



wwPDB EM Validation Summary Report ⓘ

Aug 23, 2026 – 07:49 am BST

PDB ID : 9G83 / pdb_00009g83
EMDB ID : EMD-51125
Title : Respiratory supercomplex CI1-CIII2-CIV2-(cbb3)1 from alphaproteobacterium
Authors : Yaikhomba, M.; Hirst, J.; Croll, T.I.; Spikes, T.E.; Agip, A.N.A.
Deposited on : 2024-07-22
Resolution : 6.98 Å(reported)

This is a wwPDB EM Validation Summary 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:

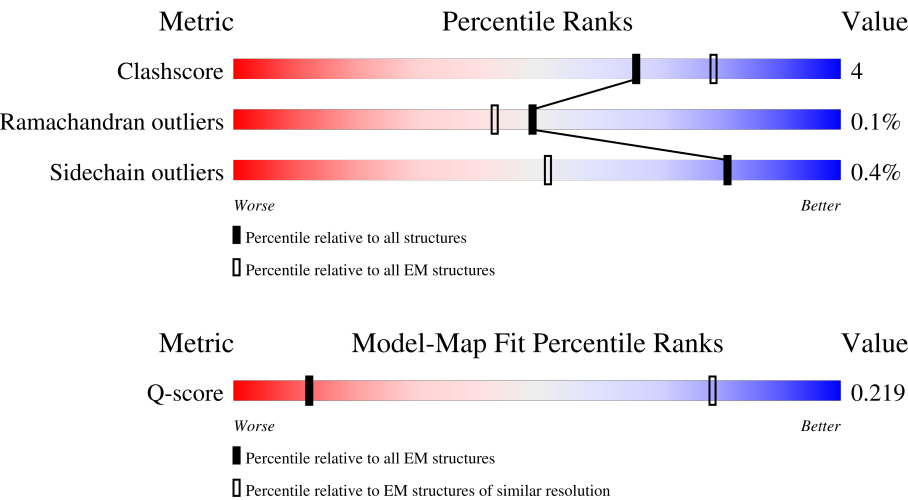
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 i

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

The reported resolution of this entry is 6.98 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.



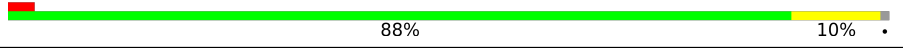
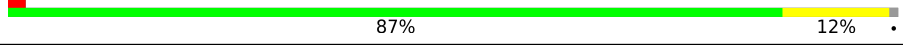
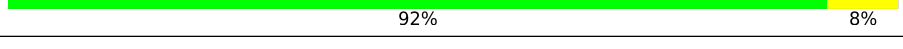
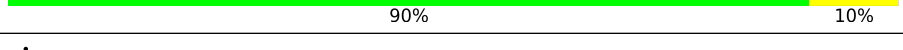
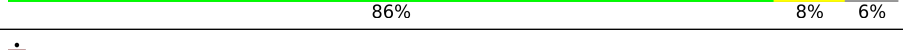
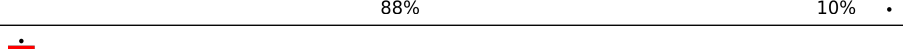
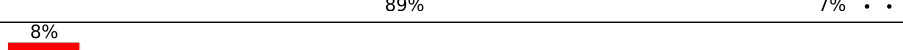
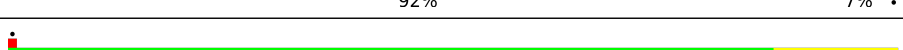
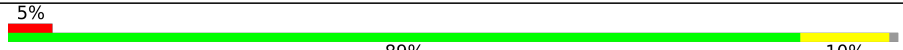
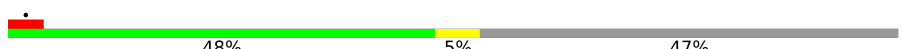
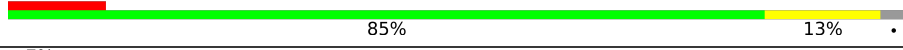
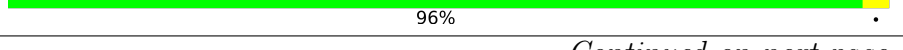
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	450 (6.48 - 7.46)

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	121	5% 90% 10%
2	B	175	6% 77% 15% 7%
3	C	208	• 86% 7% 7%
4	D	412	• 90% 9%

