



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 06:49 PM UTC

PDB ID : 7O3E / pdb_00007o3e
EMDB ID : EMD-12705
Title : Murine supercomplex CIII2CIV in the intermediate locked conformation
Authors : Vercellino, I.; Sazanov, L.A.
Deposited on : 2021-04-01
Resolution : 3.60 Å(reported)
Based on initial models : 5Z62, 5IY5, 1NTZ, 3L75

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

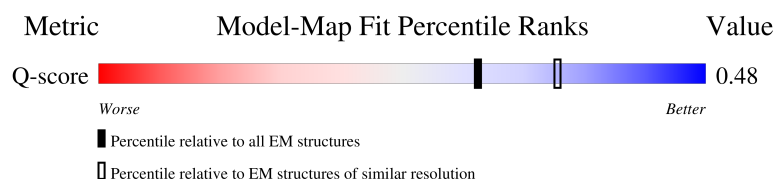
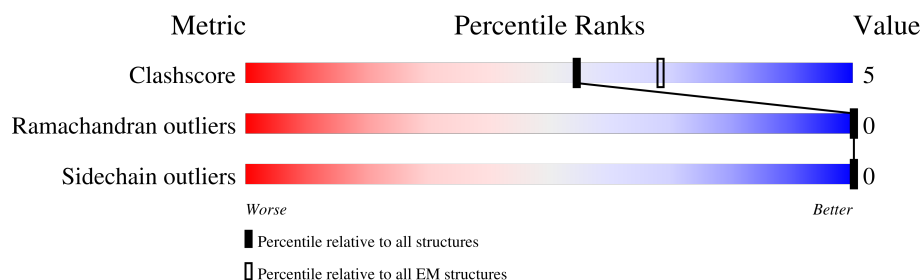
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.60 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.



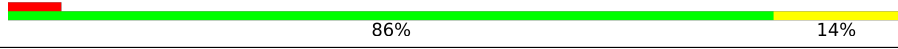
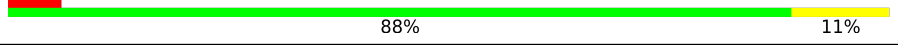
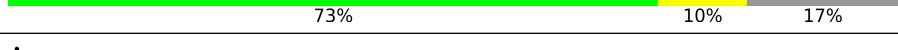
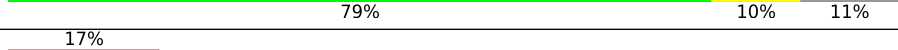
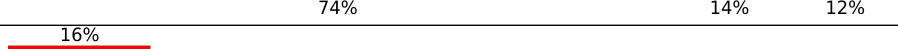
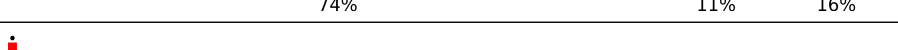
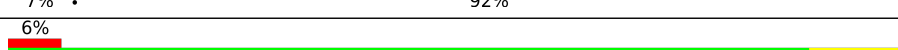
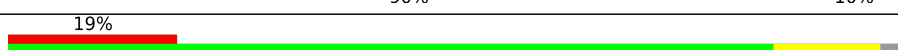
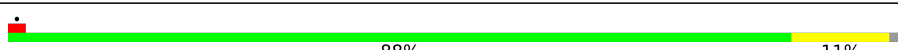
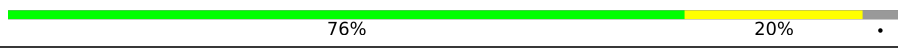
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12797 (3.10 - 4.10)

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	446	 86% 14%
1	L	446	 84% 16%
2	B	439	 81% 15% .
2	M	439	 83% 13% .

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Mol	Chain	Length	Quality of chain
3	C	381	
3	N	381	
4	D	241	
4	O	241	
5	F	110	
5	Q	110	
6	G	81	
6	R	81	
7	H	76	
7	S	76	
8	P	196	
9	T	78	
10	I	113	
11	a	514	
12	b	227	
13	c	261	
14	d	147	
15	e	109	
16	f	99	
17	g	85	
18	h	85	
19	i	75	
20	k	56	
21	l	47	
22	m	46	

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Mol	Chain	Length	Quality of chain
23	J	63	10% 44% 5% 51%
23	U	63	13% 48% • 51%

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 44039 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	446	Total	C	N	O	S	0	0
			3466	2167	611	671	17		
1	L	445	Total	C	N	O	S	0	0
			3460	2163	610	670	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	420	Total	C	N	O	S	0	0
			3154	1980	555	610	9		
2	M	420	Total	C	N	O	S	0	0
			3154	1980	555	610	9		

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	380	Total	C	N	O	S	0	0
			3045	2052	473	499	21		
3	N	380	Total	C	N	O	S	0	0
			3046	2052	473	499	22		

- Molecule 4 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	241	Total	C	N	O	S	0	0
			1919	1224	329	352	14		
4	O	240	Total	C	N	O	S	0	0
			1909	1218	327	350	14		

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	101	Total	C	N	O	S	0	0
			894	572	159	160	3		
5	Q	101	Total	C	N	O	S	0	0
			894	572	159	160	3		

- Molecule 6 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	67	Total	C	N	O		0	0
			565	364	107	94			
6	R	72	Total	C	N	O		0	0
			609	396	112	101			

- Molecule 7 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	67	Total	C	N	O	S	0	0
			554	338	102	109	5		
7	S	64	Total	C	N	O	S	0	0
			530	322	99	104	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	P	15	Total	C	N	O		0	0
			128	79	24	25			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	T	78	Total	C	N	O	S	0	0
			554	352	103	97	2		

- Molecule 10 is a protein called Cox7a2l protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	111	Total	C	N	O	S	0	0
			834	543	138	148	5		

- Molecule 11 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	a	514	Total	C	N	O	S	0	0
			4021	2691	623	675	32		

- Molecule 12 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	b	227	Total	C	N	O	S	0	0
			1817	1180	282	336	19		

- Molecule 13 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	c	259	Total	C	N	O	S	0	0
			2111	1414	338	349	10		

- Molecule 14 is a protein called Cytochrome c oxidase subunit 4 isoform 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	d	144	Total	C	N	O	S	0	0
			1195	770	199	219	7		

- Molecule 15 is a protein called Cytochrome c oxidase subunit 5A, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	e	104	Total	C	N	O	S	0	0
			842	538	141	161	2		

- Molecule 16 is a protein called Cytochrome c oxidase subunit 5B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	f	95	Total	C	N	O	S	0	0
			727	452	127	140	8		

- Molecule 17 is a protein called Cytochrome c oxidase subunit 6A2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	g	75	Total	C	N	O	S	0	0
			605	392	114	96	3		

- Molecule 18 is a protein called Cytochrome c oxidase subunit 6B1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	h	79	Total	C	N	O	S	0	0
			654	416	116	117	5		

- Molecule 19 is a protein called Cytochrome c oxidase subunit 6C.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	i	72	Total	C	N	O	S	0	0
			572	372	103	94	3		

- Molecule 20 is a protein called Cytochrome c oxidase subunit 7B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	k	49	Total	C	N	O	S	0	0
			383	248	65	68	2		

- Molecule 21 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	l	46	Total	C	N	O	S	0	0
			380	253	64	61	2		

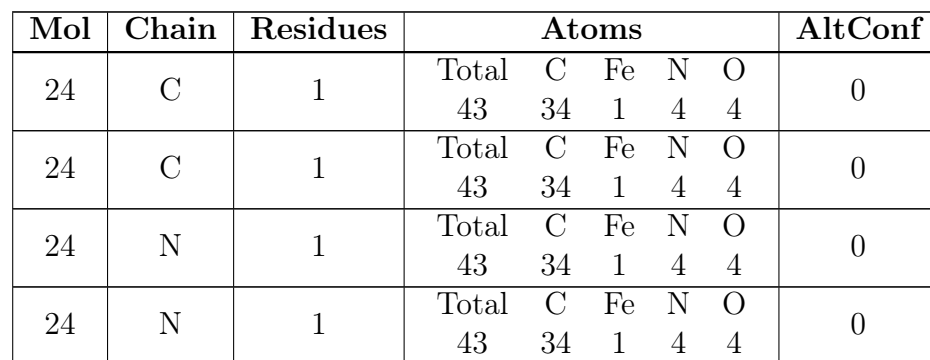
- Molecule 22 is a protein called Cytochrome c oxidase subunit 8B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	m	43	Total	C	N	O	S	0	0
			311	203	51	56	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
23	J	31	Total	C	N	O	0	0
			272	178	47	47		
23	U	31	Total	C	N	O	0	0
			272	178	47	47		

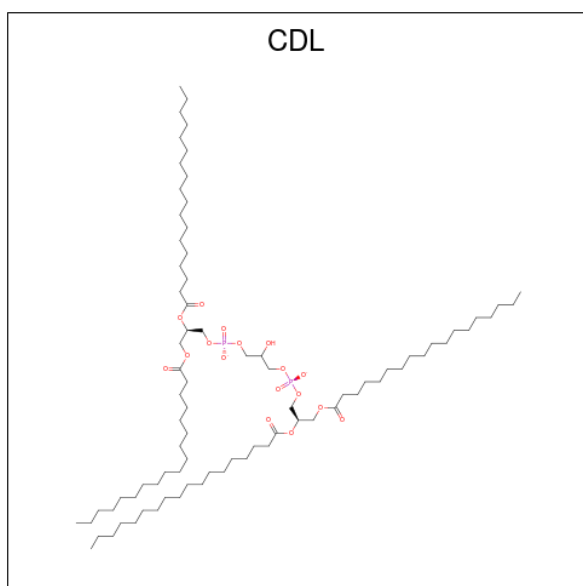
- Molecule 24 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



- ### 3PE
-
- The chemical structure of 3PE (3-phosphatidylethanolamine) is shown. It consists of a glycerol backbone esterified with two fatty acid chains (represented by zigzag lines) and a phosphate group (red P=O and O- groups) linked to an ethanolamine head group (blue N and O atoms).

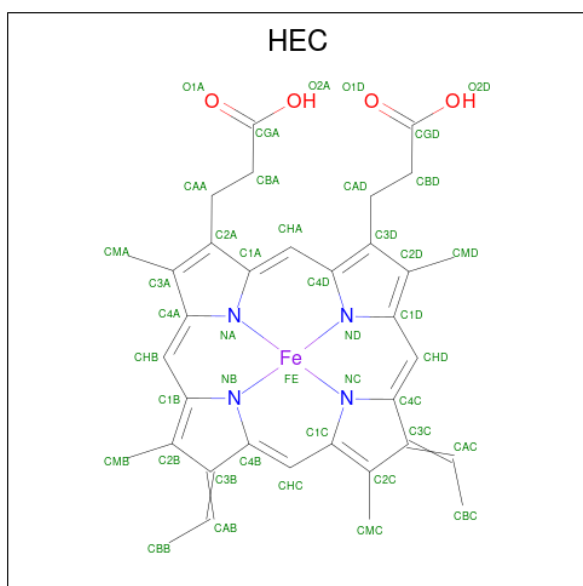
Mol	Chain	Residues	Atoms					AltConf
25	C	1	Total	C	N	O	P	0
			35	25	1	8	1	
25	F	1	Total	C	N	O	P	0
			29	19	1	8	1	
25	F	1	Total	C	N	O	P	0
			34	24	1	8	1	
25	L	1	Total	C	N	O	P	0
			23	13	1	8	1	
25	N	1	Total	C	N	O	P	0
			37	27	1	8	1	
25	N	1	Total	C	N	O	P	0
			51	41	1	8	1	
25	a	1	Total	C	N	O	P	0
			28	18	1	8	1	
25	b	1	Total	C	N	O	P	0
			29	19	1	8	1	
25	b	1	Total	C	N	O	P	0
			28	18	1	8	1	
25	c	1	Total	C	N	O	P	0
			45	35	1	8	1	
25	d	1	Total	C	N	O	P	0
			34	24	1	8	1	
25	g	1	Total	C	N	O	P	0
			25	15	1	8	1	
25	k	1	Total	C	N	O	P	0
			27	17	1	8	1	

- Molecule 26 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



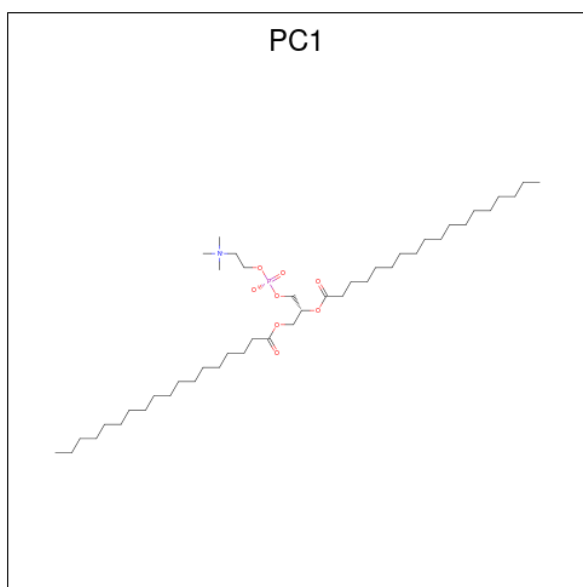
Mol	Chain	Residues	Atoms				AltConf
26	C	1	Total	C	O	P	0
			42	23	17	2	
26	D	1	Total	C	O	P	0
			56	37	17	2	
26	L	1	Total	C	O	P	0
			46	27	17	2	
26	N	1	Total	C	O	P	0
			41	22	17	2	
26	O	1	Total	C	O	P	0
			57	38	17	2	

- Molecule 27 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

- Molecule 28 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
28	L	1	Total	C	N	O	P	0
			24	14	1	8	1	
28	a	1	Total	C	N	O	P	0
			43	33	1	8	1	

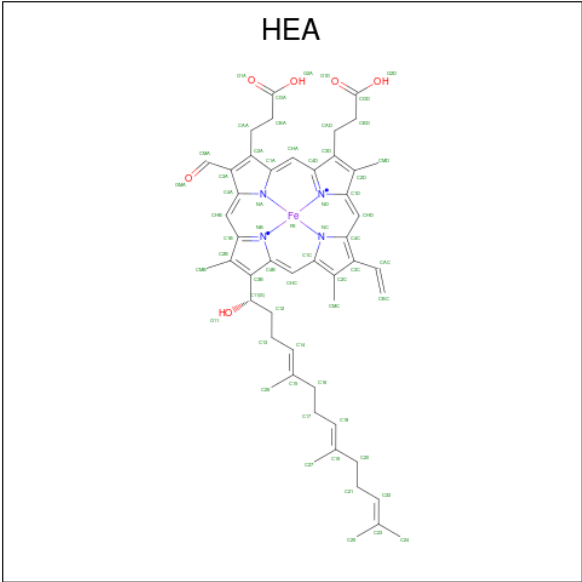
- Molecule 29 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

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

- Molecule 30 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
30	a	1	Total	Na	0
			1	1	

- Molecule 31 is HEME-A (CCD ID: HEA) (formula: C₄₉H₅₆FeN₄O₆).

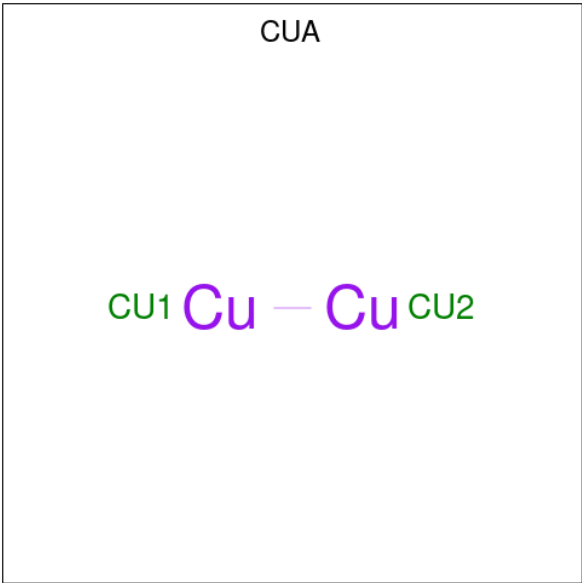


Mol	Chain	Residues	Atoms					AltConf
31	a	1	Total 60	C 49	Fe 1	N 4	O 6	0
31	a	1	Total 60	C 49	Fe 1	N 4	O 6	0

- Molecule 32 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
32	b	1	Total	Mg	0
			1	1	

- Molecule 33 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).

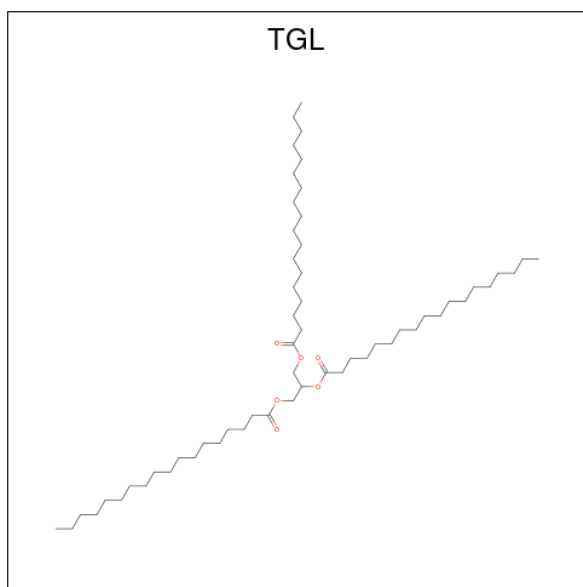


Mol	Chain	Residues	Atoms		AltConf
33	b	1	Total	Cu	0
			2	2	

- Molecule 34 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
34	f	1	Total	Zn	0
			1	1	

- Molecule 35 is TRISTEAROYLGLYCEROL (CCD ID: TGL) (formula: C₅₇H₁₁₀O₆).

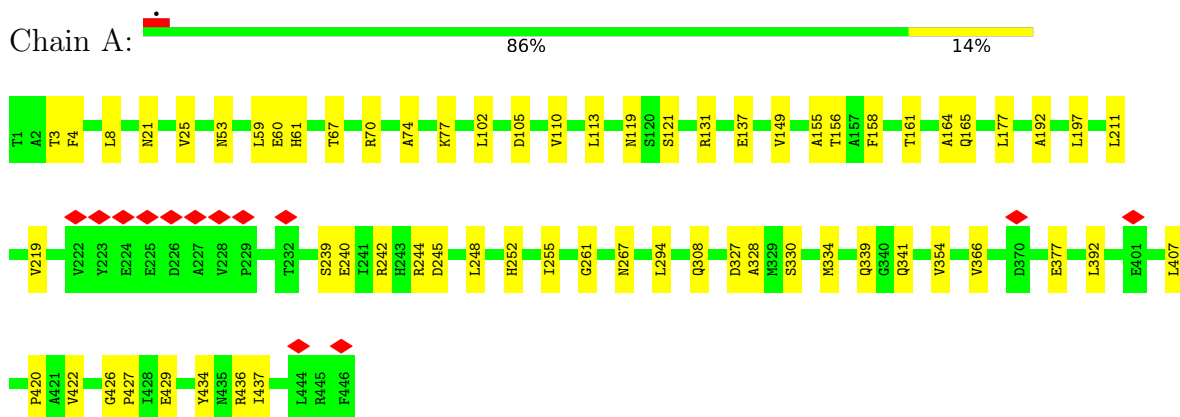


Mol	Chain	Residues	Atoms			AltConf
35	1	1	Total	C	O	0
			44	38	6	

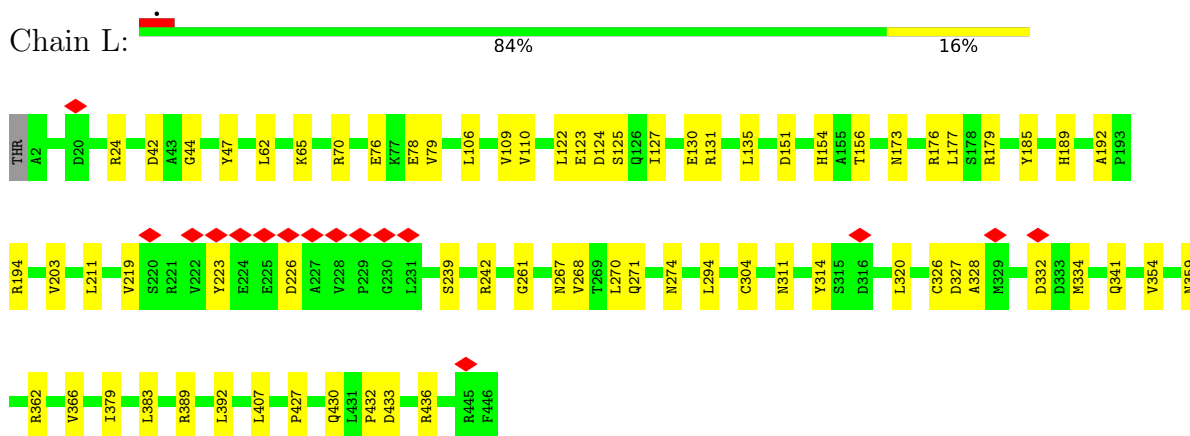
3 Residue-property plots

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

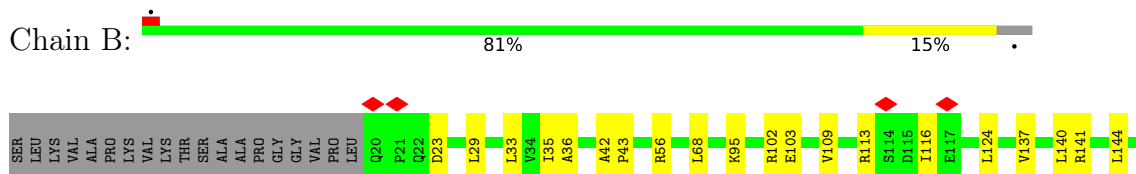
- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial

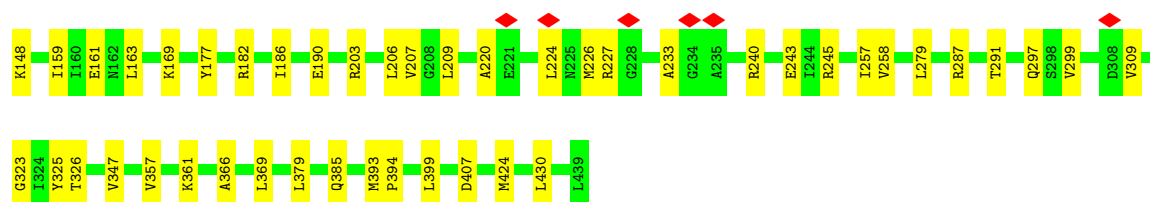


- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial



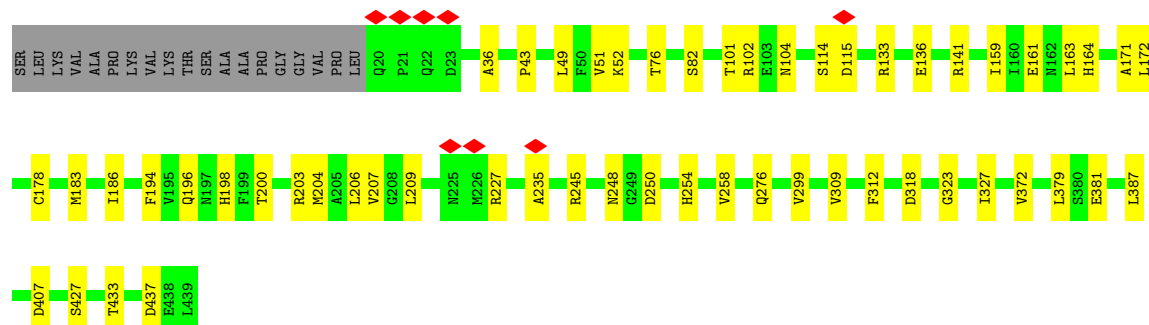
- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial





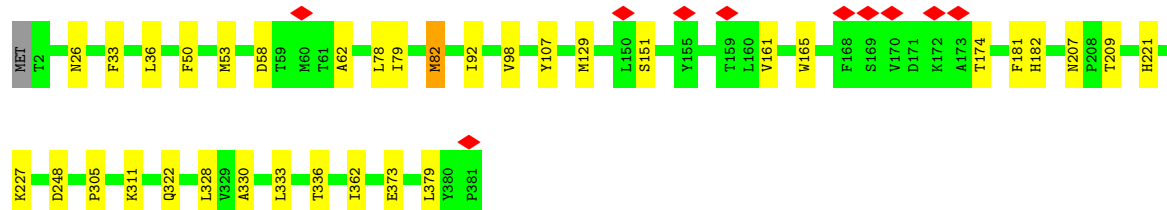
- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain M: 83% 13%



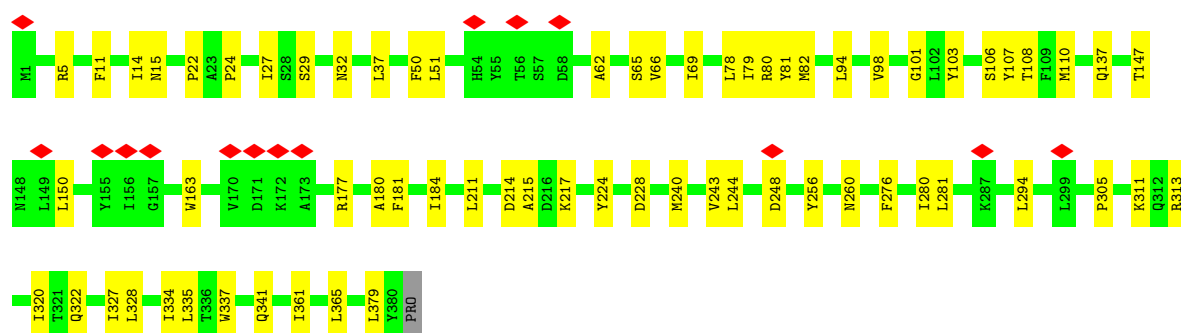
- Molecule 3: Cytochrome b

Chain C: 91% 9%



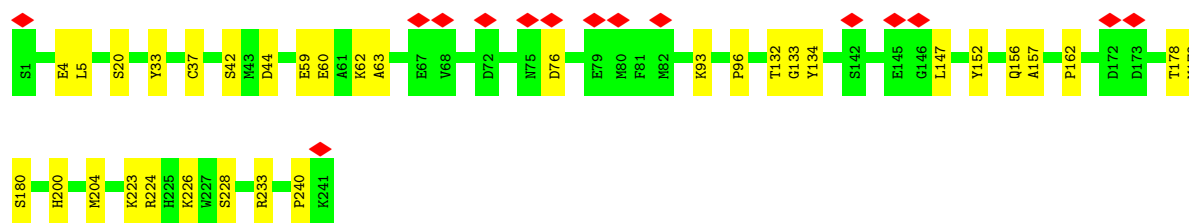
- Molecule 3: Cytochrome b

Chain N: 82% 18%

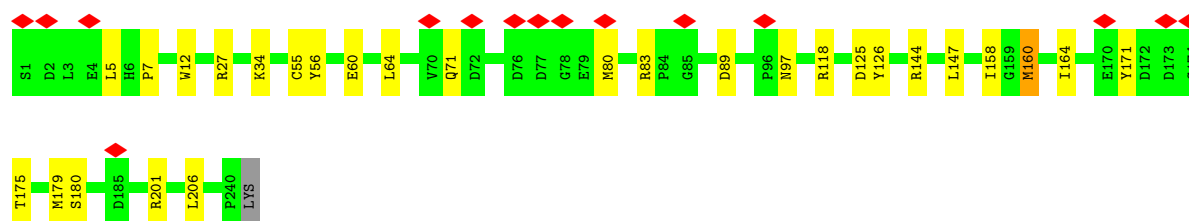
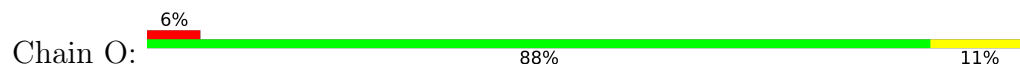


- Molecule 4: Cytochrome c1, heme protein, mitochondrial

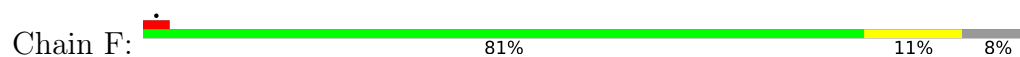
Chain D: 6% 86% 14%



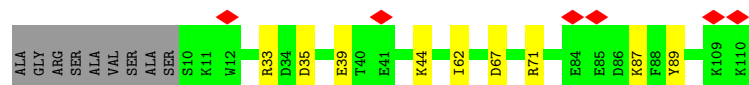
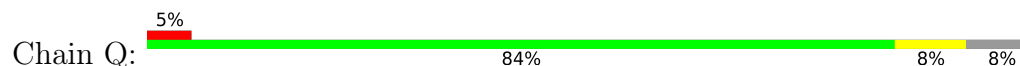
- Molecule 4: Cytochrome c1, heme protein, mitochondrial



- Molecule 5: Cytochrome b-c1 complex subunit 7



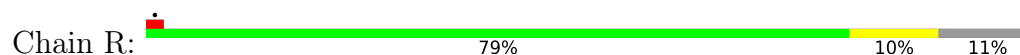
- Molecule 5: Cytochrome b-c1 complex subunit 7



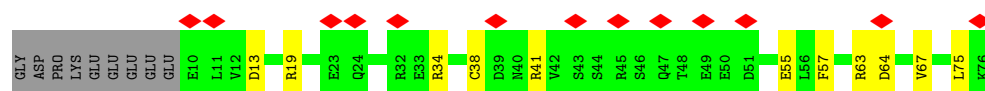
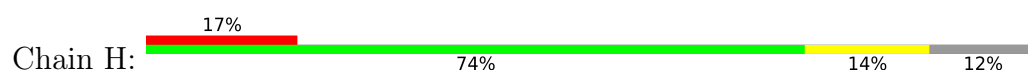
- Molecule 6: Cytochrome b-c1 complex subunit 8



