25
28	m	101	PTY	C17-C18-C19-C20
34	N	401	HEM	CAA-CBA-CGA-O1A
31	I	101	PCF	C21-C22-C23-C24
33	O	401	6PH	C2B-C2C-C2D-C2E
28	D	402	PTY	C16-C17-C18-C19
31	c	302	PCF	C34-C35-C36-C37
28	m	101	PTY	C1-C6-O7-C8
27	a	603	HEA	CAA-CBA-CGA-O1A
34	N	401	HEM	CAA-CBA-CGA-O2A
29	N	406	CN3	C1-O11-P-O13
29	N	406	CN3	O11-C1-C2-C3
27	a	603	HEA	O11-C11-C12-C13
38	C	407	9PE	C2D-C2E-C2F-C2G
28	a	604	PTY	O4-C1-C6-O7
31	T	101	PCF	C21-C22-C23-C24
27	a	603	HEA	CAA-CBA-CGA-O2A
34	C	402	HEM	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
36	C	405	CN5	C3A-C3B-C3C-C3D
35	C	404	8PE	C3C-C3D-C3E-C3F
38	N	405	9PE	C2C-C2D-C2E-C2F
35	N	404	8PE	C38-C39-C3A-C3B
28	b	302	PTY	C11-C12-C13-C14
39	E	301	7PH	C21-C22-C23-C24
37	N	403	UQ6	C12-C11-C9-C10
27	a	603	HEA	C18-C19-C20-C21
27	a	603	HEA	C3D-CAD-CBD-CGD
31	m	103	PCF	C24-C25-C26-C27
34	C	402	HEM	CAD-CBD-CGD-O2D
35	N	404	8PE	C31-C32-C33-C34
27	a	602	HEA	CAD-CBD-CGD-O2D
34	C	403	HEM	CAD-CBD-CGD-O2D
28	m	102	PTY	C17-C18-C19-C20
29	N	406	CN3	O31-C31-C32-C33
28	m	102	PTY	C12-C11-C8-O7
33	C	401	6PH	C24-C25-C26-C27
34	C	403	HEM	CAA-CBA-CGA-O1A
37	N	403	UQ6	C13-C14-C16-C17
39	E	301	7PH	C39-C3A-C3B-C3C
34	C	402	HEM	CAD-CBD-CGD-O1D
34	C	403	HEM	CAD-CBD-CGD-O1D
28	D	402	PTY	C18-C19-C20-C21
28	c	301	PTY	C12-C11-C8-O7
27	a	603	HEA	C26-C15-C16-C17
35	C	404	8PE	C33-C34-C35-C36
29	a	605	CN3	O1'-C1'-C2'-O51
29	N	406	CN3	O1'-C1'-C2'-O51
31	e	201	PCF	O11-C1-C2-O21
31	T	101	PCF	O21-C21-C22-C23
28	b	302	PTY	C34-C35-C36-C37
28	m	101	PTY	C21-C22-C23-C24
34	N	401	HEM	C4C-C3C-CAC-CBC
35	N	404	8PE	C3F-C3G-C3H-C3I
39	O	403	7PH	C23-C24-C25-C26
31	I	101	PCF	O31-C31-C32-C33
31	T	101	PCF	O31-C31-C32-C33
27	a	602	HEA	CAA-CBA-CGA-O2A
34	N	402	HEM	CAA-CBA-CGA-O1A
38	C	407	9PE	C2A-C2B-C2C-C2D
34	C	403	HEM	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
34	N	402	HEM	CAA-CBA-CGA-O2A
27	a	602	HEA	C26-C15-C16-C17
29	N	406	CN3	O51-C51-C52-C53
28	a	604	PTY	C31-C30-O4-C1
31	T	101	PCF	O32-C31-C32-C33
28	a	604	PTY	O30-C30-O4-C1
31	I	101	PCF	O32-C31-C32-C33
28	a	604	PTY	C13-C14-C15-C16
31	T	101	PCF	O22-C21-C22-C23
29	a	605	CN3	CA-O3'-P'-O2'
31	I	101	PCF	C1-O11-P-O12
31	T	101	PCF	C1-O11-P-O12
35	N	404	8PE	C11-O13-P-O12
38	C	407	9PE	C1-O11-P-O12
39	O	403	7PH	C25-C26-C27-C28
29	N	406	CN3	O52-C51-C52-C53
35	N	404	8PE	C35-C36-C37-C38
28	a	604	PTY	N1-C2-C3-O11
28	c	301	PTY	C12-C11-C8-O10
29	N	406	CN3	C56-C57-C58-C59
31	c	302	PCF	C22-C23-C24-C25
33	O	401	6PH	O22-C21-O21-C2
38	N	405	9PE	C2F-C2G-C2H-C2I
27	a	602	HEA	C3B-C11-C12-C13
28	m	101	PTY	C5-C6-O7-C8
35	N	404	8PE	C12-C11-O13-P
28	i	101	PTY	C12-C11-C8-O7
39	E	301	7PH	C23-C24-C25-C26
28	a	604	PTY	O4-C30-C31-C32
37	C	406	UQ6	C11-C12-C13-C14
37	C	406	UQ6	C13-C14-C16-C17
28	c	301	PTY	C12-C13-C14-C15
29	N	406	CN3	C55-C56-C57-C58
28	a	604	PTY	O30-C30-C31-C32

There are no ring outliers.

29 monomers are involved in 176 short contacts:

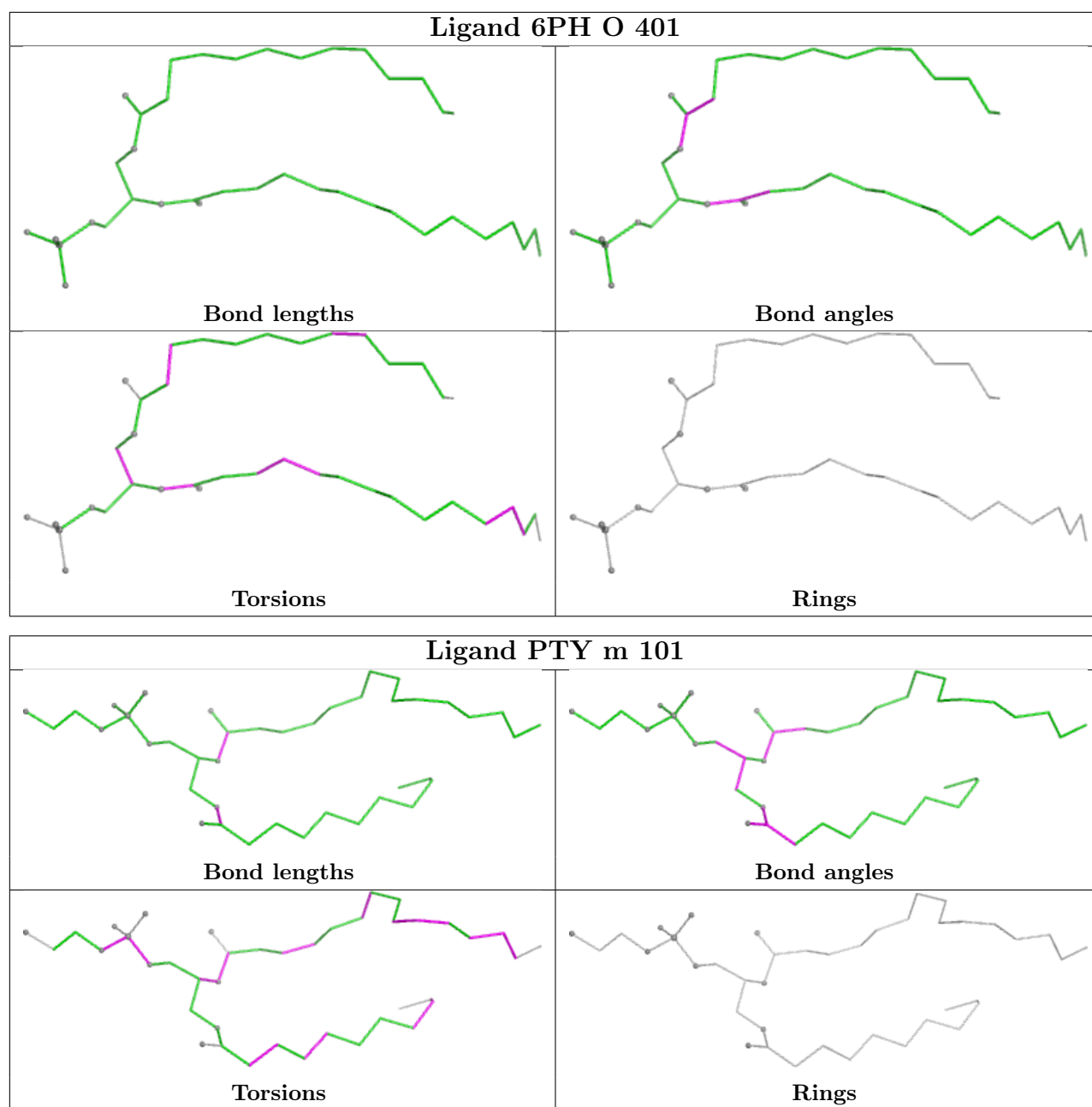
Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	O	401	6PH	4	0
28	m	101	PTY	14	0
28	m	102	PTY	18	0

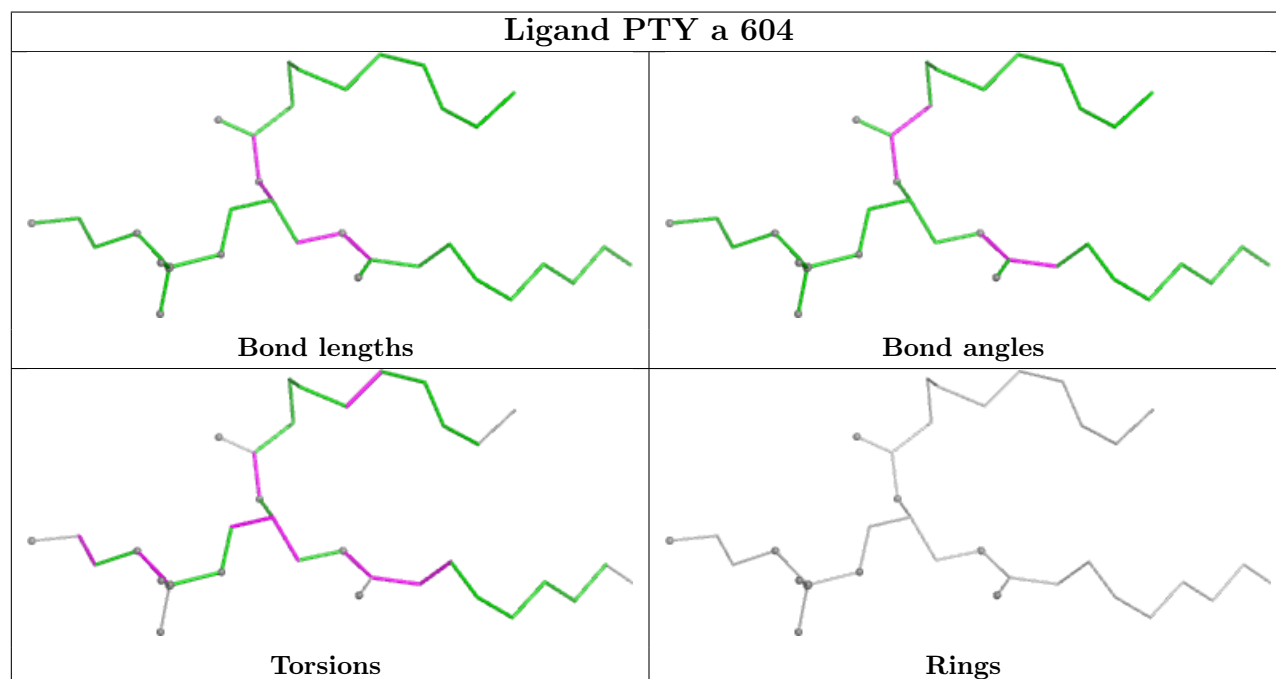
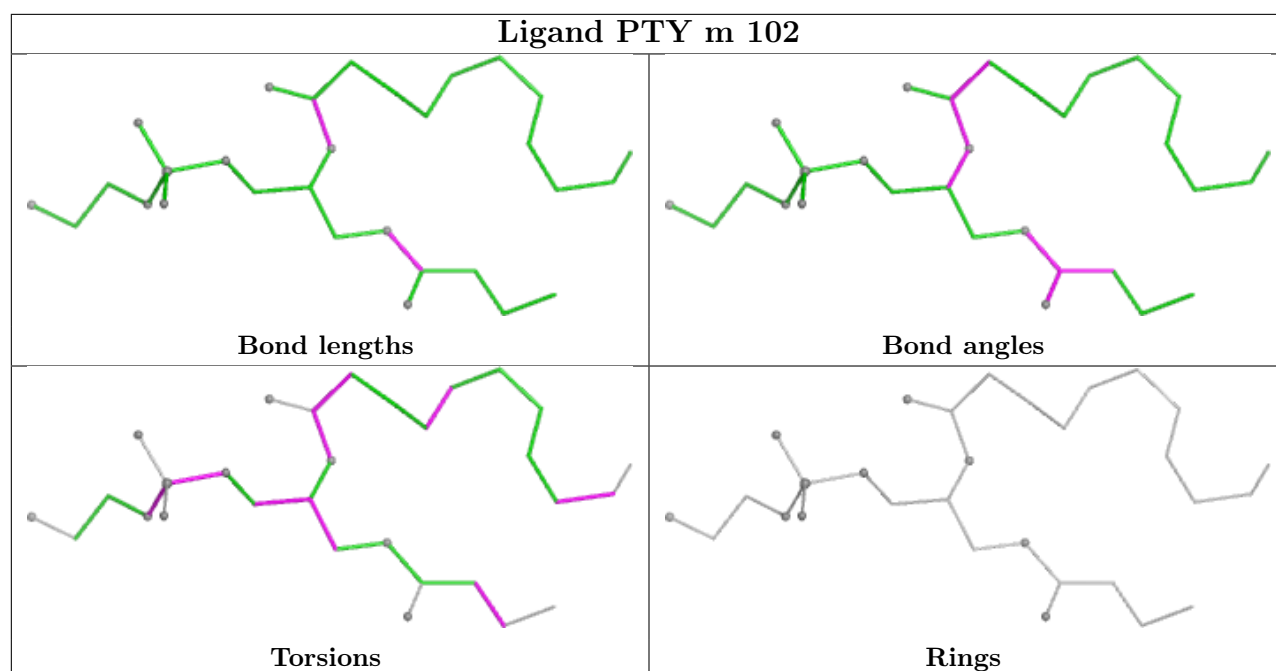
Continued on next page...

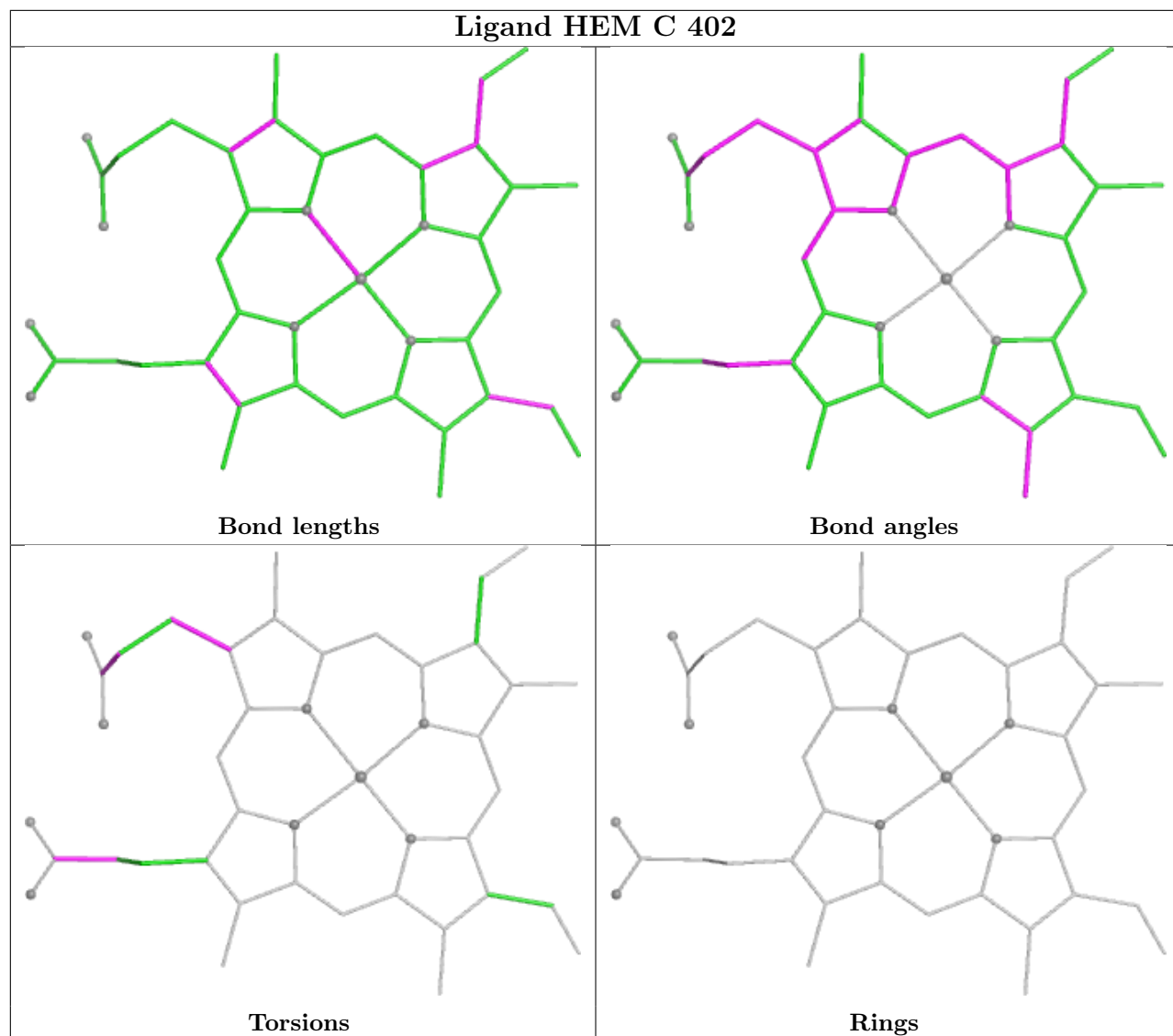
Continued from previous page...