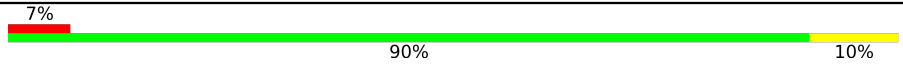
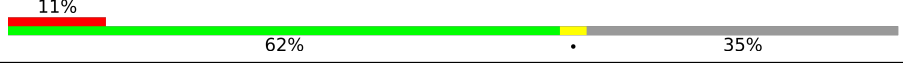
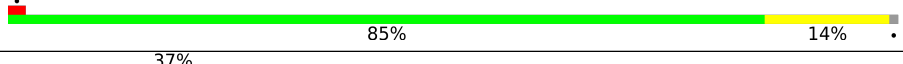
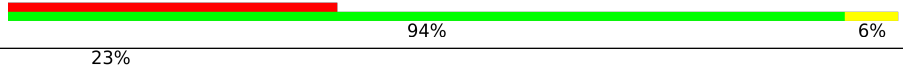
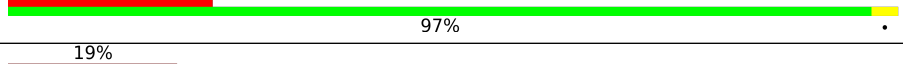
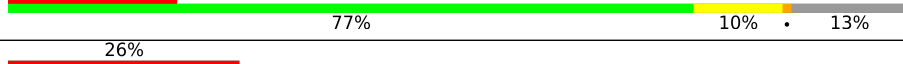
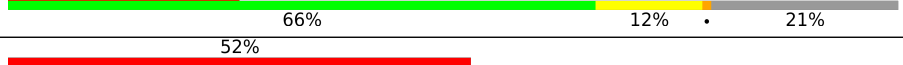
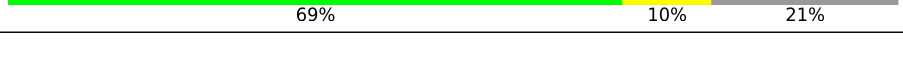
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Mol	Chain	Length	Quality of chain
5	E	239	
6	F	431	
7	G	674	
8	H	345	
9	I	163	
10	J	199	
11	K	101	
12	L	703	
13	M	513	
14	N	499	
15	P	330	
16	Q	103	
17	R	62	
18	Z	217	
19	a	440	
19	d	440	
20	b	450	
20	e	450	
21	c	195	
21	f	195	
22	g	558	
22	k	558	
23	h	298	
23	l	298	
24	i	274	

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Mol	Chain	Length	Quality of chain
24	m	274	
25	j	66	
25	n	66	
26	o	176	
26	p	176	
27	q	124	
28	r	35	
29	s	30	
30	t	539	
31	u	241	
32	v	349	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	SF4	B	1001	-	-	X	-
33	SF4	F	501	-	-	X	-
43	HEC	e	502	X	-	-	-
43	HEC	u	1000	X	-	-	-
43	HEC	v	1001	X	-	-	-
43	HEC	v	1002	X	-	-	-

2 Entry composition

There are 47 unique types of molecules in this entry. The entry contains 83417 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 NADH-quinone oxidoreductase subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	121	Total	C	N	O	S	0	0
			969	658	141	164	6		

- Molecule 2 is a protein called NADH-quinone oxidoreductase subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	162	Total	C	N	O	S	0	0
			1270	799	227	231	13		

- Molecule 3 is a protein called NADH-quinone oxidoreductase subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	194	Total	C	N	O	S	0	0
			1586	1020	274	290	2		

- Molecule 4 is a protein called NADH-quinone oxidoreductase subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	411	Total	C	N	O	S	0	0
			3277	2072	582	601	22		

- Molecule 5 is a protein called NADH dehydrogenase subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	237	Total	C	N	O	S	0	0
			1822	1155	314	340	13		

- Molecule 6 is a protein called NADH-quinone oxidoreductase subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	422	Total	C	N	O	S	0	0
			3241	2027	583	600	31		

- Molecule 7 is a protein called NADH-quinone oxidoreductase.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	665	Total	C	N	O	S	0	0
			5068	3149	917	969	33		

- Molecule 8 is a protein called NADH-quinone oxidoreductase subunit H.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	341	Total	C	N	O	S	0	0
			2722	1848	413	439	22		

- Molecule 9 is a protein called NADH-quinone oxidoreductase subunit I.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	162	Total	C	N	O	S	0	0
			1319	836	230	242	11		

- Molecule 10 is a protein called NADH-quinone oxidoreductase subunit J.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	199	Total	C	N	O	S	0	0
			1528	1014	246	257	11		

- Molecule 11 is a protein called NADH-quinone oxidoreductase subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	101	Total	C	N	O	S	0	0
			764	508	123	128	5		

- Molecule 12 is a protein called NADH dehydrogenase subunit L.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	658	Total	C	N	O	S	0	0
			5193	3458	850	852	33		

- Molecule 13 is a protein called NADH dehydrogenase subunit M.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	503	Total	C	N	O	S	0	0
			3915	2615	610	658	32		

- Molecule 14 is a protein called NADH-quinone oxidoreductase subunit N.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	480	Total	C	N	O	S	0	0
			3556	2342	565	617	32		

- Molecule 15 is a protein called NAD-dependent epimerase/dehydratase.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	328	Total	C	N	O	S	0	0
			2468	1541	463	452	12		

- Molecule 16 is a protein called ETC complex I subunit conserved region.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	103	Total	C	N	O	S	0	0
			849	523	167	156	3		

- Molecule 17 is a protein called Zinc finger CHCC-type domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	61	Total	C	N	O	S	0	0
			488	304	90	91	3		

- Molecule 18 is a protein called Protein-L-isoaspartate O-methyltransferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Z	216	Total	C	N	O	S	0	0
			1642	1033	294	306	9		

- Molecule 19 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	a	433	Total	C	N	O	S	0	0
			3504	2373	552	561	18		
19	d	434	Total	C	N	O	S	0	0
			3513	2378	553	564	18		

- Molecule 20 is a protein called Cytochrome c1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	b	239	Total	C	N	O	S	0	0
			1855	1181	311	354	9		
20	e	239	Total	C	N	O	S	0	0
			1855	1181	311	354	9		

- Molecule 21 is a protein called Ubiquinol-cytochrome c reductase iron-sulfur subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	c	180	Total	C	N	O	S	0	0
			1353	838	245	263	7		
21	f	181	Total	C	N	O	S	0	0
			1361	842	246	266	7		