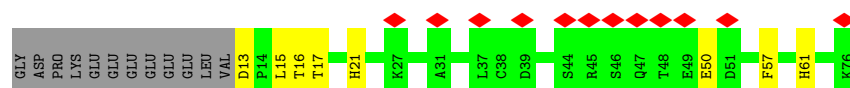
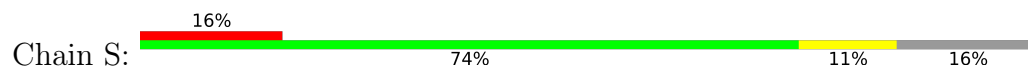
- Molecule 6: Cytochrome b-c1 complex subunit 8



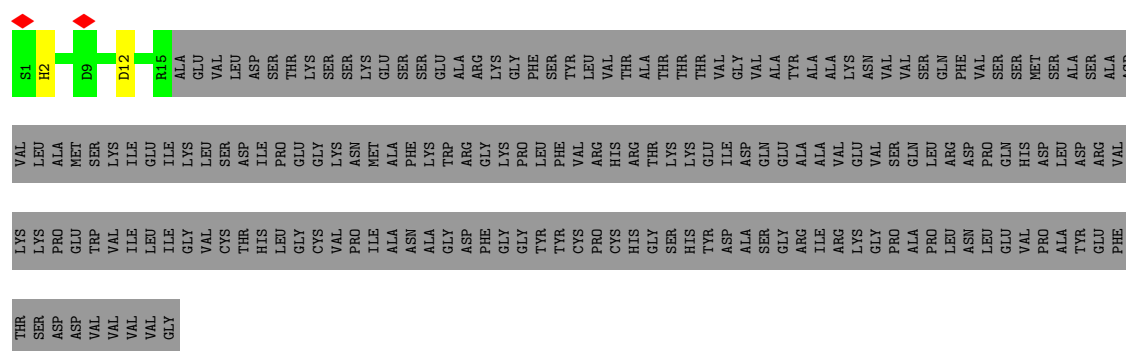
- Molecule 7: Cytochrome b-c1 complex subunit 6, mitochondrial



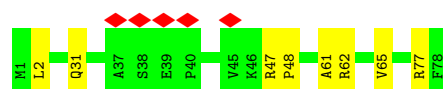
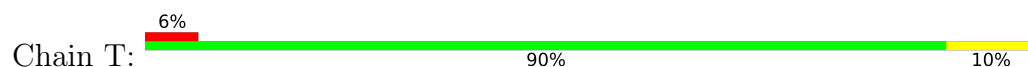
- Molecule 7: Cytochrome b-c1 complex subunit 6, mitochondrial



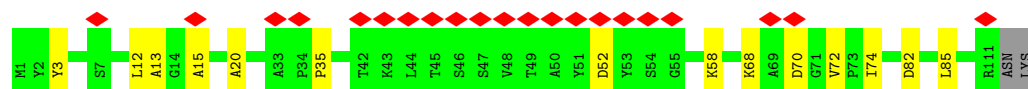
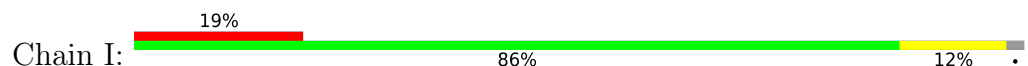
- Molecule 8: Cytochrome b-c1 complex subunit Rieske, mitochondrial



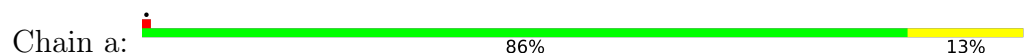
- Molecule 9: Cytochrome b-c1 complex subunit 9

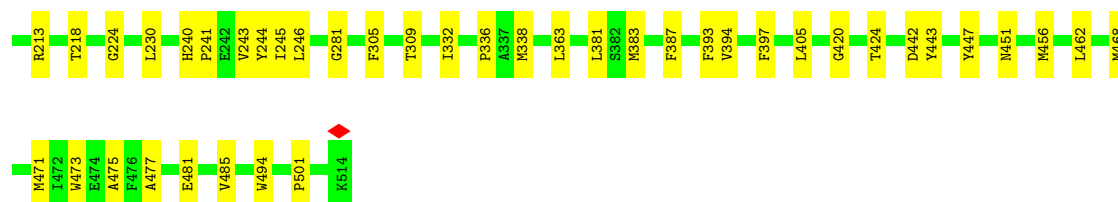


- Molecule 10: Cox7a2l protein

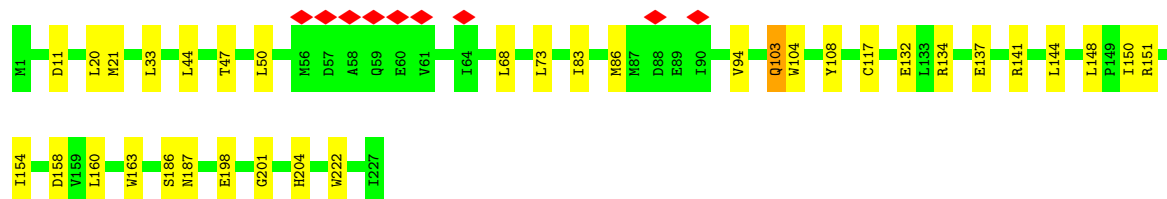
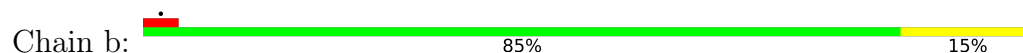


- Molecule 11: Cytochrome c oxidase subunit 1

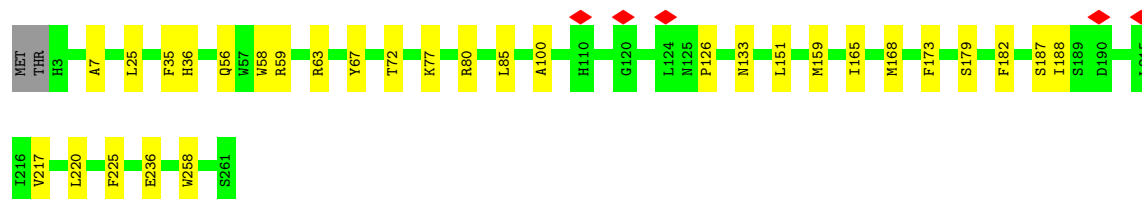
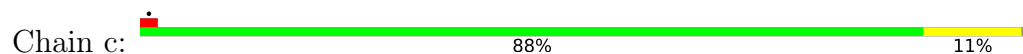




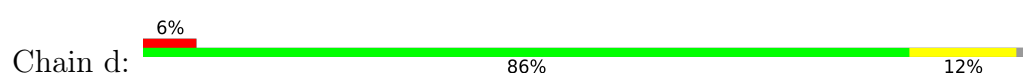
• Molecule 12: Cytochrome c oxidase subunit 2



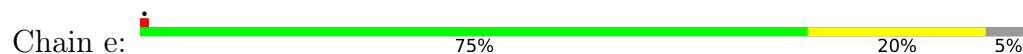
• Molecule 13: Cytochrome c oxidase subunit 3



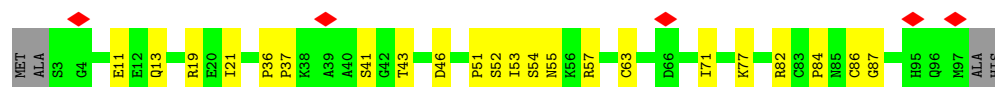
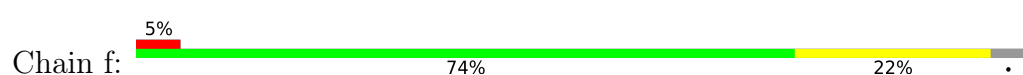
• Molecule 14: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



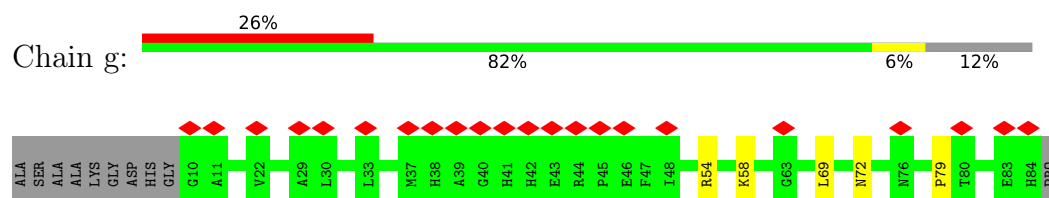
• Molecule 15: Cytochrome c oxidase subunit 5A, mitochondrial



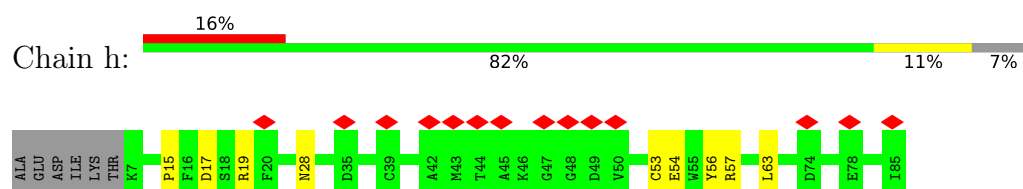
• Molecule 16: Cytochrome c oxidase subunit 5B, mitochondrial



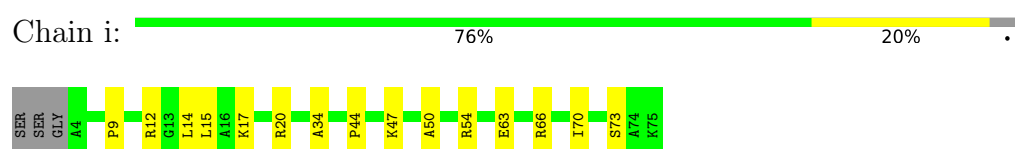
- Molecule 17: Cytochrome c oxidase subunit 6A2, mitochondrial



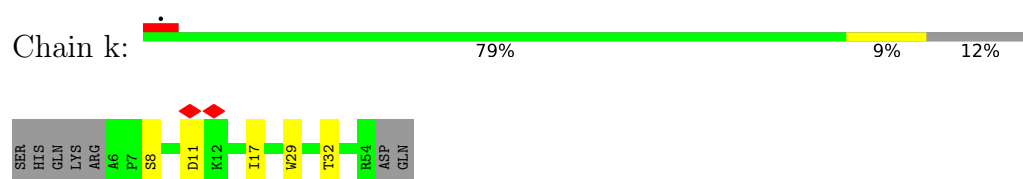
- Molecule 18: Cytochrome c oxidase subunit 6B1



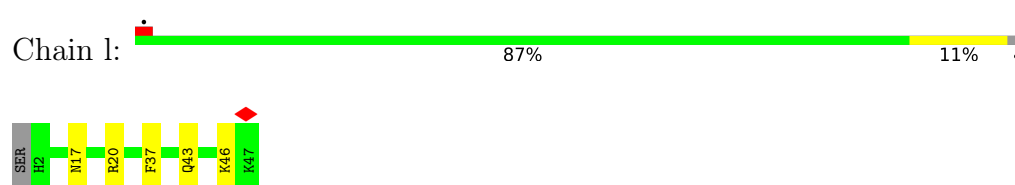
- Molecule 19: Cytochrome c oxidase subunit 6C



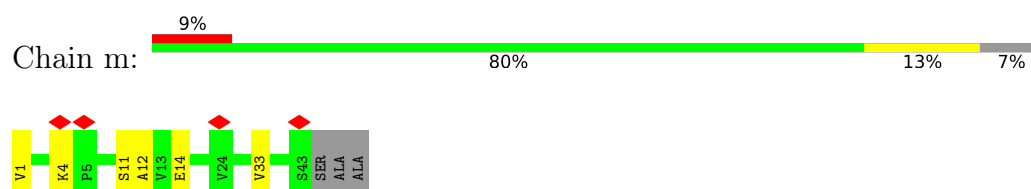
- Molecule 20: Cytochrome c oxidase subunit 7B, mitochondrial



- Molecule 21: Cytochrome c oxidase subunit 7C, mitochondrial

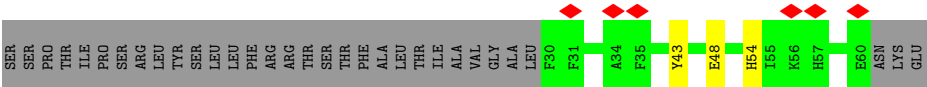


- Molecule 22: Cytochrome c oxidase subunit 8B, mitochondrial



- Molecule 23: Cytochrome b-c1 complex subunit 9





● Molecule 23: Cytochrome b-c1 complex subunit 9



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	8426	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 ($e^-/\text{\AA}^2$)	90.66	Depositor
Minimum defocus (nm)	200	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.330	Depositor
Minimum map value	-0.026	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	161.728, 214.92801, 180.88	wwPDB
Map dimensions	170, 202, 152	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.064, 1.064, 1.064	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.21	0/3536	0.49	0/4803
1	L	0.20	0/3530	0.47	0/4793
2	B	0.21	0/3205	0.47	0/4332
2	M	0.19	0/3205	0.44	0/4332
3	C	0.23	0/3147	0.53	1/4299 (0.0%)
3	N	0.25	0/3147	0.60	2/4297 (0.0%)
4	D	0.20	0/1978	0.51	0/2685
4	O	0.20	0/1968	0.49	0/2674
5	F	0.20	0/916	0.43	0/1226
5	Q	0.19	0/916	0.42	0/1226
6	G	0.27	0/578	0.54	0/777
6	R	0.29	0/627	0.63	0/848
7	H	0.22	0/561	0.59	0/751
7	S	0.27	0/537	0.73	0/718
8	P	0.13	0/131	0.31	0/176
9	T	0.20	0/565	0.52	0/772
10	I	0.25	0/856	0.66	1/1164 (0.1%)
11	a	0.30	0/4162	0.59	1/5686 (0.0%)
12	b	0.28	0/1863	0.65	3/2542 (0.1%)
13	c	0.27	0/2195	0.59	0/3000
14	d	0.24	0/1229	0.55	0/1659
15	e	0.26	0/860	0.61	0/1167
16	f	0.25	0/744	0.57	0/1009
17	g	0.19	0/632	0.43	0/866
18	h	0.24	0/674	0.64	0/910
19	i	0.26	0/584	0.58	0/778
20	k	0.22	0/396	0.49	0/541
21	l	0.28	0/393	0.58	0/527
22	m	0.26	0/318	0.51	0/433
23	J	0.20	0/281	0.57	0/375
23	U	0.21	0/281	0.53	0/375
All	All	0.23	0/44015	0.54	8/59741 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
4	O	0	1
All	All	0	2

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	180	ALA	CA-C-N	-6.28	112.19	122.54
3	N	180	ALA	C-N-CA	-6.28	112.19	122.54
12	b	103	GLN	CA-C-N	6.24	131.45	122.35
12	b	103	GLN	C-N-CA	6.24	131.45	122.35
11	a	107	PRO	CA-N-CD	-5.62	104.14	112.00
3	C	82	MET	N-CA-CB	5.43	118.10	110.12
10	I	68	LYS	CB-CG-CD	5.15	123.15	111.30
12	b	68	LEU	CA-CB-CG	5.07	134.06	116.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	330	SER	Peptide
4	O	160	MET	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3466	0	3377	39	0
1	L	3460	0	3367	42	0
2	B	3154	0	3158	38	0
2	M	3154	0	3158	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	3045	0	3107	24	0
3	N	3046	0	3112	44	0
4	D	1919	0	1867	23	0
4	O	1909	0	1854	22	0
5	F	894	0	882	9	0
5	Q	894	0	882	6	0
6	G	565	0	577	6	0
6	R	609	0	614	7	0
7	H	554	0	535	7	0
7	S	530	0	509	6	0
8	P	128	0	120	2	0
9	T	554	0	590	7	0
10	I	834	0	823	8	0
11	a	4021	0	3998	58	0
12	b	1817	0	1822	25	0
13	c	2111	0	2047	25	0
14	d	1195	0	1161	16	0
15	e	842	0	838	17	0
16	f	727	0	703	14	0
17	g	605	0	570	4	0
18	h	654	0	622	5	0
19	i	572	0	596	12	0
20	k	383	0	367	6	0
21	l	380	0	378	4	0
22	m	311	0	329	5	0
23	J	272	0	251	2	0
23	U	272	0	251	1	0
24	C	86	0	60	2	0
24	N	86	0	60	2	0
25	C	35	0	44	0	0
25	F	63	0	74	1	0
25	L	23	0	20	0	0
25	N	88	0	130	3	0
25	a	28	0	30	0	0
25	b	57	0	62	0	0
25	c	45	0	67	2	0
25	d	34	0	42	1	0
25	g	25	0	24	3	0
25	k	27	0	28	2	0
26	C	42	0	28	0	0
26	D	56	0	56	2	0
26	L	46	0	36	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	N	41	0	26	0	0
26	O	57	0	58	2	0
27	D	43	0	30	0	0
27	O	43	0	30	0	0
28	L	24	0	22	0	0
28	a	43	0	60	0	0
29	a	1	0	0	0	0
30	a	1	0	0	0	0
31	a	120	0	108	3	0
32	b	1	0	0	0	0
33	b	2	0	0	0	0
34	f	1	0	0	0	0
35	l	44	0	63	0	0
All	All	44039	0	43623	446	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 5.