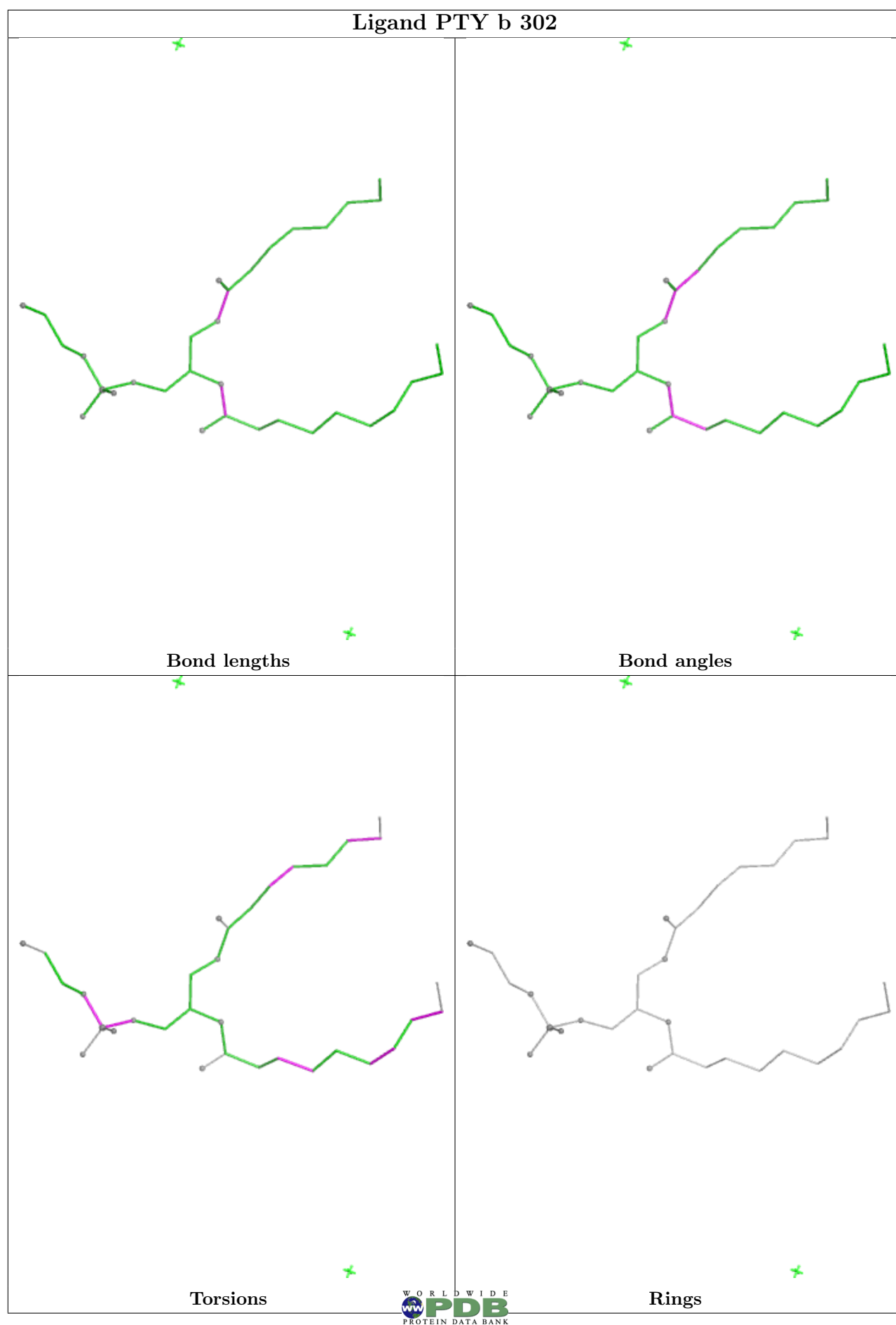
Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	a	604	PTY	11	0
28	b	302	PTY	2	0
36	C	405	CN5	2	0
31	e	201	PCF	8	0
29	a	605	CN3	1	0
31	m	103	PCF	1	0
39	O	403	7PH	4	0
28	c	301	PTY	40	0
34	O	402	HEM	3	0
29	N	406	CN3	2	0
34	D	401	HEM	3	0
40	P	301	FES	2	0
35	N	404	8PE	2	0
31	T	101	PCF	2	0
34	N	401	HEM	1	0
27	a	603	HEA	1	0
40	E	302	FES	1	0
37	C	406	UQ6	2	0
39	E	301	7PH	2	0
27	a	602	HEA	6	0
28	D	402	PTY	39	0
34	C	403	HEM	1	0
35	C	404	8PE	2	0
28	i	101	PTY	18	0
31	I	101	PCF	1	0
31	c	302	PCF	1	0

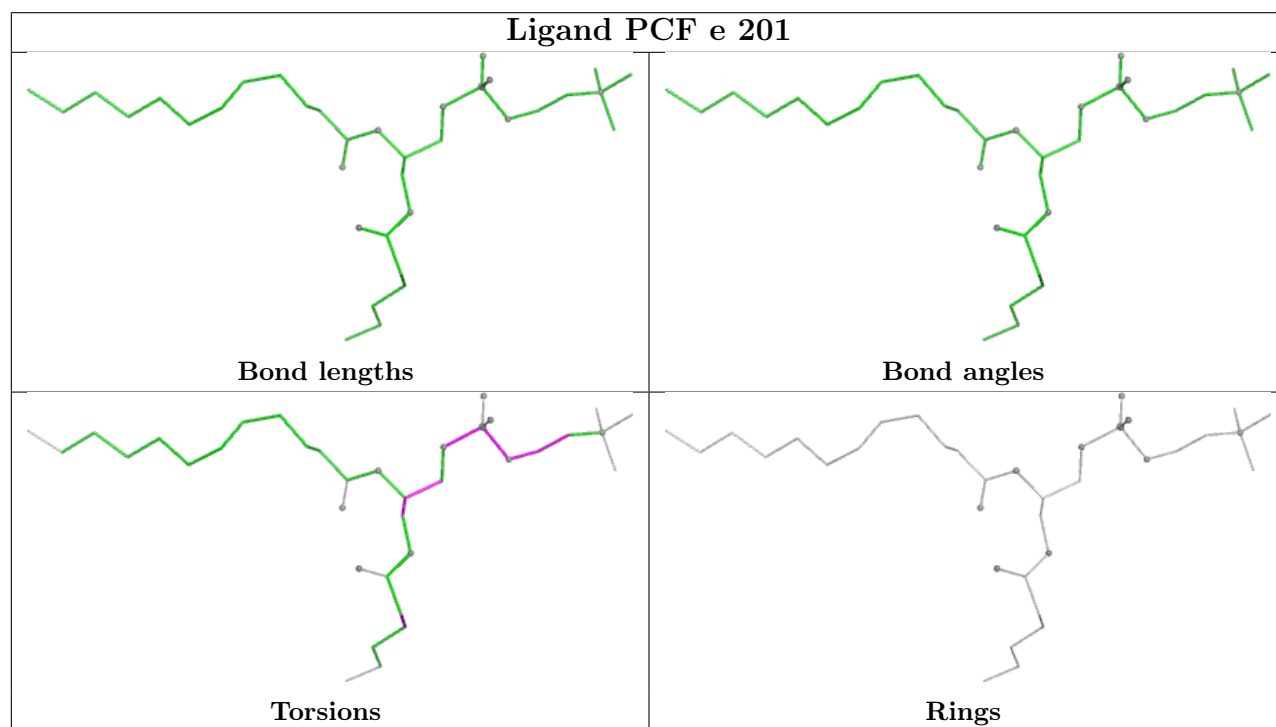
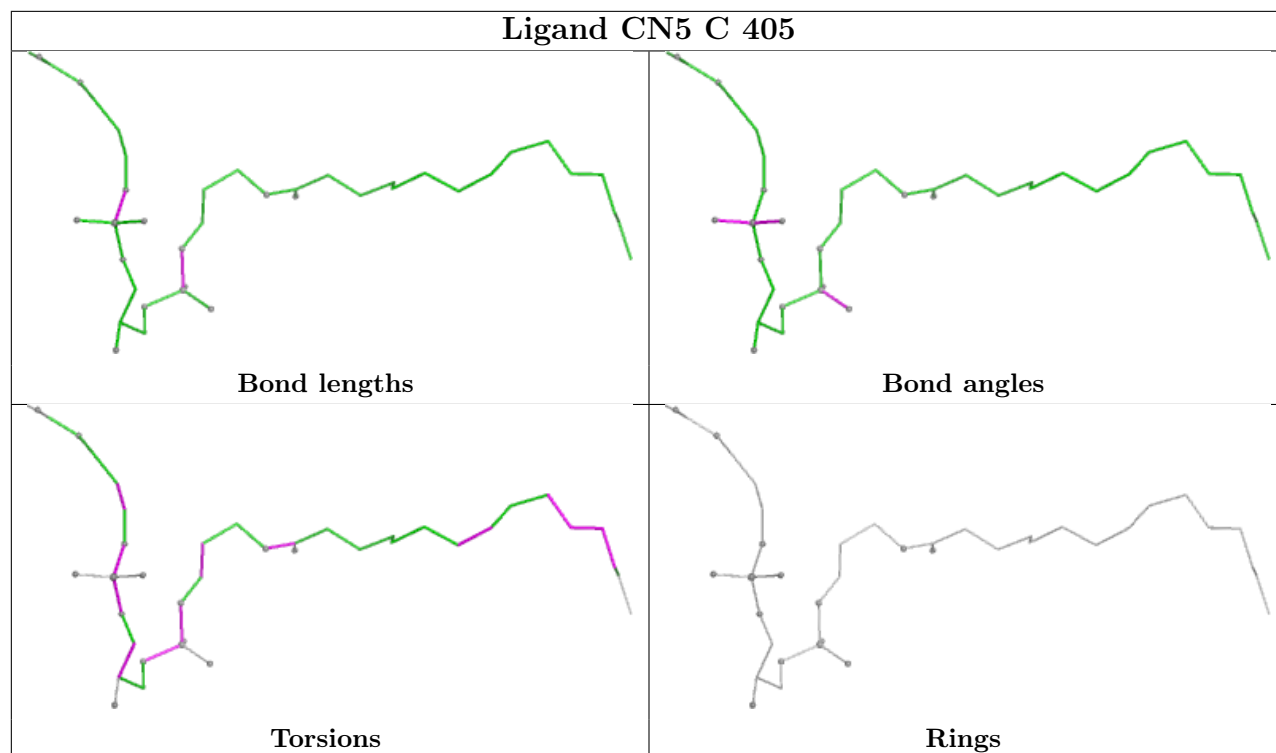
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

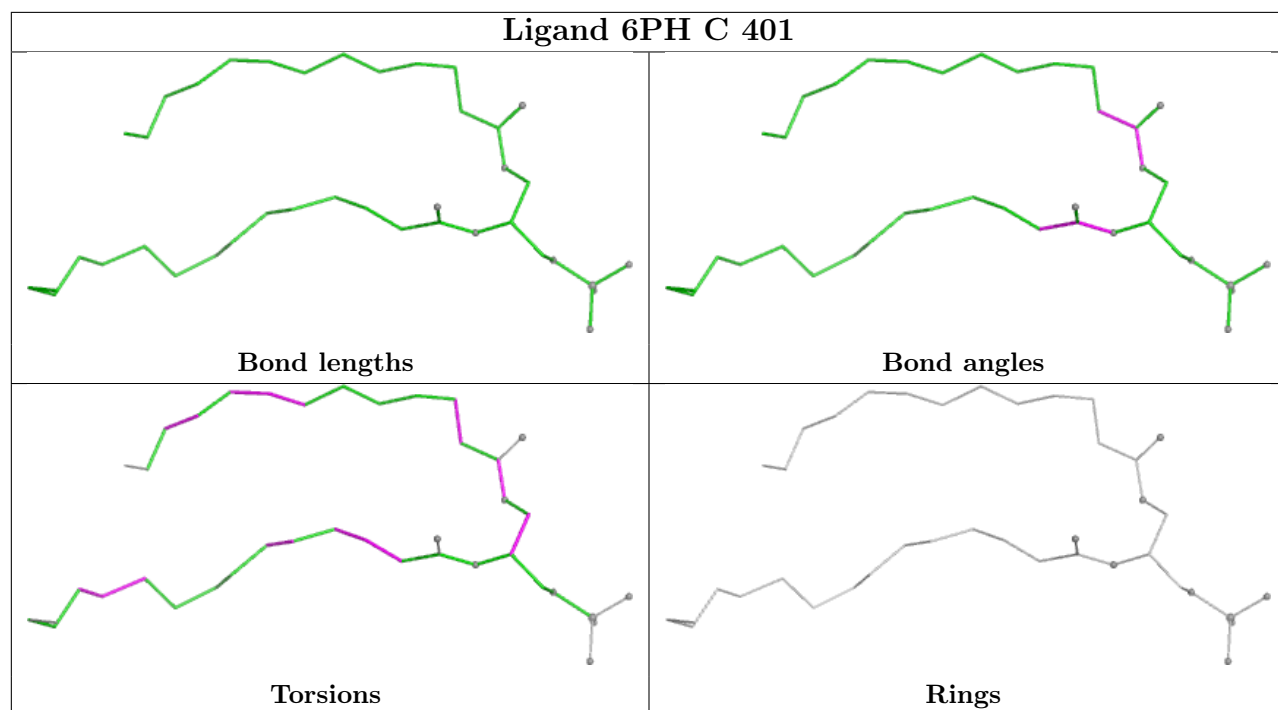
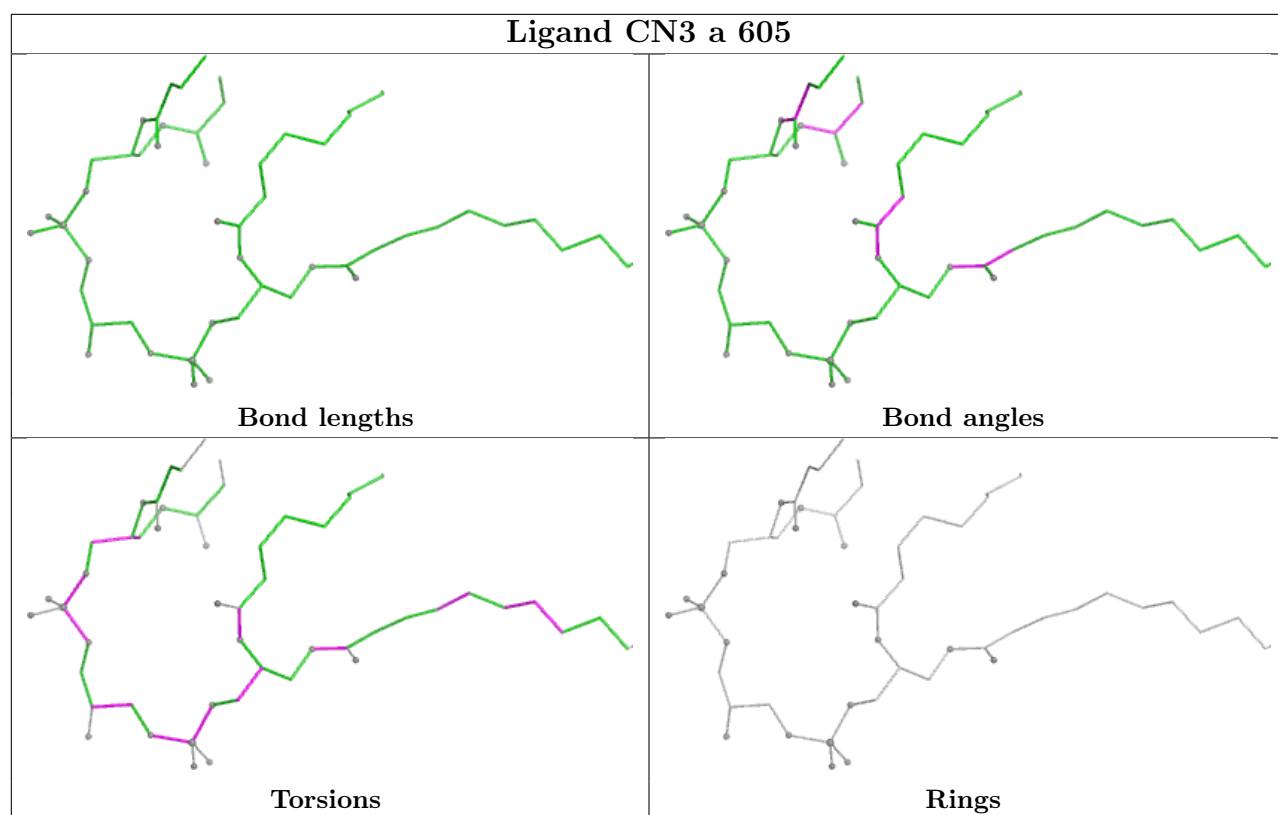