- Molecule 22 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	g	544	Total	C	N	O	S	0	0
			4322	2890	684	715	33		
22	k	544	Total	C	N	O	S	0	0
			4322	2890	684	715	33		

- Molecule 23 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	h	252	Total	C	N	O	S	0	0
			1976	1295	319	354	8		
23	l	252	Total	C	N	O	S	0	0
			1976	1295	319	354	8		

- Molecule 24 is a protein called cytochrome-c oxidase.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	i	273	Total	C	N	O	S	0	0
			2183	1483	341	348	11		
24	m	273	Total	C	N	O	S	0	0
			2183	1483	341	348	11		

- Molecule 25 is a protein called Aa3 type cytochrome c oxidase subunit IV.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	j	43	Total	C	N	O	S	0	0
			332	214	58	59	1		
25	n	43	Total	C	N	O	S	0	0
			332	214	58	59	1		

- Molecule 26 is a protein called Cytochrome c, class I.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	o	43	Total	C	N	O	S	0	0
			315	210	48	55	2		
26	p	44	Total	C	N	O	S	0	0
			321	213	49	57	2		

- Molecule 27 is a protein called NADH:ubiquinone oxidoreductase 17.2 kD subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	q	123	Total	C	N	O	S	0	0
			1018	651	181	185	1		

- Molecule 28 is a protein called Transmembrane helix of unknown identity.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	r	35	Total	C	N	O	0	0
			175	105	35	35		

- Molecule 29 is a protein called Transmembrane helix of unknown identity.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	s	30	Total	C	N	O	0	0
			150	90	30	30		

- Molecule 30 is a protein called cytochrome-c oxidase.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	t	470	Total	C	N	O	S	0	0
			3732	2498	596	616	22		

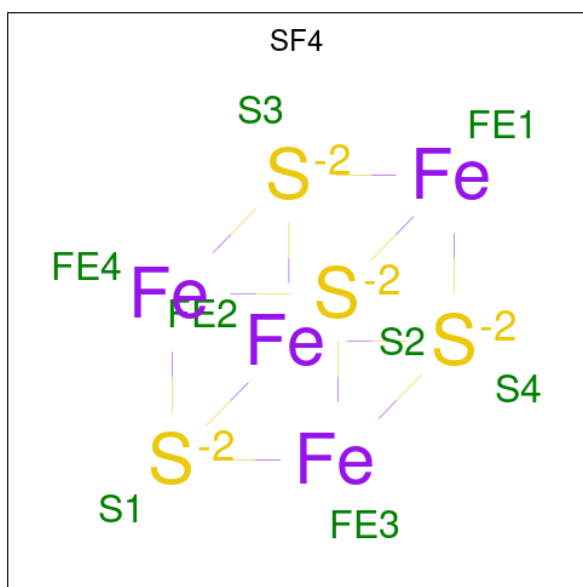
- Molecule 31 is a protein called Cytochrome c oxidase, cbb3-type, subunit II.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	u	191	Total	C	N	O	S	0	0
			1517	969	261	277	10		

- Molecule 32 is a protein called Cbb3-type cytochrome c oxidase subunit CcoP.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	v	276	Total	C	N	O	S	0	0
			2095	1326	356	406	7		

- Molecule 33 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).

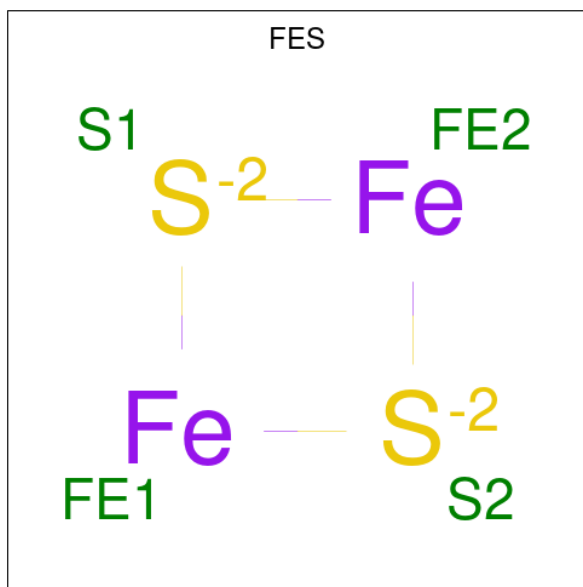


Mol	Chain	Residues	Atoms			AltConf
33	B	1	Total	Fe	S	0
			8	4	4	
33	F	1	Total	Fe	S	
			8	4	4	
33	G	1	Total	Fe	S	
			8	4	4	
33	G	1	Total	Fe	S	0
			8	4	4	
33	I	1	Total	Fe	S	
			8	4	4	
33	I	1	Total	Fe	S	
			8	4	4	

- Molecule 34 is SODIUM ION (CCD ID: NA) (formula: Na).