All (446) 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)
11:a:240:HIS:NE2	11:a:244:TYR:CE2	1.72	1.49
11:a:240:HIS:CD2	11:a:244:TYR:CE2	2.21	1.27
11:a:240:HIS:CD2	11:a:244:TYR:HE2	1.72	0.89
11:a:240:HIS:CD2	11:a:244:TYR:CD2	2.66	0.84
11:a:240:HIS:NE2	11:a:244:TYR:HE2	1.40	0.79
11:a:240:HIS:NE2	11:a:244:TYR:CZ	2.27	0.72
14:d:121:LYS:O	14:d:125:ASP:HB2	1.89	0.72
11:a:194:LEU:HB2	11:a:245:ILE:HD11	1.74	0.70
7:H:34:ARG:HG3	7:H:55:GLU:HG3	1.73	0.70
4:D:233:ARG:HA	6:G:16:TYR:O	1.91	0.69
14:d:53:ARG:HH12	15:e:103:GLU:HG3	1.58	0.67
2:B:226:MET:HG2	2:B:227:ARG:HG3	1.77	0.66
21:l:37:PHE:HB3	22:m:33:VAL:HG11	1.78	0.66
2:B:220:ALA:HA	2:B:224:LEU:HD23	1.80	0.63
4:O:71:GLN:HE21	4:O:80:MET:HG3	1.64	0.62
11:a:107:PRO:HB3	13:c:25:LEU:HB2	1.81	0.62
11:a:116:SER:O	21:l:43:GLN:NE2	2.32	0.61
3:N:107:TYR:HB2	3:N:305:PRO:HG3	1.80	0.61
3:C:107:TYR:HB2	3:C:305:PRO:HG3	1.82	0.60
13:c:56:GLN:OE1	13:c:59:ARG:NH2	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:181:PHE:HA	3:N:184:ILE:HG12	1.84	0.60
3:C:129:MET:HE1	3:C:181:PHE:HB3	1.84	0.60
12:b:11:ASP:HA	12:b:21:MET:HE1	1.83	0.59
4:O:34:LYS:HE3	4:O:64:LEU:HD22	1.85	0.58
2:M:141:ARG:NH1	2:M:186:ILE:O	2.37	0.58
3:N:379:LEU:HD13	5:Q:33:ARG:HH12	1.68	0.58
3:C:58:ASP:O	3:C:62:ALA:N	2.35	0.58
14:d:53:ARG:HH11	15:e:104:LEU:HD23	1.67	0.57
14:d:89:ILE:HG22	20:k:29:TRP:HE1	1.70	0.57
12:b:141:ARG:NH1	19:i:70:ILE:O	2.35	0.57
13:c:151:LEU:HD22	13:c:159:MET:HE1	1.86	0.57
2:M:36:ALA:HB3	2:M:207:VAL:HG12	1.85	0.57
16:f:43:THR:HG23	16:f:46:ASP:H	1.70	0.57
10:I:3:TYR:HA	10:I:13:ALA:O	2.05	0.56
14:d:23:PRO:HG3	15:e:37:VAL:HG21	1.87	0.56
4:O:12:TRP:NE1	4:O:125:ASP:OD1	2.35	0.56
11:a:170:ASN:HD21	13:c:77:LYS:HB3	1.69	0.56
3:N:147:THR:HA	3:N:150:LEU:HG	1.88	0.56
15:e:41:LEU:O	15:e:74:LYS:NZ	2.39	0.56
2:B:257:ILE:HG13	2:B:424:MET:HG3	1.86	0.56
3:C:98:VAL:HG22	24:C:402:HEM:HBC2	1.87	0.56
4:O:71:GLN:O	4:O:83:ARG:NH1	2.38	0.56
9:T:65:VAL:HB	9:T:77:ARG:HB3	1.88	0.56
16:f:63:CYS:SG	16:f:86:CYS:HB3	2.46	0.56
21:l:17:ASN:HB3	21:l:20:ARG:HG2	1.88	0.55
2:B:42:ALA:O	2:B:113:ARG:NH1	2.38	0.55
15:e:53:ARG:NH2	15:e:95:GLU:OE2	2.38	0.55
19:i:17:LYS:HA	19:i:20:ARG:HG2	1.88	0.55
10:I:52:ASP:O	10:I:58:LYS:NZ	2.39	0.55
7:S:61:HIS:HB2	4:O:5:LEU:HD11	1.89	0.55
2:B:203:ARG:HH12	2:B:233:ALA:HB2	1.70	0.55
4:D:233:ARG:O	5:F:71:ARG:NH2	2.40	0.55
2:M:52:LYS:O	2:M:203:ARG:NH2	2.40	0.55
11:a:144:ASP:OD1	11:a:213:ARG:NE	2.40	0.55
4:D:224:ARG:NH1	26:D:301:CDL:O1	2.40	0.54
2:B:243:GLU:HG3	2:B:424:MET:HB3	1.88	0.54
2:B:299:VAL:HG21	2:B:309:VAL:HG21	1.89	0.54
11:a:447:TYR:O	11:a:451:ASN:ND2	2.39	0.54
1:L:261:GLY:O	1:L:267:ASN:ND2	2.40	0.54
13:c:187:SER:HA	25:g:101:3PE:H111	1.88	0.54
1:L:173:ASN:HA	1:L:176:ARG:HG2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:VAL:HG22	1:A:407:LEU:HD13	1.89	0.54
15:e:8:ASP:OD2	19:i:12:ARG:NH1	2.37	0.54
1:A:261:GLY:O	1:A:267:ASN:ND2	2.41	0.54
3:N:103:TYR:OH	3:N:322:GLN:NE2	2.40	0.54
3:N:163:TRP:O	3:N:177:ARG:NH1	2.40	0.54
11:a:485:VAL:HG11	11:a:494:TRP:HB3	1.90	0.54
1:A:21:ASN:HB3	1:A:192:ALA:HB1	1.90	0.53
3:N:98:VAL:HG22	24:N:402:HEM:HBC2	1.90	0.53
3:N:328:LEU:HB2	3:N:361:ILE:HG21	1.91	0.53
4:D:200:HIS:CE1	4:D:204:MET:HE3	2.43	0.53
1:A:158:PHE:O	1:A:161:THR:OG1	2.27	0.53
3:C:50:PHE:HA	3:C:53:MET:HG2	1.91	0.53
5:F:67:ASP:O	5:F:71:ARG:NH1	2.41	0.53
2:B:113:ARG:HA	2:B:116:ILE:HD11	1.90	0.53
2:B:141:ARG:NH1	2:B:186:ILE:O	2.42	0.53
2:M:104:ASN:HD22	2:M:387:LEU:HD12	1.73	0.53
2:B:169:LYS:HE3	2:B:240:ARG:HB3	1.90	0.53
11:a:12:HIS:ND1	11:a:80:ASN:O	2.38	0.53
3:N:5:ARG:O	3:N:15:ASN:ND2	2.42	0.53
3:N:240:MET:HA	3:N:243:VAL:HB	1.90	0.53
1:A:308:GLN:NE2	9:T:31:GLN:OE1	2.42	0.53
2:B:36:ALA:HB3	2:B:207:VAL:HG22	1.91	0.53
3:N:214:ASP:HB3	6:R:8:ALA:HB2	1.91	0.53
11:a:332:ILE:HG23	11:a:338:MET:HE2	1.91	0.53
4:O:83:ARG:NH2	4:O:89:ASP:OD1	2.42	0.53
4:O:158:ILE:HG13	4:O:160:MET:H	1.73	0.53
1:A:244:ARG:NH2	1:A:429:GLU:OE1	2.42	0.52
3:C:78:LEU:HG	3:C:82:MET:HE2	1.91	0.52
11:a:243:VAL:HA	11:a:246:LEU:HD12	1.91	0.52
1:L:106:LEU:HD11	1:L:203:VAL:HG23	1.90	0.52
3:N:78:LEU:HG	3:N:82:MET:HE2	1.90	0.52
11:a:173:PRO:HD2	11:a:176:MET:HE2	1.91	0.52
23:U:42:ILE:HG23	4:O:206:LEU:HD21	1.91	0.52
2:B:385:GLN:HA	9:T:2:LEU:HD12	1.91	0.52
2:B:407:ASP:N	2:B:407:ASP:OD1	2.42	0.52
4:D:59:GLU:O	4:D:62:LYS:HB3	2.10	0.52
2:M:102:ARG:NH2	2:M:161:GLU:OE1	2.42	0.52
2:M:76:THR:HG22	2:M:82:SER:H	1.75	0.52
1:A:25:VAL:HG22	1:A:197:LEU:HB3	1.92	0.51
3:N:244:LEU:HD12	4:O:201:ARG:HG3	1.92	0.51
15:e:56:ARG:HG2	15:e:96:LEU:HD22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:70:ARG:NH1	1:L:78:GLU:OE1	2.43	0.51
1:L:354:VAL:HG22	1:L:407:LEU:HD13	1.93	0.51
3:N:66:VAL:HA	3:N:69:ILE:HD12	1.92	0.51
18:h:53:CYS:HB2	18:h:56:TYR:HD2	1.75	0.51
2:B:68:LEU:HD13	2:B:144:LEU:HD23	1.93	0.51
10:I:15:ALA:HB3	10:I:20:ALA:HB2	1.92	0.51
10:I:74:ILE:O	13:c:63:ARG:NH1	2.44	0.51
15:e:91:PRO:O	15:e:95:GLU:HB3	2.10	0.51
22:m:11:SER:OG	22:m:14:GLU:OE1	2.25	0.51
1:L:62:LEU:HD13	1:L:122:LEU:HD22	1.90	0.51
1:L:106:LEU:HA	1:L:109:VAL:HG12	1.93	0.51
10:I:70:ASP:HB3	10:I:72:VAL:HG12	1.91	0.51
11:a:62:ALA:HB2	31:a:603:HEA:HBD1	1.93	0.51
3:N:50:PHE:HB3	3:N:79:ILE:HD12	1.92	0.51
4:D:4:GLU:OE2	4:D:156:GLN:NE2	2.44	0.51
2:M:133:ARG:HB2	2:M:136:GLU:HG3	1.92	0.51
6:R:40:ARG:NH1	26:O:301:CDL:OA3	2.43	0.51
2:M:102:ARG:NH1	2:M:172:LEU:O	2.44	0.51
13:c:7:ALA:HB1	13:c:72:THR:HG21	1.93	0.51
2:B:309:VAL:HG13	2:B:326:THR:HG22	1.93	0.51
2:M:171:ALA:HB2	2:M:235:ALA:HB3	1.93	0.51
1:A:61:HIS:NE2	1:A:137:GLU:OE1	2.41	0.50
1:A:105:ASP:OD1	1:A:105:ASP:N	2.43	0.50
1:L:24:ARG:HD2	1:L:383:LEU:HD23	1.93	0.50
12:b:94:VAL:HG21	12:b:148:LEU:HD22	1.93	0.50
3:N:215:ALA:HA	6:R:10:ILE:HD11	1.92	0.50
3:N:327:ILE:HG23	25:N:405:3PE:H2C2	1.93	0.50
11:a:51:ASP:OD2	11:a:55:ASN:ND2	2.40	0.50
2:B:369:LEU:HD11	2:B:399:LEU:HD11	1.92	0.50
1:A:245:ASP:OD1	6:G:11:ARG:NH1	2.42	0.50
1:A:131:ARG:NH2	1:A:177:LEU:O	2.45	0.50
19:i:14:LEU:HA	19:i:17:LYS:HG2	1.94	0.50
3:N:37:LEU:HD11	3:N:94:LEU:HA	1.92	0.50
11:a:35:ILE:HG13	11:a:462:LEU:HD13	1.93	0.50
13:c:72:THR:HG23	16:f:21:ILE:HD13	1.94	0.49
4:D:20:SER:OG	23:J:43:TYR:OH	2.29	0.49
1:L:42:ASP:O	1:L:194:ARG:NH1	2.45	0.49
11:a:485:VAL:HG23	22:m:1:VAL:HG22	1.94	0.49
1:A:155:ALA:HA	1:A:164:ALA:HB1	1.95	0.49
11:a:117:MET:O	21:l:46:LYS:NZ	2.45	0.49
1:A:60:GLU:OE2	2:B:287:ARG:NH2	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:248:ASP:HB2	4:O:118:ARG:HH21	1.77	0.49
3:N:311:LYS:HD2	3:N:379:LEU:HD21	1.94	0.49
5:Q:35:ASP:OD1	5:Q:89:TYR:OH	2.28	0.49
12:b:94:VAL:HG11	12:b:148:LEU:HD13	1.95	0.49
12:b:132:GLU:HB3	12:b:137:GLU:HG3	1.93	0.49
2:M:196:GLN:O	2:M:227:ARG:NH2	2.45	0.49
3:C:330:ALA:HB2	6:G:51:PRO:HB3	1.95	0.49
2:M:248:ASN:ND2	2:M:250:ASP:OD2	2.45	0.49
13:c:165:ILE:HA	13:c:168:MET:HG2	1.95	0.49
3:N:211:LEU:HD13	5:Q:62:ILE:HD12	1.95	0.48
11:a:38:ARG:NH2	11:a:451:ASN:O	2.45	0.48
4:O:144:ARG:HH21	4:O:147:LEU:HD11	1.78	0.48
1:A:366:VAL:HG11	2:B:43:PRO:HB2	1.95	0.48
3:C:207:ASN:ND2	3:C:209:THR:OG1	2.46	0.48
3:N:24:PRO:O	3:N:224:TYR:OH	2.29	0.48
2:M:200:THR:HA	2:M:227:ARG:HE	1.77	0.48
5:Q:67:ASP:OD1	5:Q:71:ARG:NH1	2.46	0.48
20:k:8:SER:N	20:k:11:ASP:OD2	2.47	0.48
3:N:32:ASN:ND2	3:N:228:ASP:OD1	2.44	0.48
12:b:108:TYR:O	12:b:117:CYS:HA	2.13	0.48
25:k:101:3PE:H332	25:k:101:3PE:H242	1.94	0.48
4:D:60:GLU:O	4:D:63:ALA:HB3	2.14	0.48
16:f:55:ASN:HA	16:f:77:LYS:HE3	1.96	0.48
5:F:12:TRP:HE3	25:F:201:3PE:H352	1.77	0.48
11:a:383:MET:O	11:a:387:PHE:HB2	2.14	0.48
3:N:361:ILE:HA	3:N:365:LEU:HB2	1.96	0.48
1:L:110:VAL:HG21	1:L:211:LEU:HB3	1.96	0.48
1:L:366:VAL:HG11	2:M:43:PRO:HB2	1.95	0.48
3:N:108:THR:OG1	3:N:313:ARG:NH2	2.47	0.48
16:f:54:SER:OG	16:f:55:ASN:N	2.46	0.48
1:A:67:THR:HG23	1:A:70:ARG:H	1.79	0.47
4:D:178:THR:OG1	7:H:13:ASP:OD1	2.30	0.47
3:N:81:TYR:OH	4:O:118:ARG:NH1	2.45	0.47
14:d:52:SER:OG	14:d:55:GLU:OE1	2.24	0.47
4:D:180:SER:HB3	7:H:75:LEU:HD11	1.96	0.47
1:L:242:ARG:NH2	1:L:432:PRO:O	2.46	0.47
20:k:29:TRP:HA	20:k:32:THR:HG22	1.95	0.47
2:B:23:ASP:OD1	2:B:23:ASP:N	2.46	0.47
4:D:5:LEU:HB2	7:H:57:PHE:HD2	1.79	0.47
17:g:69:LEU:HD22	25:g:101:3PE:H331	1.95	0.47
1:A:240:GLU:OE2	1:A:242:ARG:NH1	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:137:VAL:HA	2:B:140:LEU:HD23	1.96	0.47
11:a:481:GLU:H	22:m:4:LYS:HB3	1.79	0.47
15:e:71:VAL:HG11	15:e:85:VAL:HG11	1.97	0.47
15:e:90:ARG:HD2	15:e:93:LEU:HD12	1.97	0.47
1:A:436:ARG:NH2	3:C:221:HIS:O	2.47	0.47
3:N:276:PHE:HB2	3:N:335:LEU:HB3	1.96	0.47
12:b:33:LEU:HB2	19:i:34:ALA:HB2	1.95	0.47
12:b:44:LEU:O	12:b:47:THR:OG1	2.32	0.47
12:b:186:SER:OG	12:b:187:ASN:N	2.46	0.47
1:L:131:ARG:NH2	1:L:177:LEU:O	2.48	0.47
1:L:156:THR:O	1:L:239:SER:OG	2.31	0.47
3:N:320:ILE:HD11	25:N:405:3PE:H122	1.96	0.47
13:c:179:SER:HA	13:c:182:PHE:HD2	1.80	0.47
14:d:83:GLY:HA3	20:k:17:ILE:HG22	1.97	0.47
1:L:42:ASP:OD1	1:L:42:ASP:N	2.41	0.47
1:L:366:VAL:HG22	1:L:392:LEU:HD21	1.97	0.47
6:R:67:GLU:O	6:R:71:ARG:NH1	2.46	0.47
16:f:51:PRO:O	16:f:57:ARG:NH1	2.44	0.47
3:C:92:ILE:HG21	26:D:301:CDL:H791	1.96	0.47
5:F:35:ASP:OD1	5:F:89:TYR:OH	2.31	0.47
1:L:122:LEU:O	1:L:179:ARG:NH1	2.48	0.47
2:M:299:VAL:HG21	2:M:309:VAL:HG21	1.97	0.47
25:d:201:3PE:H342	25:d:201:3PE:H252	1.97	0.47
13:c:63:ARG:HA	13:c:67:TYR:HD2	1.79	0.47
14:d:112:ASP:N	14:d:112:ASP:OD1	2.48	0.47
1:A:294:LEU:HB2	1:A:341:GLN:HG3	1.97	0.46
1:L:76:GLU:HA	1:L:79:VAL:HG12	1.98	0.46
2:M:159:ILE:HD11	2:M:427:SER:HB3	1.97	0.46
11:a:82:LEU:HB3	11:a:86:MET:HE3	1.96	0.46
18:h:28:ASN:HB3	18:h:63:LEU:HD21	1.97	0.46
2:M:209:LEU:HG	2:M:379:LEU:HD13	1.96	0.46
14:d:69:ALA:HB1	15:e:109:VAL:HG22	1.95	0.46
4:D:147:LEU:HD23	4:D:157:ALA:HB1	1.96	0.46
1:L:328:ALA:HB2	1:L:427:PRO:HB2	1.96	0.46
4:D:132:THR:HA	4:D:179:MET:HE2	1.97	0.46
2:M:258:VAL:HA	2:M:323:GLY:HA3	1.98	0.46
11:a:13:LYS:NZ	11:a:501:PRO:O	2.39	0.46
2:M:194:PHE:O	2:M:198:HIS:HB2	2.16	0.46
11:a:443:TYR:O	12:b:134:ARG:NH2	2.48	0.46
13:c:126:PRO:HG3	13:c:258:TRP:HA	1.96	0.46
13:c:80:ARG:NH2	13:c:236:GLU:OE1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:279:LEU:HD21	2:B:347:VAL:HG21	1.98	0.46
3:N:101:GLY:HA2	3:N:106:SER:HB2	1.96	0.46
11:a:456:MET:HG2	14:d:96:LEU:HD11	1.97	0.46
4:O:164:ILE:HG12	4:O:179:MET:HG3	1.98	0.46
7:S:17:THR:O	7:S:21:HIS:ND1	2.42	0.46
1:A:327:ASP:OD1	1:A:327:ASP:N	2.46	0.46
11:a:473:TRP:O	11:a:477:ALA:N	2.49	0.46
13:c:225:PHE:O	16:f:13:GLN:NE2	2.47	0.46
4:D:224:ARG:O	4:D:228:SER:HB3	2.15	0.46
12:b:50:LEU:HB2	19:i:15:LEU:HD13	1.98	0.46
12:b:160:LEU:HB3	12:b:198:GLU:HG2	1.98	0.46
15:e:31:LYS:NZ	16:f:84:PRO:O	2.34	0.46
1:A:74:ALA:O	1:A:77:LYS:HB2	2.16	0.45
1:A:328:ALA:HB2	1:A:427:PRO:HB2	1.97	0.45
3:C:379:LEU:HD11	5:F:33:ARG:HD2	1.98	0.45
4:D:240:PRO:HA	10:I:35:PRO:HD3	1.98	0.45
12:b:154:ILE:HD13	12:b:163:TRP:HB3	1.98	0.45
13:c:217:VAL:HA	13:c:220:LEU:HG	1.97	0.45
4:D:133:GLY:HA3	4:D:152:TYR:HE2	1.81	0.45
6:G:67:GLU:HG3	6:G:71:ARG:HH21	1.81	0.45
1:L:270:LEU:HD13	1:L:320:LEU:HD22	1.98	0.45
7:S:13:ASP:O	7:S:16:THR:OG1	2.33	0.45
1:A:377:GLU:HG3	10:I:12:LEU:HG	1.98	0.45
2:B:95:LYS:O	2:B:109:VAL:HA	2.16	0.45
2:B:258:VAL:HA	2:B:323:GLY:HA3	1.99	0.45
11:a:12:HIS:HB3	11:a:92:MET:HG2	1.99	0.45
1:L:433:ASP:OD1	1:L:433:ASP:N	2.47	0.45
11:a:230:LEU:HD11	13:c:100:ALA:HA	1.98	0.45
16:f:11:GLU:O	16:f:19:ARG:NH2	2.50	0.45
1:A:67:THR:HA	1:A:121:SER:H	1.80	0.45
1:A:248:LEU:HD12	1:A:426:GLY:HA2	1.98	0.45
2:B:102:ARG:NH2	2:B:161:GLU:OE1	2.45	0.45
11:a:82:LEU:O	11:a:86:MET:N	2.45	0.45
11:a:172:LYS:HB2	11:a:172:LYS:HE2	1.85	0.45
11:a:240:HIS:HE2	11:a:244:TYR:HH	1.62	0.45
3:C:165:TRP:O	3:C:174:THR:OG1	2.34	0.45
8:P:12:ASP:O	6:R:24:ARG:NH2	2.50	0.45
15:e:81:ILE:HD13	19:i:9:PRO:HG2	1.97	0.45
16:f:52:SER:OG	16:f:53:ILE:N	2.50	0.45
3:C:50:PHE:HB3	3:C:79:ILE:HG21	1.99	0.45
11:a:241:PRO:O	11:a:245:ILE:HG12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:a:442:ASP:OD2	12:b:134:ARG:NH1	2.43	0.45
3:C:182:HIS:CE1	24:C:401:HEM:NC	2.85	0.45
4:D:76:ASP:OD2	4:O:97:ASN:N	2.43	0.45
18:h:54:GLU:O	18:h:57:ARG:HB3	2.16	0.45
4:O:171:TYR:HD2	4:O:175:THR:HB	1.82	0.45
4:D:93:LYS:HE3	4:D:96:PRO:HA	1.99	0.44
1:L:359:ASN:OD1	1:L:362:ARG:NH1	2.50	0.44
7:S:57:PHE:HB3	4:O:5:LEU:HD13	1.98	0.44
12:b:144:LEU:HD23	12:b:150:ILE:HD13	1.98	0.44
15:e:42:VAL:HG11	15:e:81:ILE:HG21	1.99	0.44
5:F:94:LEU:O	5:F:98:ILE:HG12	2.18	0.44
16:f:82:ARG:HB3	16:f:87:GLY:HA2	1.98	0.44
1:A:3:THR:OG1	1:A:4:PHE:N	2.51	0.44
3:C:151:SER:HB2	3:C:161:VAL:HG21	1.98	0.44
4:D:33:TYR:HA	4:D:37:CYS:HB3	1.98	0.44
2:M:318:ASP:OD1	2:M:318:ASP:N	2.50	0.44
19:i:50:ALA:O	19:i:54:ARG:HB2	2.17	0.44
7:H:19:ARG:HB2	7:H:63:ARG:HD3	1.99	0.44
3:N:337:TRP:CD1	3:N:341:GLN:HE21	2.36	0.44
6:R:72:LYS:HE3	7:S:50:GLU:HG2	1.99	0.44
11:a:50:ASP:OD1	11:a:50:ASP:N	2.43	0.44
11:a:363:LEU:HD22	12:b:20:LEU:HD22	1.98	0.44
13:c:182:PHE:HB3	17:g:72:ASN:HD21	1.82	0.44
23:J:48:GLU:HA	23:J:54:HIS:HE1	1.83	0.44
5:F:31:LEU:HD11	5:F:65:ALA:HB2	1.99	0.44
11:a:194:LEU:HD11	11:a:281:GLY:HA2	1.99	0.44
31:a:604:HEA:H253	12:b:73:LEU:HG	1.99	0.44
4:O:7:PRO:HG3	4:O:126:TYR:HB2	2.00	0.44
4:O:27:ARG:HB2	4:O:55:CYS:HB3	2.00	0.44
1:A:149:VAL:HG21	1:A:252:HIS:HB2	2.00	0.44
1:A:53:ASN:HD21	1:A:165:GLN:HB2	1.82	0.44
1:L:223:TYR:HB3	1:L:226:ASP:HA	2.00	0.44
2:M:372:VAL:HG12	2:M:381:GLU:HG2	2.00	0.44
3:N:24:PRO:HD2	3:N:27:ILE:HD11	1.98	0.44
11:a:381:LEU:HD13	31:a:603:HEA:HAC	2.00	0.44
14:d:82:VAL:O	14:d:86:MET:HG2	2.17	0.44
2:M:51:VAL:HG22	2:M:204:MET:HG2	2.00	0.44
25:N:405:3PE:H282	6:R:54:VAL:HG21	2.00	0.44
11:a:162:ILE:HA	13:c:85:LEU:HD23	2.00	0.44
2:M:437:ASP:OD1	2:M:437:ASP:N	2.51	0.43
3:N:281:LEU:HD11	3:N:294:LEU:HD11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:T:62:ARG:HH21	9:T:77:ARG:HE	1.64	0.43
12:b:222:TRP:HB2	19:i:73:SER:HB2	1.99	0.43
11:a:162:ILE:HG12	13:c:85:LEU:HB3	1.99	0.43
2:B:56:ARG:NH1	2:B:103:GLU:OE2	2.52	0.43
3:C:26:ASN:HD21	3:C:207:ASN:HB2	1.82	0.43
3:C:322:GLN:OE1	6:G:47:ARG:NH1	2.51	0.43
2:B:245:ARG:HB3	2:B:430:LEU:HD13	2.00	0.43
2:M:101:THR:OG1	2:M:102:ARG:N	2.52	0.43
3:N:110:MET:HE1	3:N:305:PRO:HB3	2.00	0.43
16:f:36:PRO:HA	16:f:37:PRO:HD3	1.79	0.43
2:B:29:LEU:HD12	2:B:33:LEU:HD23	1.99	0.43
4:D:226:LYS:HA	4:D:226:LYS:HD2	1.89	0.43
2:M:115:ASP:OD2	2:M:115:ASP:N	2.51	0.43
1:L:294:LEU:HB2	1:L:341:GLN:HG3	2.00	0.43
2:M:36:ALA:O	2:M:207:VAL:HA	2.18	0.43
13:c:188:ILE:HD12	25:g:101:3PE:H31	2.00	0.43
4:O:71:GLN:NE2	4:O:80:MET:HG3	2.29	0.43
1:L:192:ALA:HB2	1:L:219:VAL:HG11	2.01	0.43
1:A:156:THR:O	1:A:239:SER:OG	2.35	0.43
3:C:227:LYS:HD3	4:D:223:LYS:HE3	2.00	0.43
11:a:393:PHE:O	11:a:397:PHE:HB2	2.18	0.43
12:b:158:ASP:OD1	12:b:158:ASP:N	2.42	0.43
16:f:71:ILE:HD12	16:f:84:PRO:HG2	2.00	0.43
2:B:124:LEU:HD23	2:B:124:LEU:HA	1.89	0.43
7:H:64:ASP:HA	7:H:67:VAL:HG12	2.01	0.43
1:L:327:ASP:OD1	1:L:327:ASP:N	2.45	0.43
2:M:178:CYS:HB2	2:M:183:MET:HE3	2.01	0.43
2:B:35:ILE:HD13	2:B:206:LEU:HB3	2.01	0.43
1:L:379:ILE:HG12	1:L:389:ARG:HD3	2.01	0.43
2:M:49:LEU:HD13	2:M:206:LEU:HD13	2.01	0.43
2:M:407:ASP:OD1	2:M:407:ASP:N	2.50	0.43
9:T:47:ARG:HD2	9:T:48:PRO:HD2	2.01	0.43
10:I:82:ASP:HA	10:I:85:LEU:HD23	2.01	0.43
1:A:102:LEU:HD21	2:B:366:ALA:HA	2.01	0.42
3:C:33:PHE:O	3:C:36:LEU:HB2	2.19	0.42
1:A:110:VAL:HG11	1:A:211:LEU:HB3	2.01	0.42
5:Q:39:GLU:O	5:Q:44:LYS:NZ	2.52	0.42
3:N:11:PHE:HA	3:N:14:ILE:HG12	2.01	0.42
11:a:144:ASP:OD2	13:c:36:HIS:NE2	2.36	0.42
11:a:336:PRO:HB2	11:a:394:VAL:HG11	2.01	0.42
14:d:93:ALA:HB2	20:k:29:TRP:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:274:ASN:HD21	1:L:311:ASN:HB2	1.85	0.42
12:b:83:ILE:HA	12:b:86:MET:HB2	2.02	0.42
1:L:65:LYS:HA	1:L:65:LYS:HD3	1.90	0.42
2:M:114:SER:OG	2:M:115:ASP:N	2.53	0.42
2:B:291:THR:O	2:B:297:GLN:NE2	2.52	0.42
2:B:357:VAL:HG12	2:B:361:LYS:HE3	2.02	0.42
1:L:268:VAL:O	1:L:271:GLN:HB2	2.19	0.42
11:a:240:HIS:HD2	11:a:244:TYR:CD2	2.32	0.42
3:C:311:LYS:HE3	3:C:311:LYS:HB3	1.85	0.42
1:L:44:GLY:H	1:L:47:TYR:HD2	1.66	0.42
1:L:124:ASP:HA	1:L:127:ILE:HG22	2.02	0.42
3:N:22:PRO:HB2	3:N:217:LYS:HE3	2.02	0.42
3:N:137:GLN:HE22	3:N:260:ASN:H	1.68	0.42
12:b:103:GLN:HG3	12:b:104:TRP:CE3	2.54	0.42
1:L:436:ARG:HD2	1:L:436:ARG:HA	1.76	0.42
4:D:42:SER:OG	4:D:44:ASP:OD1	2.36	0.42
11:a:240:HIS:HD2	11:a:244:TYR:CE2	2.20	0.42
13:c:35:PHE:O	17:g:58:LYS:NZ	2.52	0.42
15:e:66:ARG:HA	15:e:69:GLU:HB2	2.02	0.42
2:B:159:ILE:HG21	2:B:325:TYR:HE1	1.85	0.41
6:G:41:THR:O	6:G:45:ILE:HB	2.21	0.41
2:M:102:ARG:HH12	2:M:164:HIS:HB3	1.85	0.41
3:N:137:GLN:NE2	3:N:260:ASN:H	2.17	0.41
7:S:15:LEU:HD23	4:O:180:SER:HB3	2.01	0.41
13:c:58:TRP:CG	25:c:301:3PE:H251	2.55	0.41
1:A:8:LEU:HD12	1:A:392:LEU:HB3	2.02	0.41
3:N:80:ARG:HH22	3:N:256:TYR:HE1	1.67	0.41
11:a:23:GLY:HA3	11:a:73:MET:HG3	2.01	0.41
12:b:198:GLU:O	12:b:204:HIS:CE1	2.73	0.41
1:A:192:ALA:HB2	1:A:219:VAL:HB	2.02	0.41
1:A:255:ILE:HG12	1:A:422:VAL:HG13	2.03	0.41
11:a:140:GLY:O	11:a:213:ARG:NH2	2.53	0.41
7:H:38:CYS:HA	7:H:41:ARG:HG2	2.02	0.41
2:M:163:LEU:HD11	2:M:258:VAL:HG22	2.02	0.41
11:a:420:GLY:O	11:a:424:THR:OG1	2.30	0.41
1:L:123:GLU:OE1	1:L:125:SER:N	2.53	0.41
1:L:185:TYR:O	1:L:189:HIS:HB2	2.20	0.41
2:M:254:HIS:CE1	2:M:327:ILE:HD12	2.56	0.41
2:B:393:MET:HA	2:B:394:PRO:HD3	1.95	0.41
11:a:468:MET:HA	11:a:471:MET:HG3	2.03	0.41
12:b:151:ARG:NH2	18:h:15:PRO:O	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:d:33:LEU:HB2	14:d:38:LYS:HE3	2.02	0.41
14:d:53:ARG:NH1	15:e:103:GLU:O	2.53	0.41
18:h:17:ASP:OD2	18:h:19:ARG:NH1	2.54	0.41
19:i:44:PRO:HA	19:i:47:LYS:HG2	2.03	0.41
2:B:182:ARG:NH2	2:B:190:GLU:OE1	2.40	0.41
3:C:328:LEU:HD11	3:C:362:ILE:HD13	2.02	0.41
3:N:29:SER:O	3:N:32:ASN:HB2	2.21	0.41
16:f:41:SER:OG	16:f:46:ASP:O	2.34	0.41
3:N:334:ILE:HD13	3:N:334:ILE:HA	1.96	0.41
12:b:21:MET:HE3	12:b:21:MET:HB2	1.96	0.41
14:d:89:ILE:HG22	20:k:29:TRP:NE1	2.35	0.41
25:k:101:3PE:H322	22:m:12:ALA:HA	2.01	0.41
4:O:27:ARG:HH21	4:O:56:TYR:HA	1.86	0.41
1:A:339:GLN:NE2	1:A:437:ILE:O	2.54	0.41
3:C:333:LEU:HA	3:C:336:THR:HG22	2.03	0.41
4:D:134:TYR:CG	4:D:162:PRO:HG3	2.55	0.41
1:L:65:LYS:NZ	1:L:130:GLU:OE2	2.53	0.41
1:L:135:LEU:HD23	1:L:135:LEU:HA	1.90	0.41
1:L:304:CYS:HA	1:L:326:CYS:HB3	2.03	0.41
2:M:245:ARG:HH21	2:M:433:THR:HB	1.85	0.41
2:M:312:PHE:HA	9:T:61:ALA:HA	2.02	0.41
3:N:29:SER:HB2	26:O:301:CDL:H721	2.02	0.41
11:a:218:THR:HG21	11:a:224:GLY:HA3	2.02	0.41
19:i:63:GLU:HA	19:i:66:ARG:HG2	2.03	0.41
2:B:209:LEU:HD12	2:B:379:LEU:HB2	2.02	0.41
3:C:248:ASP:OD1	3:C:248:ASP:N	2.54	0.41
2:M:276:GLN:HE21	9:T:61:ALA:HB1	1.85	0.41
13:c:58:TRP:CE3	25:c:301:3PE:H271	2.56	0.41
1:A:113:LEU:HD23	1:A:113:LEU:HA	1.92	0.40
1:L:151:ASP:OD2	8:P:2:HIS:NE2	2.51	0.40
11:a:197:LEU:HD23	11:a:197:LEU:HA	1.95	0.40
12:b:104:TRP:HZ2	12:b:201:GLY:HA3	1.85	0.40
15:e:86:ILE:HD13	15:e:86:ILE:HA	1.92	0.40
1:L:304:CYS:HB3	1:L:334:MET:SD	2.62	0.40
11:a:305:PHE:O	11:a:309:THR:HG23	2.20	0.40
13:c:133:ASN:HB2	13:c:173:PHE:CD1	2.56	0.40
1:A:334:MET:HE3	1:A:334:MET:HB2	1.89	0.40
1:A:420:PRO:O	1:A:434:TYR:OH	2.32	0.40
2:B:163:LEU:HD11	2:B:258:VAL:HG22	2.04	0.40
5:F:109:LYS:HE3	5:F:109:LYS:HB3	1.82	0.40
3:N:51:LEU:HD13	24:N:401:HEM:HBA1	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:62:ALA:O	3:N:65:SER:OG	2.32	0.40
11:a:191:THR:HG23	11:a:245:ILE:HG23	2.03	0.40
4:O:56:TYR:HD2	4:O:60:GLU:HB3	1.86	0.40
2:B:148:LYS:HG3	2:B:177:TYR:HB3	2.03	0.40
1:L:154:HIS:NE2	1:L:314:TYR:OH	2.47	0.40
3:N:280:ILE:H	3:N:280:ILE:HG13	1.76	0.40
5:Q:87:LYS:HB2	5:Q:87:LYS:HE2	1.92	0.40
11:a:30:GLY:C	11:a:65:MET:HE2	2.46	0.40
19:i:17:LYS:HE2	19:i:17:LYS:HB2	1.94	0.40
1:A:59:LEU:HD23	1:A:59:LEU:HA	1.99	0.40
1:A:67:THR:OG1	1:A:119:ASN:O	2.30	0.40
3:C:373:GLU:OE2	5:F:20:TYR:OH	2.37	0.40
1:L:332:ASP:HB2	1:L:430:GLN:HG2	2.03	0.40
11:a:405:LEU:HD23	11:a:475:ALA:HB2	2.04	0.40
14:d:114:ASP:OD1	14:d:114:ASP:N	2.51	0.40
17:g:54:ARG:HB3	17:g:79:PRO:HG3	2.04	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	444/446 (100%)	423 (95%)	21 (5%)	0	100	100
1	L	443/446 (99%)	426 (96%)	17 (4%)	0	100	100
2	B	418/439 (95%)	398 (95%)	20 (5%)	0	100	100
2	M	418/439 (95%)	400 (96%)	18 (4%)	0	100	100
3	C	378/381 (99%)	365 (97%)	13 (3%)	0	100	100
3	N	378/381 (99%)	359 (95%)	19 (5%)	0	100	100
4	D	239/241 (99%)	226 (95%)	13 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	O	238/241 (99%)	227 (95%)	11 (5%)	0	100	100
5	F	99/110 (90%)	99 (100%)	0	0	100	100
5	Q	99/110 (90%)	99 (100%)	0	0	100	100
6	G	63/81 (78%)	60 (95%)	3 (5%)	0	100	100
6	R	70/81 (86%)	66 (94%)	4 (6%)	0	100	100
7	H	65/76 (86%)	62 (95%)	3 (5%)	0	100	100
7	S	62/76 (82%)	57 (92%)	5 (8%)	0	100	100
8	P	13/196 (7%)	12 (92%)	1 (8%)	0	100	100
9	T	76/78 (97%)	66 (87%)	10 (13%)	0	100	100
10	I	109/113 (96%)	96 (88%)	13 (12%)	0	100	100
11	a	512/514 (100%)	498 (97%)	14 (3%)	0	100	100
12	b	225/227 (99%)	210 (93%)	15 (7%)	0	100	100
13	c	257/261 (98%)	250 (97%)	7 (3%)	0	100	100
14	d	142/147 (97%)	132 (93%)	10 (7%)	0	100	100
15	e	102/109 (94%)	97 (95%)	5 (5%)	0	100	100
16	f	93/99 (94%)	84 (90%)	9 (10%)	0	100	100
17	g	73/85 (86%)	67 (92%)	6 (8%)	0	100	100
18	h	77/85 (91%)	75 (97%)	2 (3%)	0	100	100
19	i	70/75 (93%)	67 (96%)	3 (4%)	0	100	100
20	k	47/56 (84%)	47 (100%)	0	0	100	100
21	l	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
22	m	41/46 (89%)	38 (93%)	3 (7%)	0	100	100
23	J	29/63 (46%)	28 (97%)	1 (3%)	0	100	100
23	U	29/63 (46%)	25 (86%)	4 (14%)	0	100	100
All	All	5353/5812 (92%)	5102 (95%)	251 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	373/373 (100%)	373 (100%)	0	100	100
1	L	372/373 (100%)	372 (100%)	0	100	100
2	B	330/344 (96%)	330 (100%)	0	100	100
2	M	330/344 (96%)	330 (100%)	0	100	100
3	C	332/333 (100%)	332 (100%)	0	100	100
3	N	332/333 (100%)	332 (100%)	0	100	100
4	D	206/206 (100%)	206 (100%)	0	100	100
4	O	205/206 (100%)	205 (100%)	0	100	100
5	F	93/98 (95%)	93 (100%)	0	100	100
5	Q	93/98 (95%)	93 (100%)	0	100	100
6	G	61/73 (84%)	61 (100%)	0	100	100
6	R	66/73 (90%)	66 (100%)	0	100	100
7	H	64/72 (89%)	64 (100%)	0	100	100
7	S	61/72 (85%)	61 (100%)	0	100	100
8	P	15/166 (9%)	15 (100%)	0	100	100
9	T	58/58 (100%)	58 (100%)	0	100	100
10	I	82/95 (86%)	82 (100%)	0	100	100
11	a	425/425 (100%)	425 (100%)	0	100	100
12	b	210/210 (100%)	210 (100%)	0	100	100
13	c	225/227 (99%)	225 (100%)	0	100	100
14	d	127/128 (99%)	127 (100%)	0	100	100
15	e	91/95 (96%)	91 (100%)	0	100	100
16	f	81/83 (98%)	81 (100%)	0	100	100
17	g	62/67 (92%)	62 (100%)	0	100	100
18	h	70/75 (93%)	70 (100%)	0	100	100
19	i	54/56 (96%)	54 (100%)	0	100	100
20	k	39/46 (85%)	39 (100%)	0	100	100
21	l	39/40 (98%)	39 (100%)	0	100	100
22	m	33/34 (97%)	33 (100%)	0	100	100
23	J	26/54 (48%)	26 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	U	26/54 (48%)	26 (100%)	0	100	100
All	All	4581/4911 (93%)	4581 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	A	53	ASN
1	A	69	ASN
1	A	119	ASN
1	A	341	GLN
2	B	251	ASN
2	B	277	HIS
2	B	297	GLN
2	B	343	GLN
2	B	401	GLN
3	C	345	HIS
4	D	31	GLN
4	D	181	GLN
1	L	126	GLN
1	L	305	GLN
1	L	368	HIS
2	M	143	GLN
2	M	162	ASN
2	M	174	ASN
2	M	290	ASN
2	M	297	GLN
2	M	329	GLN
2	M	338	ASN
2	M	343	GLN
2	M	358	GLN
3	N	308	HIS
10	I	57	ASN
11	a	170	ASN
11	a	214	ASN
11	a	331	ASN
11	a	360	ASN
11	a	368	HIS
11	a	491	ASN

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Mol	Chain	Res	Type
11	a	496	HIS
13	c	76	GLN
14	d	76	ASN
16	f	81	GLN
17	g	66	ASN
19	i	22	HIS
20	k	15	ASN
22	m	15	GLN
4	O	6	HIS