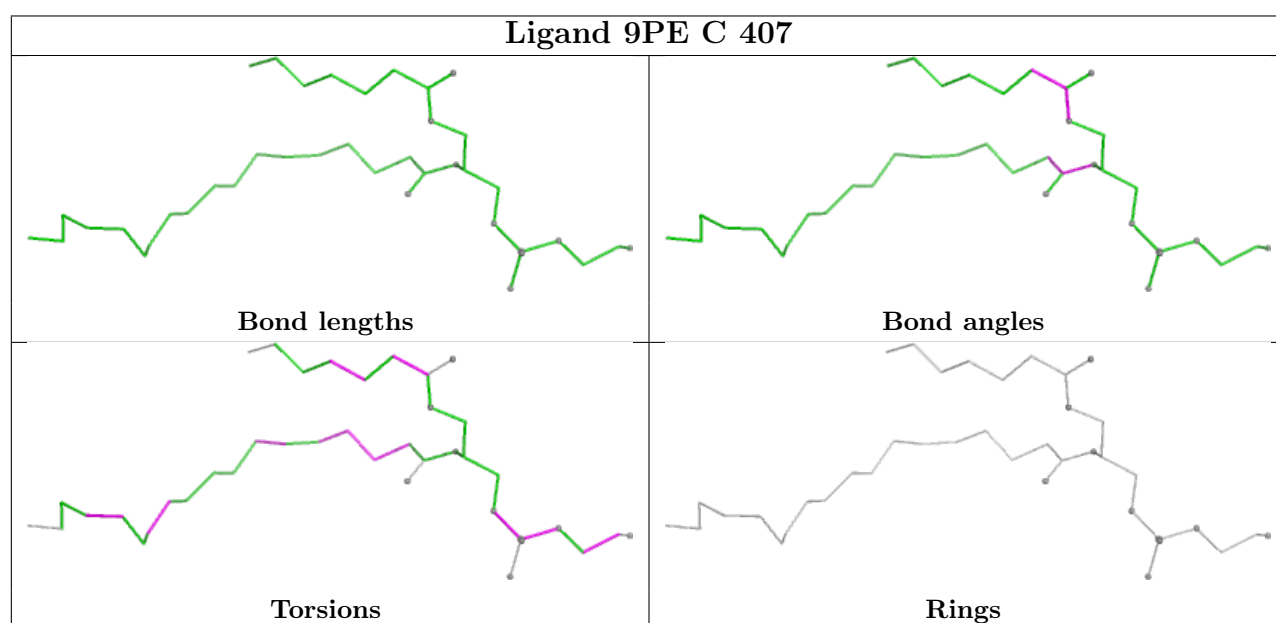
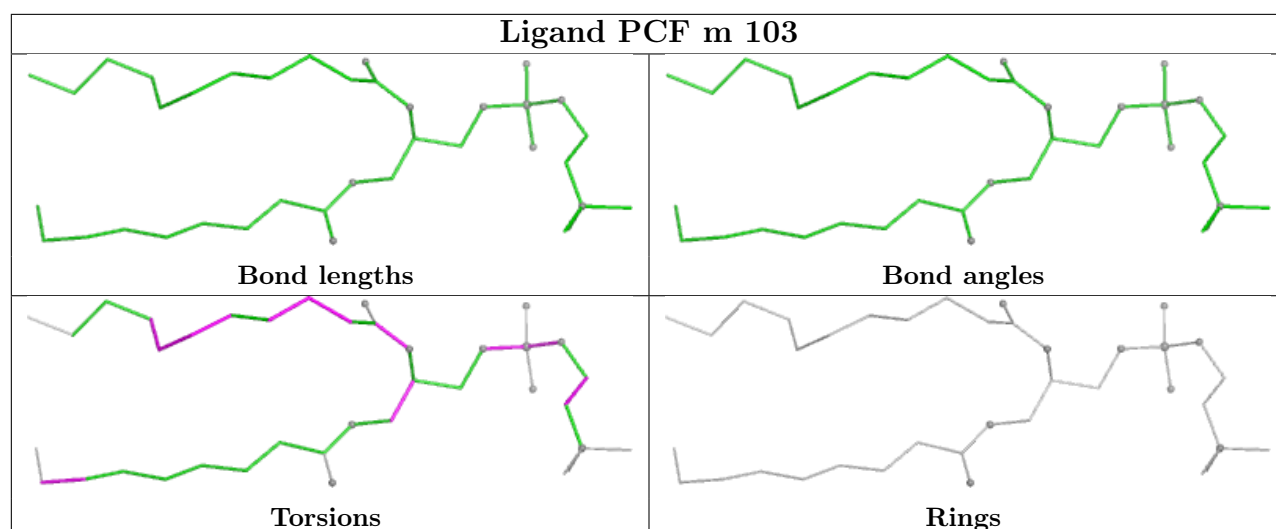


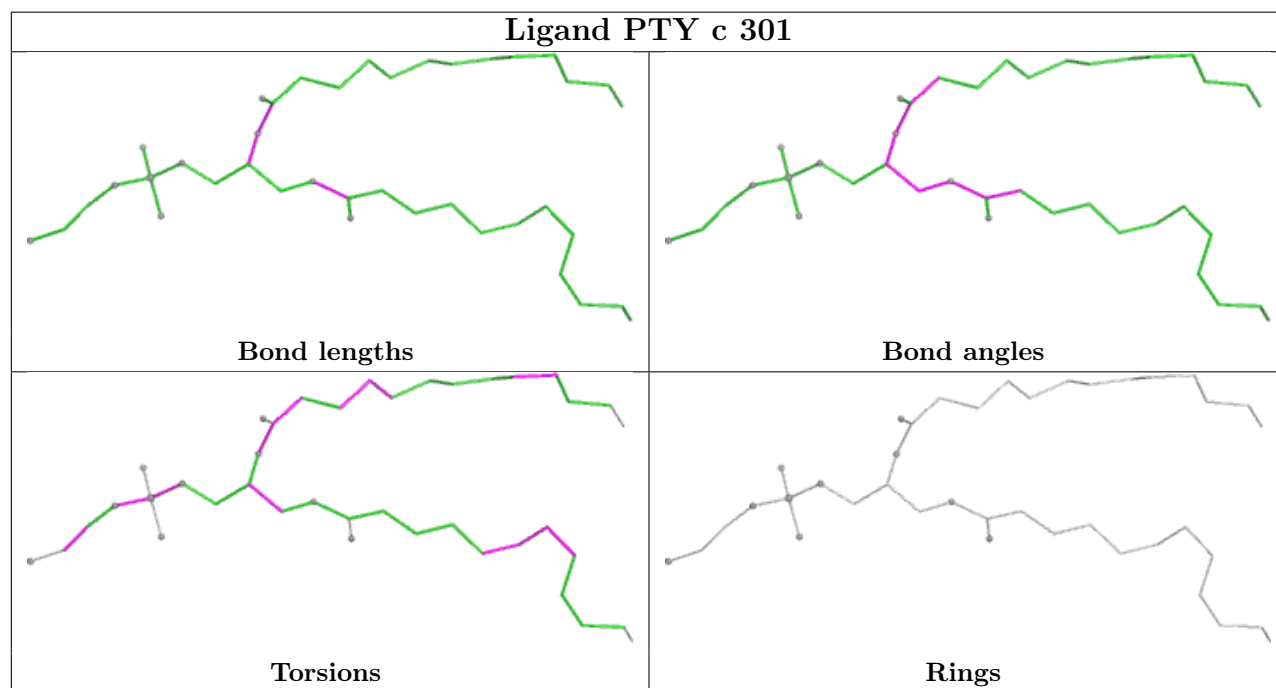
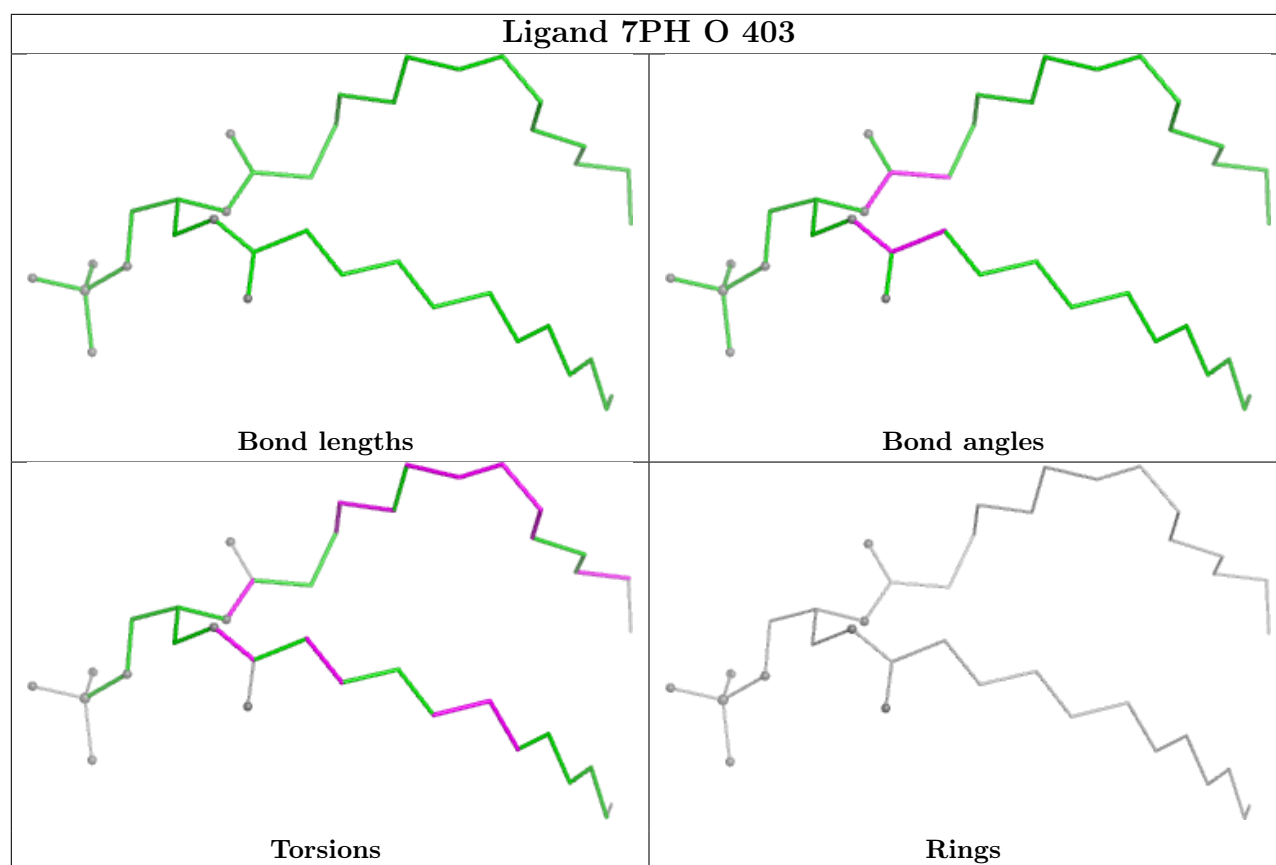