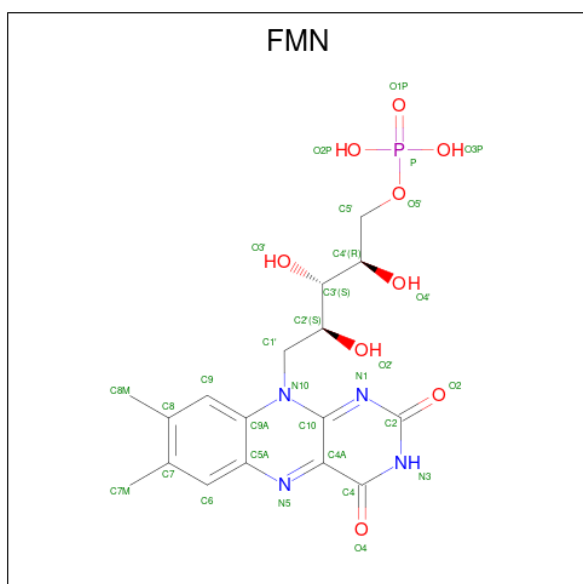
Mol	Chain	Residues	Atoms		AltConf
34	D	1	Total	Na	0
			1	1	

- Molecule 35 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



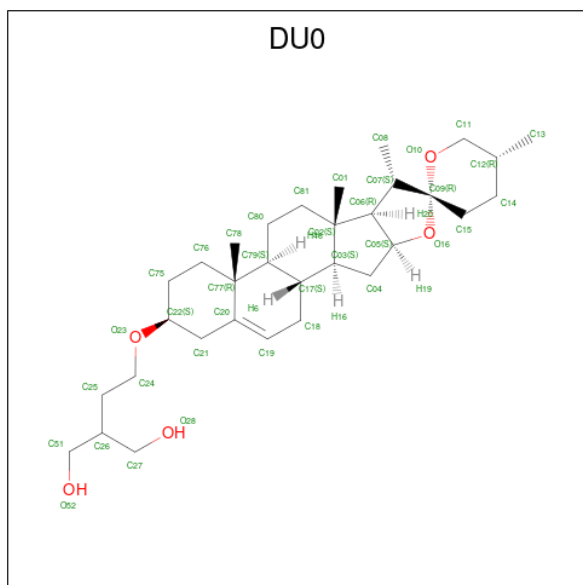
Mol	Chain	Residues	Atoms			AltConf
35	E	1	Total	Fe	S	0
			4	2	2	
35	G	1	Total	Fe	S	0
			4	2	2	
35	c	1	Total	Fe	S	0
			4	2	2	
35	f	1	Total	Fe	S	0
			4	2	2	

- Molecule 36 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: C₁₇H₂₁N₄O₉P) (labeled as "Ligand of Interest" by depositor).



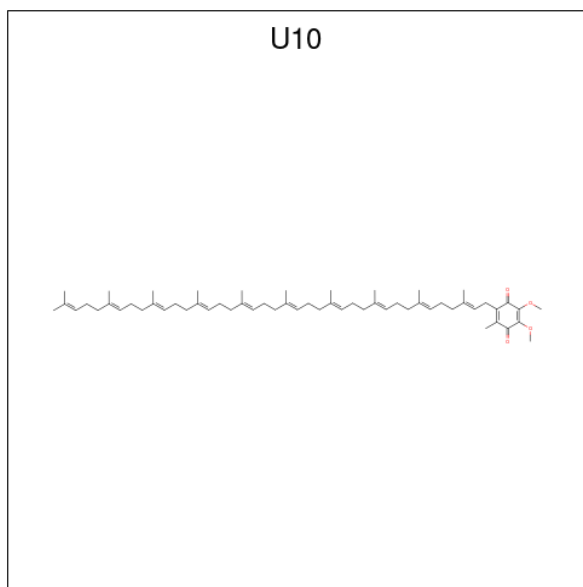
Mol	Chain	Residues	Atoms					AltConf
36	F	1	Total 31	C 17	N 4	O 9	P 1	0

- Molecule 37 is 2-[2-[(1 {S},2 {S},4 {S},5' {R},6 {R},7 {S},8 {R},9 {S},12 {S},13 {R},16 {S})-5',7,9,13-tetramethylspiro[5-oxapentacyclo[10.8.0.0^{2,9}.0^{4,8}.0^{13,18}]]icos-18-ene-6,2'-oxane]-16-yl]oxyethyl]propane-1,3-diol (CCD ID: DU0) (formula: C₃₂H₅₂O₅).



Mol	Chain	Residues	Atoms			AltConf
37	H	1	Total 37	C 32	O 5	0
37	N	1	Total 37	C 32	O 5	0
37	f	1	Total 37	C 32	O 5	0

- Molecule 38 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$).

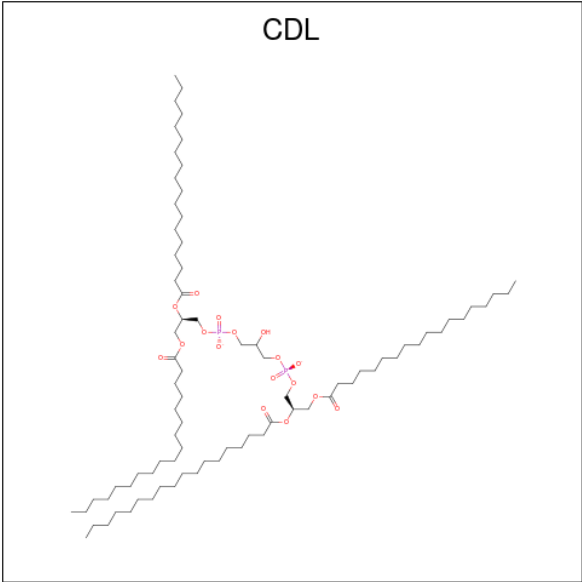


Mol	Chain	Residues	Atoms			AltConf
38	H	1	Total	C	O	0
			63	59	4	
38	a	1	Total	C	O	0
			63	59	4	
38	a	1	Total	C	O	0
			63	59	4	
38	d	1	Total	C	O	0
			63	59	4	
38	d	1	Total	C	O	0
			63	59	4	

- Molecule 39 is ZINC ION (CCD ID: ZN) (formula: Zn).