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 34 ligands modelled in this entry, 4 are monoatomic - leaving 30 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	$\# Z > 2$
25	3PE	b	302	-	28,28,50	0.39	0	31,33,55	0.36	0
25	3PE	d	201	-	33,33,50	0.39	0	36,38,55	0.62	1 (2%)
27	HEC	D	302	4	46,50,50	1.83	7 (15%)	58,82,82	1.94	6 (10%)
26	CDL	O	301	-	56,56,99	0.38	0	62,68,111	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	CUA	b	303	12	0,1,1	-	-	-		
25	3PE	N	405	-	50,50,50	0.30	0	53,55,55	0.30	0
26	CDL	N	404	-	40,40,99	0.46	0	46,52,111	0.60	1 (2%)
24	HEM	N	402	3	50,50,50	1.33	6 (12%)	67,82,82	1.65	13 (19%)
25	3PE	L	502	-	22,22,50	0.44	0	25,27,55	0.40	0
25	3PE	C	403	-	34,34,50	0.36	0	37,39,55	0.37	0
27	HEC	O	302	4	46,50,50	1.84	7 (15%)	58,82,82	1.96	5 (8%)
26	CDL	C	404	-	41,41,99	0.44	0	47,53,111	0.36	0
26	CDL	L	503	-	45,45,99	0.44	0	51,57,111	0.56	1 (1%)
25	3PE	k	101	-	26,26,50	0.41	0	29,31,55	0.49	0
25	3PE	F	201	-	28,28,50	0.39	0	31,33,55	0.41	0
31	HEA	a	604	11	67,67,67	1.38	7 (10%)	81,103,103	2.15	27 (33%)
26	CDL	D	301	-	55,55,99	0.38	0	61,67,111	0.33	0
31	HEA	a	603	11	67,67,67	1.36	7 (10%)	81,103,103	2.23	28 (34%)
25	3PE	b	304	-	27,27,50	0.40	0	30,32,55	0.40	0
25	3PE	F	202	-	33,33,50	0.37	0	36,38,55	0.32	0
24	HEM	C	402	3	50,50,50	1.33	7 (14%)	67,82,82	1.58	12 (17%)
28	PC1	a	605	-	42,42,53	0.33	0	48,50,61	0.35	0
25	3PE	g	101	-	24,24,50	0.44	0	27,29,55	0.70	1 (3%)
25	3PE	N	403	-	36,36,50	0.35	0	39,41,55	0.34	0
35	TGL	l	601	-	43,43,62	0.20	0	46,46,65	0.24	0
25	3PE	c	301	-	44,44,50	0.32	0	47,49,55	0.37	0
24	HEM	C	401	3	50,50,50	1.31	8 (16%)	67,82,82	1.62	12 (17%)
28	PC1	L	501	-	23,23,53	0.45	0	29,31,61	0.70	1 (3%)
25	3PE	a	606	-	27,27,50	0.40	0	30,32,55	0.46	0
24	HEM	N	401	3	50,50,50	1.29	8 (16%)	67,82,82	1.65	12 (17%)

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
25	3PE	b	302	-	-	7/32/32/54	-
25	3PE	d	201	-	-	8/37/37/54	-
27	HEC	D	302	4	-	4/14/54/54	-
26	CDL	O	301	-	-	19/67/67/110	-
25	3PE	N	405	-	-	13/54/54/54	-
26	CDL	N	404	-	-	11/51/51/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	HEM	N	402	3	-	10/14/54/54	-
25	3PE	L	502	-	-	9/26/26/54	-
25	3PE	C	403	-	-	9/38/38/54	-
27	HEC	O	302	4	-	4/14/54/54	-
26	CDL	C	404	-	-	11/52/52/110	-
26	CDL	L	503	-	-	14/56/56/110	-
25	3PE	k	101	-	-	6/30/30/54	-
25	3PE	F	201	-	-	5/32/32/54	-
31	HEA	a	604	11	-	8/36/76/76	-
26	CDL	D	301	-	-	18/66/66/110	-
31	HEA	a	603	11	-	12/36/76/76	-
25	3PE	b	304	-	-	6/31/31/54	-
25	3PE	F	202	-	-	9/37/37/54	-
24	HEM	C	402	3	-	7/14/54/54	-
28	PC1	a	605	-	-	7/46/46/57	-
25	3PE	g	101	-	-	9/28/28/54	-
25	3PE	N	403	-	-	4/40/40/54	-
35	TGL	l	601	-	-	4/46/46/65	-
25	3PE	c	301	-	-	7/48/48/54	-
24	HEM	C	401	3	-	7/14/54/54	-
28	PC1	L	501	-	-	8/27/27/57	-
25	3PE	a	606	-	-	11/31/31/54	-
24	HEM	N	401	3	-	7/14/54/54	-

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	D	302	HEC	CAC-C3C	6.22	1.55	1.35
27	O	302	HEC	CAC-C3C	6.19	1.55	1.35
27	D	302	HEC	CAB-C3B	6.14	1.54	1.35
27	O	302	HEC	CAB-C3B	6.10	1.54	1.35
27	O	302	HEC	C3D-C2D	5.70	1.53	1.38
27	D	302	HEC	C3D-C2D	5.52	1.53	1.38
31	a	604	HEA	C3B-C2B	4.40	1.44	1.34
31	a	603	HEA	C3B-C2B	4.28	1.44	1.34
24	C	402	HEM	C4D-ND	-3.89	1.33	1.40
31	a	604	HEA	C3D-C2D	3.88	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	a	603	HEA	C3D-C2D	3.73	1.44	1.36
24	C	401	HEM	C4D-ND	-3.72	1.33	1.40
31	a	603	HEA	C3A-C2A	3.66	1.45	1.37
24	N	402	HEM	C4D-ND	-3.66	1.33	1.40
24	N	401	HEM	C4D-ND	-3.51	1.34	1.40
31	a	604	HEA	C3A-C2A	3.36	1.44	1.37
24	N	402	HEM	C1B-NB	-3.18	1.34	1.40
24	C	401	HEM	C1B-NB	-3.12	1.34	1.40
24	N	401	HEM	C1B-NB	-3.10	1.34	1.40
24	C	402	HEM	C1B-NB	-3.07	1.34	1.40
31	a	604	HEA	C4B-C3B	3.05	1.50	1.44
24	N	402	HEM	C1C-C2C	-3.00	1.39	1.45
24	C	402	HEM	C1D-ND	-2.95	1.33	1.38
31	a	603	HEA	C4B-C3B	2.91	1.49	1.44
24	C	402	HEM	C1C-C2C	-2.89	1.39	1.45
24	N	402	HEM	C1D-ND	-2.78	1.33	1.38
24	C	401	HEM	C1D-ND	-2.74	1.33	1.38
24	N	401	HEM	C1D-ND	-2.70	1.33	1.38
31	a	603	HEA	C1D-ND	-2.62	1.35	1.40
24	N	401	HEM	C1C-C2C	-2.47	1.40	1.45
24	C	401	HEM	C1C-C2C	-2.44	1.40	1.45
24	N	402	HEM	FE-NB	2.43	2.02	1.94
24	C	402	HEM	FE-NB	2.35	2.02	1.94
31	a	604	HEA	C1D-ND	-2.29	1.36	1.40
24	N	401	HEM	FE-NB	2.26	2.01	1.94
31	a	603	HEA	C1C-C2C	2.26	1.48	1.43
24	C	401	HEM	FE-NB	2.20	2.01	1.94
24	C	401	HEM	C4B-NB	-2.18	1.34	1.38
24	N	401	HEM	FE-ND	2.15	2.01	1.94
24	N	401	HEM	C3C-C4C	-2.13	1.42	1.46
24	C	402	HEM	C4B-NB	-2.13	1.34	1.38
31	a	604	HEA	C4D-C3D	2.10	1.48	1.45
24	C	401	HEM	C3C-C4C	-2.10	1.42	1.46
31	a	604	HEA	C1C-C2C	2.10	1.48	1.43
31	a	603	HEA	C4D-C3D	2.10	1.48	1.45
24	C	402	HEM	C3C-C4C	-2.09	1.42	1.46
27	D	302	HEC	C3B-C2B	-2.09	1.34	1.41
24	C	401	HEM	FE-ND	2.09	2.01	1.94
27	O	302	HEC	CMB-C2B	2.08	1.55	1.50
24	N	401	HEM	C4B-NB	-2.07	1.34	1.38
27	D	302	HEC	C3C-C2C	-2.06	1.34	1.41
27	O	302	HEC	CMC-C2C	2.06	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	N	402	HEM	C4B-NB	-2.05	1.34	1.38
27	D	302	HEC	CMC-C2C	2.05	1.55	1.50
27	O	302	HEC	C3C-C2C	-2.05	1.34	1.41
27	O	302	HEC	C3B-C2B	-2.04	1.34	1.41
27	D	302	HEC	CMB-C2B	2.03	1.54	1.50

All (120) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	O	302	HEC	CBC-CAC-C3C	-8.71	110.02	127.43
27	D	302	HEC	CBC-CAC-C3C	-8.49	110.46	127.43
27	O	302	HEC	CBB-CAB-C3B	-8.42	110.60	127.43
27	D	302	HEC	CBB-CAB-C3B	-8.30	110.83	127.43
31	a	603	HEA	C3A-C2A-C1A	-6.84	100.58	107.05
31	a	604	HEA	C3A-C2A-C1A	-6.46	100.93	107.05
31	a	603	HEA	C2A-C1A-NA	5.15	115.30	110.32
31	a	604	HEA	C2A-C1A-NA	4.98	115.13	110.32
24	N	401	HEM	CHC-C4B-NB	4.94	129.73	124.42
24	C	401	HEM	CHC-C4B-NB	4.86	129.65	124.42
31	a	604	HEA	CMC-C2C-C3C	4.82	137.88	126.55
31	a	603	HEA	CMC-C2C-C3C	4.76	137.75	126.55
31	a	603	HEA	C3D-C4D-ND	4.63	114.83	110.35
31	a	603	HEA	CMD-C2D-C1D	-4.59	117.86	125.03
24	C	402	HEM	CHC-C4B-NB	4.56	129.33	124.42
31	a	604	HEA	C3D-C4D-ND	4.53	114.73	110.35
24	N	402	HEM	CHC-C4B-NB	4.50	129.26	124.42
24	C	401	HEM	CHD-C4C-NC	4.50	129.35	124.45
24	N	401	HEM	CHD-C4C-NC	4.44	129.28	124.45
31	a	604	HEA	CMC-C2C-C1C	-4.37	118.77	125.42
24	C	402	HEM	CHD-C4C-NC	4.28	129.11	124.45
31	a	603	HEA	CMC-C2C-C1C	-4.20	119.02	125.42
24	N	402	HEM	CHB-C1B-NB	4.19	129.55	124.37
31	a	604	HEA	CMB-C2B-C1B	-4.17	118.52	125.03
24	C	401	HEM	CHB-C1B-NB	4.17	129.52	124.37
24	N	402	HEM	CHD-C4C-NC	4.16	128.98	124.45
31	a	603	HEA	CMB-C2B-C1B	-4.07	118.68	125.03
24	N	401	HEM	CHB-C1B-NB	4.00	129.32	124.37
31	a	603	HEA	C4D-C3D-C2D	-3.98	101.09	106.89
27	O	302	HEC	C4D-ND-C1D	3.81	112.04	105.82
31	a	604	HEA	CHA-C1A-C2A	-3.81	118.85	124.86
31	a	604	HEA	CMD-C2D-C1D	-3.80	119.09	125.03
24	C	402	HEM	CHB-C1B-NB	3.79	129.05	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	603	HEA	CHA-C1A-C2A	-3.72	118.99	124.86
31	a	604	HEA	C4D-C3D-C2D	-3.66	101.57	106.89
27	D	302	HEC	C4D-ND-C1D	3.57	111.64	105.82
31	a	603	HEA	C13-C12-C11	-3.45	108.89	114.39
31	a	603	HEA	CHA-C4D-C3D	-3.41	119.80	124.77
24	N	402	HEM	C4D-ND-C1D	3.40	109.23	105.21
31	a	603	HEA	C3C-C2C-C1C	-3.35	103.23	107.17
31	a	603	HEA	CMD-C2D-C3D	3.33	135.16	126.15
31	a	604	HEA	CHA-C4D-C3D	-3.31	119.95	124.77
24	C	402	HEM	C4D-ND-C1D	3.29	109.10	105.21
31	a	604	HEA	C3C-C2C-C1C	-3.24	103.35	107.17
24	N	402	HEM	CHD-C1D-ND	3.14	127.80	124.42
31	a	603	HEA	C26-C15-C16	3.12	120.64	115.23
31	a	604	HEA	CMB-C2B-C3B	3.07	136.21	130.28
31	a	604	HEA	CMD-C2D-C3D	3.05	134.40	126.15
31	a	604	HEA	CAD-C3D-C4D	3.04	129.99	124.70
24	C	401	HEM	C1B-NB-C4B	3.00	108.76	105.21
31	a	603	HEA	CAD-C3D-C4D	2.94	129.83	124.70
31	a	603	HEA	CAA-CBA-CGA	-2.92	105.93	113.67
31	a	603	HEA	CMB-C2B-C3B	2.89	135.86	130.28
24	N	401	HEM	C1B-NB-C4B	2.87	108.61	105.21
24	N	402	HEM	CHA-C4D-ND	2.85	127.90	124.37
31	a	604	HEA	CHB-C1B-C2B	-2.80	120.60	125.03
24	C	401	HEM	C4D-ND-C1D	2.80	108.52	105.21
24	N	401	HEM	CHA-C1A-NA	2.77	128.89	123.86
24	C	401	HEM	CHA-C4D-ND	2.75	127.77	124.37
24	N	401	HEM	CHD-C1D-ND	2.74	127.38	124.42
31	a	603	HEA	CHB-C1B-C2B	-2.74	120.70	125.03
24	N	401	HEM	C4D-ND-C1D	2.73	108.44	105.21
24	C	402	HEM	C1B-NB-C4B	2.72	108.43	105.21
24	N	401	HEM	CHA-C4D-ND	2.69	127.69	124.37
31	a	604	HEA	C2B-C1B-NB	2.65	112.97	109.90
24	C	401	HEM	CHA-C1A-NA	2.65	128.66	123.86
24	C	402	HEM	CHD-C1D-ND	2.61	127.23	124.42
24	N	402	HEM	CHB-C1B-C2B	-2.60	119.56	126.95
31	a	603	HEA	C17-C18-C19	-2.52	121.86	127.62
24	C	401	HEM	CHD-C1D-ND	2.52	127.13	124.42
31	a	603	HEA	C27-C19-C20	2.51	119.58	115.23
27	O	302	HEC	CAD-C3D-C4D	2.50	129.83	124.94
24	C	402	HEM	CHA-C1A-NA	2.47	128.34	123.86
31	a	603	HEA	OMA-CMA-C3A	-2.47	120.05	125.62
31	a	604	HEA	C26-C15-C16	2.46	119.49	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	N	402	HEM	CAD-CBD-CGD	-2.45	107.16	113.67
26	N	404	CDL	CA4-OA6-CA5	2.45	123.66	117.80
25	g	101	3PE	C2-O21-C21	2.45	123.65	117.80
31	a	604	HEA	C4B-C3B-C2B	-2.44	103.33	107.44
24	C	402	HEM	CHA-C4D-ND	2.43	127.37	124.37
26	L	503	CDL	CB4-OB6-CB5	2.39	123.52	117.80
24	C	402	HEM	C4A-CHB-C1B	-2.38	120.64	126.25
24	C	402	HEM	C1C-CHC-C4B	-2.37	120.97	126.02
24	N	402	HEM	CHA-C1A-NA	2.36	128.15	123.86
27	D	302	HEC	C2A-C1A-NA	-2.36	108.05	110.32
31	a	604	HEA	C3B-C4B-NB	2.35	112.55	109.84
24	N	402	HEM	C1C-CHC-C4B	-2.35	121.02	126.02
24	N	402	HEM	C1B-NB-C4B	2.35	107.98	105.21
31	a	604	HEA	CHC-C1C-C2C	-2.34	120.62	127.43
24	C	401	HEM	CHB-C1B-C2B	-2.31	120.39	126.95
31	a	604	HEA	C12-C13-C14	-2.30	106.11	112.16
31	a	603	HEA	C3C-C4C-NC	2.30	111.74	109.80
28	L	501	PC1	C2-O21-C21	2.30	123.29	117.80
31	a	604	HEA	CAA-CBA-CGA	-2.29	107.58	113.67
25	d	201	3PE	C2-O21-C21	2.28	123.25	117.80
31	a	603	HEA	CHB-C1B-NB	2.28	126.87	124.42
24	N	402	HEM	C4A-CHB-C1B	-2.27	120.91	126.25
24	N	401	HEM	CHB-C1B-C2B	-2.25	120.55	126.95
31	a	604	HEA	C26-C15-C14	-2.24	117.88	123.63
24	C	402	HEM	CHB-C1B-C2B	-2.24	120.59	126.95
31	a	604	HEA	CAD-CBD-CGD	-2.23	107.75	113.67
31	a	604	HEA	C27-C19-C20	2.23	119.09	115.23
24	N	401	HEM	C1C-CHC-C4B	-2.22	121.31	126.02
24	N	401	HEM	C4A-CHB-C1B	-2.19	121.09	126.25
24	C	401	HEM	C1C-CHC-C4B	-2.19	121.37	126.02
31	a	603	HEA	C2B-C1B-NB	2.19	112.43	109.90
27	O	302	HEC	C2A-C1A-NA	-2.18	108.22	110.32
31	a	603	HEA	C4B-C3B-C2B	-2.18	103.78	107.44
31	a	603	HEA	C13-C14-C15	-2.16	122.67	127.62
24	C	401	HEM	C4A-CHB-C1B	-2.15	121.19	126.25
24	C	402	HEM	C4C-CHD-C1D	-2.15	121.46	126.02
31	a	604	HEA	C21-C22-C23	-2.14	120.49	127.64
27	D	302	HEC	CMC-C2C-C1C	-2.14	122.16	125.42
31	a	603	HEA	C25-C23-C24	2.13	119.48	114.59
31	a	604	HEA	C25-C23-C24	2.11	119.44	114.59
24	N	402	HEM	C2A-C1A-NA	-2.08	107.85	110.15
31	a	603	HEA	CHC-C1C-C2C	-2.07	121.41	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	N	401	HEM	C3B-C4B-NB	-2.05	108.00	109.47
27	D	302	HEC	CAA-CBA-CGA	-2.04	108.24	113.67
24	C	401	HEM	C3B-C4B-NB	-2.01	108.03	109.47

There are no chirality outliers.

All (254) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	C	401	HEM	C2B-C3B-CAB-CBB
24	C	401	HEM	C4B-C3B-CAB-CBB
24	C	401	HEM	C2C-C3C-CAC-CBC
24	C	401	HEM	C4C-C3C-CAC-CBC
24	C	402	HEM	C2B-C3B-CAB-CBB
24	C	402	HEM	C4B-C3B-CAB-CBB
24	C	402	HEM	C2C-C3C-CAC-CBC
24	C	402	HEM	C4C-C3C-CAC-CBC
24	N	401	HEM	C2B-C3B-CAB-CBB
24	N	401	HEM	C4B-C3B-CAB-CBB
24	N	401	HEM	C2C-C3C-CAC-CBC
24	N	401	HEM	C4C-C3C-CAC-CBC
24	N	402	HEM	C2B-C3B-CAB-CBB
24	N	402	HEM	C2C-C3C-CAC-CBC
24	N	402	HEM	C4C-C3C-CAC-CBC
25	C	403	3PE	C1-O11-P-O14
25	C	403	3PE	O13-C11-C12-N
25	F	201	3PE	C1-O11-P-O12
25	F	201	3PE	C1-O11-P-O13
25	F	201	3PE	C1-O11-P-O14
25	F	201	3PE	O13-C11-C12-N
25	F	202	3PE	C1-O11-P-O12
25	F	202	3PE	C1-O11-P-O13
25	F	202	3PE	O13-C11-C12-N
25	L	502	3PE	C1-O11-P-O13
25	L	502	3PE	C1-O11-P-O14
25	L	502	3PE	C11-O13-P-O11
25	L	502	3PE	C11-O13-P-O12
25	L	502	3PE	C11-O13-P-O14
25	N	403	3PE	C1-O11-P-O14
25	N	405	3PE	C1-O11-P-O13
25	N	405	3PE	C1-O11-P-O14
25	N	405	3PE	C11-O13-P-O11
25	N	405	3PE	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
25	N	405	3PE	O13-C11-C12-N
25	a	606	3PE	C1-O11-P-O12
25	a	606	3PE	C1-O11-P-O13
25	a	606	3PE	C1-O11-P-O14
25	a	606	3PE	O13-C11-C12-N
25	b	302	3PE	C1-O11-P-O12
25	b	302	3PE	C1-O11-P-O13
25	b	302	3PE	C11-O13-P-O11
25	b	302	3PE	C11-O13-P-O14
25	b	302	3PE	O13-C11-C12-N
25	b	304	3PE	C11-O13-P-O11
25	b	304	3PE	C11-O13-P-O12
25	c	301	3PE	O13-C11-C12-N
25	d	201	3PE	C1-O11-P-O12
25	d	201	3PE	C1-O11-P-O13
25	d	201	3PE	C1-O11-P-O14
25	d	201	3PE	C11-O13-P-O11
25	g	101	3PE	C11-O13-P-O11
25	g	101	3PE	C11-O13-P-O12
25	g	101	3PE	O13-C11-C12-N
25	k	101	3PE	C1-O11-P-O13
25	k	101	3PE	C2-C1-O11-P
25	k	101	3PE	O13-C11-C12-N
26	C	404	CDL	CB2-OB2-PB2-OB3
26	C	404	CDL	CB2-OB2-PB2-OB4
26	C	404	CDL	CB2-OB2-PB2-OB5
26	C	404	CDL	CB3-OB5-PB2-OB2
26	C	404	CDL	CB3-OB5-PB2-OB3
26	D	301	CDL	CA2-OA2-PA1-OA5
26	D	301	CDL	CB2-OB2-PB2-OB3
26	D	301	CDL	CB2-OB2-PB2-OB5
26	D	301	CDL	CB3-OB5-PB2-OB2
26	D	301	CDL	CB3-OB5-PB2-OB3
26	D	301	CDL	CB3-OB5-PB2-OB4
26	L	503	CDL	CA2-OA2-PA1-OA3
26	L	503	CDL	CA2-OA2-PA1-OA4
26	L	503	CDL	CA2-OA2-PA1-OA5
26	L	503	CDL	CB3-OB5-PB2-OB2
26	L	503	CDL	CB3-OB5-PB2-OB3
26	N	404	CDL	CA2-OA2-PA1-OA4
26	N	404	CDL	CA2-OA2-PA1-OA5
26	N	404	CDL	CB2-OB2-PB2-OB3

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Mol	Chain	Res	Type	Atoms
26	O	301	CDL	CA3-OA5-PA1-OA3
26	O	301	CDL	CB2-OB2-PB2-OB3
26	O	301	CDL	CB2-OB2-PB2-OB5
26	O	301	CDL	OB5-CB3-CB4-OB6
27	D	302	HEC	C2C-C3C-CAC-CBC
27	O	302	HEC	C2C-C3C-CAC-CBC
28	L	501	PC1	C11-O13-P-O12
28	L	501	PC1	C11-O13-P-O11
28	L	501	PC1	C1-O11-P-O14
28	a	605	PC1	C11-O13-P-O14
28	a	605	PC1	C11-O13-P-O11
28	a	605	PC1	C1-O11-P-O14
31	a	603	HEA	C2A-C3A-CMA-OMA
31	a	603	HEA	C4A-C3A-CMA-OMA
31	a	604	HEA	C2A-C3A-CMA-OMA
31	a	603	HEA	C15-C16-C17-C18
31	a	604	HEA	C15-C16-C17-C18
26	O	301	CDL	C1-CA2-OA2-PA1
25	a	606	3PE	C2-C1-O11-P
26	L	503	CDL	C33-C34-C35-C36
35	l	601	TGL	CC3-CC4-CC5-CC6
25	N	405	3PE	C3B-C3C-C3D-C3E
28	a	605	PC1	C28-C29-C2A-C2B
31	a	603	HEA	C1A-C2A-CAA-CBA
25	F	202	3PE	C36-C37-C38-C39
25	d	201	3PE	C22-C23-C24-C25
31	a	604	HEA	C19-C20-C21-C22
24	N	402	HEM	C4B-C3B-CAB-CBB
24	N	401	HEM	C2A-CAA-CBA-CGA
26	O	301	CDL	CB2-C1-CA2-OA2
25	N	405	3PE	C33-C34-C35-C36
25	a	606	3PE	O11-C1-C2-C3
26	C	404	CDL	OB5-CB3-CB4-CB6
26	O	301	CDL	OB5-CB3-CB4-CB6
25	F	202	3PE	C32-C33-C34-C35
25	C	403	3PE	C1-C2-C3-O31
25	N	405	3PE	C3D-C3E-C3F-C3G
31	a	603	HEA	C11-C12-C13-C14
31	a	603	HEA	C3A-C2A-CAA-CBA
25	a	606	3PE	O11-C1-C2-O21
26	C	404	CDL	OB5-CB3-CB4-OB6
25	C	403	3PE	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
25	c	301	3PE	C23-C24-C25-C26
31	a	604	HEA	C1A-C2A-CAA-CBA
25	L	502	3PE	C32-C33-C34-C35
25	k	101	3PE	C21-C22-C23-C24
25	F	202	3PE	C1-C2-C3-O31
26	N	404	CDL	OB5-CB3-CB4-OB6
26	O	301	CDL	C1-CB2-OB2-PB2
35	l	601	TGL	OG2-CB1-CB2-CB3
25	C	403	3PE	O21-C2-C3-O31
26	L	503	CDL	OB5-CB3-CB4-CB6
24	N	402	HEM	C2A-CAA-CBA-CGA
26	O	301	CDL	O1-C1-CA2-OA2
26	L	503	CDL	OB5-CB3-CB4-OB6
26	N	404	CDL	OA5-CA3-CA4-OA6
31	a	603	HEA	O11-C11-C12-C13
25	b	304	3PE	O21-C2-C3-O31
25	c	301	3PE	C31-C32-C33-C34
28	L	501	PC1	O13-C11-C12-N
28	a	605	PC1	O13-C11-C12-N
25	a	606	3PE	C22-C23-C24-C25
25	g	101	3PE	O11-C1-C2-C3
26	N	404	CDL	OB5-CB3-CB4-CB6
26	D	301	CDL	C73-C74-C75-C76
25	N	405	3PE	C2-C1-O11-P
27	D	302	HEC	C4B-C3B-CAB-CBB
27	D	302	HEC	C4C-C3C-CAC-CBC
27	O	302	HEC	C4B-C3B-CAB-CBB
31	a	604	HEA	C4A-C3A-CMA-OMA
26	C	404	CDL	C12-C11-CA5-OA7
25	F	202	3PE	O21-C2-C3-O31
25	b	302	3PE	O21-C2-C3-O31
26	O	301	CDL	OA6-CA4-CA6-OA8
25	b	302	3PE	C1-C2-C3-O31
25	F	202	3PE	C11-O13-P-O14
25	L	502	3PE	C1-O11-P-O12
25	N	405	3PE	C1-O11-P-O12
25	N	405	3PE	C11-O13-P-O12
25	a	606	3PE	C11-O13-P-O14
25	b	304	3PE	C11-O13-P-O14
25	c	301	3PE	C11-O13-P-O14
25	d	201	3PE	C11-O13-P-O14
25	g	101	3PE	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
25	k	101	3PE	C1-O11-P-O14
26	D	301	CDL	CA2-OA2-PA1-OA3
26	D	301	CDL	CA3-OA5-PA1-OA2
26	D	301	CDL	CA3-OA5-PA1-OA3
26	D	301	CDL	CA3-OA5-PA1-OA4
26	D	301	CDL	CB2-OB2-PB2-OB4
26	L	503	CDL	CA3-OA5-PA1-OA2
26	L	503	CDL	CA3-OA5-PA1-OA3
26	L	503	CDL	CA3-OA5-PA1-OA4
26	O	301	CDL	CA2-OA2-PA1-OA3
26	O	301	CDL	CA2-OA2-PA1-OA4
26	O	301	CDL	CA2-OA2-PA1-OA5
26	O	301	CDL	CB2-OB2-PB2-OB4
27	D	302	HEC	C2B-C3B-CAB-CBB
27	O	302	HEC	C2B-C3B-CAB-CBB
28	L	501	PC1	C11-O13-P-O14
28	L	501	PC1	C1-O11-P-O13
25	c	301	3PE	C2-C1-O11-P
25	g	101	3PE	C2-C1-O11-P
26	C	404	CDL	C1-CB2-OB2-PB2
26	L	503	CDL	C1-CA2-OA2-PA1
26	L	503	CDL	C1-CB2-OB2-PB2
26	O	301	CDL	CB4-CB3-OB5-PB2
28	L	501	PC1	C2-C1-O11-P
26	D	301	CDL	C71-C72-C73-C74
26	D	301	CDL	C1-CA2-OA2-PA1
31	a	604	HEA	C3A-C2A-CAA-CBA
25	N	405	3PE	C32-C33-C34-C35
26	C	404	CDL	C12-C11-CA5-OA6
31	a	604	HEA	CAD-CBD-CGD-O1D
31	a	604	HEA	CAD-CBD-CGD-O2D
24	C	401	HEM	C2A-CAA-CBA-CGA
31	a	603	HEA	CAD-CBD-CGD-O1D
31	a	603	HEA	CAD-CBD-CGD-O2D
26	L	503	CDL	C32-C33-C34-C35
24	N	401	HEM	CAD-CBD-CGD-O1D
24	N	402	HEM	CAD-CBD-CGD-O1D
24	N	402	HEM	CAD-CBD-CGD-O2D
26	N	404	CDL	C52-C51-CB5-OB6
26	D	301	CDL	O1-C1-CA2-OA2
26	N	404	CDL	CA4-CA3-OA5-PA1
24	C	402	HEM	C3D-CAD-CBD-CGD