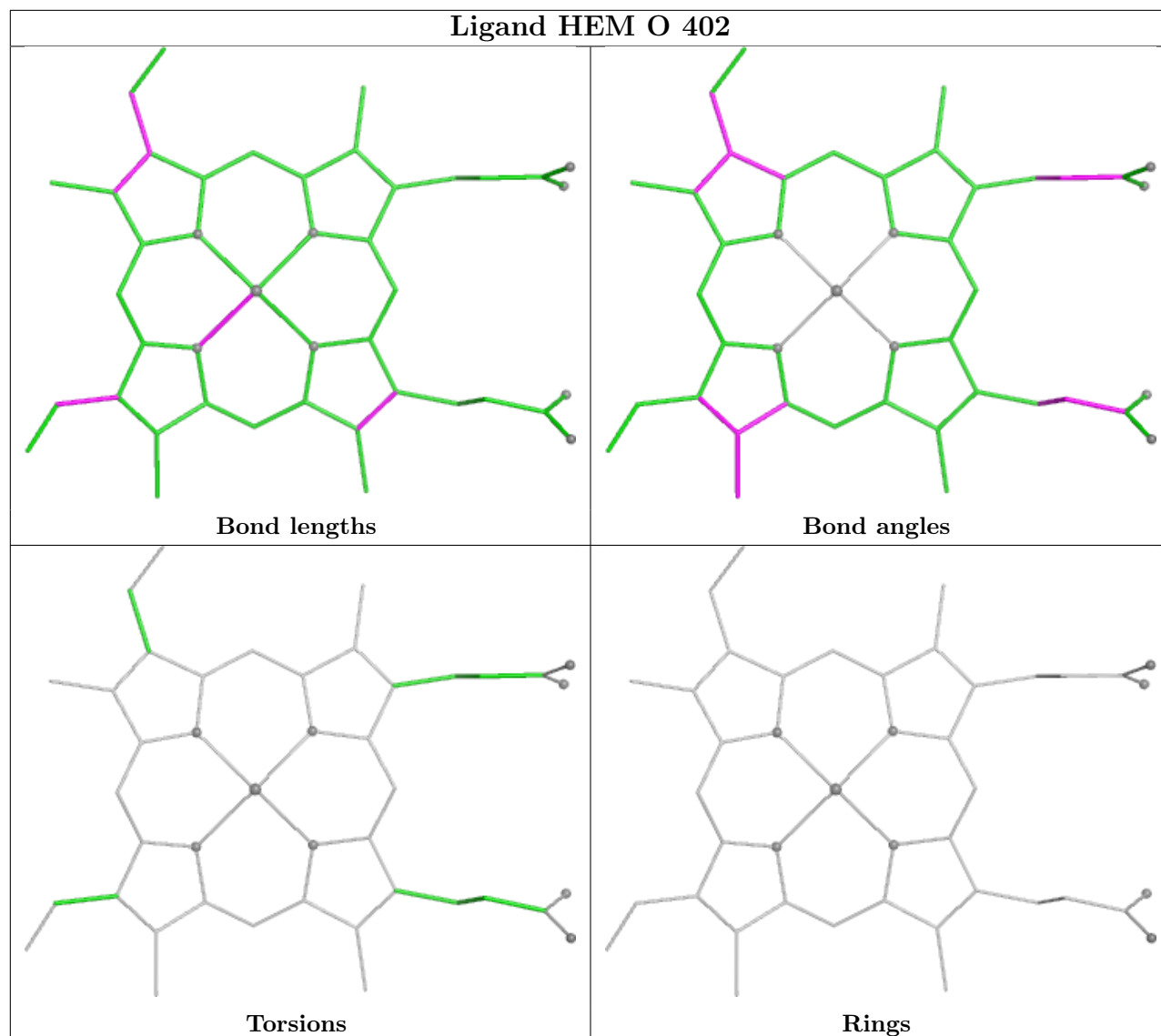


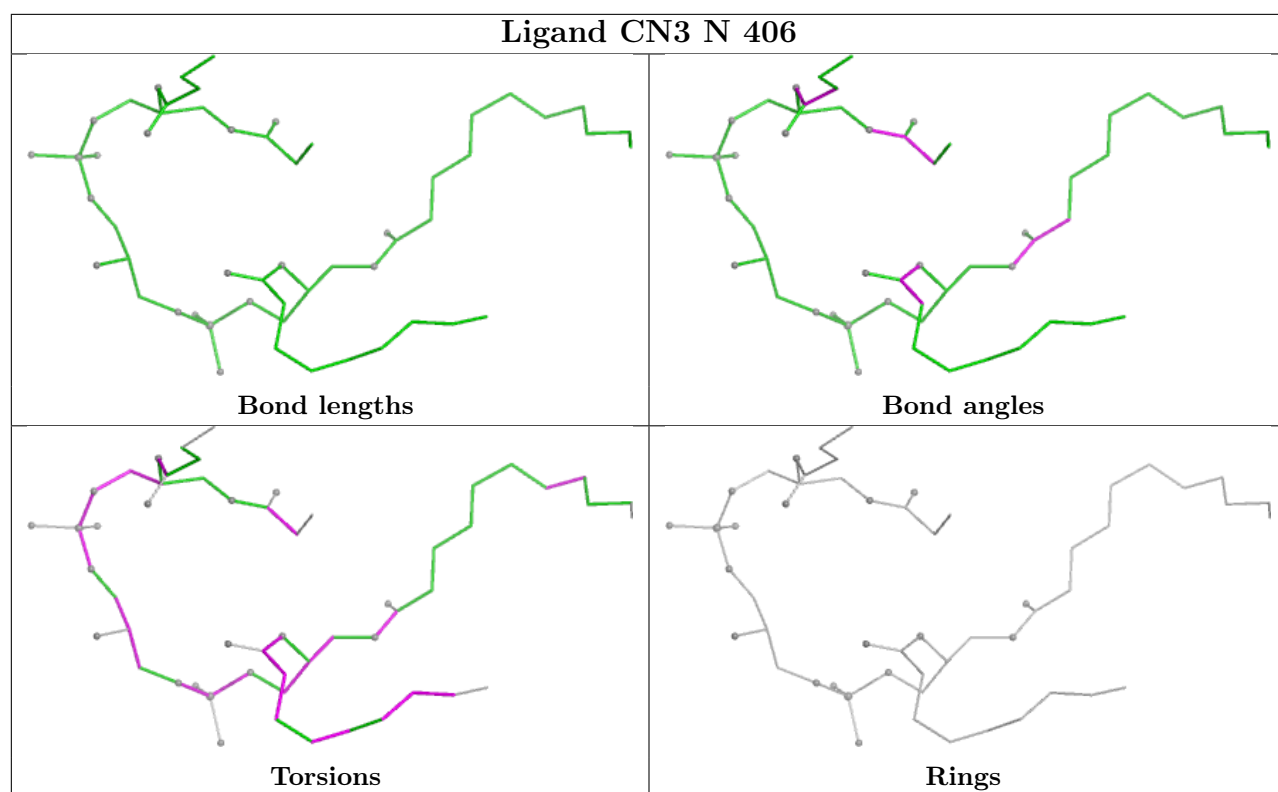


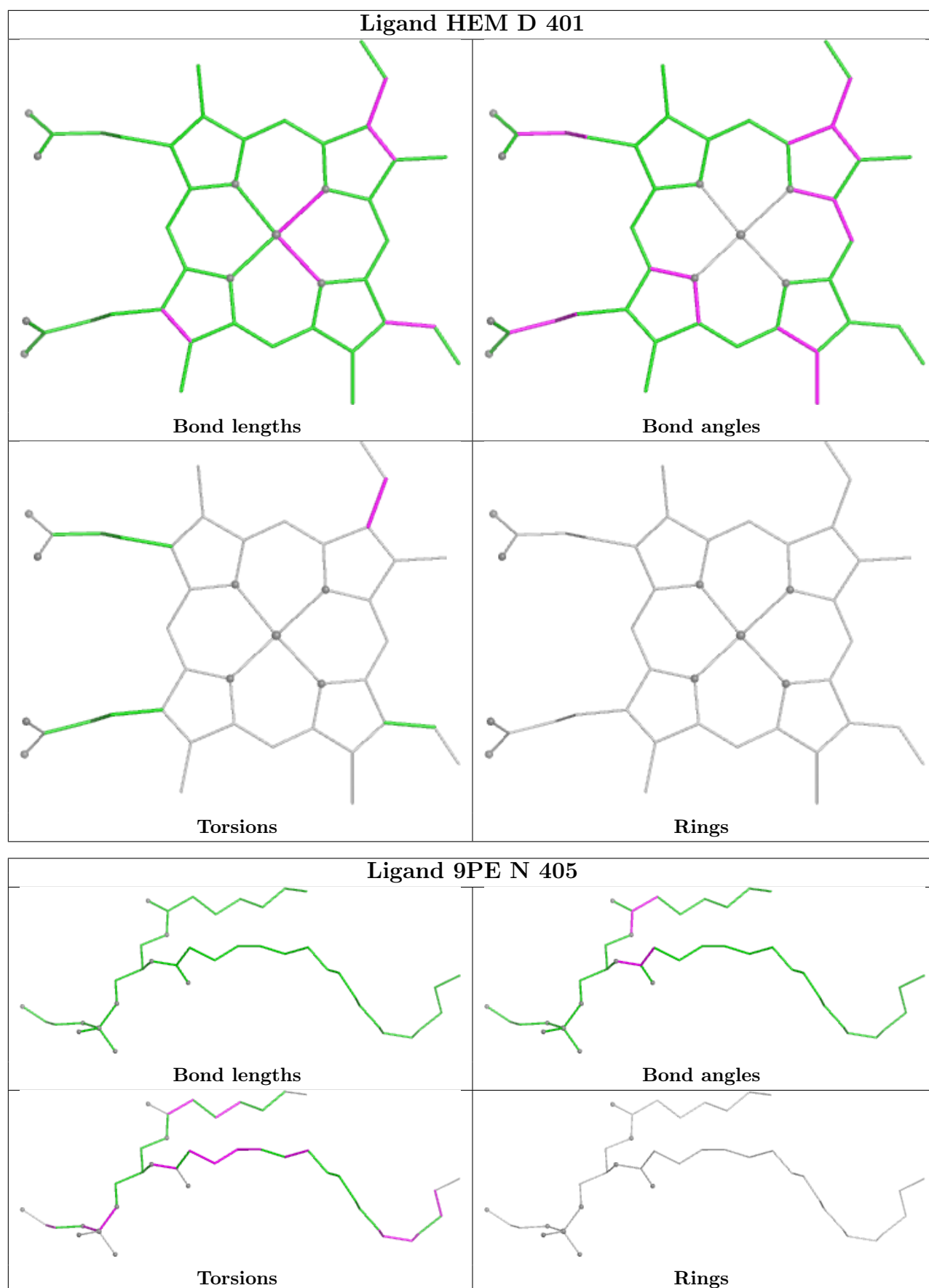


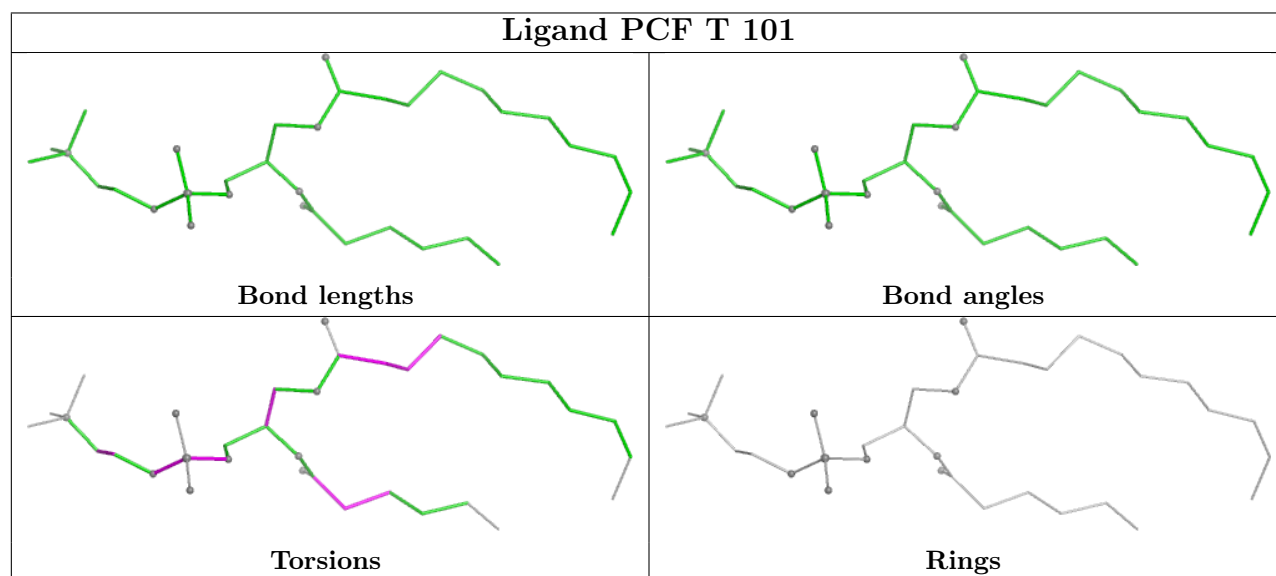
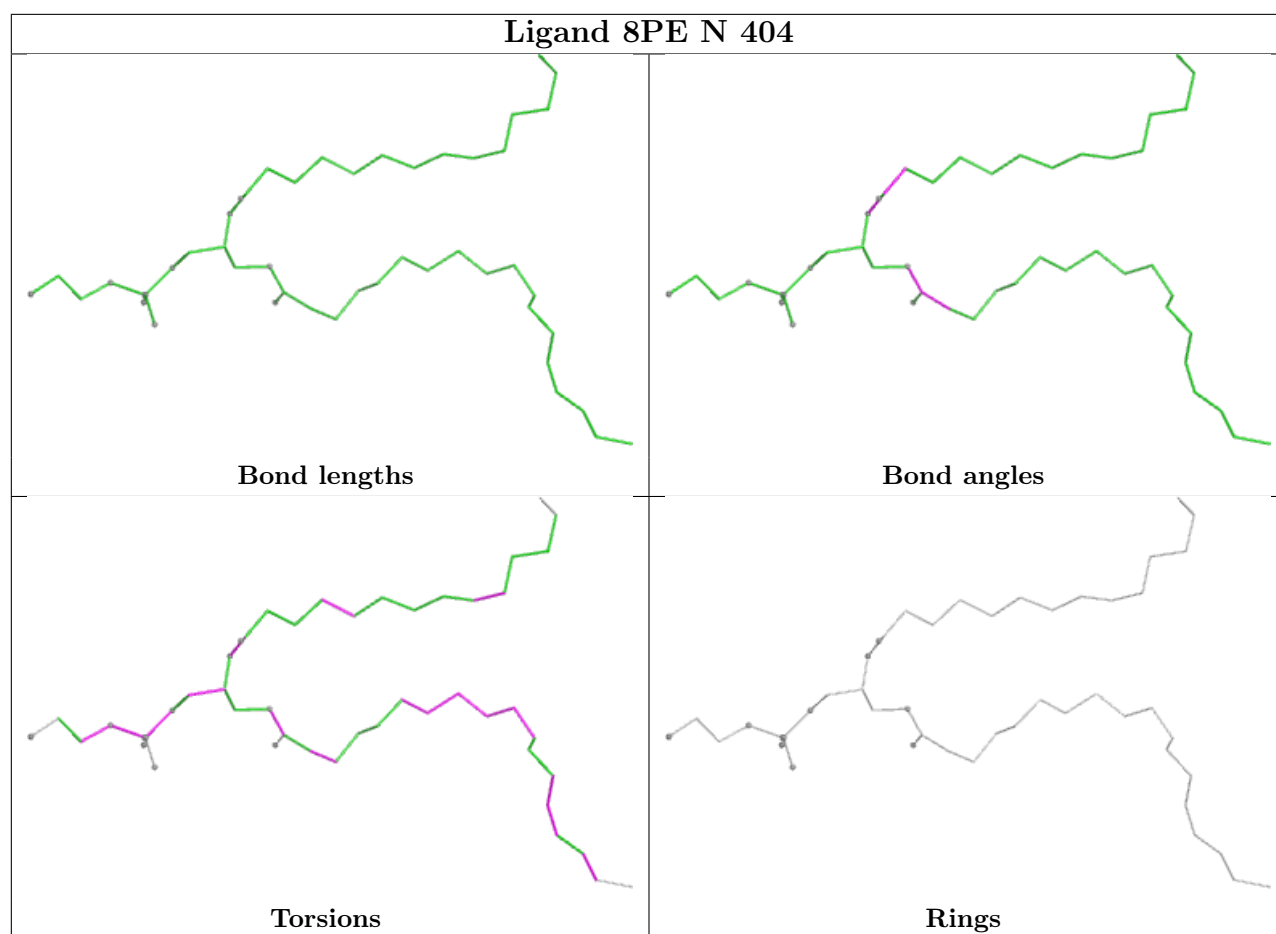