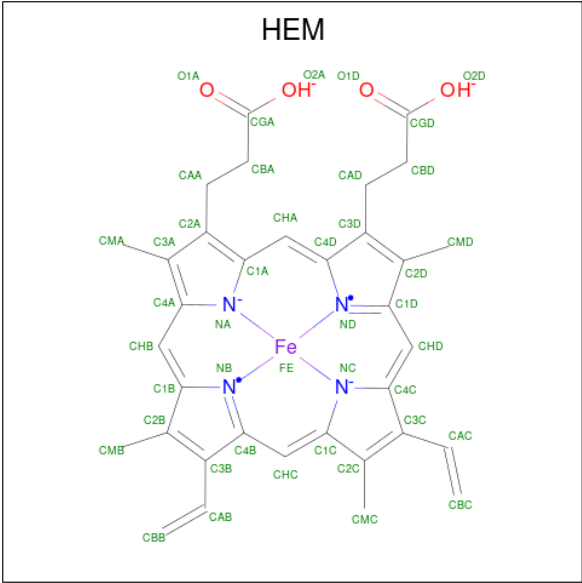
Mol	Chain	Residues	Atoms		AltConf
39	R	1	Total	Zn	0
			1	1	

- Molecule 40 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
40	a	1	100	81	17	2	0

- Molecule 41 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
			Total	C	Fe	N	O	
41	a	1	43	34	1	4	4	0
41	a	1	43	34	1	4	4	0

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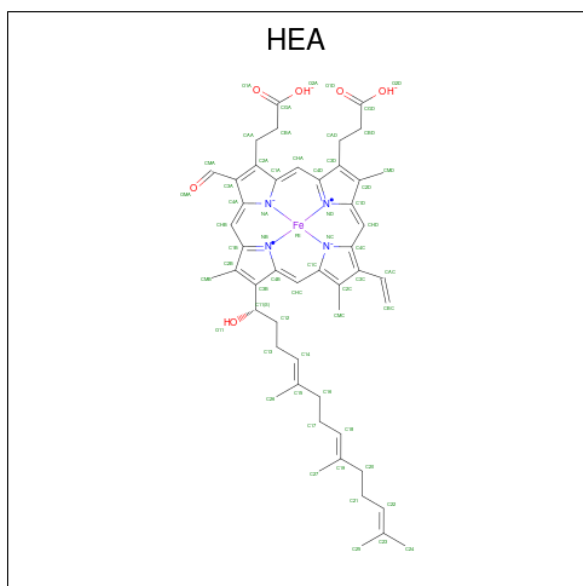
Mol	Chain	Residues	Atoms				AltConf	
41	d	1	Total 43	C 34	Fe 1	N 4	O 4	0
41	d	1	Total 43	C 34	Fe 1	N 4	O 4	0
41	t	1	Total 43	C 34	Fe 1	N 4	O 4	0
41	t	1	Total 43	C 34	Fe 1	N 4	O 4	0

- | Mol | Chain | Residues | Atoms | AltConf |
|-----|-------|----------|--------------|---------|
| 42 | b | 1 | Total 1 Ca 1 | 0 |
| 42 | e | 1 | Total 1 Ca 1 | 0 |
| 42 | g | 1 | Total 1 Ca 1 | 0 |
| 42 | k | 1 | Total 1 Ca 1 | 0 |
| 42 | t | 2 | Total 2 Ca 2 | 0 |

- [illegible]

Mol	Chain	Residues	Atoms					AltConf
43	b	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
43	e	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
43	u	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
43	v	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
43	v	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 44 is HEME-A (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
44	g	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
44	g	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
44	k	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
44	k	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

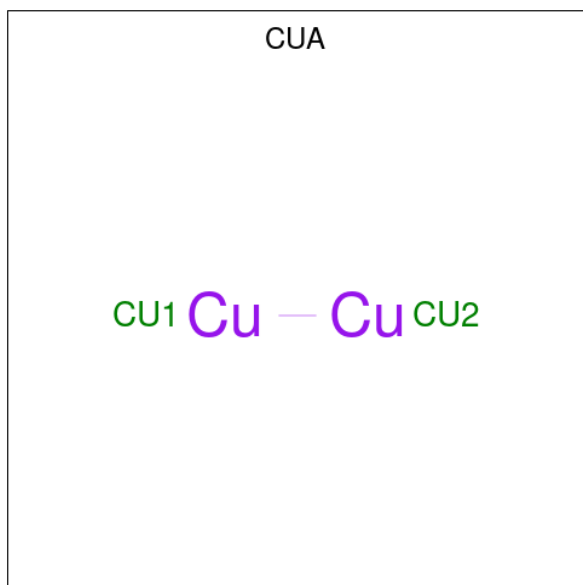
- Molecule 45 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
45	g	1	Total 1	Cu 1	0
45	k	1	Total 1	Cu 1	0
45	t	1	Total 1	Cu 1	0

- Molecule 46 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		AltConf
46	g	1	Total 1	Mn 1	0

- Molecule 47 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).