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Mol	Chain	Res	Type	Atoms
24	N	401	HEM	CAD-CBD-CGD-O2D
24	N	402	HEM	CAA-CBA-CGA-O2A
26	D	301	CDL	C72-C73-C74-C75
25	g	101	3PE	O31-C31-C32-C33
24	C	402	HEM	CAA-CBA-CGA-O2A
25	C	403	3PE	C27-C28-C29-C2A
24	N	402	HEM	CAA-CBA-CGA-O1A
24	N	402	HEM	C3D-CAD-CBD-CGD
25	F	202	3PE	O11-C1-C2-O21
24	C	401	HEM	CAD-CBD-CGD-O1D
35	l	601	TGL	OB1-CB1-CB2-CB3
26	N	404	CDL	OA5-CA3-CA4-CA6
25	k	101	3PE	O21-C2-C3-O31
24	C	402	HEM	CAA-CBA-CGA-O1A
26	N	404	CDL	C52-C51-CB5-OB7
35	l	601	TGL	OG1-CA1-CA2-CA3
26	D	301	CDL	C52-C51-CB5-OB6
25	g	101	3PE	C3-C2-O21-C21
25	N	403	3PE	C27-C28-C29-C2A
26	C	404	CDL	C32-C31-CA7-OA8
31	a	603	HEA	CAA-CBA-CGA-O1A
25	g	101	3PE	O11-C1-C2-O21
25	F	201	3PE	C1-C2-C3-O31
25	a	606	3PE	C1-C2-C3-O31
25	b	304	3PE	C1-C2-C3-O31
26	O	301	CDL	C72-C71-CB7-OB8
25	C	403	3PE	C24-C25-C26-C27
25	a	606	3PE	O21-C2-C3-O31
25	N	405	3PE	C2B-C2C-C2D-C2E
25	d	201	3PE	C31-C32-C33-C34
31	a	603	HEA	C27-C19-C20-C21
25	N	403	3PE	O31-C31-C32-C33
28	a	605	PC1	C27-C28-C29-C2A
25	C	403	3PE	O31-C31-C32-C33
24	C	401	HEM	CAD-CBD-CGD-O2D
25	L	502	3PE	O31-C31-C32-C33
26	O	301	CDL	C52-C51-CB5-OB6
25	d	201	3PE	C1-C2-O21-C21
28	L	501	PC1	C1-C2-O21-C21
25	b	304	3PE	O31-C31-C32-C33
26	N	404	CDL	C12-C11-CA5-OA6
25	C	403	3PE	O32-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
26	D	301	CDL	C1-CB2-OB2-PB2
31	a	603	HEA	CAA-CBA-CGA-O2A
27	O	302	HEC	C4C-C3C-CAC-CBC
28	a	605	PC1	C22-C23-C24-C25
25	L	502	3PE	O32-C31-C32-C33
25	N	403	3PE	O32-C31-C32-C33
26	O	301	CDL	C72-C71-CB7-OB9
25	c	301	3PE	C21-C22-C23-C24
26	O	301	CDL	C52-C51-CB5-OB7
25	c	301	3PE	C32-C33-C34-C35

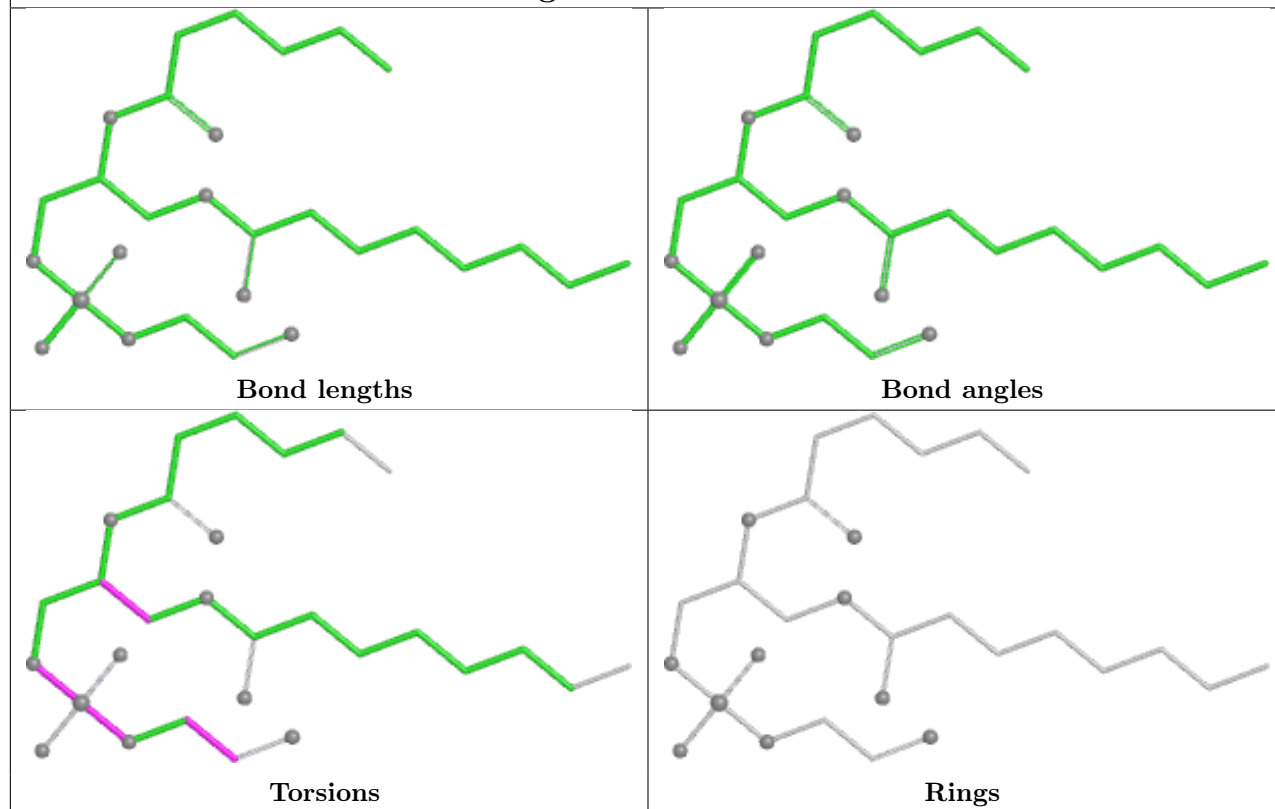
There are no ring outliers.

14 monomers are involved in 23 short contacts:

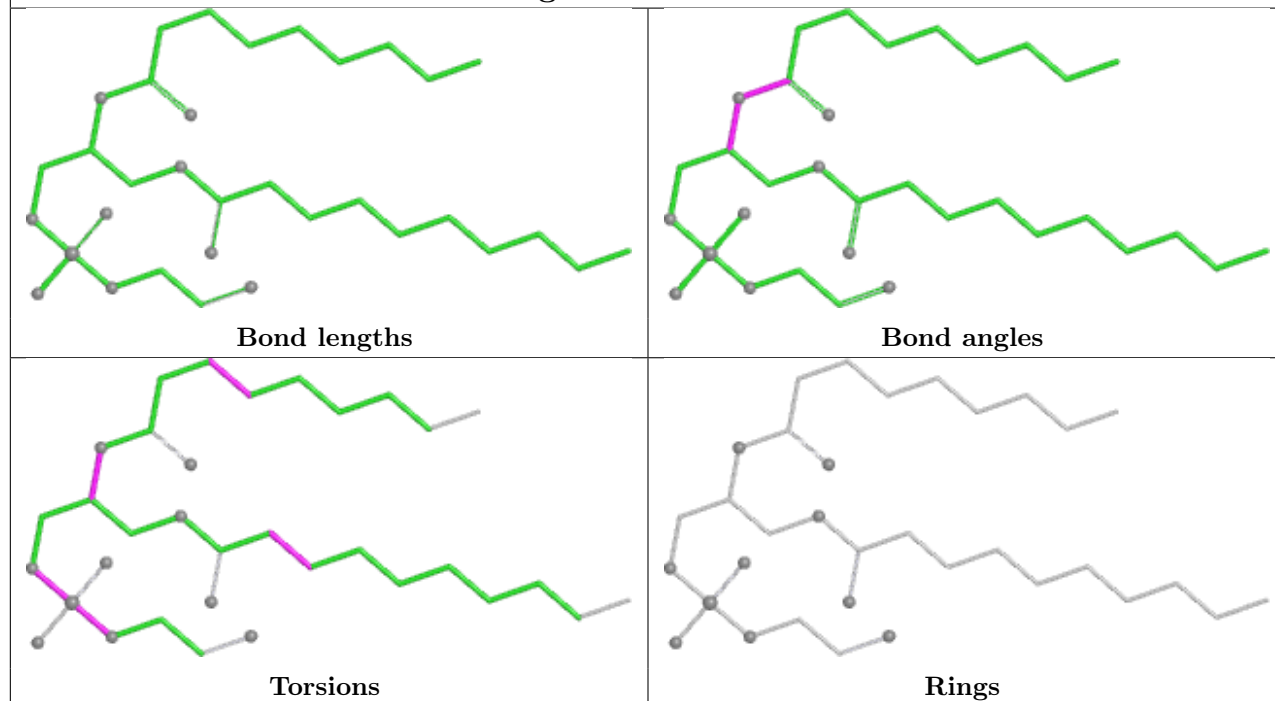
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	d	201	3PE	1	0
26	O	301	CDL	2	0
25	N	405	3PE	3	0
24	N	402	HEM	1	0
25	k	101	3PE	2	0
25	F	201	3PE	1	0
31	a	604	HEA	1	0
26	D	301	CDL	2	0
31	a	603	HEA	2	0
24	C	402	HEM	1	0
25	g	101	3PE	3	0
25	c	301	3PE	2	0
24	C	401	HEM	1	0
24	N	401	HEM	1	0

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.

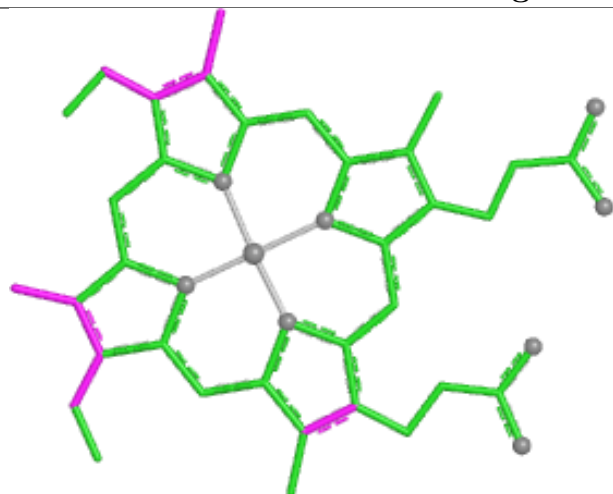
Ligand 3PE b 302



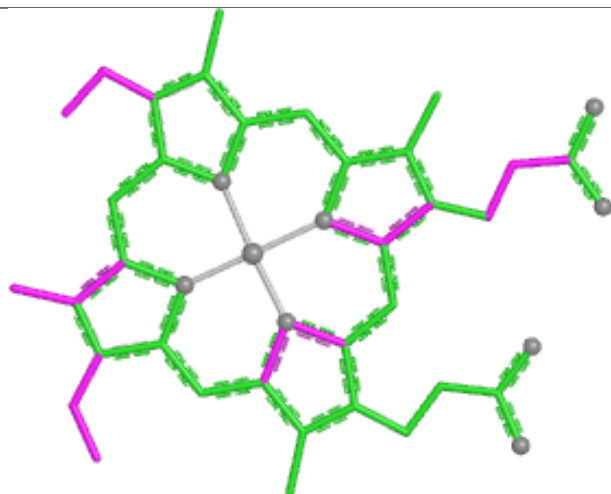
Ligand 3PE d 201



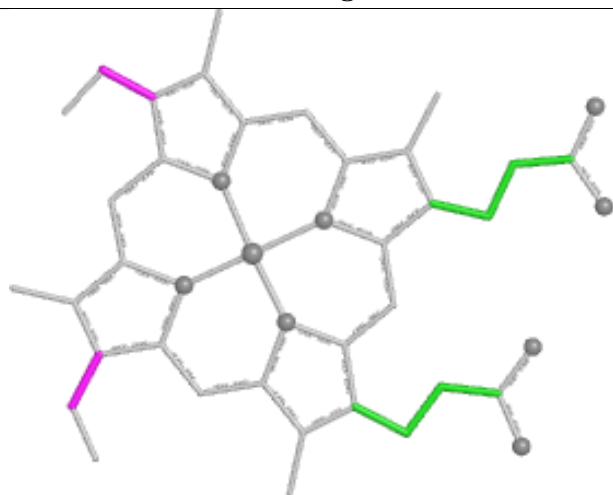
Ligand HEC D 302



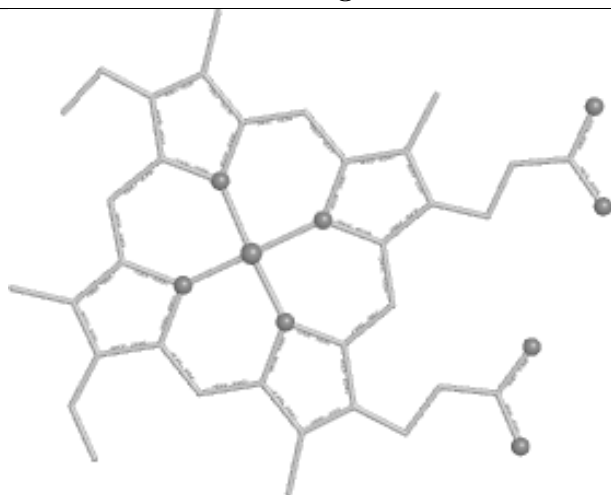
Bond lengths



Bond angles

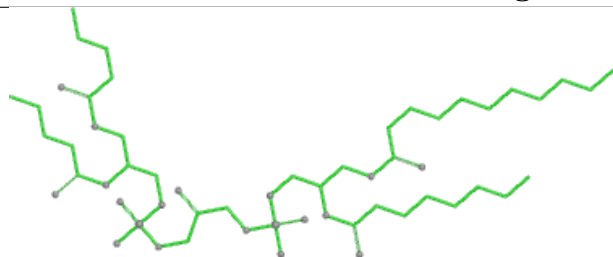


Torsions

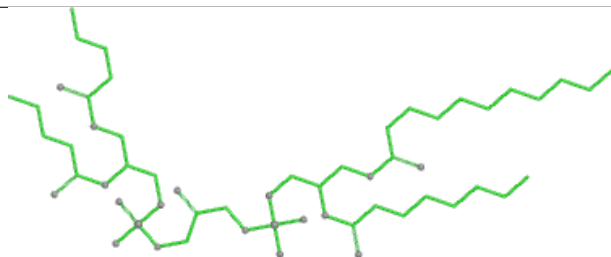


Rings

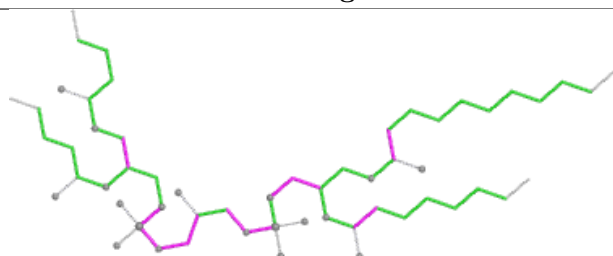
Ligand CDL O 301



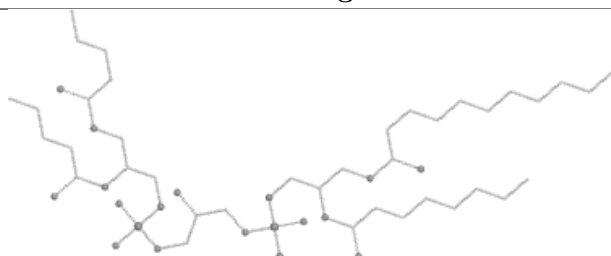
Bond lengths



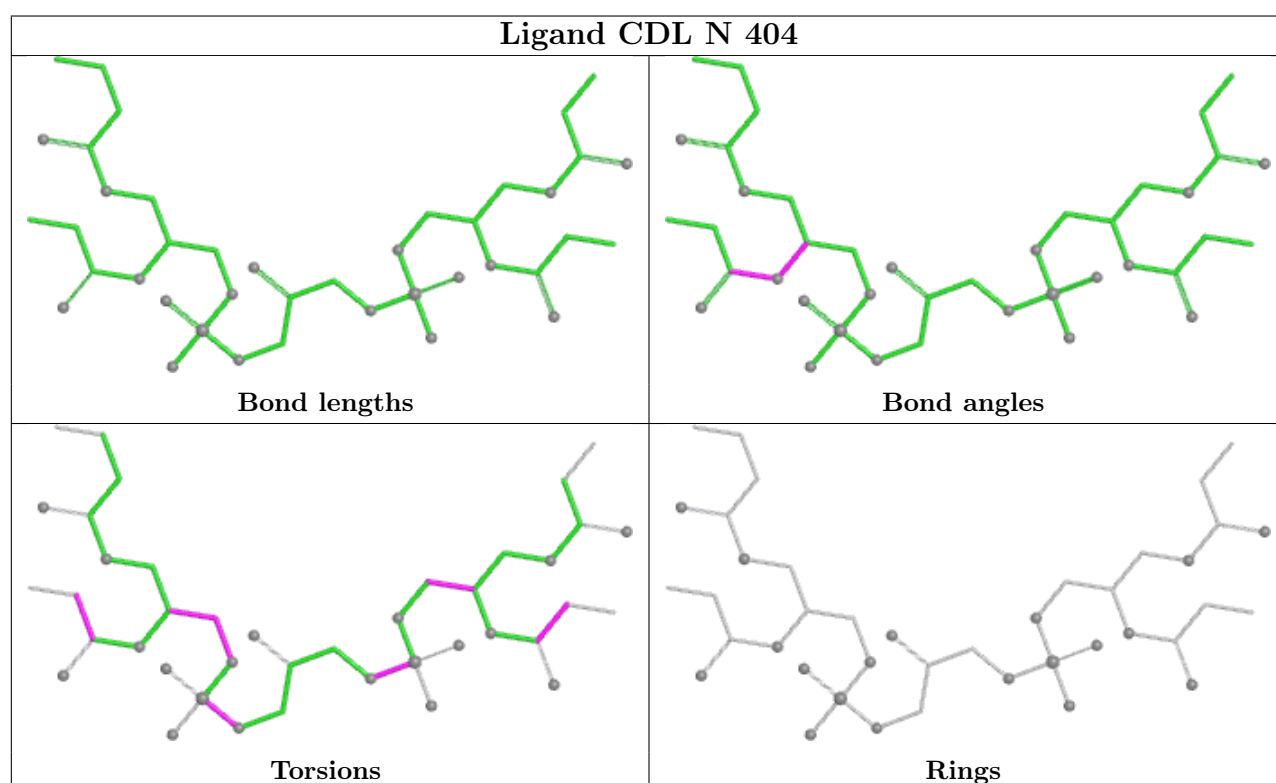
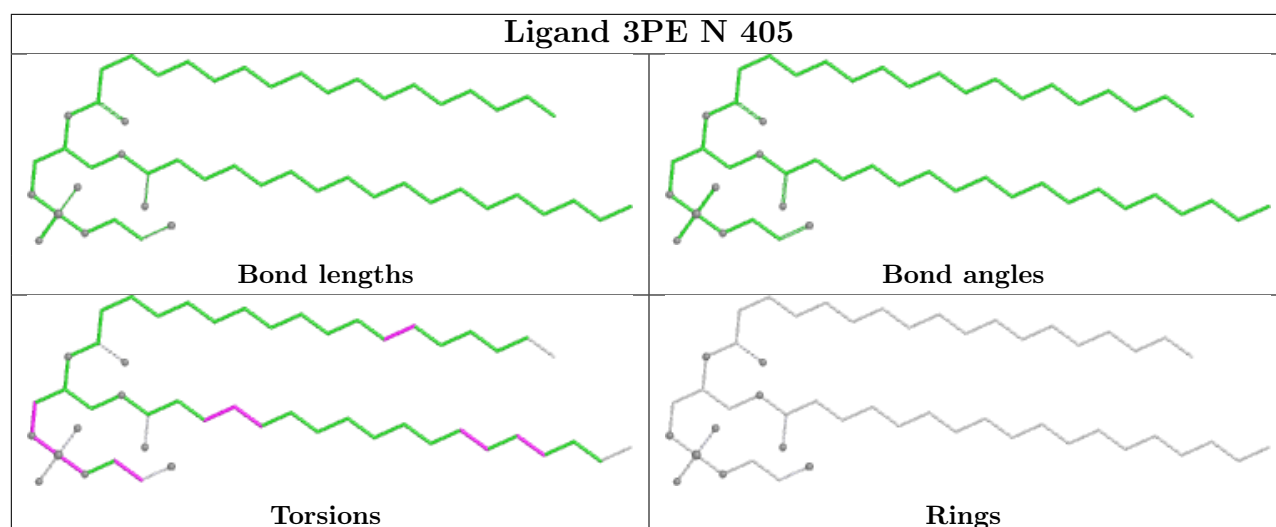
Bond angles