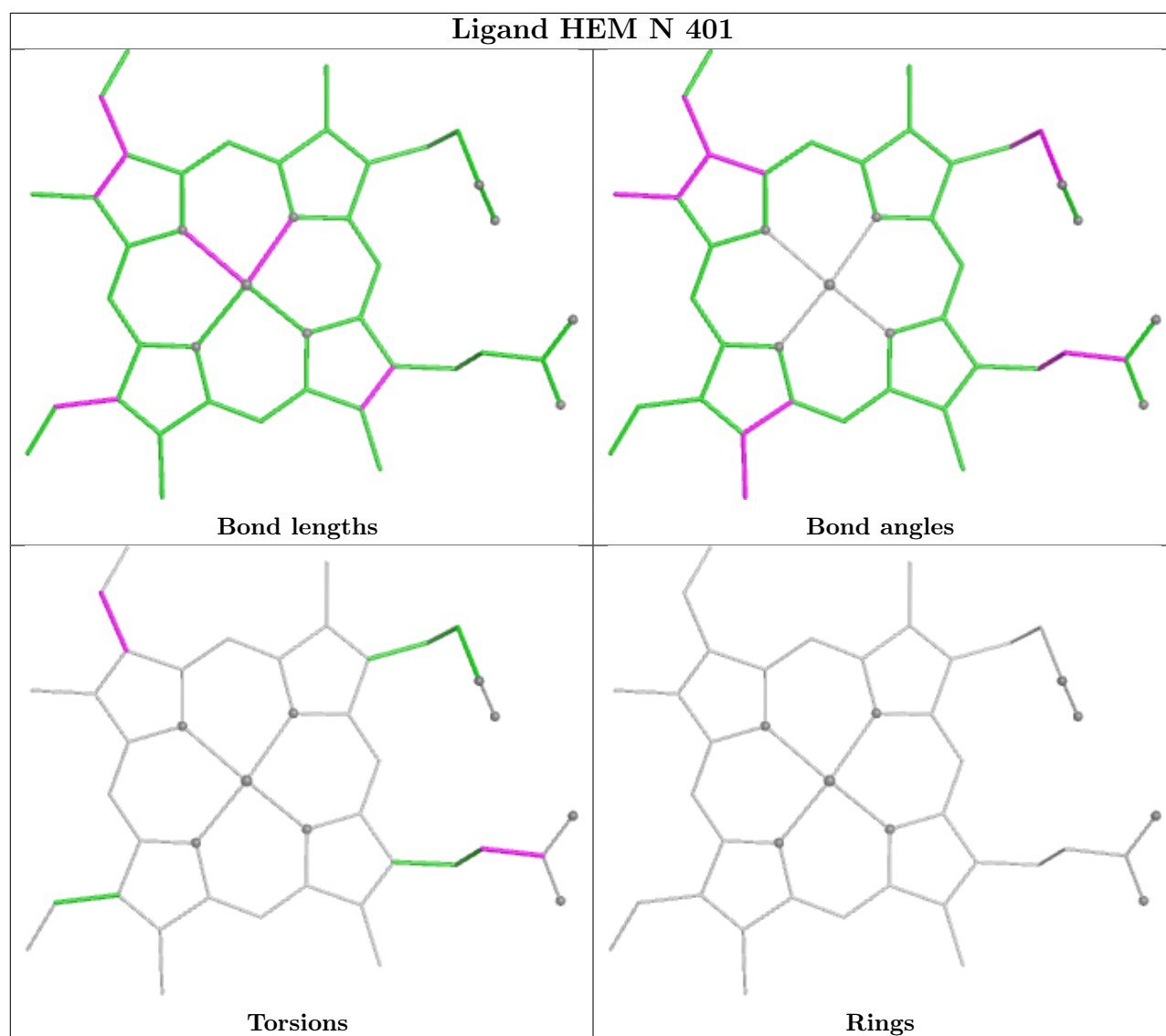


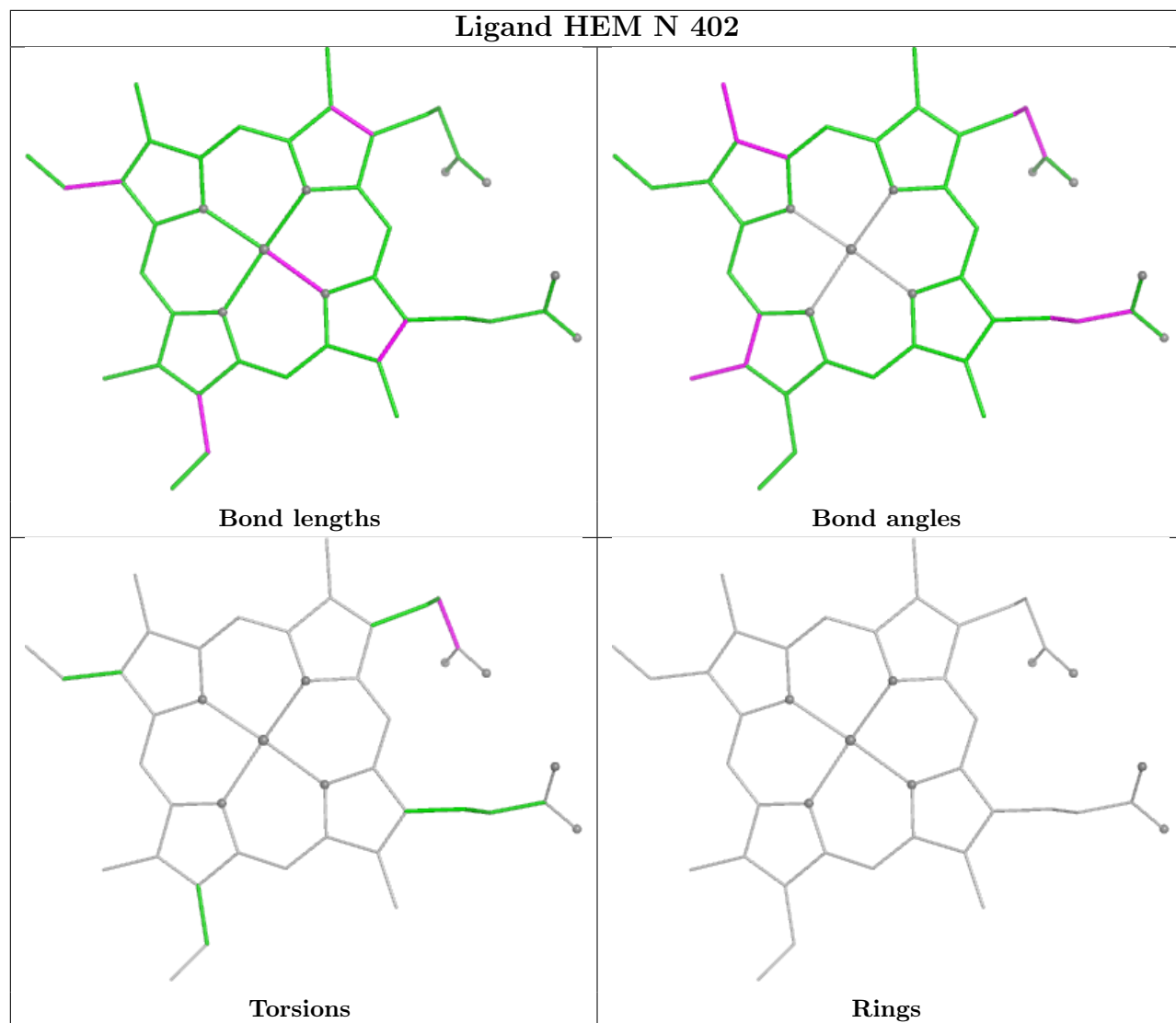


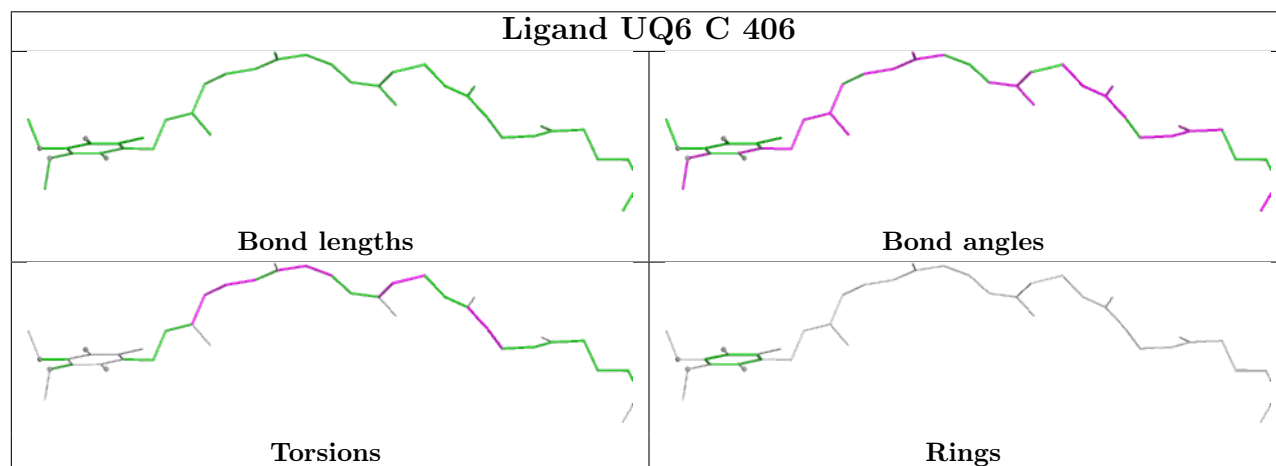
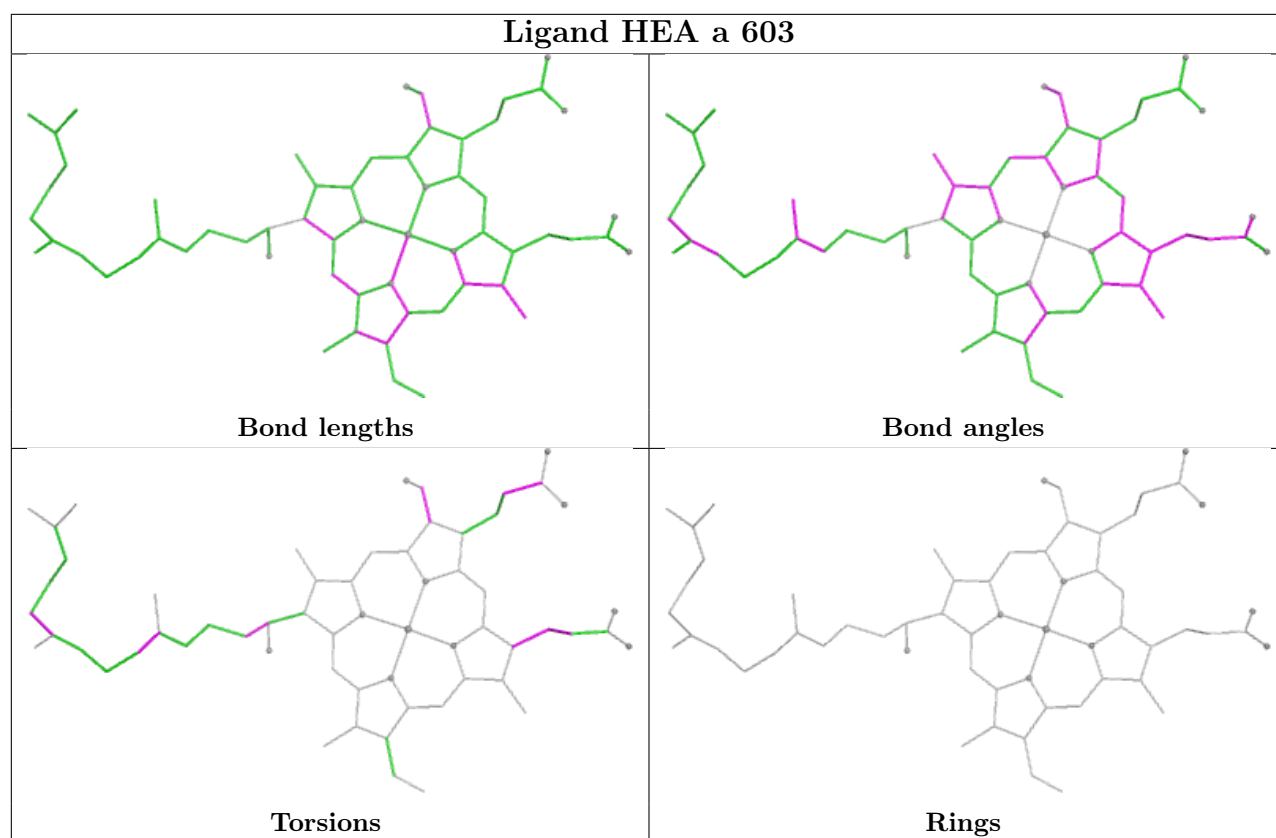


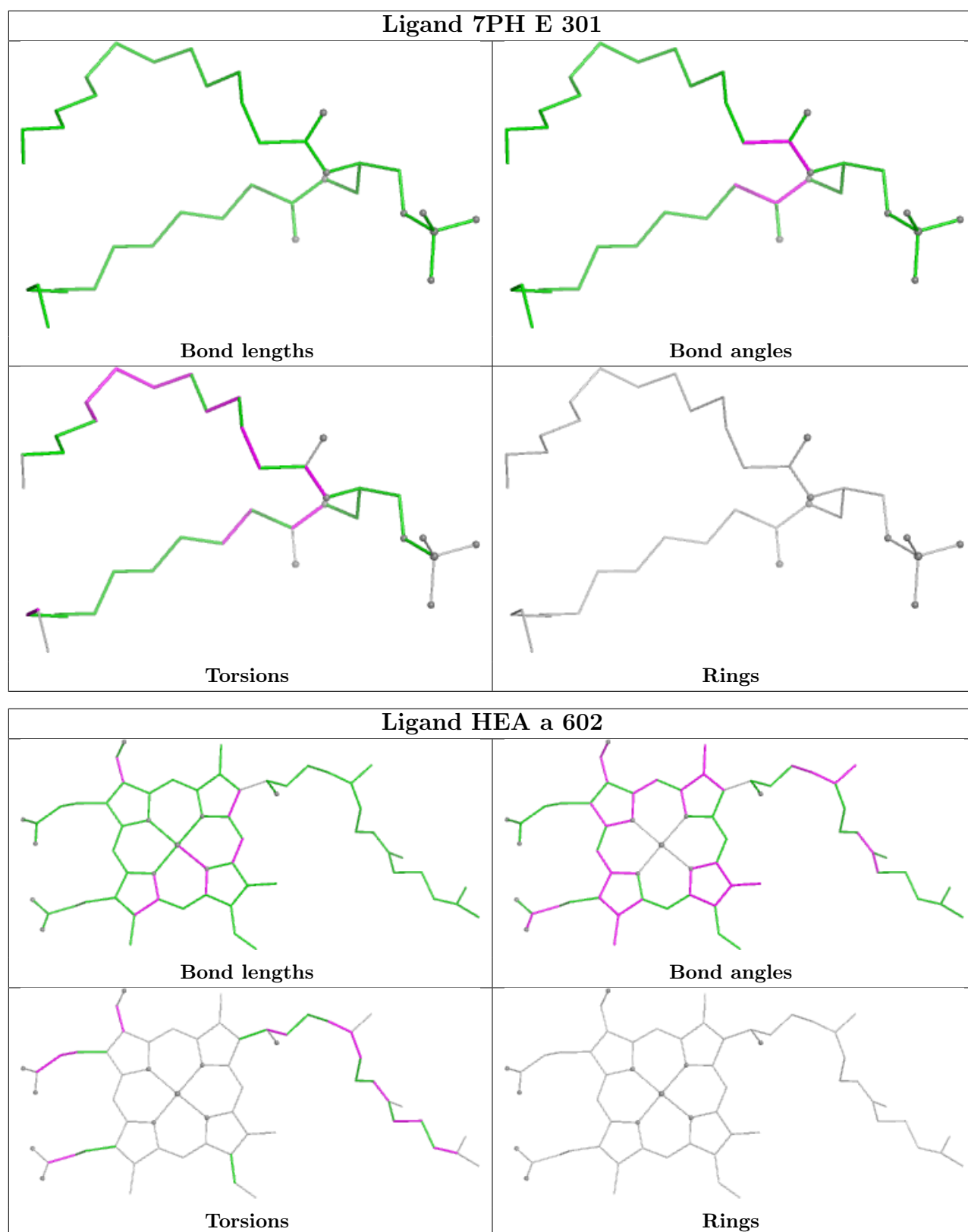


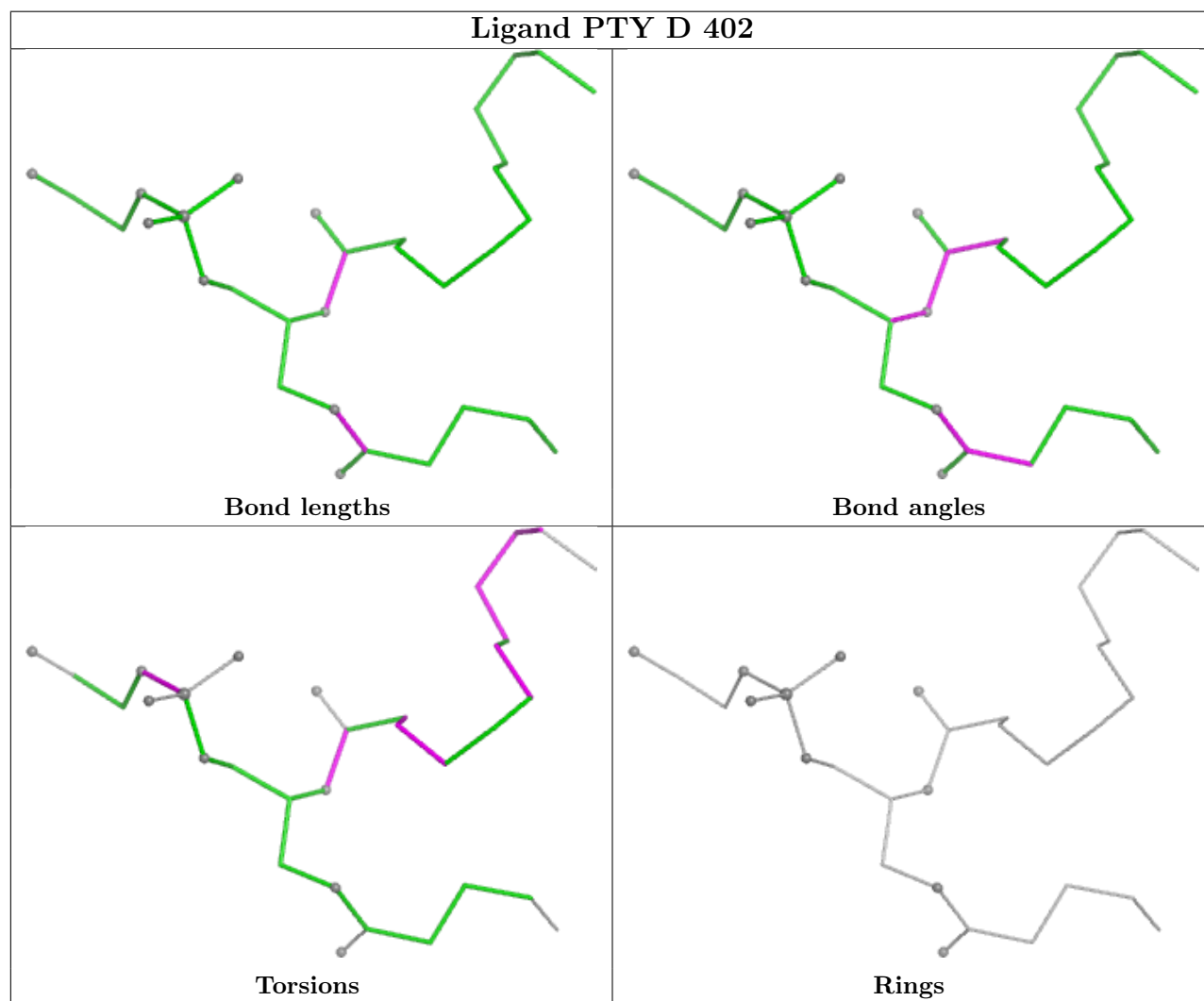
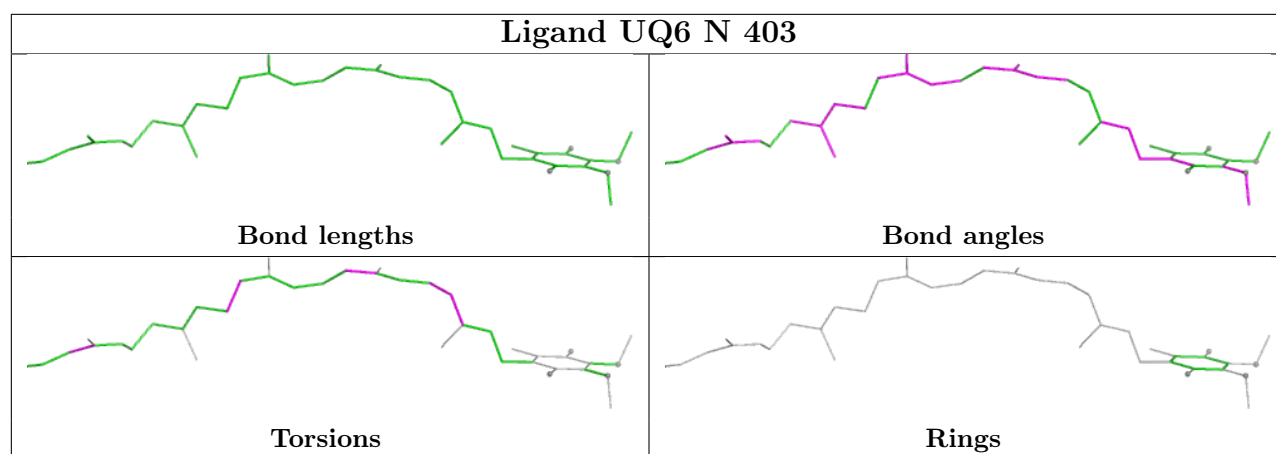