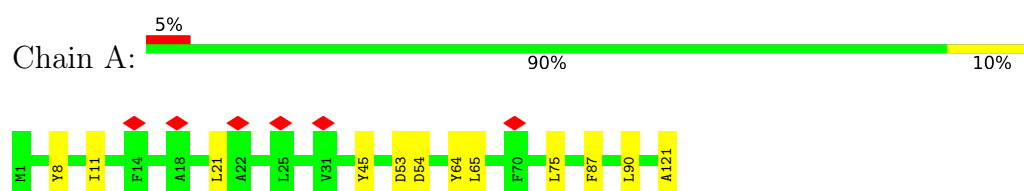


Mol	Chain	Residues	Atoms		AltConf
47	h	1	Total 2	Cu 2	0
47	l	1	Total 2	Cu 2	0

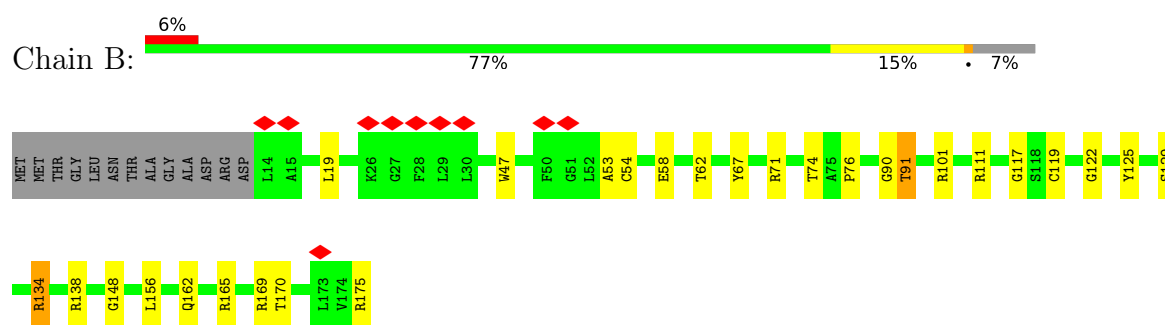
3 Residue-property plots [i](#)

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.

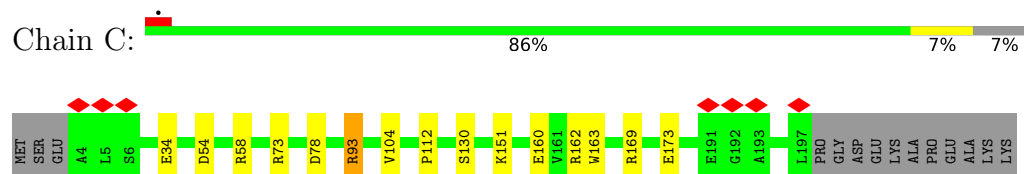
- Molecule 1: NADH-quinone oxidoreductase subunit A



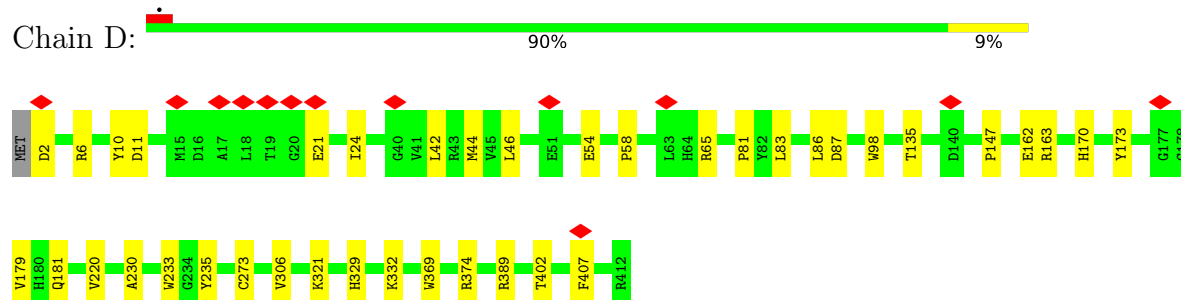
- Molecule 2: NADH-quinone oxidoreductase subunit B



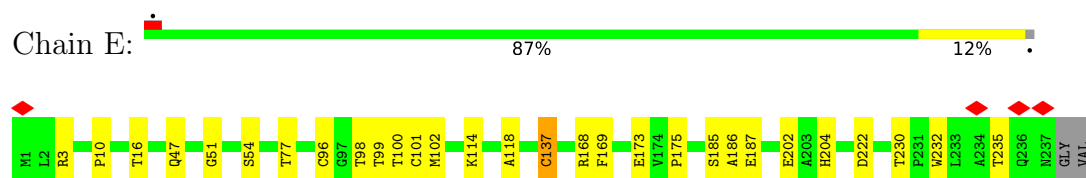
- Molecule 3: NADH-quinone oxidoreductase subunit C