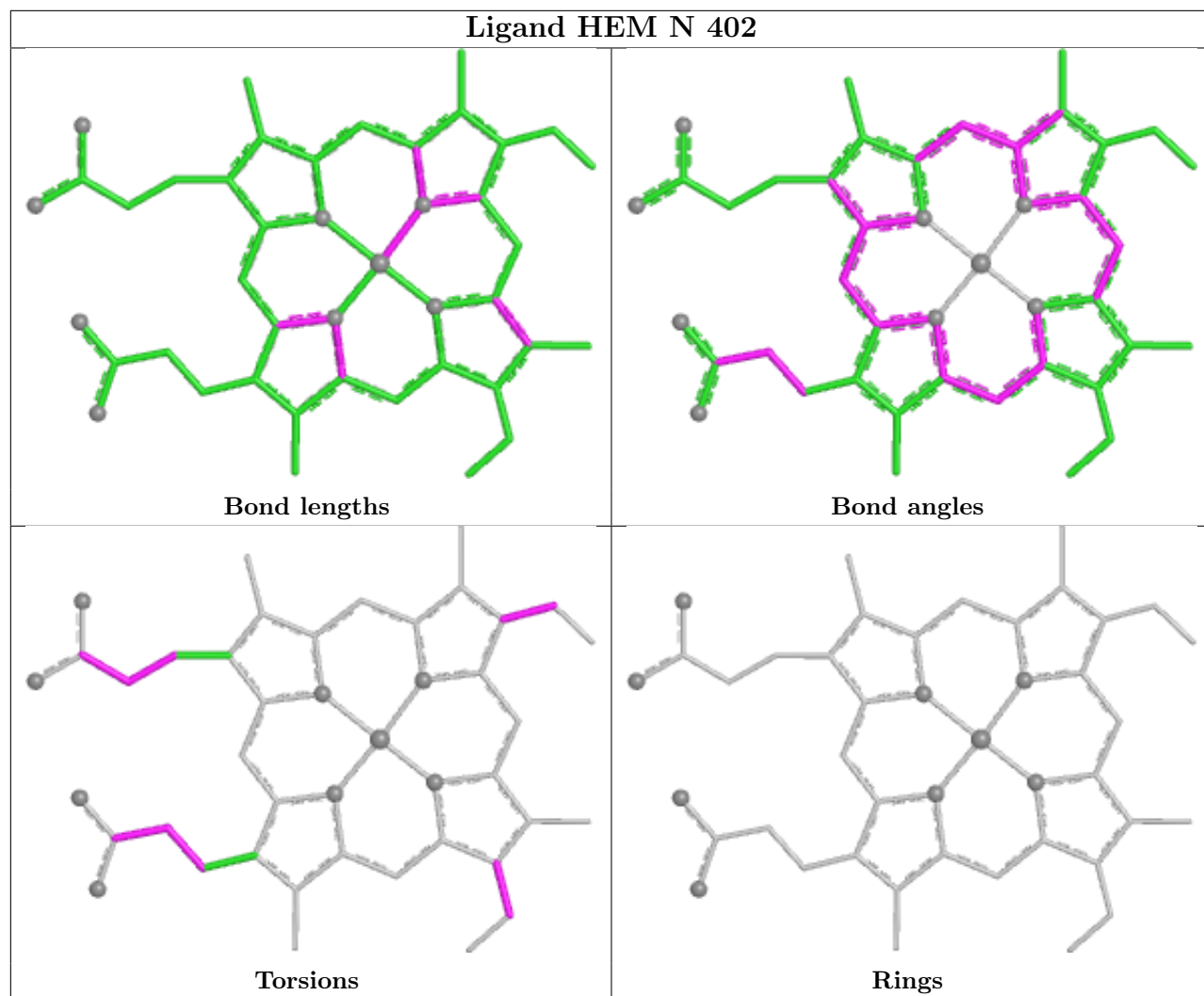


Torsions

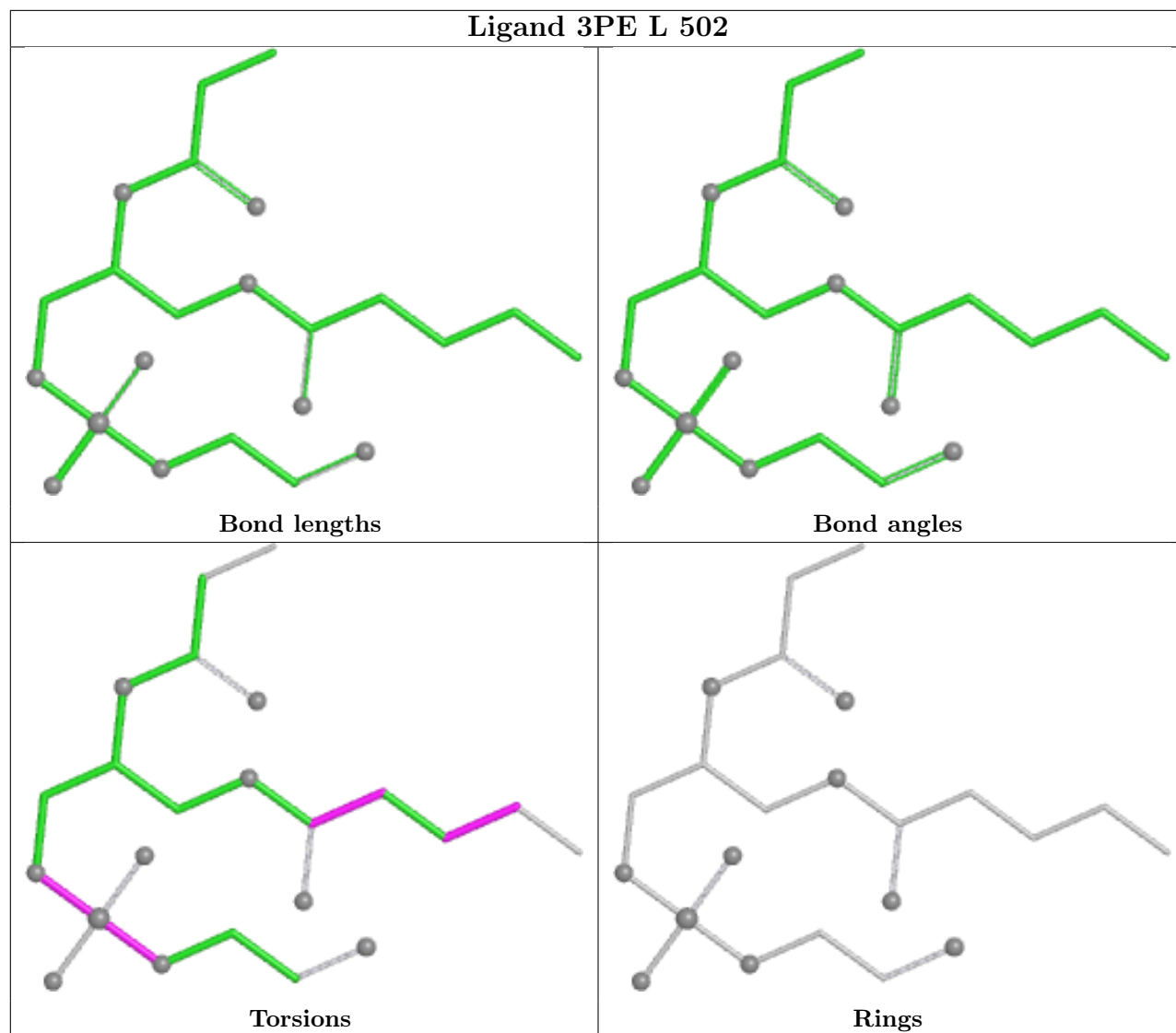


Rings

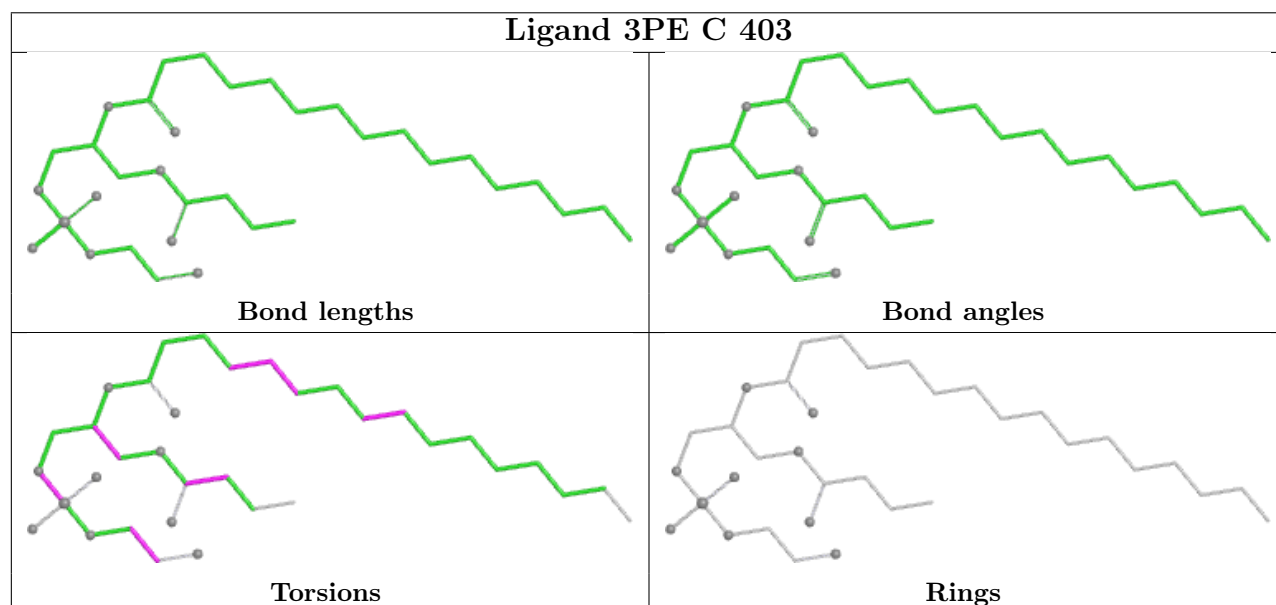


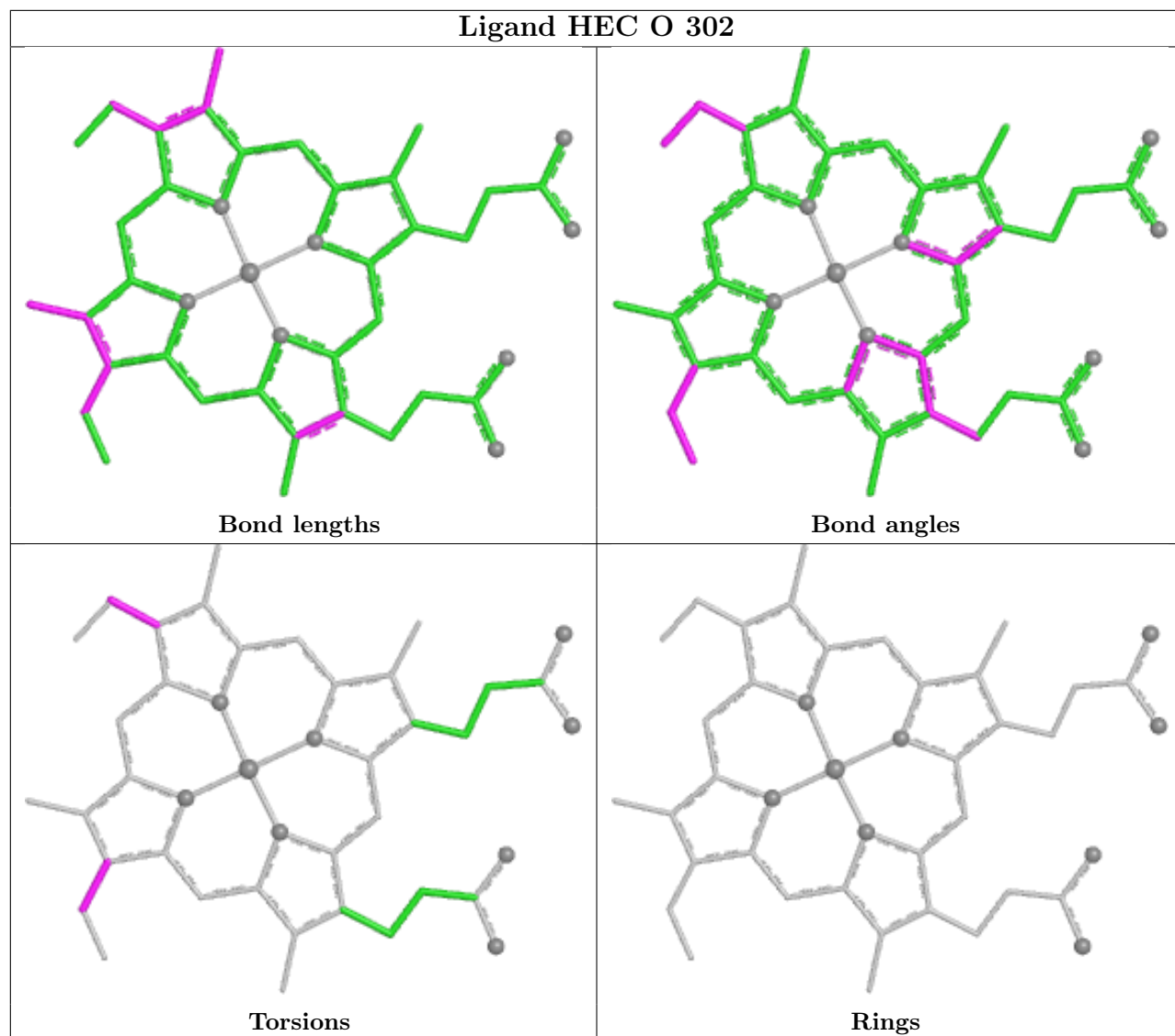


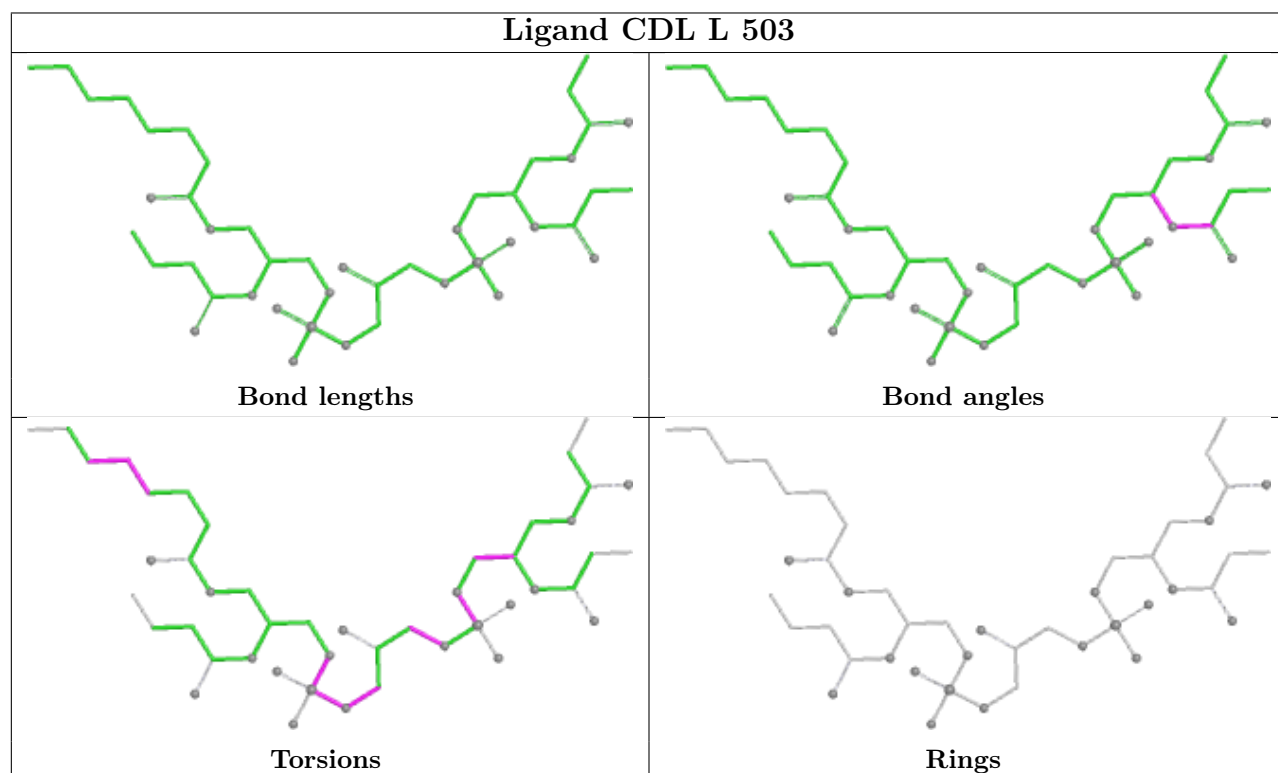
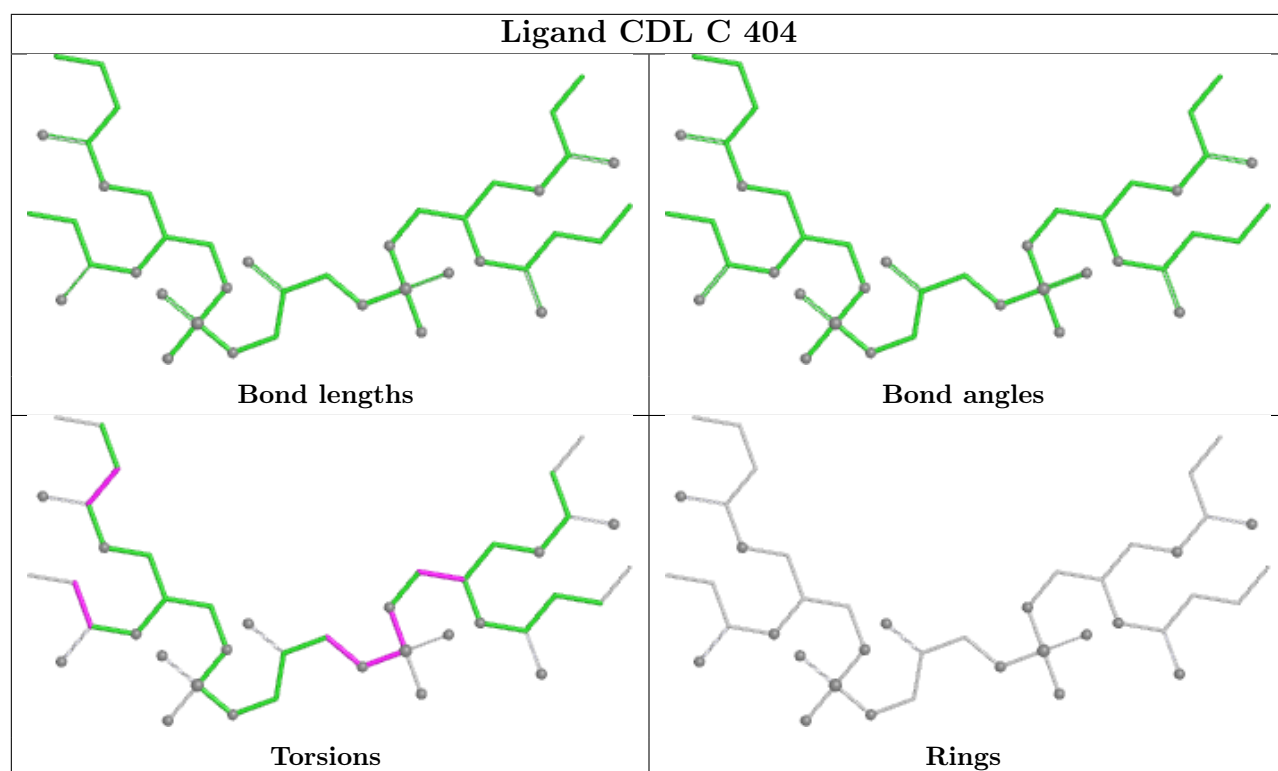
Ligand 3PE L 502



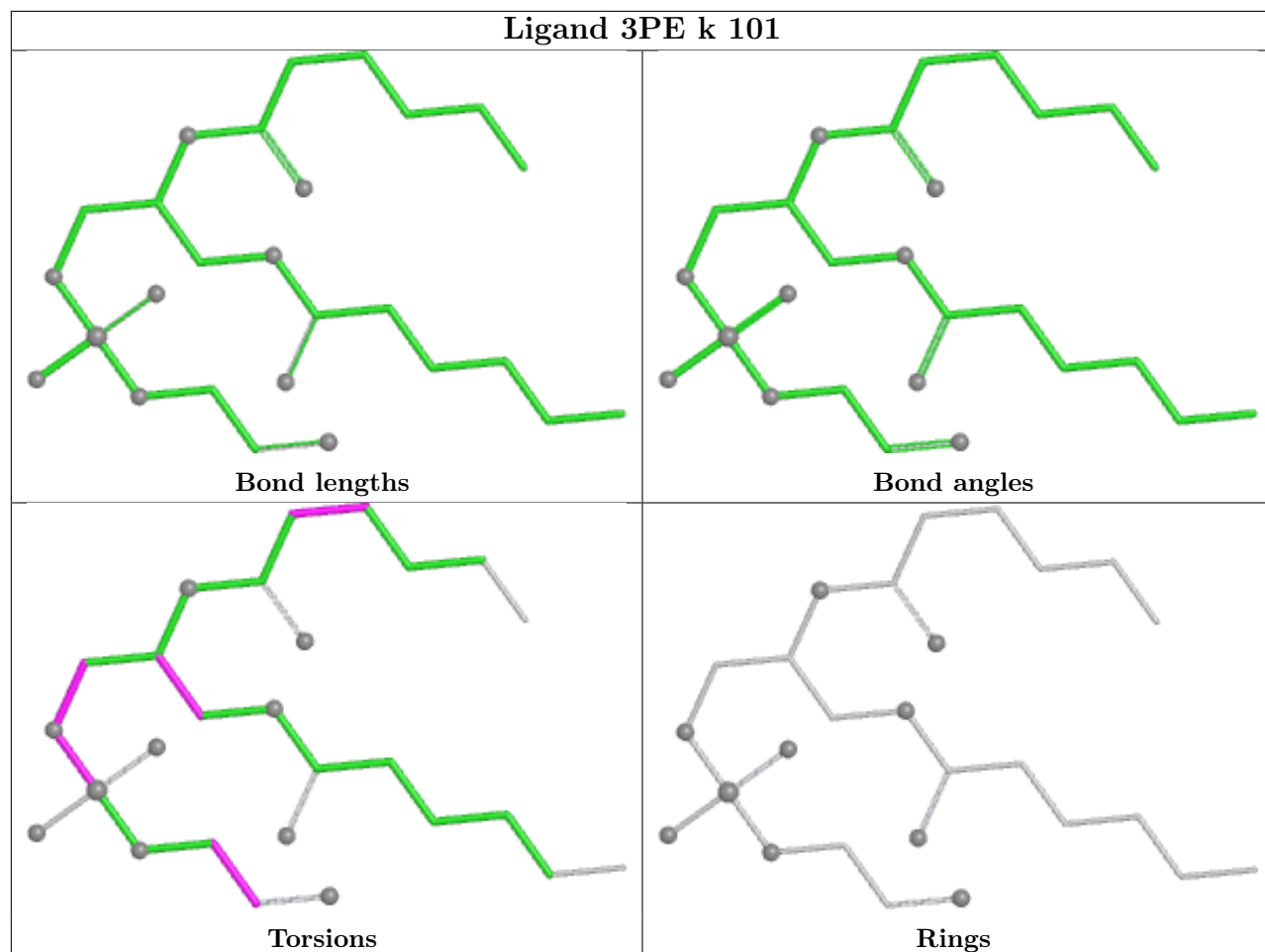
Ligand 3PE C 403



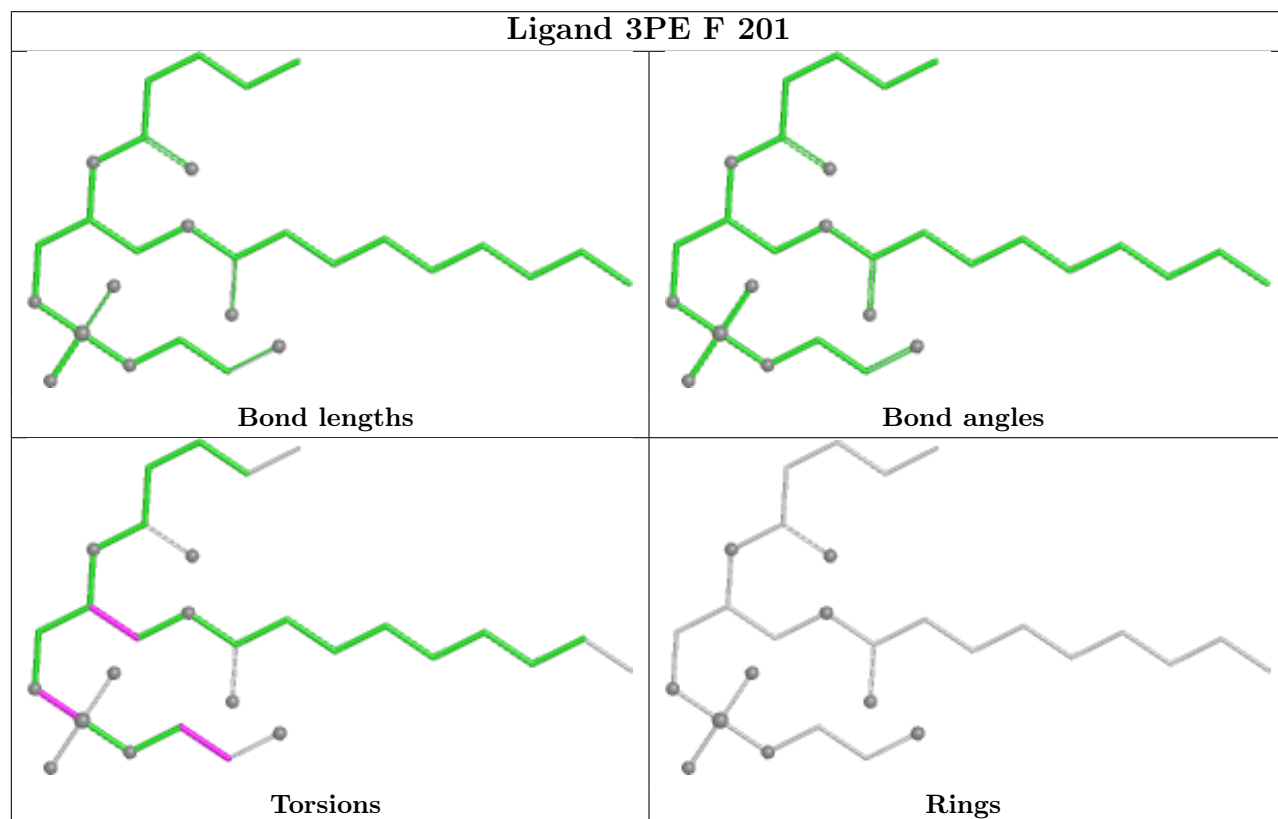


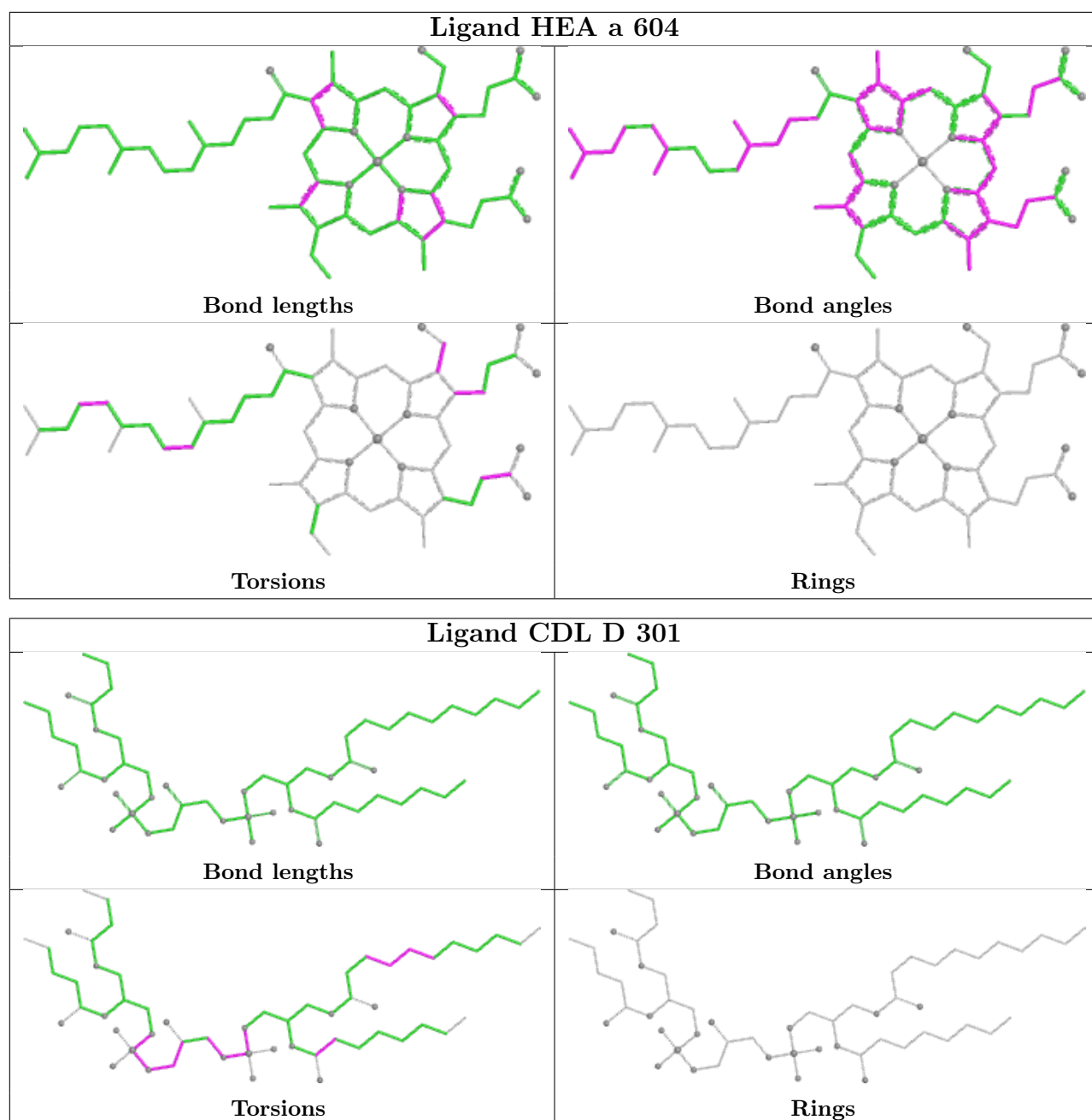


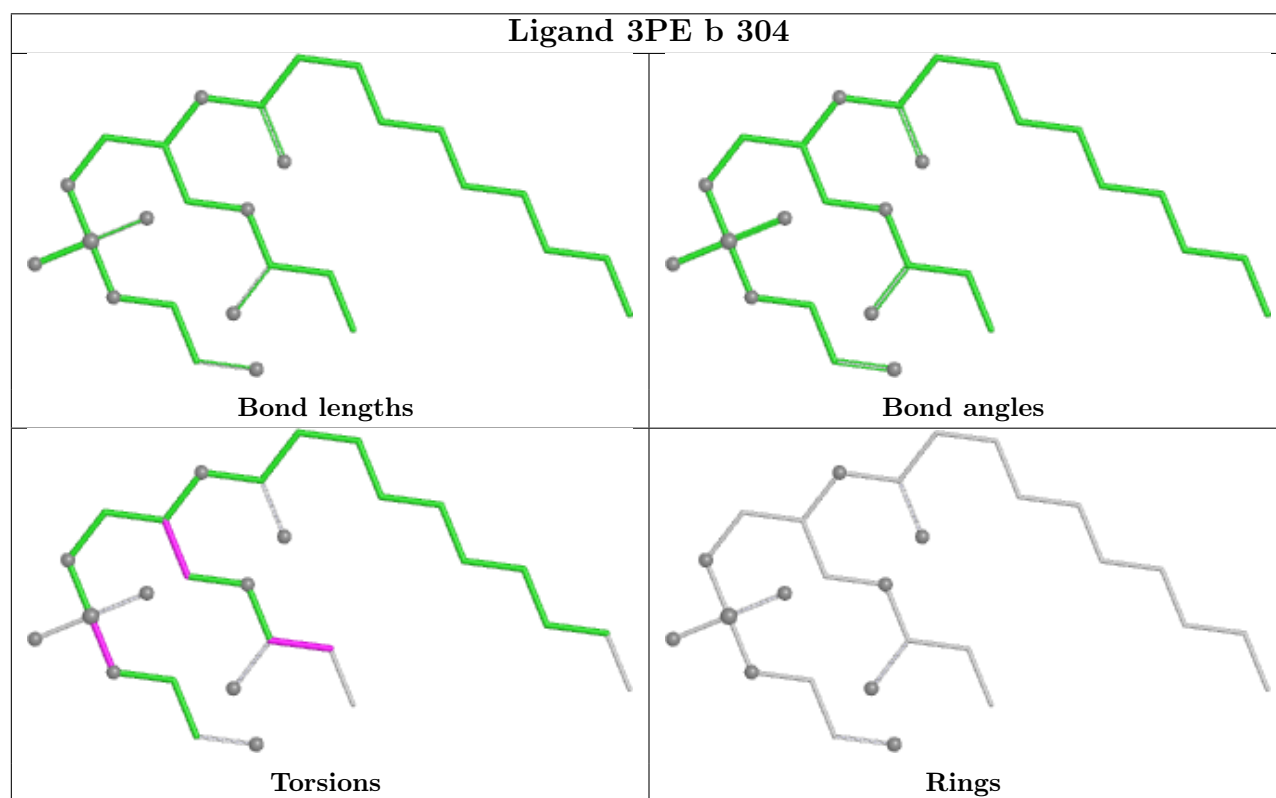
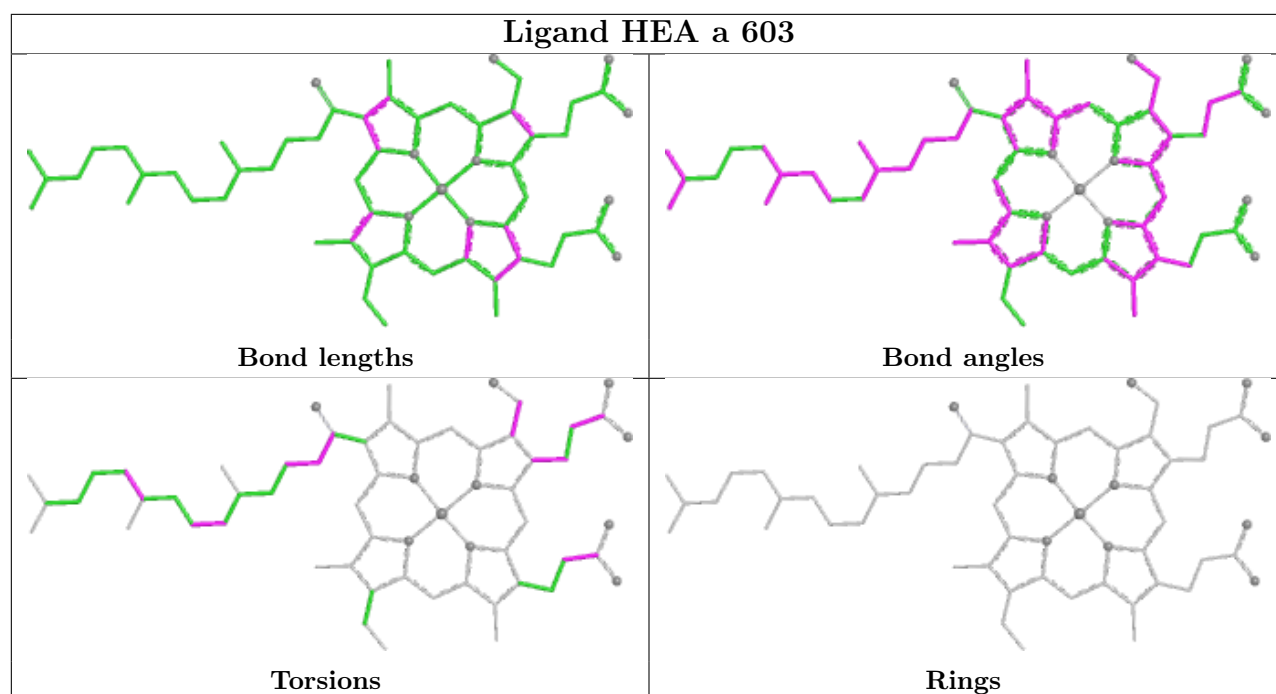
Ligand 3PE k 101