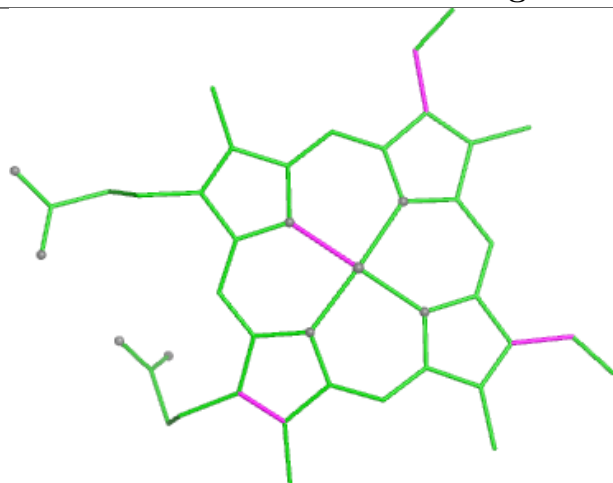




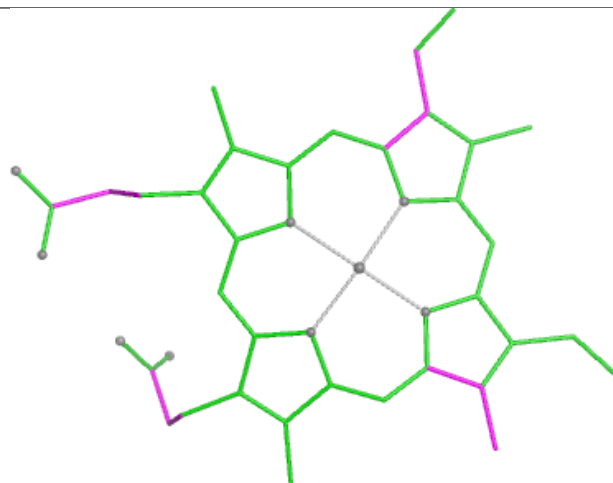




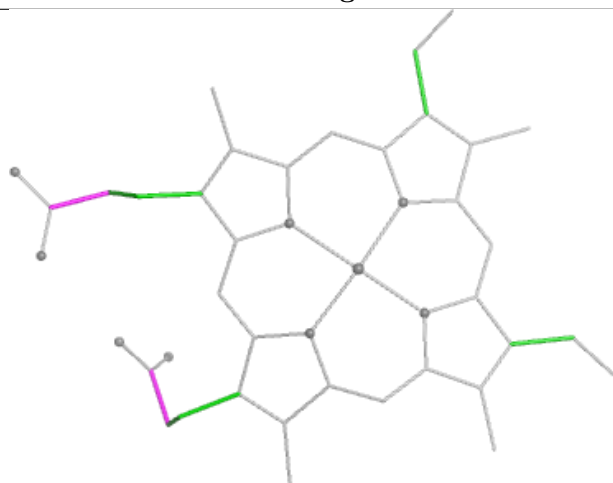
Ligand HEM C 403



Bond lengths



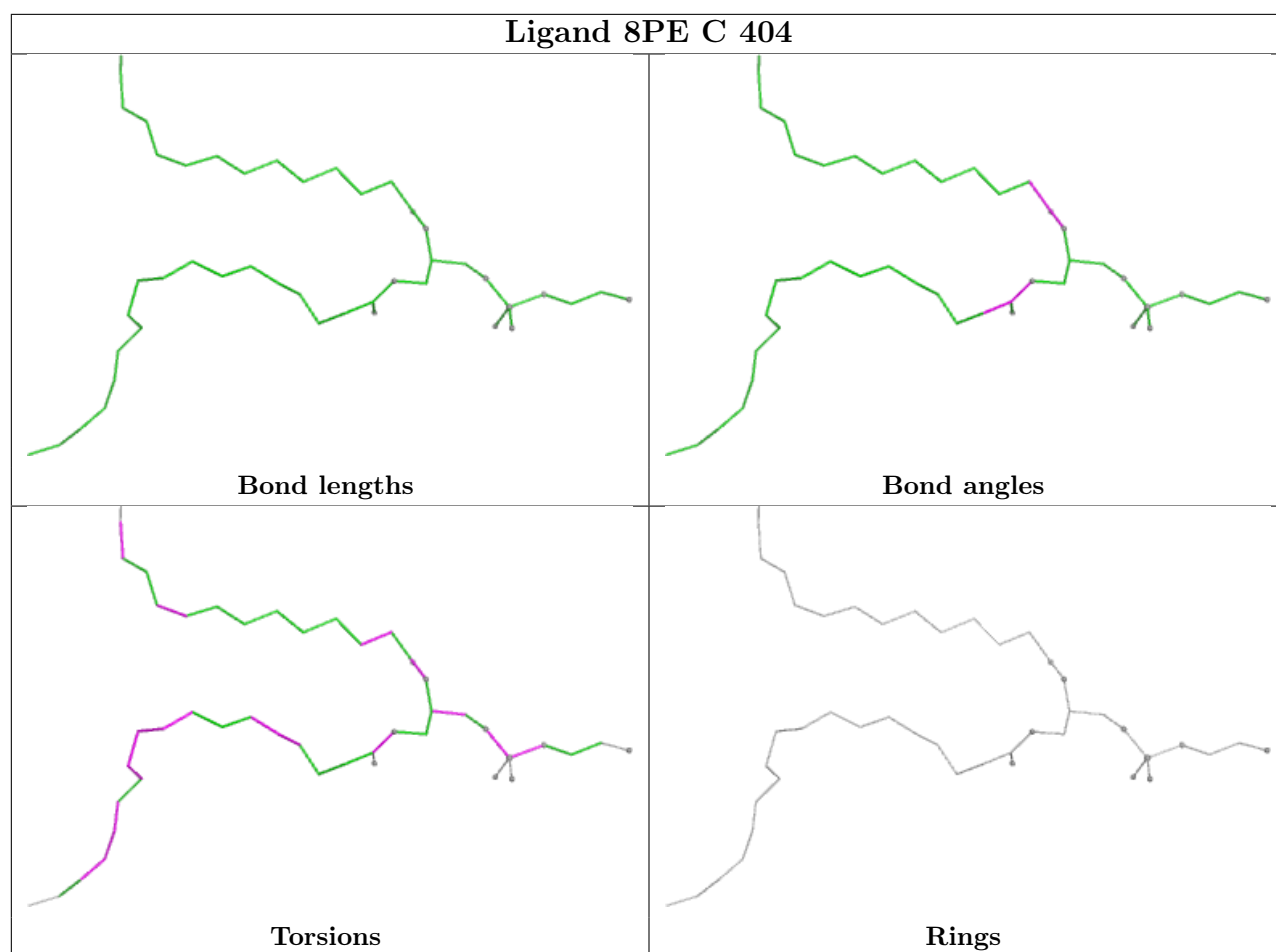
Bond angles

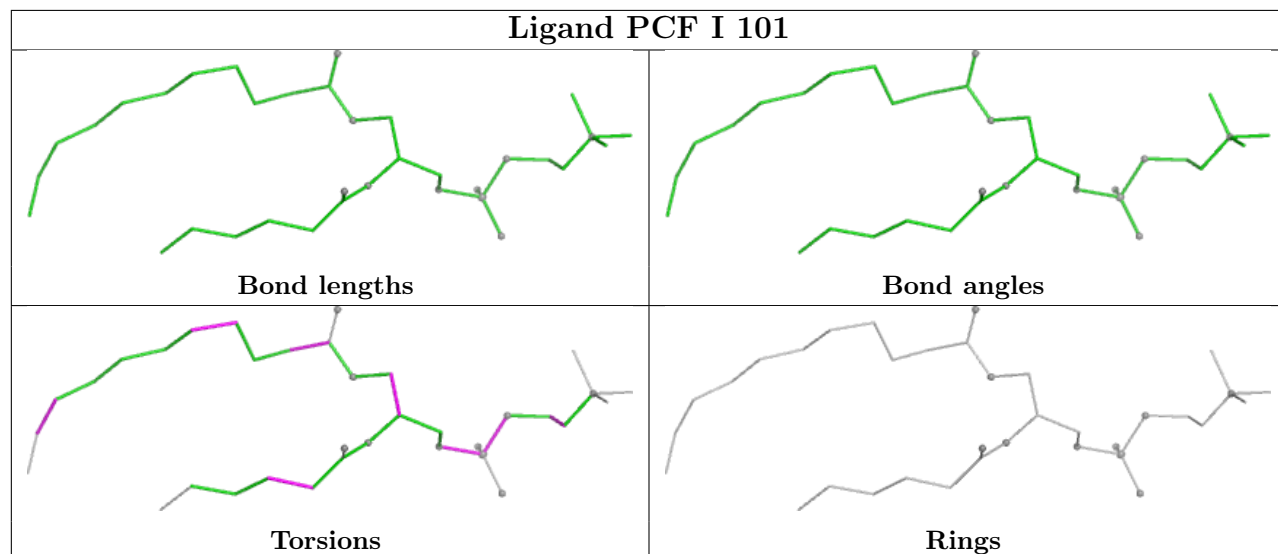
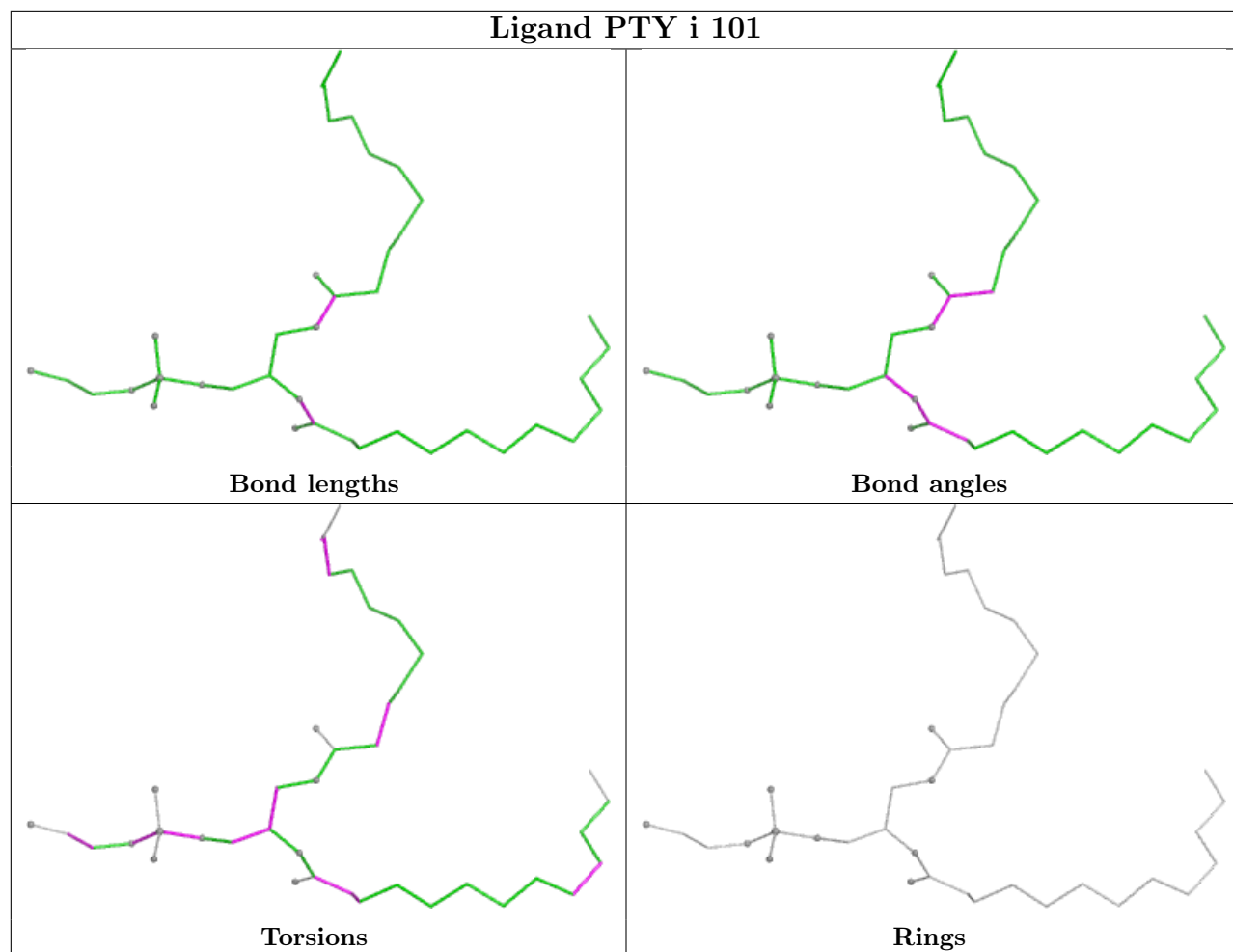


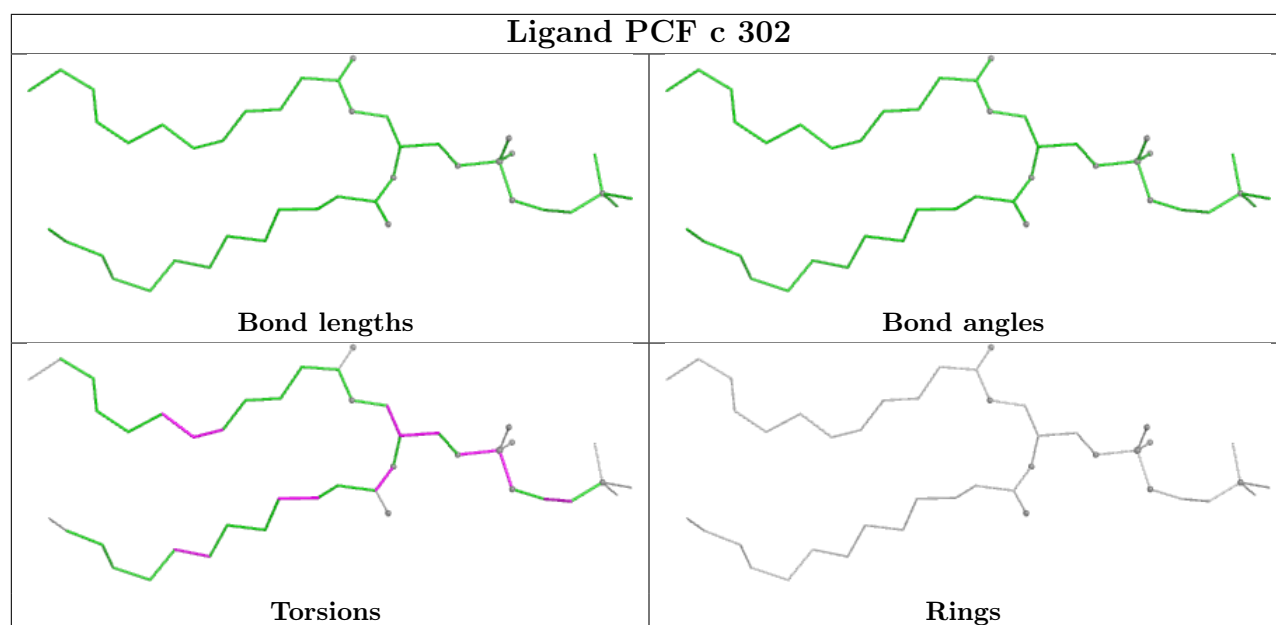
Torsions



Rings







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

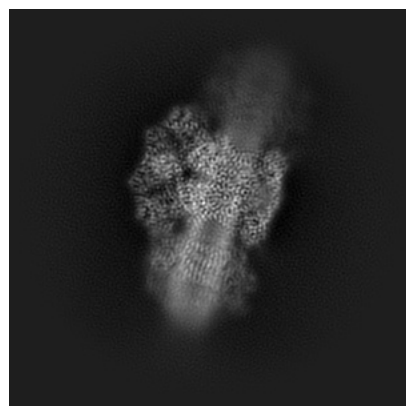
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10847. These allow visual inspection of the internal detail of the map and identification of artifacts.

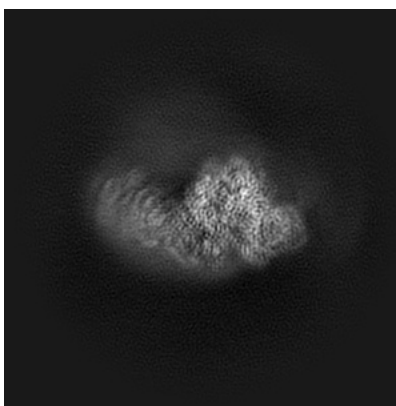
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

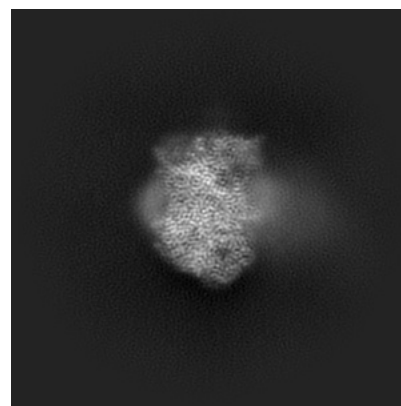
6.1.1 Primary map



X

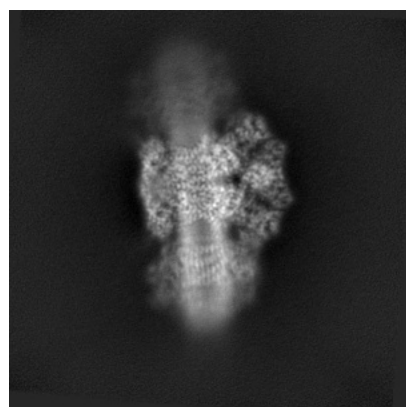


Y

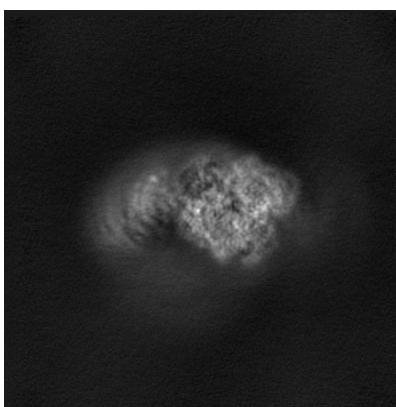


Z

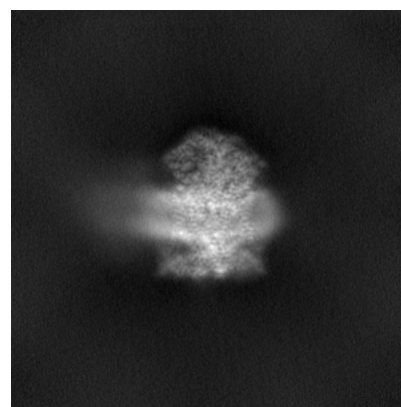
6.1.2 Raw map



X



Y

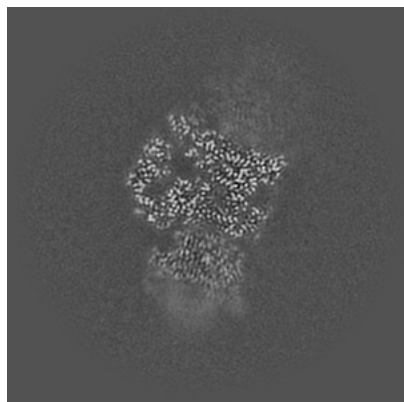


Z

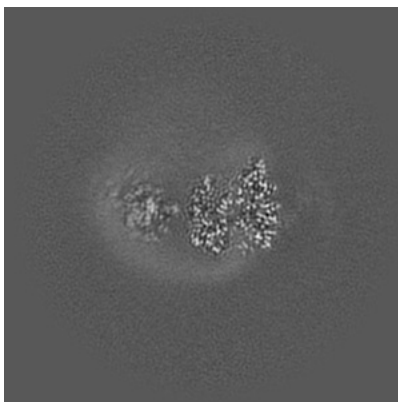
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