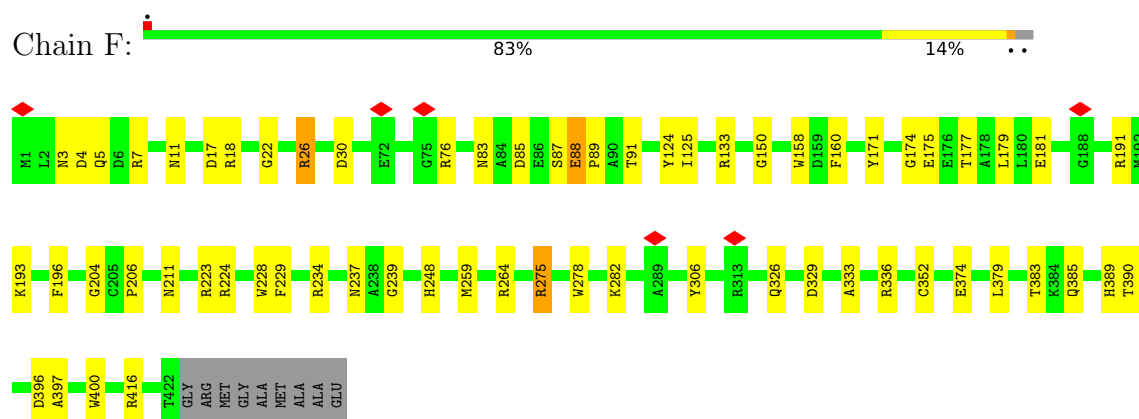
- Molecule 4: NADH-quinone oxidoreductase subunit D



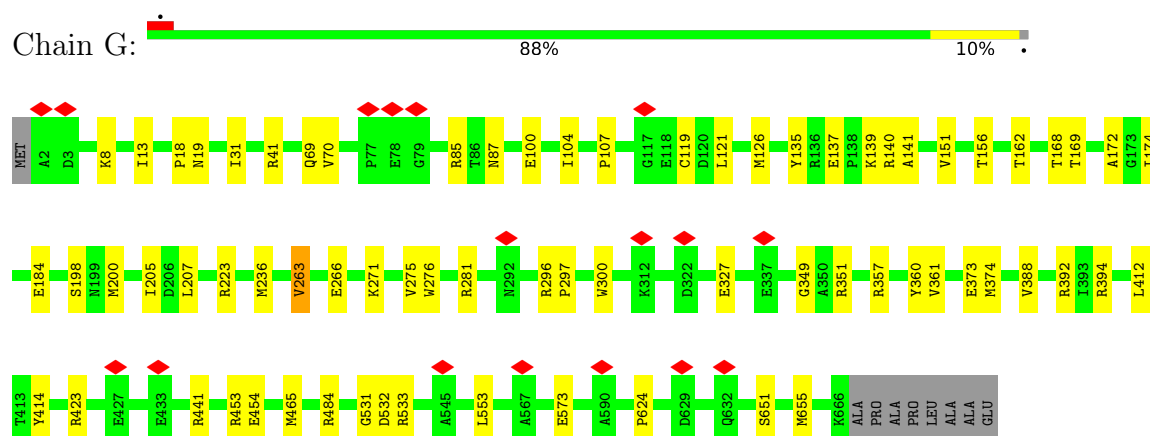
- Molecule 5: NADH dehydrogenase subunit E



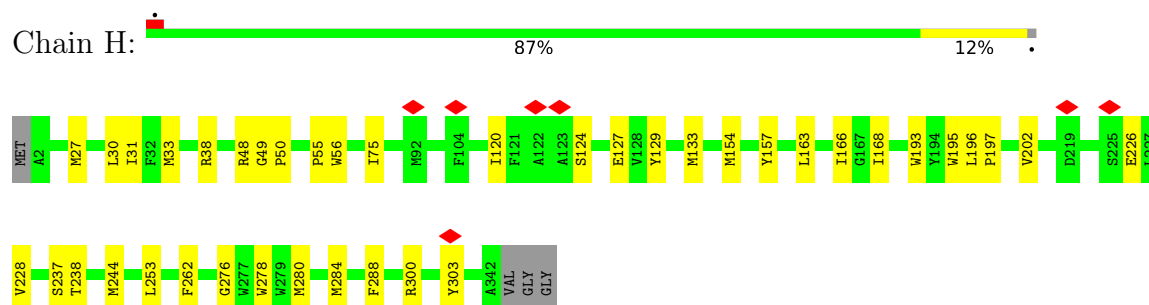
- Molecule 6: NADH-quinone oxidoreductase subunit F