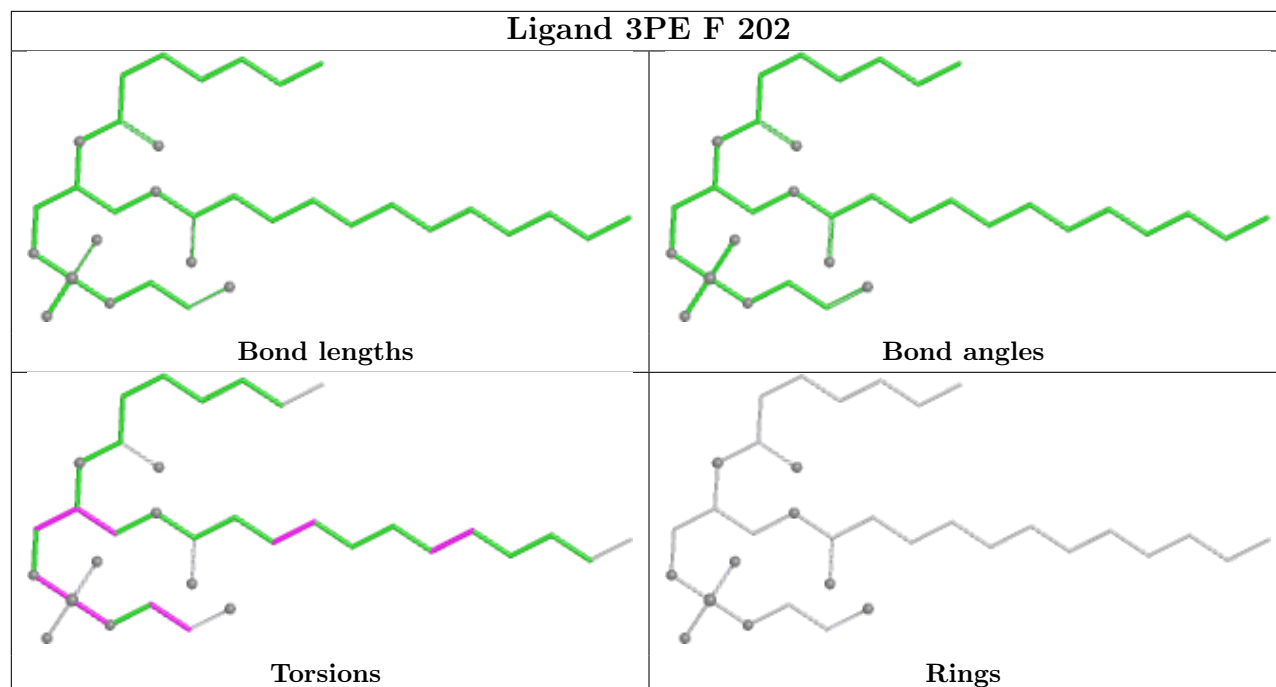
Ligand 3PE F 201



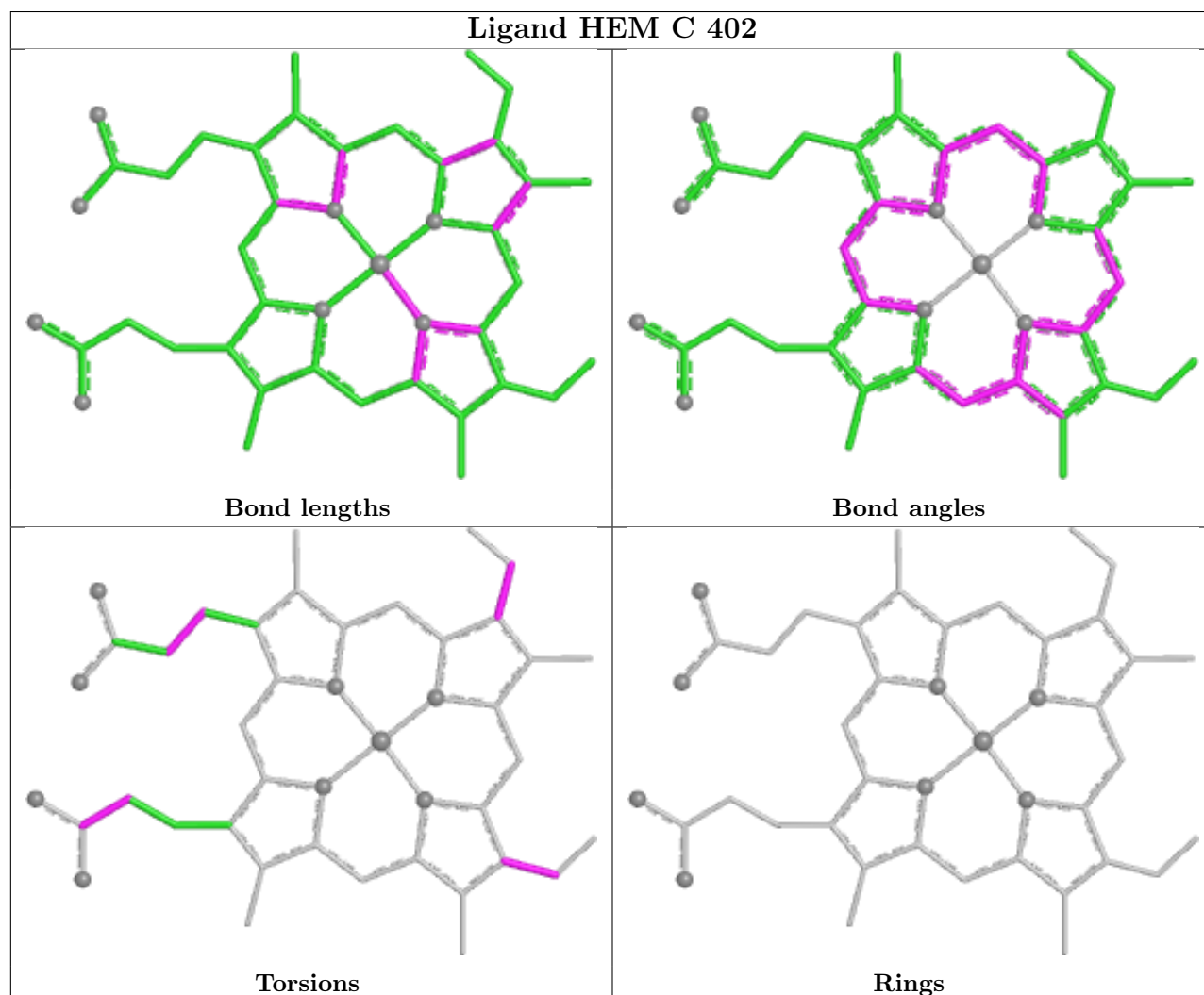


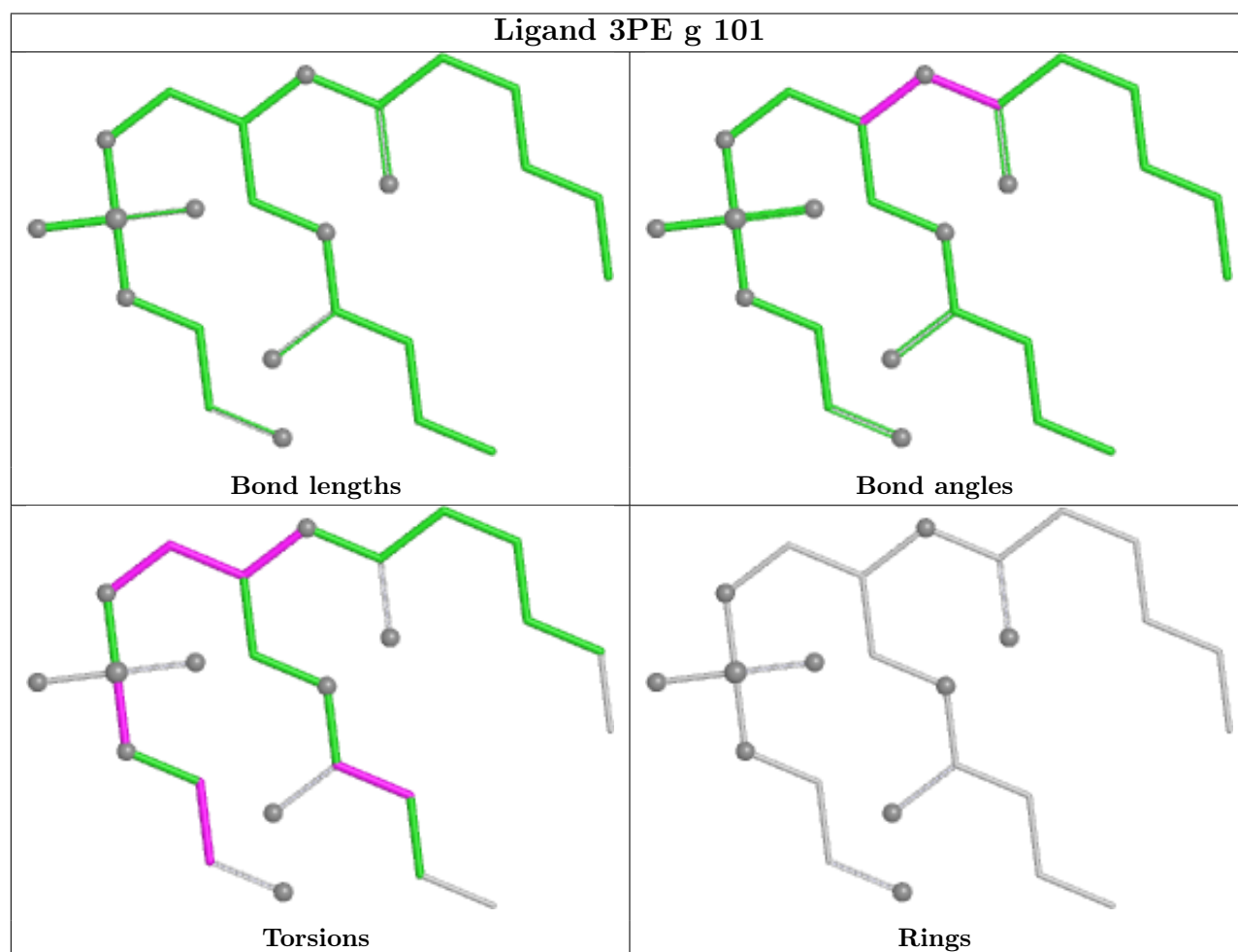
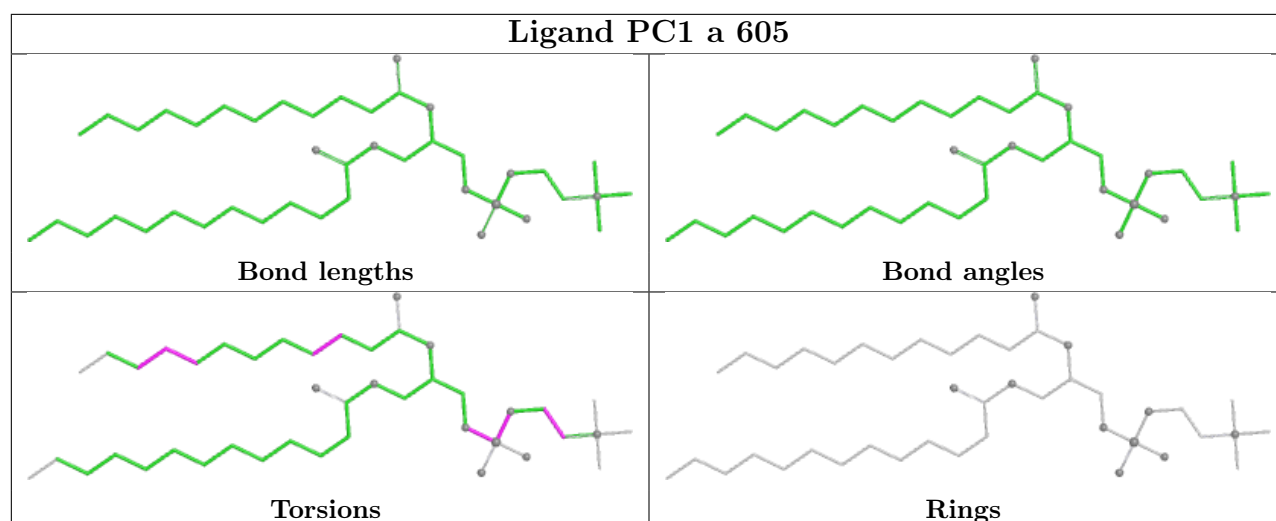


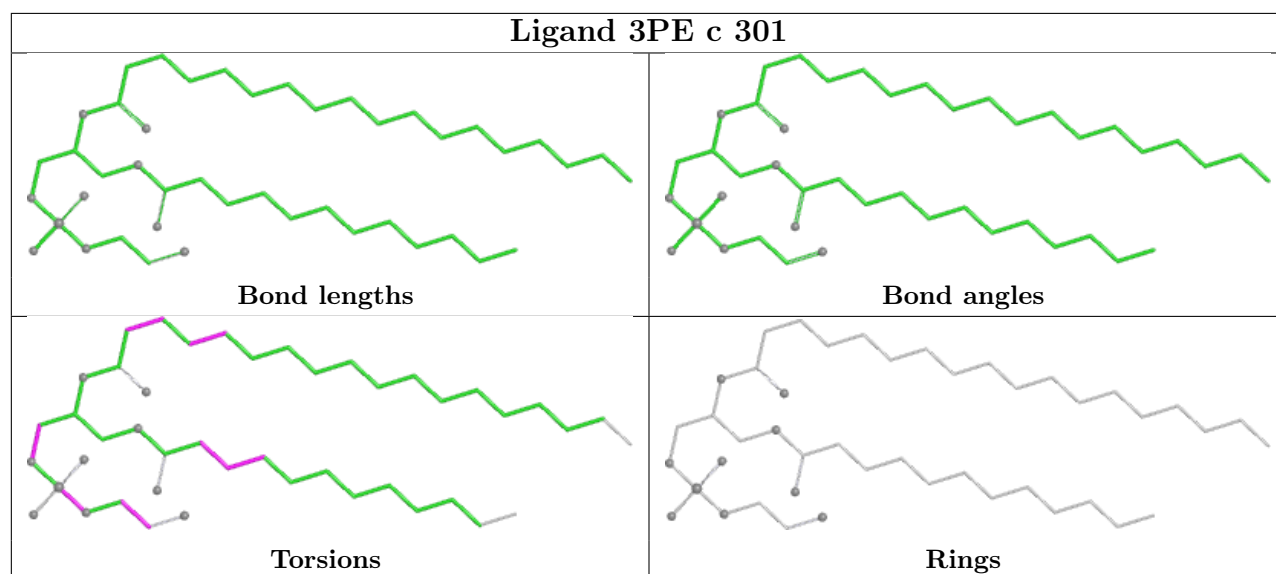
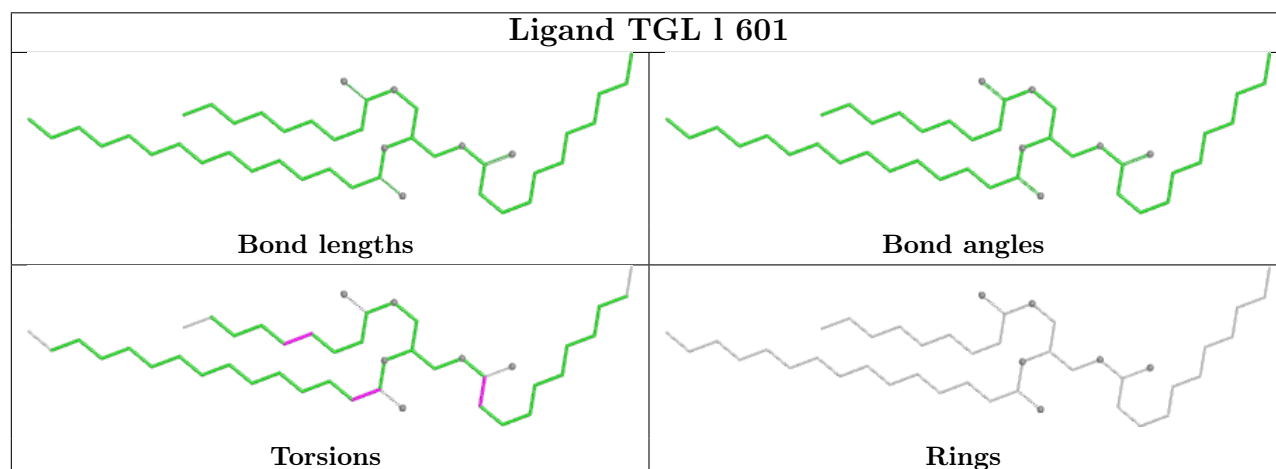
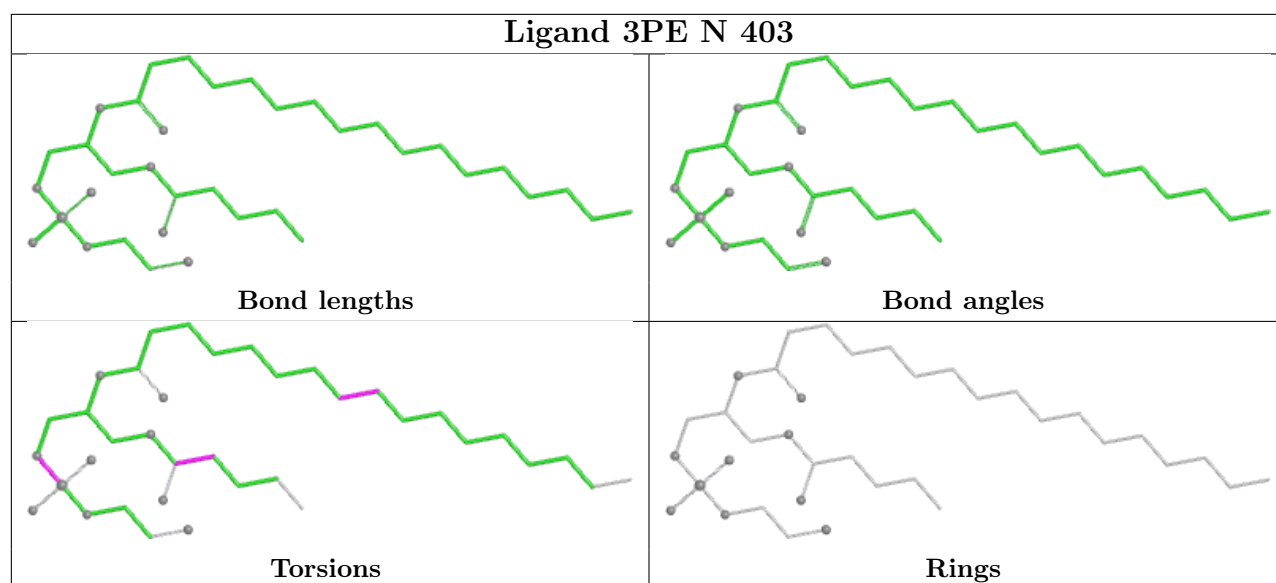
Ligand 3PE F 202

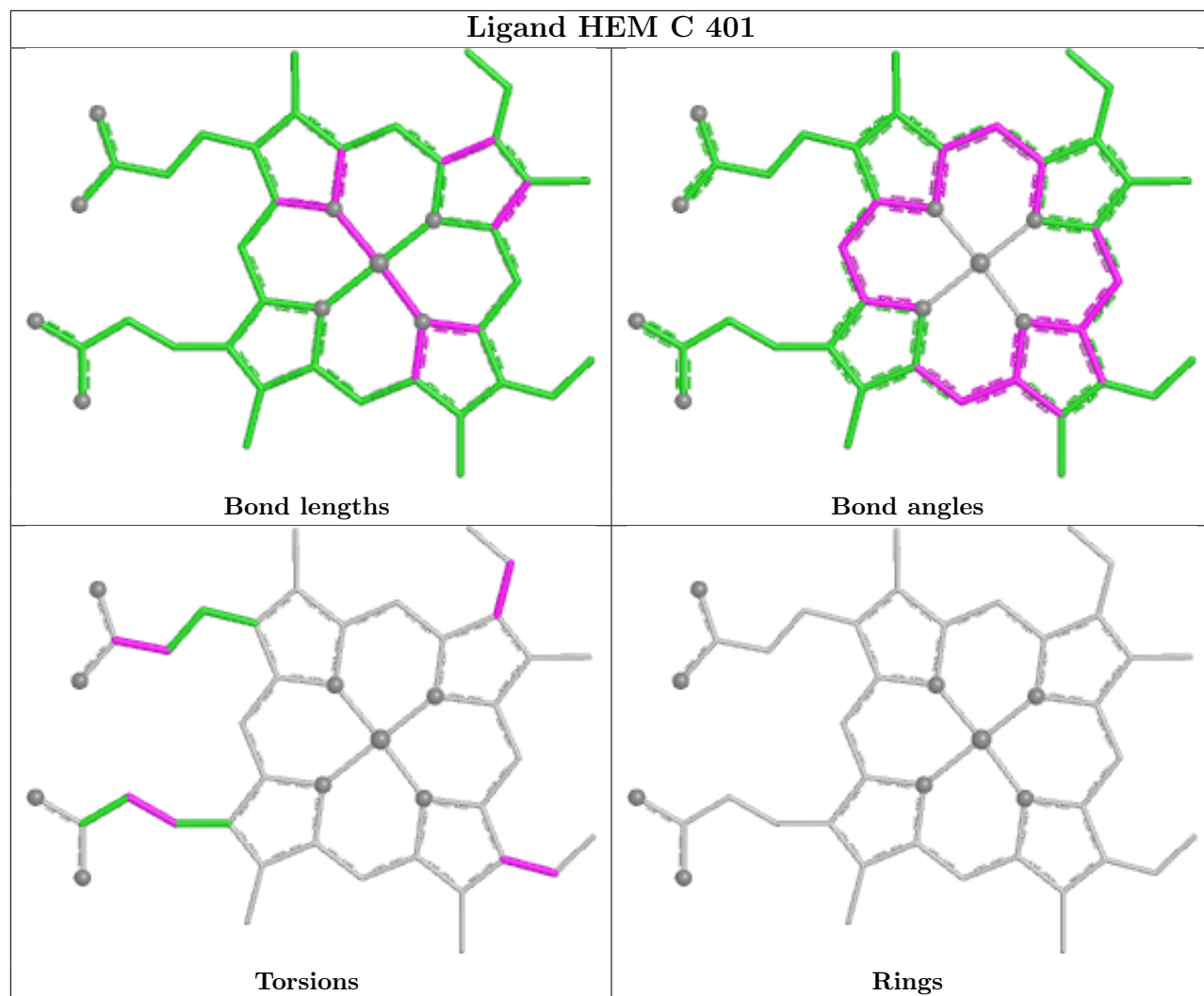


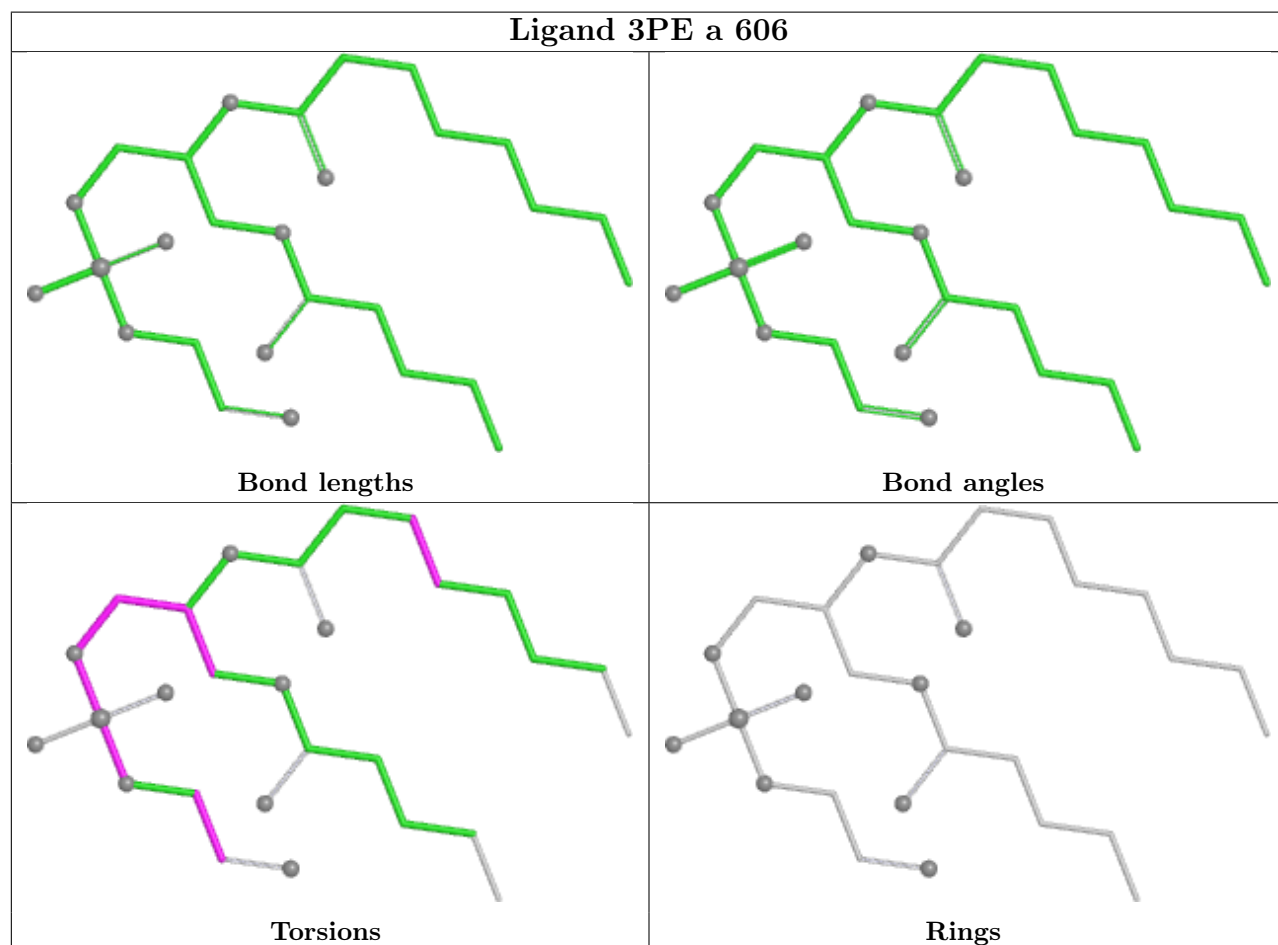
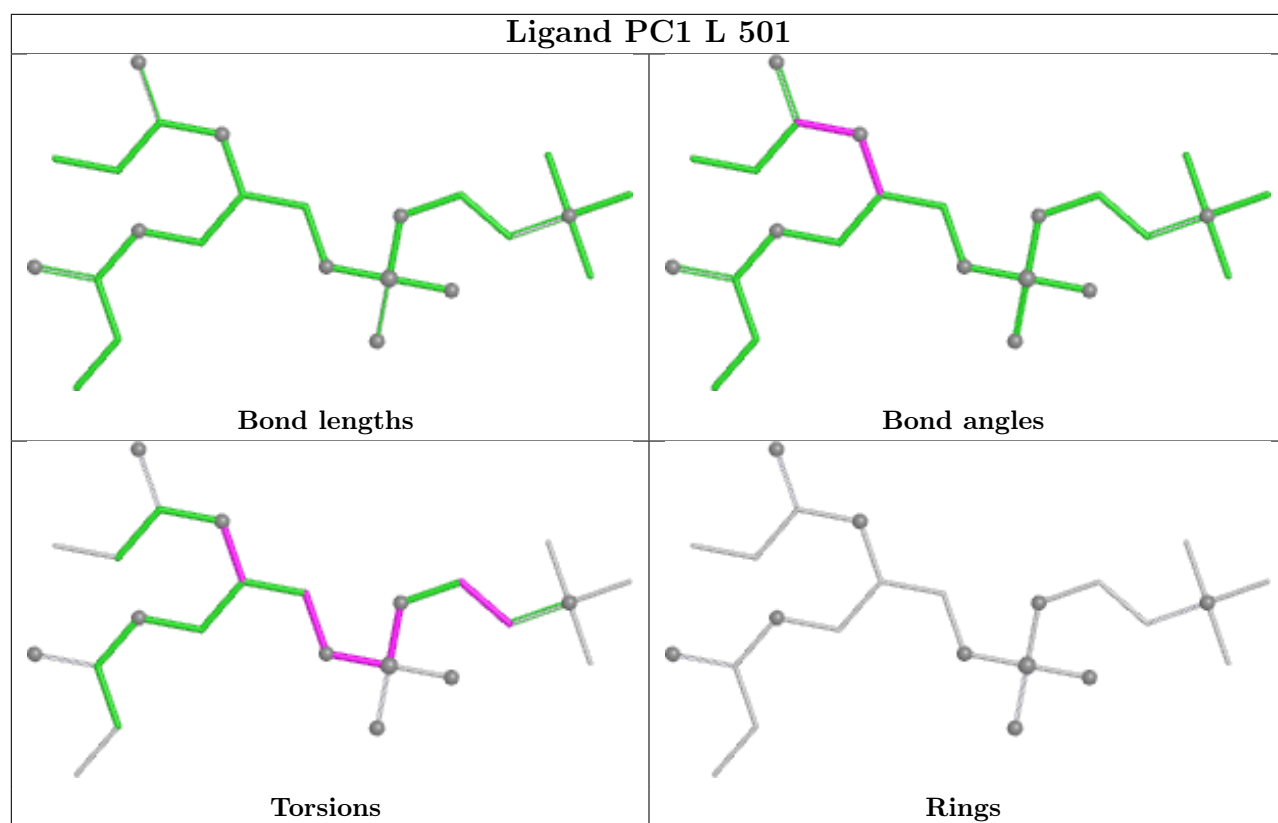
Ligand HEM C 402

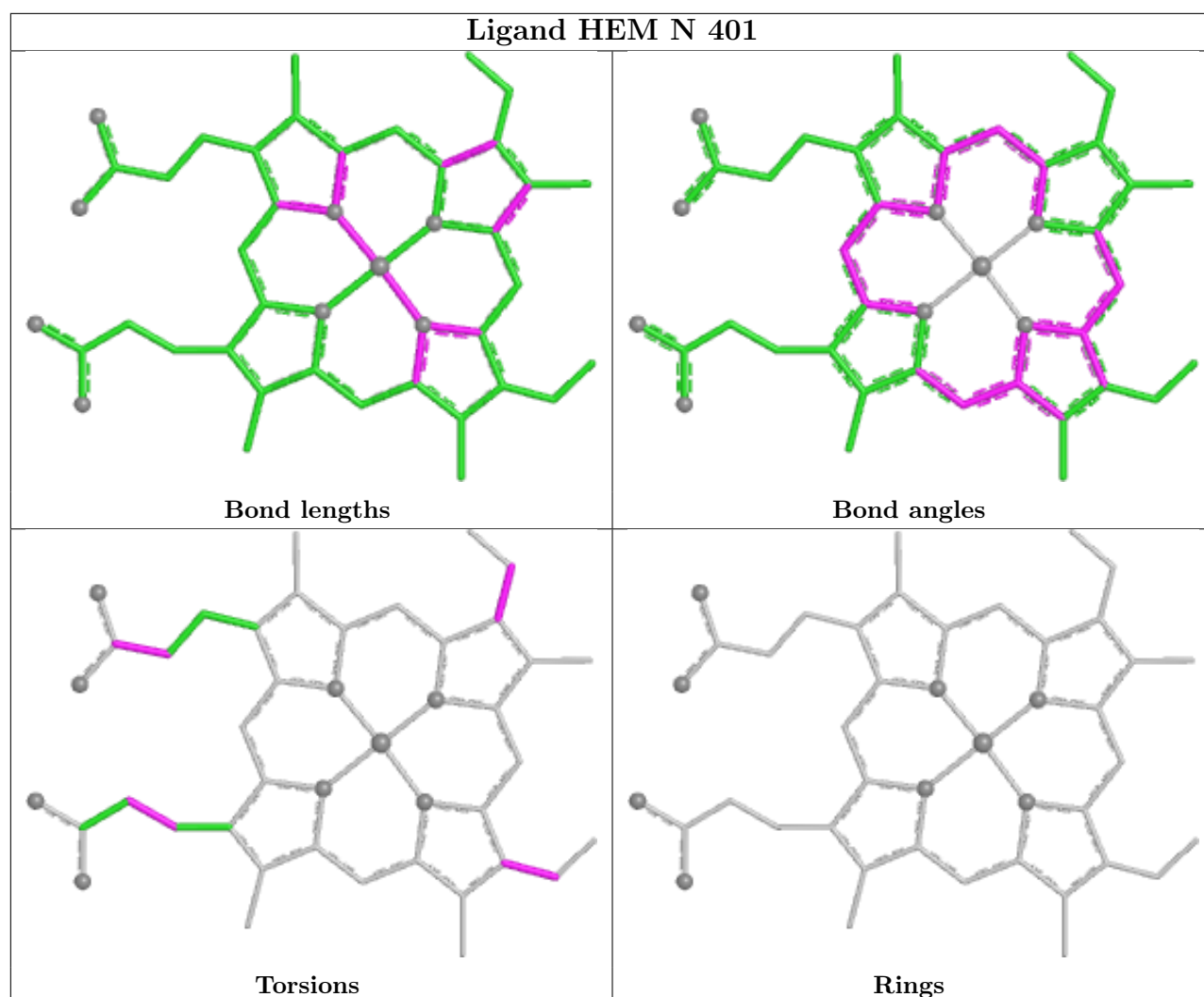












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

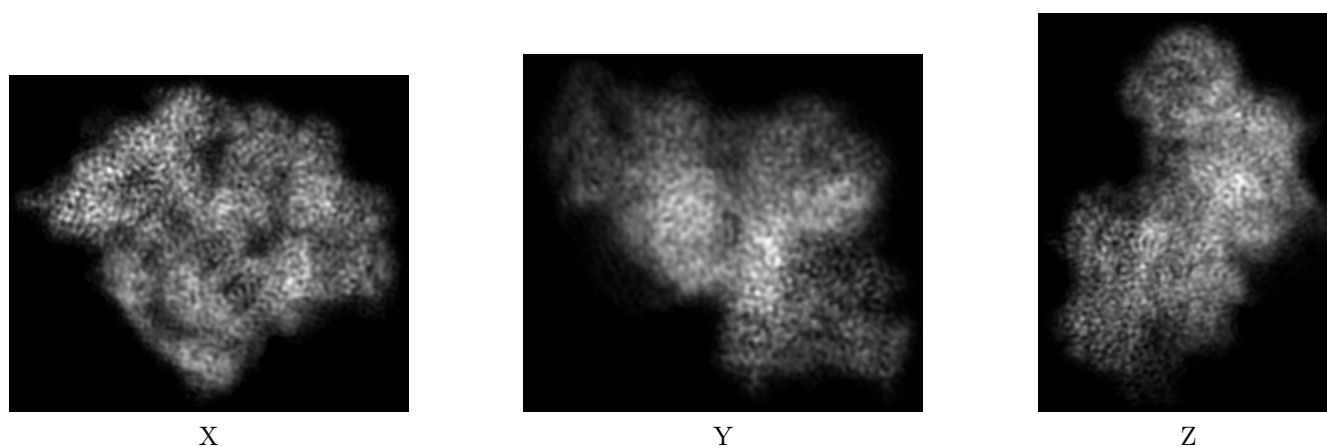
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12705. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