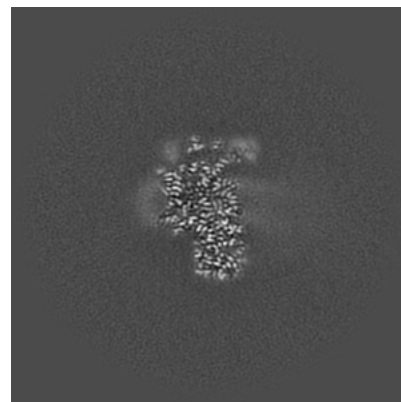
6.2.1 Primary map



X Index: 185

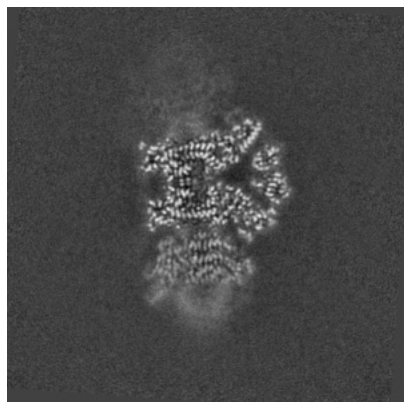


Y Index: 185

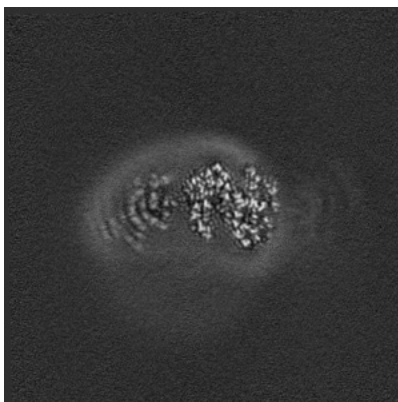


Z Index: 185

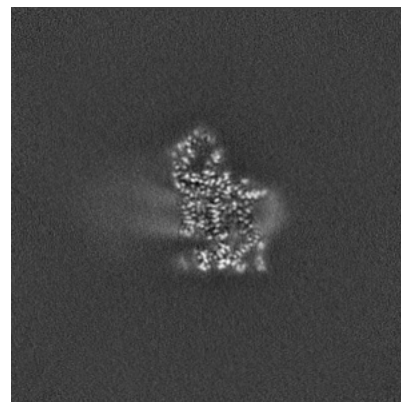
6.2.2 Raw map



X Index: 185



Y Index: 185

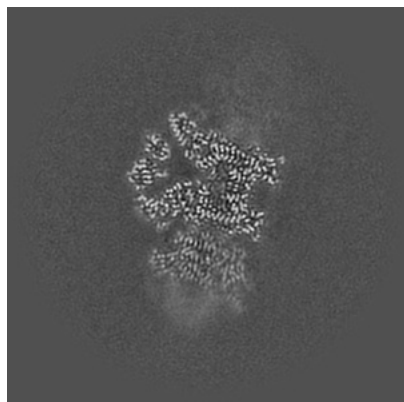


Z Index: 185

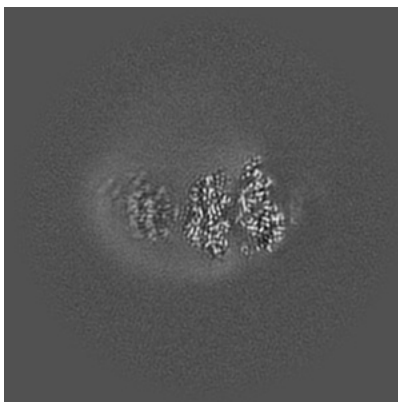
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

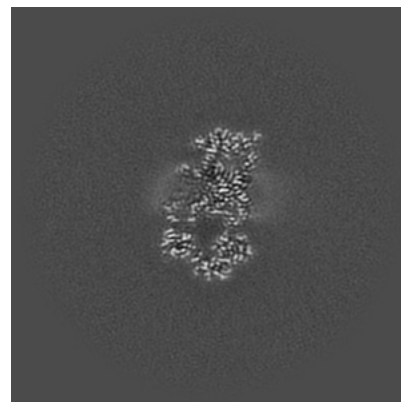
6.3.1 Primary map



X Index: 182

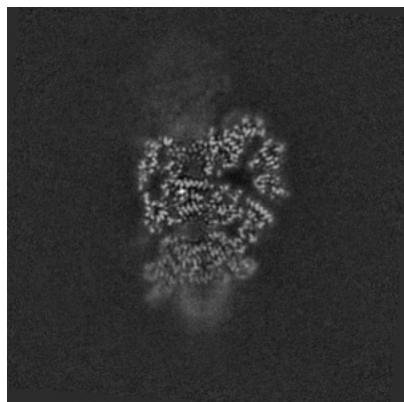


Y Index: 180

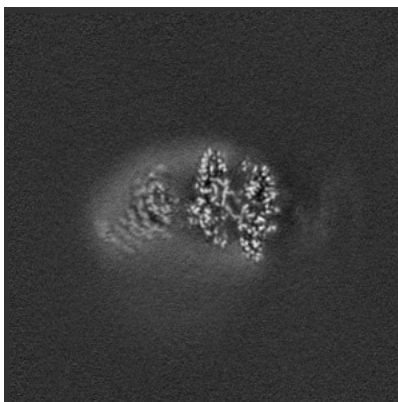


Z Index: 221

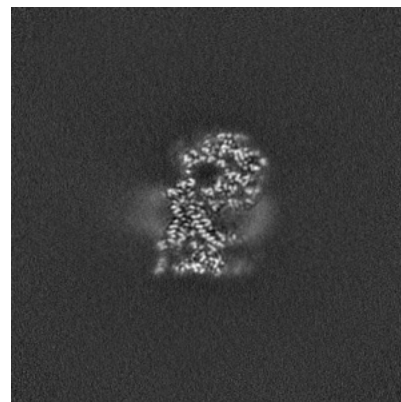
6.3.2 Raw map



X Index: 191



Y Index: 197

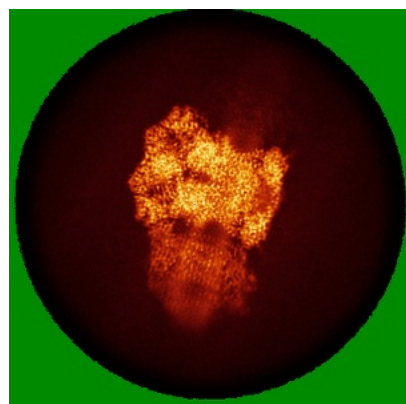


Z Index: 223

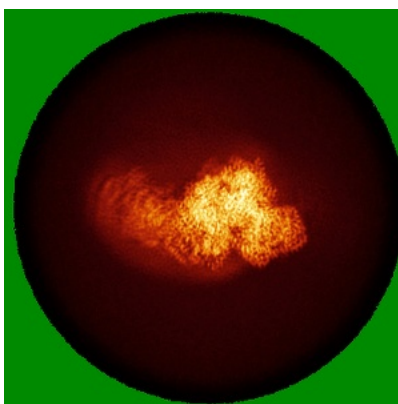
The images above show the largest variance slices of the map in three orthogonal directions.

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

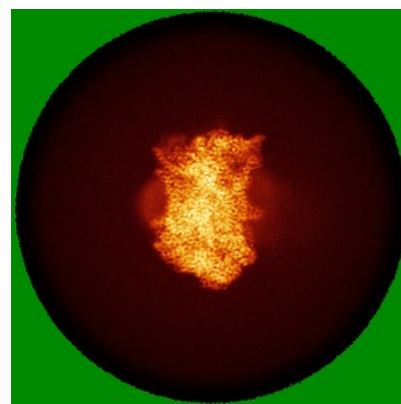
6.4.1 Primary map



X

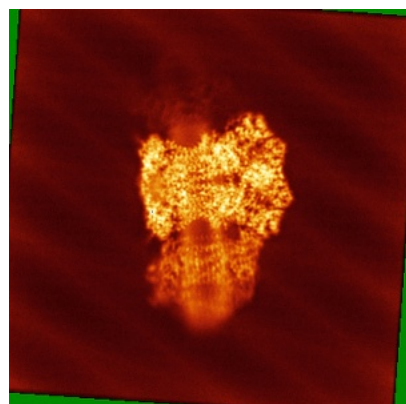


Y

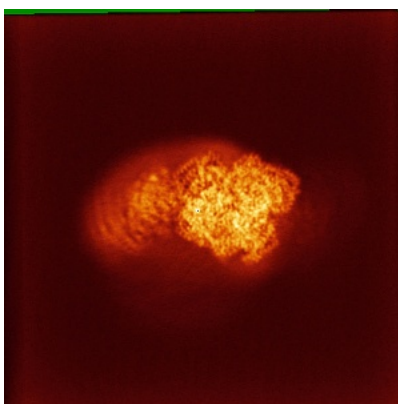


Z

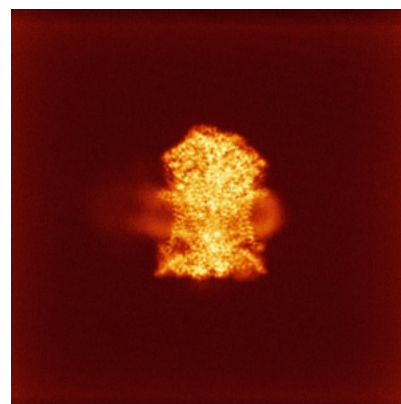
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.25. 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.

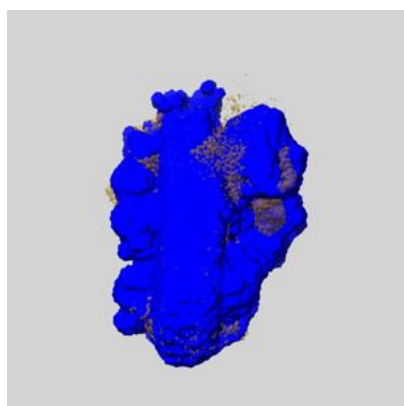
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

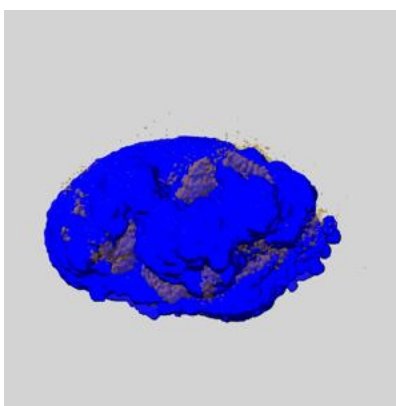
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

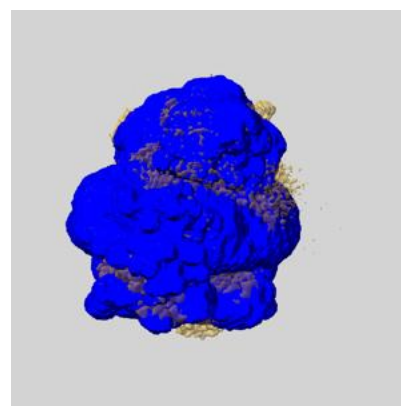
6.6.1 emd_10847_msk_1.map [i](#)



X



Y

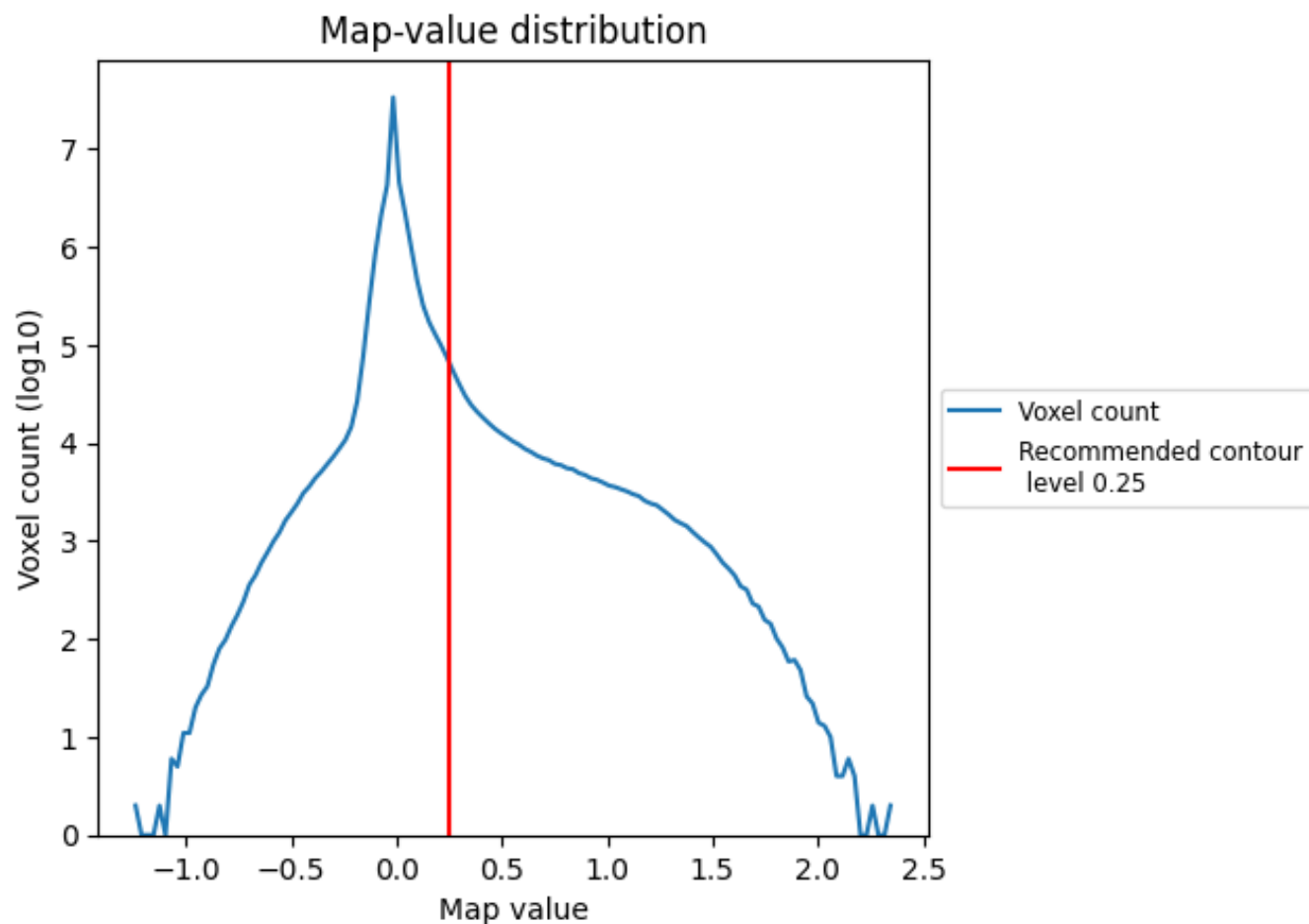


Z

7 Map analysis [i](#)

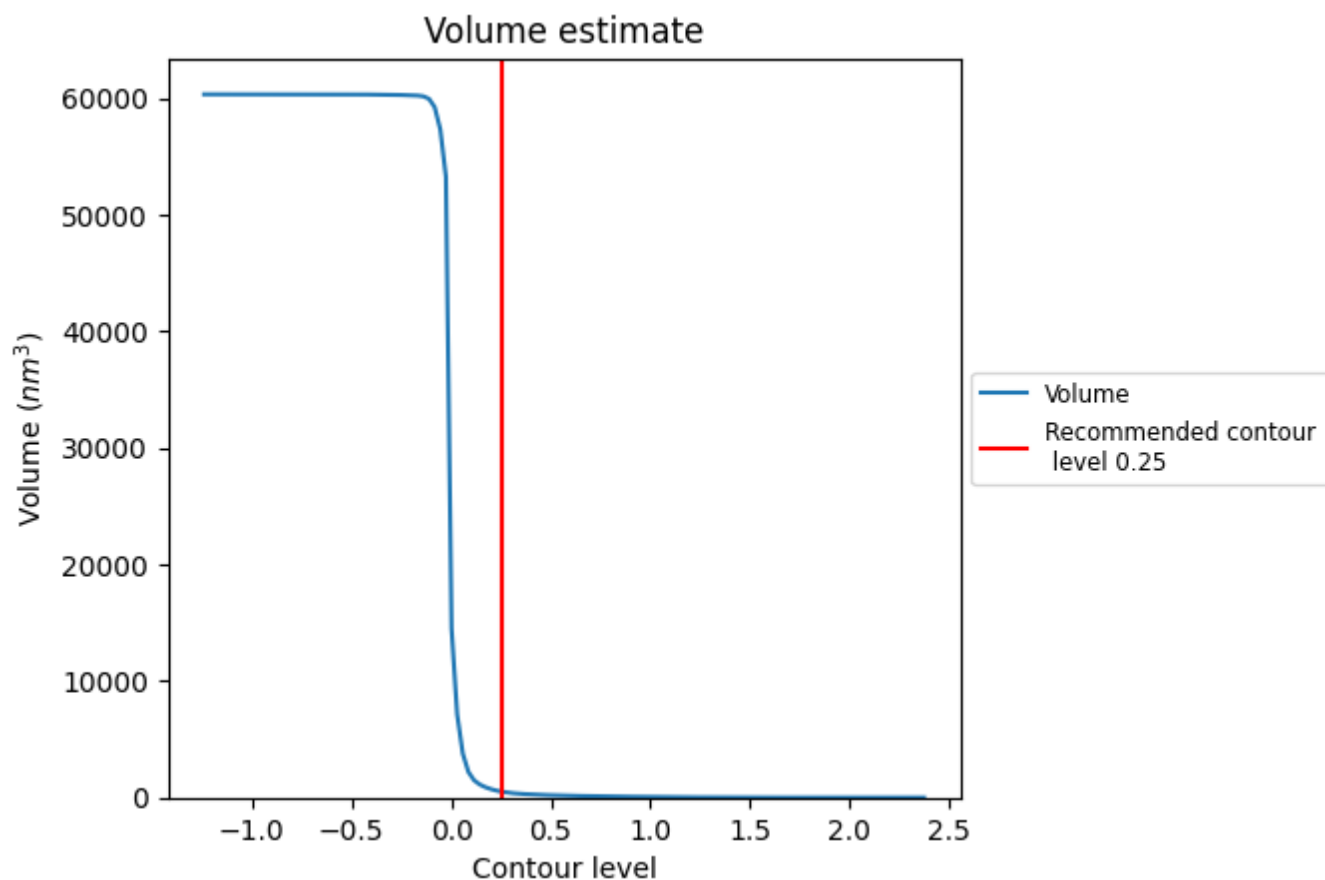
This section contains the results of statistical analysis of the map.

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.

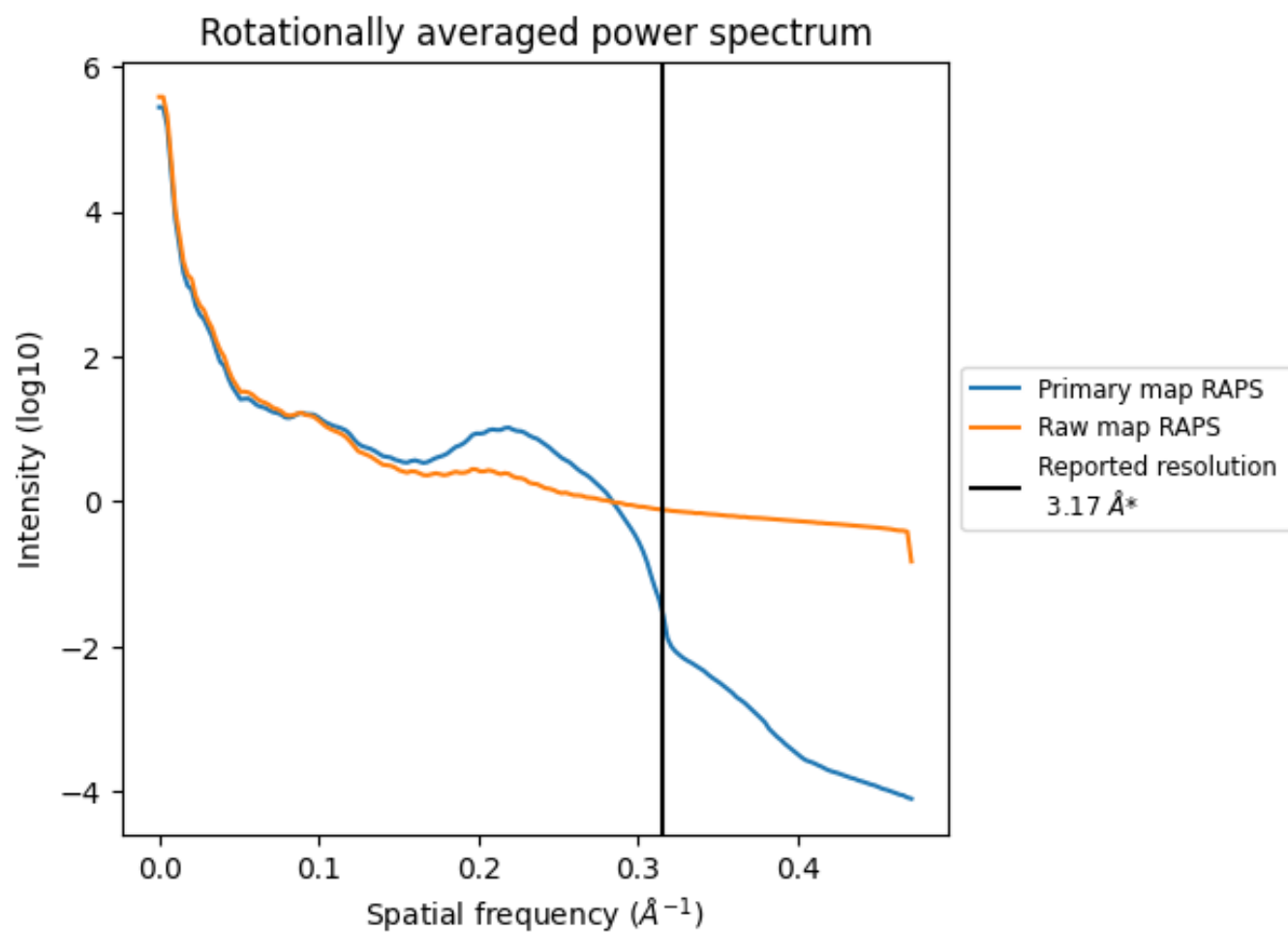
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 517 nm³; this corresponds to an approximate mass of 467 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 ⓘ

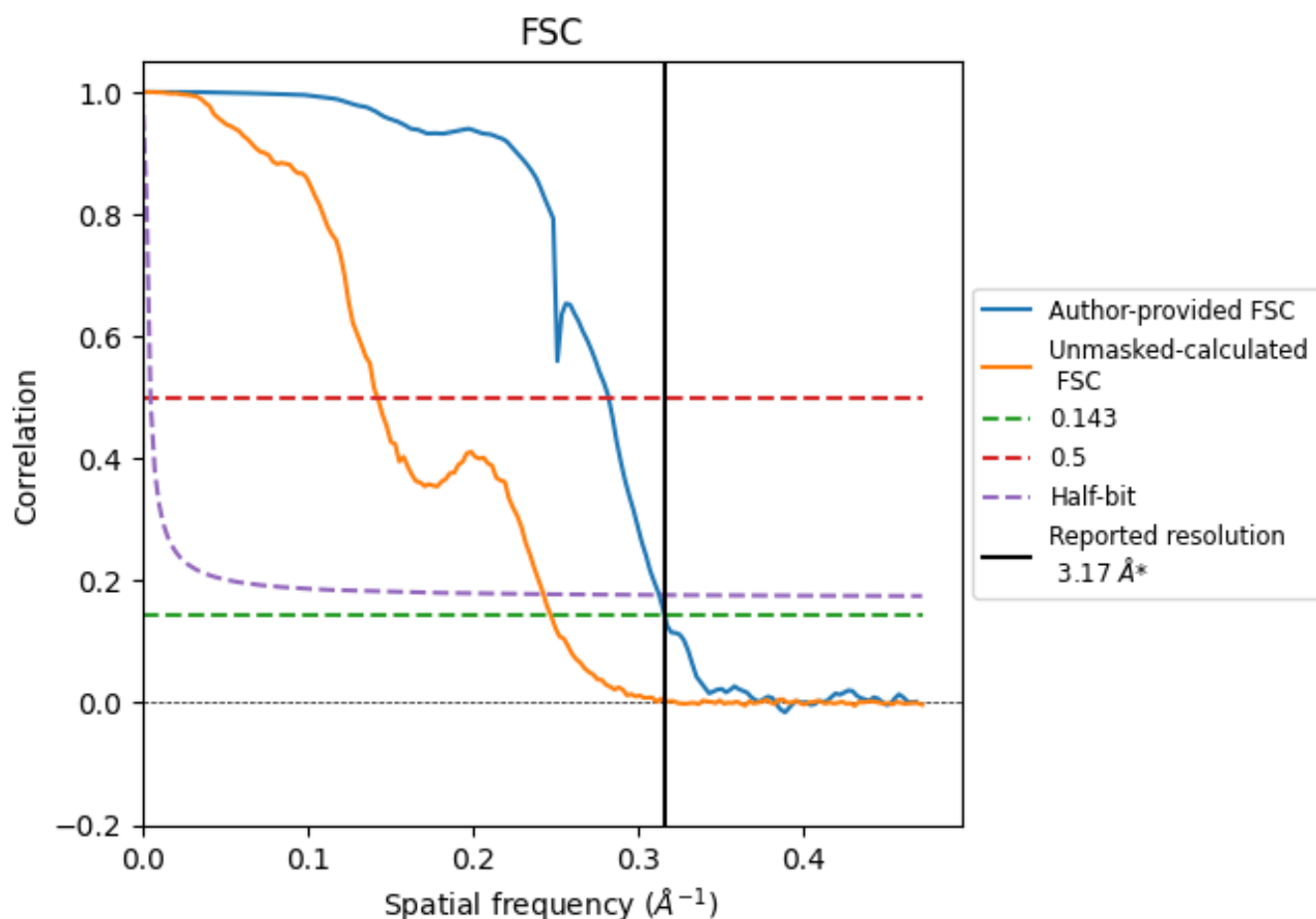


*Reported resolution corresponds to spatial frequency of $0.315 \text{ \AA}^{-1}$

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 0.315 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

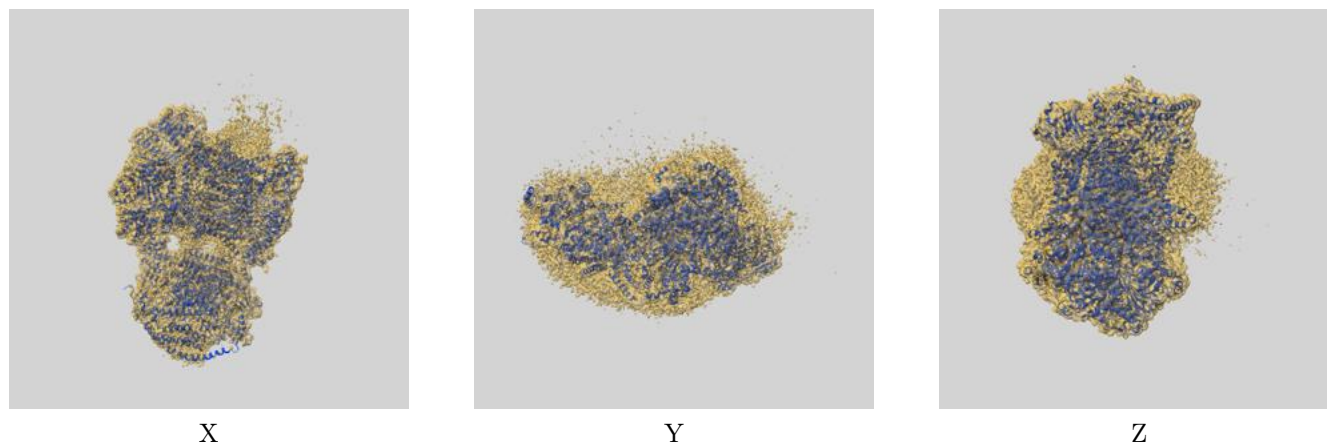
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.17	-	-
Author-provided FSC curve	3.16	3.55	3.20
Unmasked-calculated*	4.05	7.03	4.12

*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 4.05 differs from the reported value 3.17 by more than 10 %

9 Map-model fit [i](#)

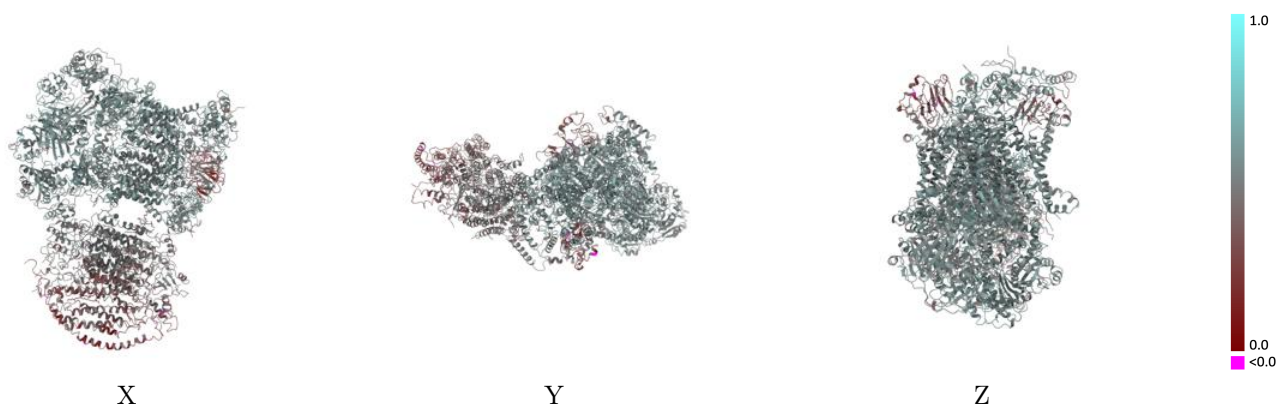
This section contains information regarding the fit between EMDB map EMD-10847 and PDB model 6YMX. Per-residue inclusion information can be found in section [3](#) on page [18](#).

9.1 Map-model overlay [i](#)



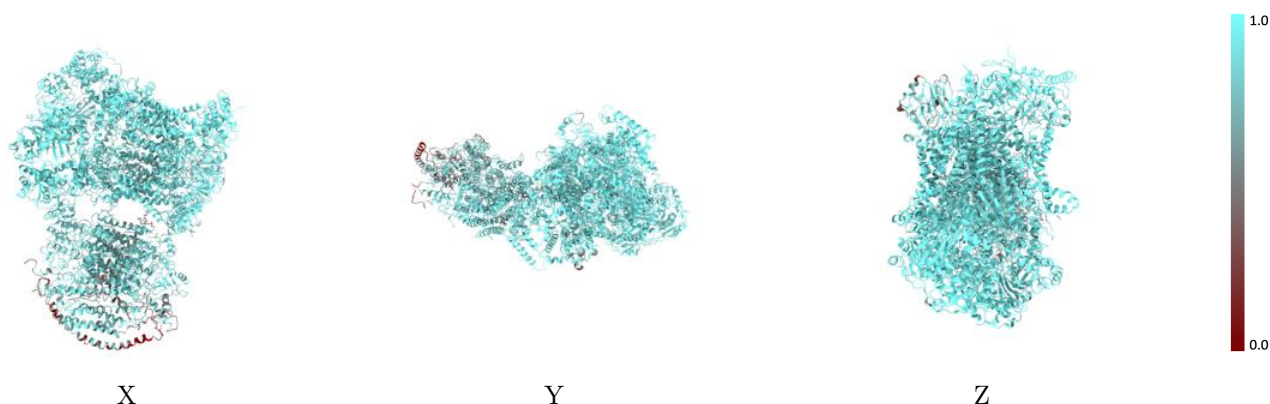
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



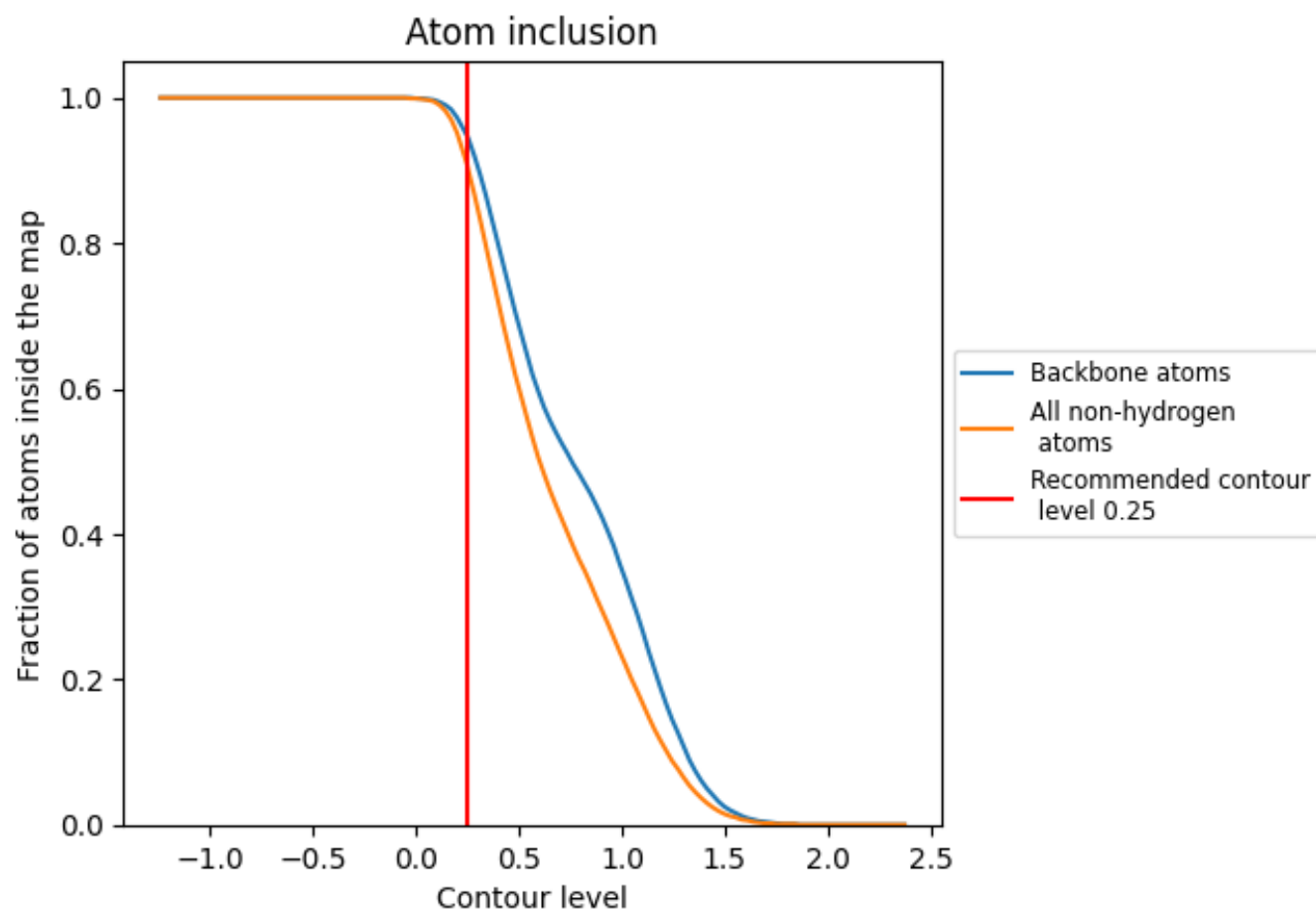
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.25).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 91% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9070	 0.4950
A	 0.9640	 0.5440
B	 0.9640	 0.5480
C	 0.9550	 0.5530
D	 0.9490	 0.5420
E	 0.9030	 0.4140
F	 0.9400	 0.5010
G	 0.9540	 0.5420
H	 0.9590	 0.5410
I	 0.9490	 0.5450
L	 0.9640	 0.5370
M	 0.9670	 0.5430
N	 0.9600	 0.5550
O	 0.9660	 0.5490
P	 0.8230	 0.3840
Q	 0.9500	 0.4930
R	 0.9610	 0.5480
S	 0.9570	 0.5330
T	 0.9680	 0.5420
U	 0.9740	 0.5350
V	 0.9170	 0.5200
a	 0.8710	 0.4650
b	 0.8660	 0.4320
c	 0.7780	 0.3600
d	 0.7970	 0.4140
e	 0.8960	 0.4860
f	 0.9280	 0.4360
g	 0.7460	 0.3590
h	 0.8060	 0.4330
i	 0.8800	 0.4280
j	 0.6680	 0.3610
k	 0.3500	 0.2600
m	 0.8170	 0.4300