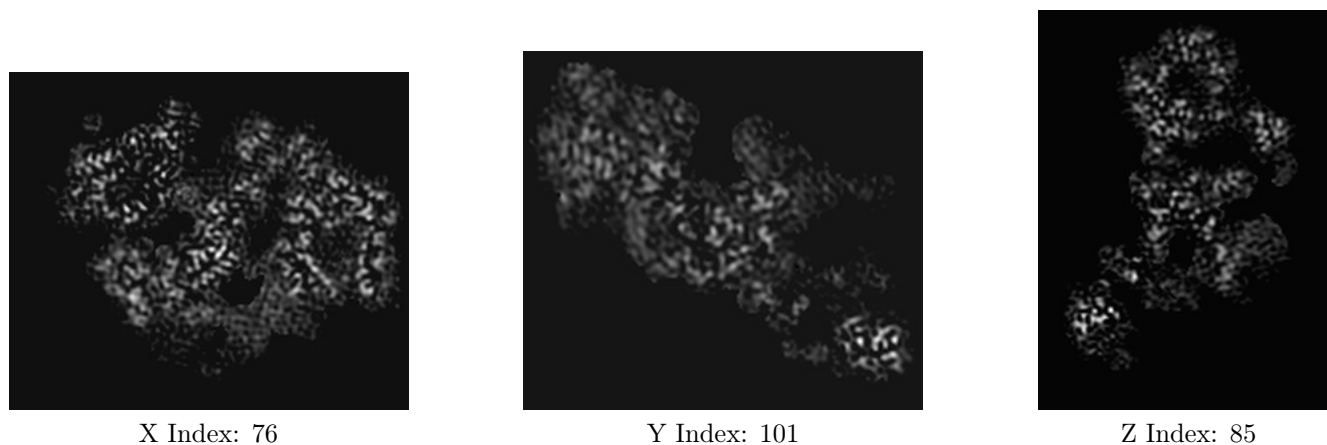
6.1.1 Primary map



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

6.2 Central slices [i](#)

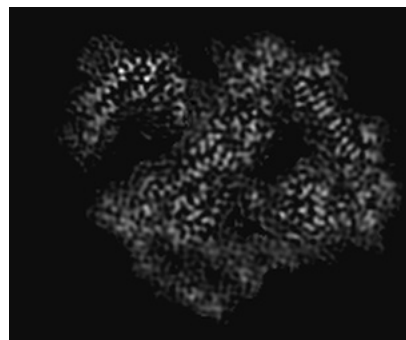
6.2.1 Primary map



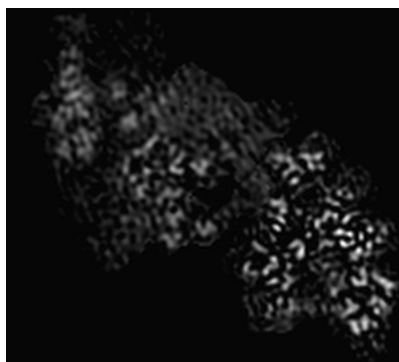
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

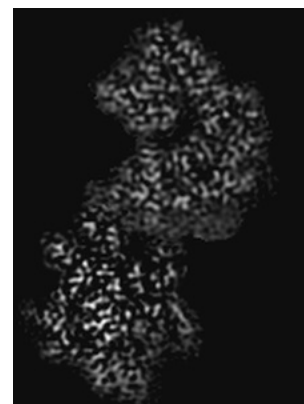
6.3.1 Primary map



X Index: 87



Y Index: 87

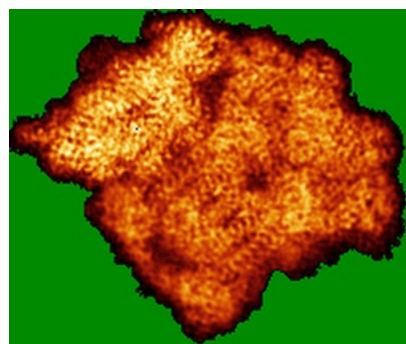


Z Index: 104

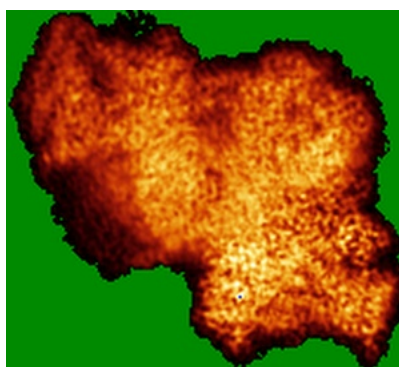
The images above show the largest variance slices of the map in three orthogonal directions.

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

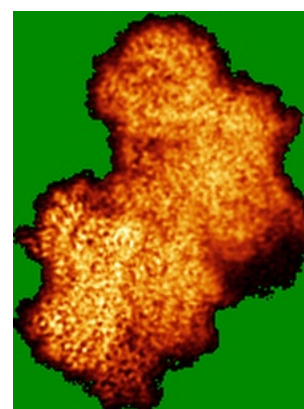
6.4.1 Primary map



X



Y

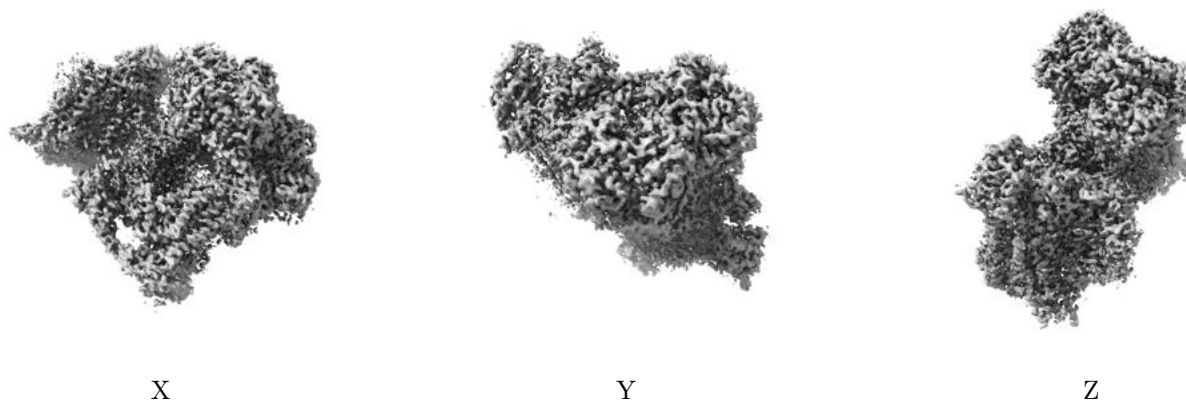


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

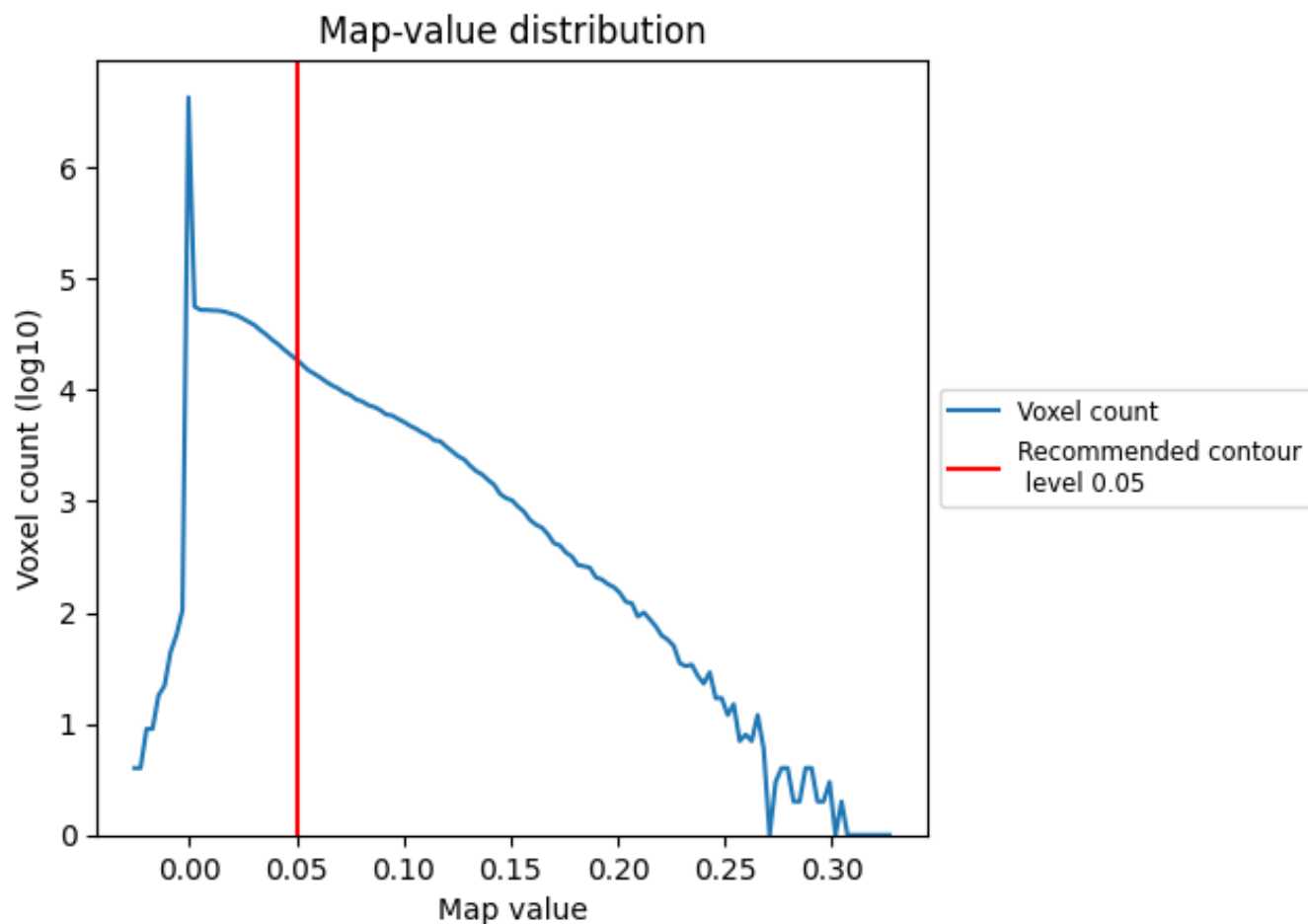
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

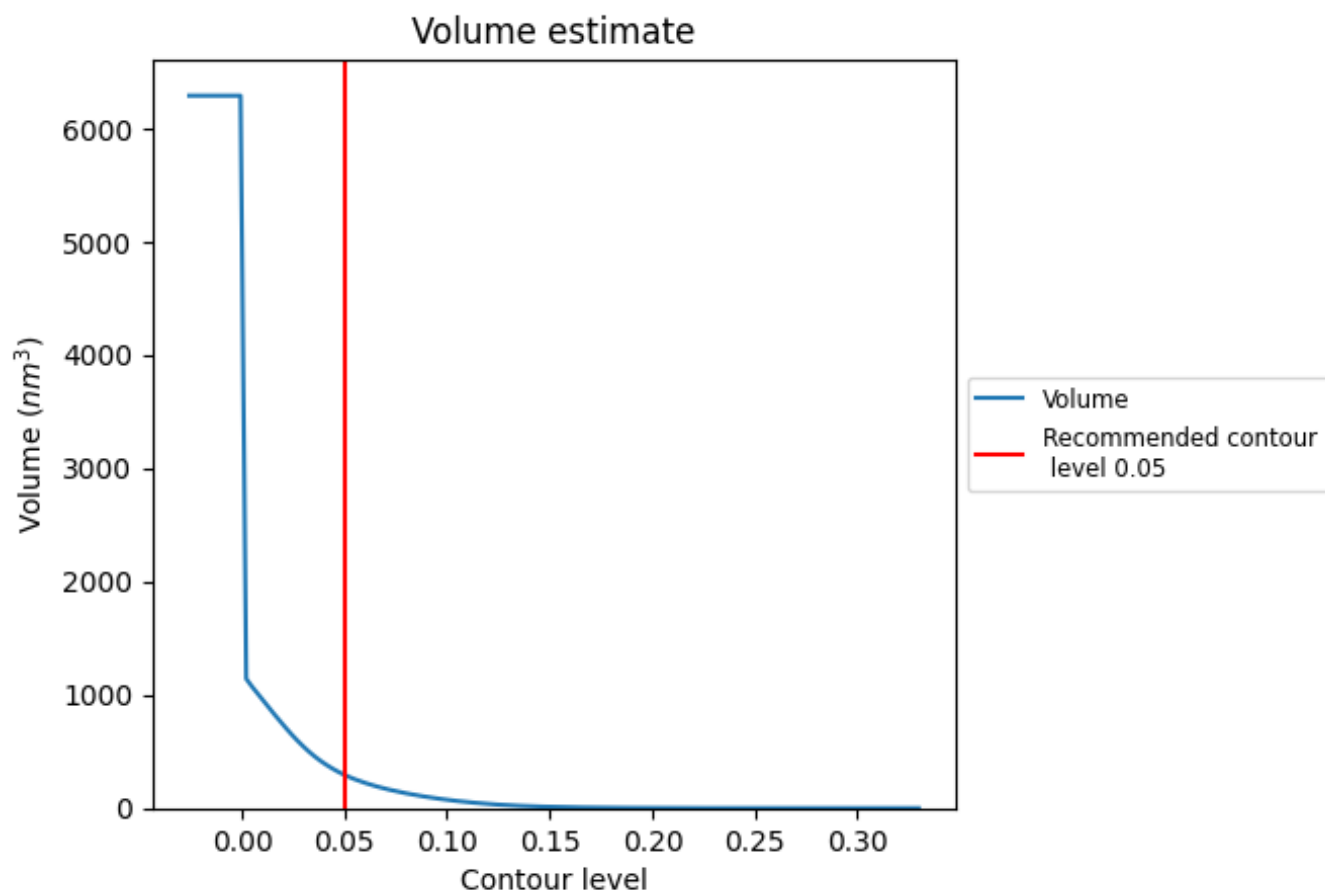
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

7.2 Volume estimate [i](#)



The volume at the recommended contour level is 294 nm³; this corresponds to an approximate mass of 266 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

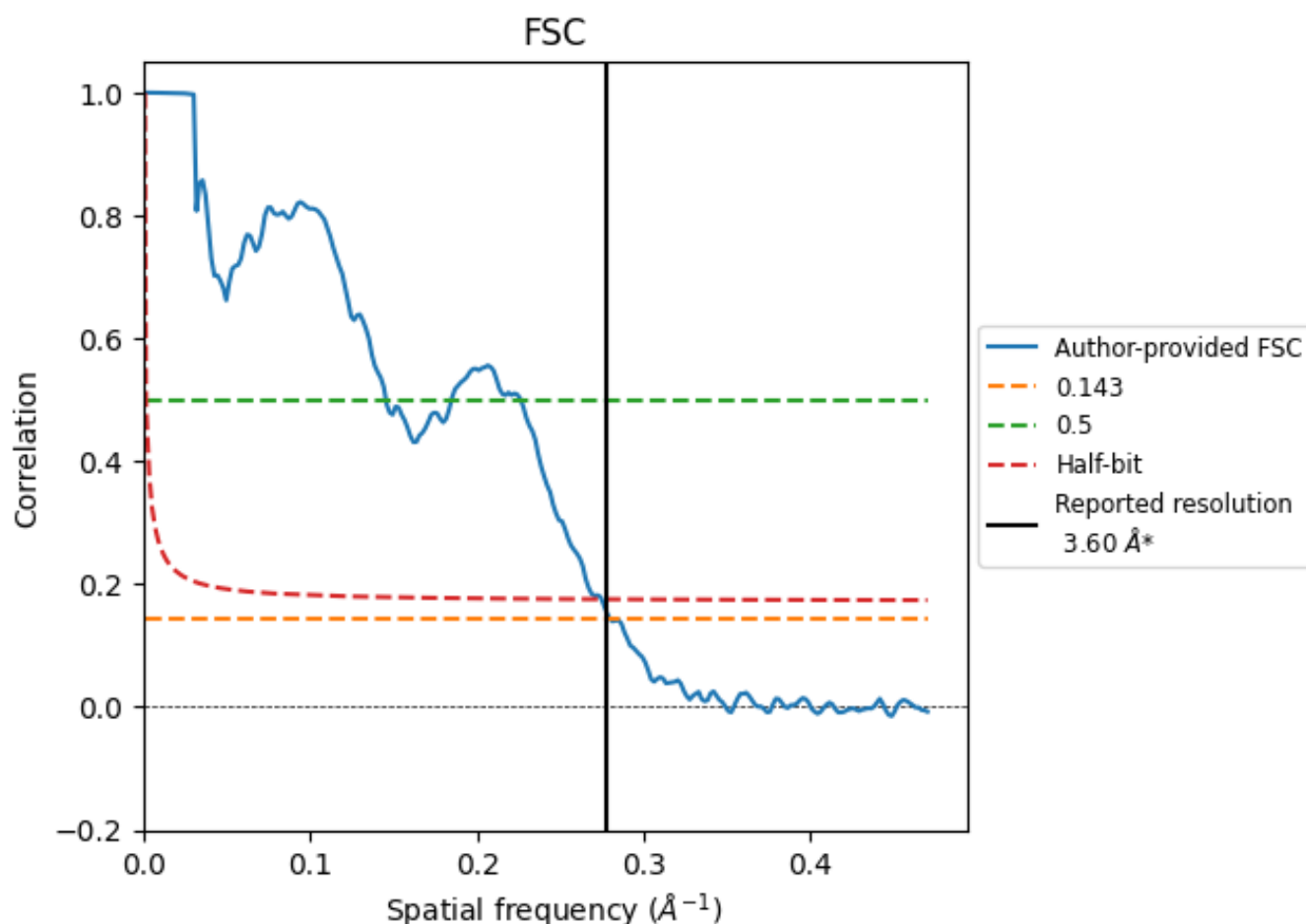
7.3 Rotationally averaged power spectrum [i](#)

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

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.278 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

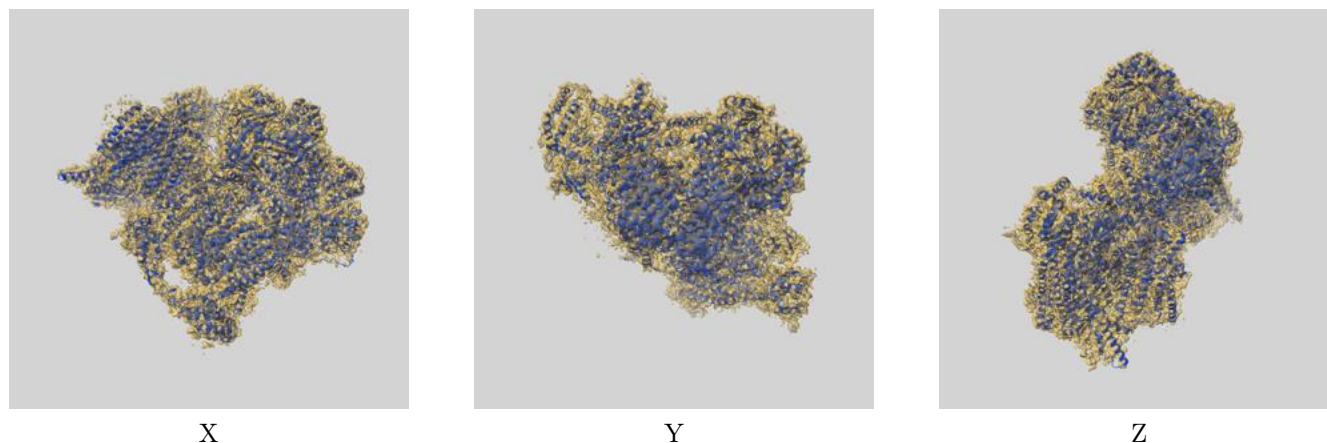
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.57	6.87	3.64
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

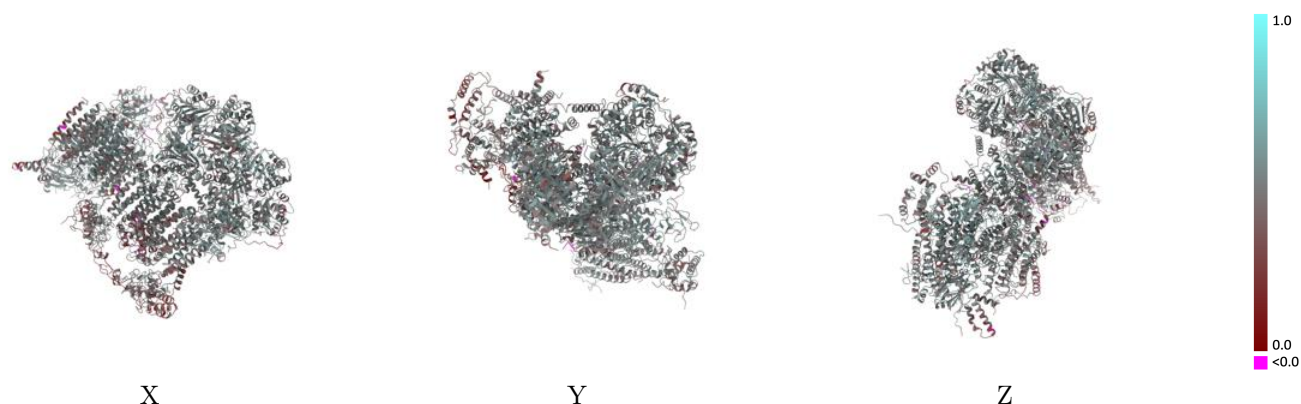
This section contains information regarding the fit between EMDB map EMD-12705 and PDB model 7O3E. Per-residue inclusion information can be found in [section 3](#) on [page 15](#).

9.1 Map-model overlay [i](#)



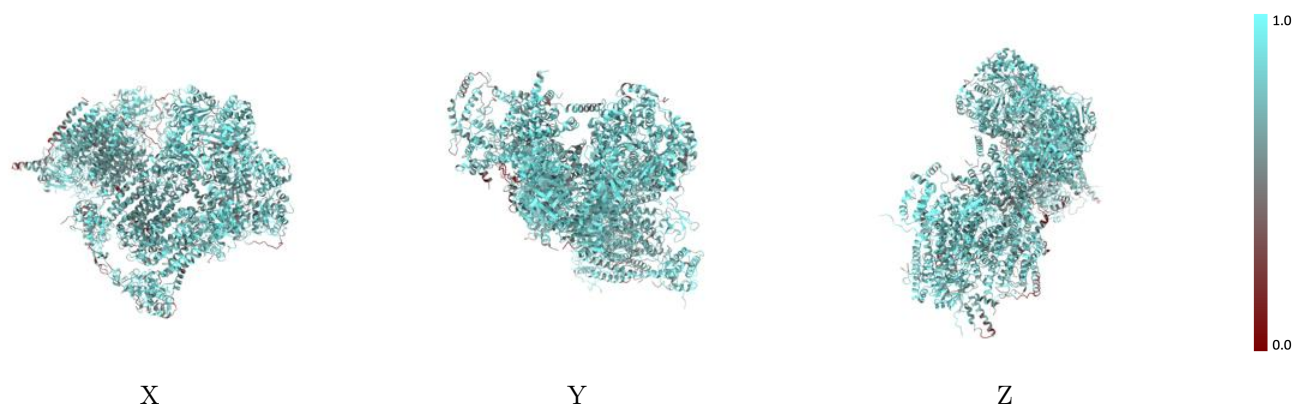
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



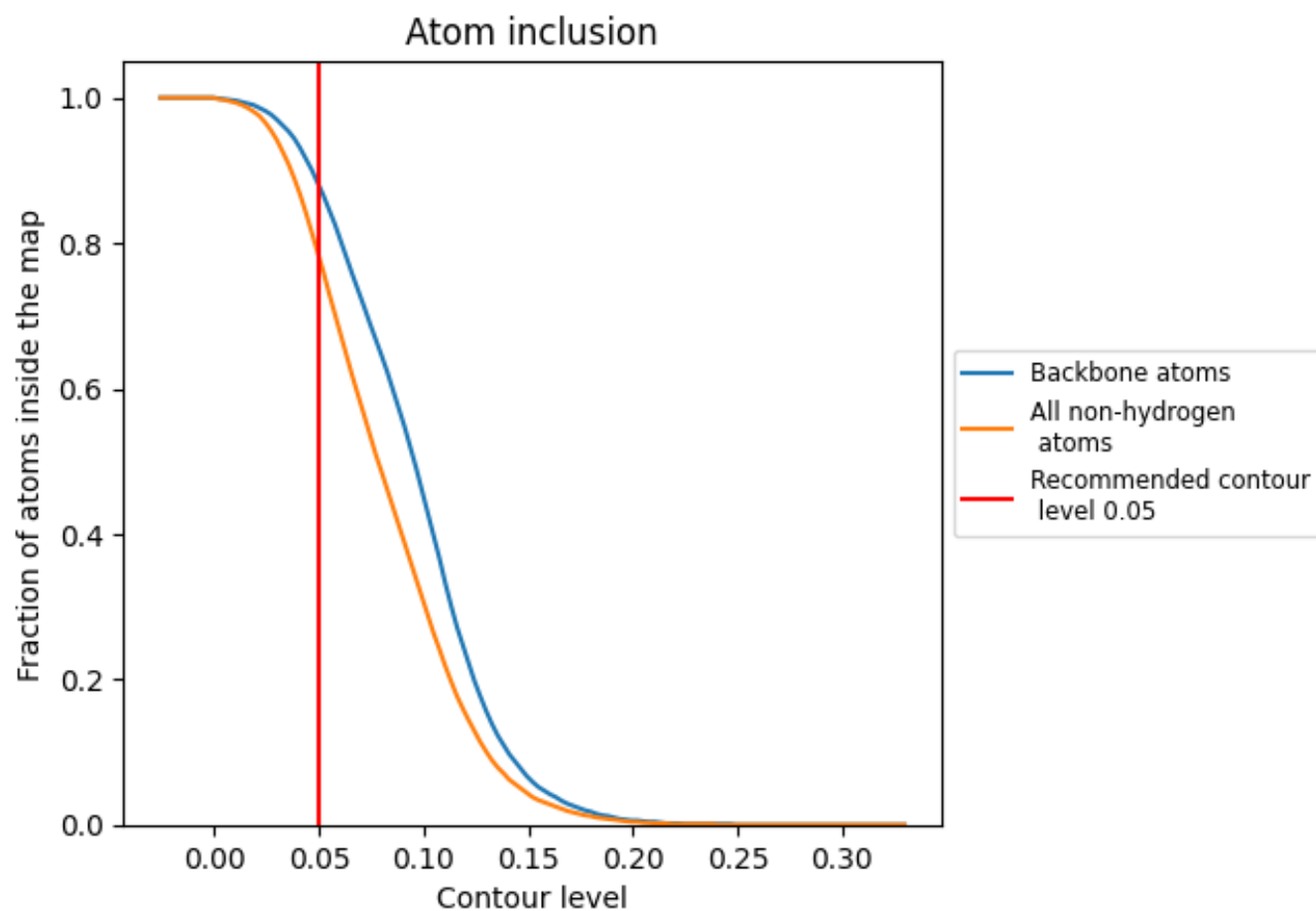
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).

9.4 Atom inclusion ⓘ



At the recommended contour level, 88% of all backbone atoms, 78% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7820	 0.4800
A	 0.8050	 0.4950
B	 0.8170	 0.5000
C	 0.7750	 0.4670
D	 0.7710	 0.4430
F	 0.8000	 0.5140
G	 0.7880	 0.4790
H	 0.6530	 0.3540
I	 0.6590	 0.4410
J	 0.6440	 0.3610
L	 0.7820	 0.4840
M	 0.8110	 0.4950
N	 0.7580	 0.4620
O	 0.7760	 0.4420
P	 0.7970	 0.4970
Q	 0.8120	 0.4900
R	 0.8070	 0.4860
S	 0.6350	 0.3400
T	 0.7650	 0.4710
U	 0.6630	 0.3520
a	 0.8280	 0.5380
b	 0.8190	 0.5060
c	 0.7800	 0.4830
d	 0.7790	 0.4760
e	 0.8540	 0.4710
f	 0.7920	 0.5030
g	 0.5490	 0.4340
h	 0.6630	 0.4290
i	 0.8290	 0.4730
k	 0.7710	 0.4920
l	 0.7770	 0.5350
m	 0.7150	 0.4380