- Molecule 7: NADH-quinone oxidoreductase

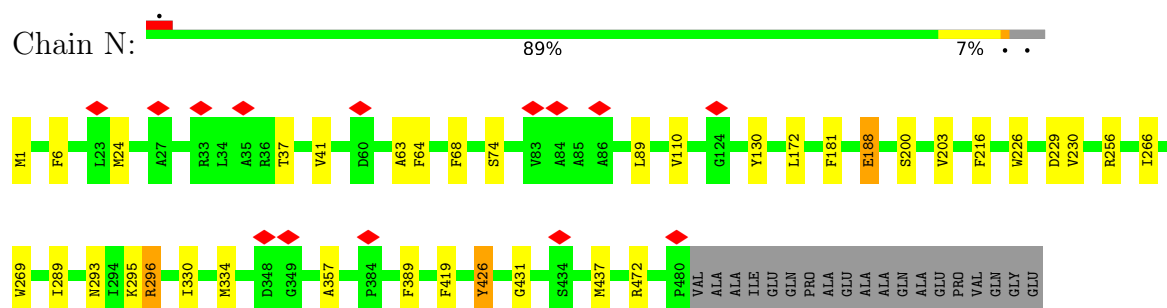


- Molecule 8: NADH-quinone oxidoreductase subunit H

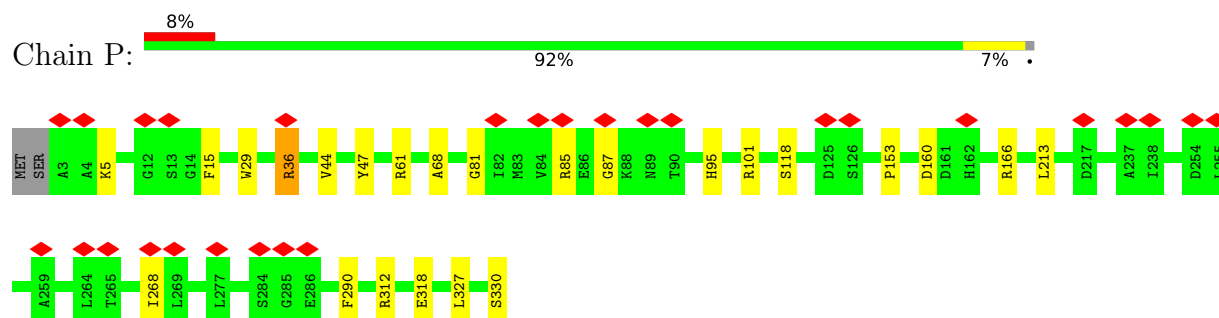


- Molecule 9: NADH-quinone oxidoreductase subunit I

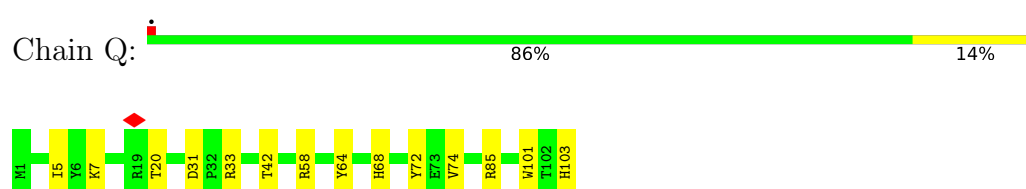
- Molecule 14: NADH-quinone oxidoreductase subunit N



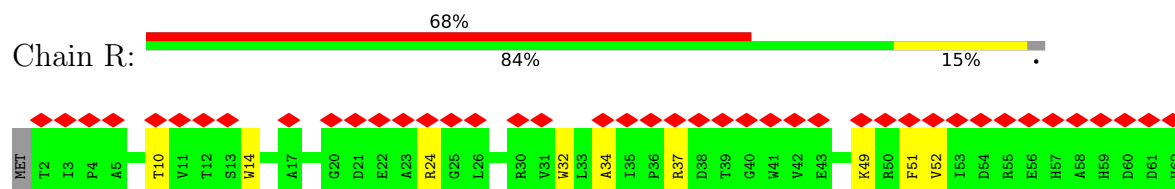
- Molecule 15: NAD-dependent epimerase/dehydratase



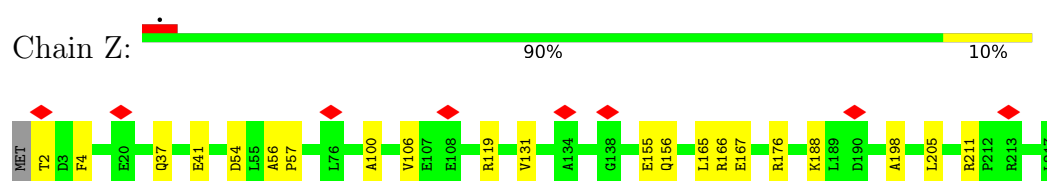
- Molecule 16: ETC complex I subunit conserved region



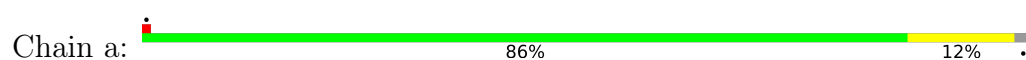
- Molecule 17: Zinc finger CHCC-type domain-containing protein



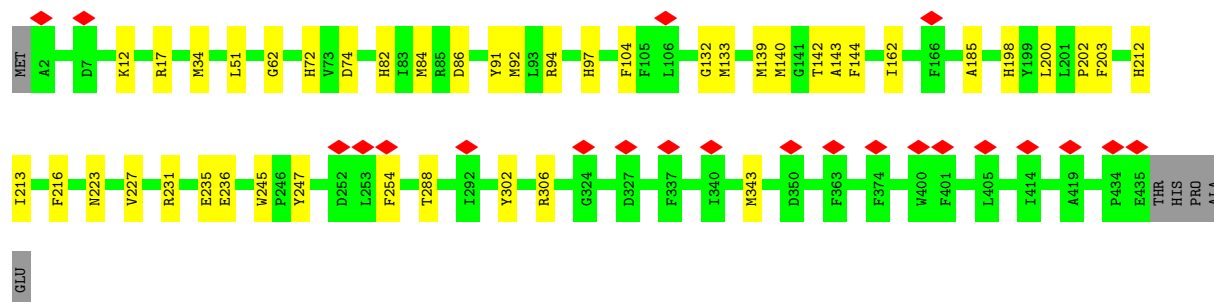
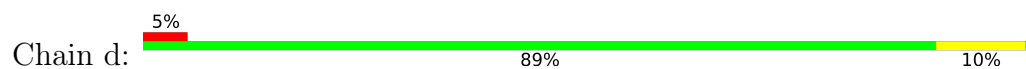
- Molecule 18: Protein-L-isoaspartate O-methyltransferase



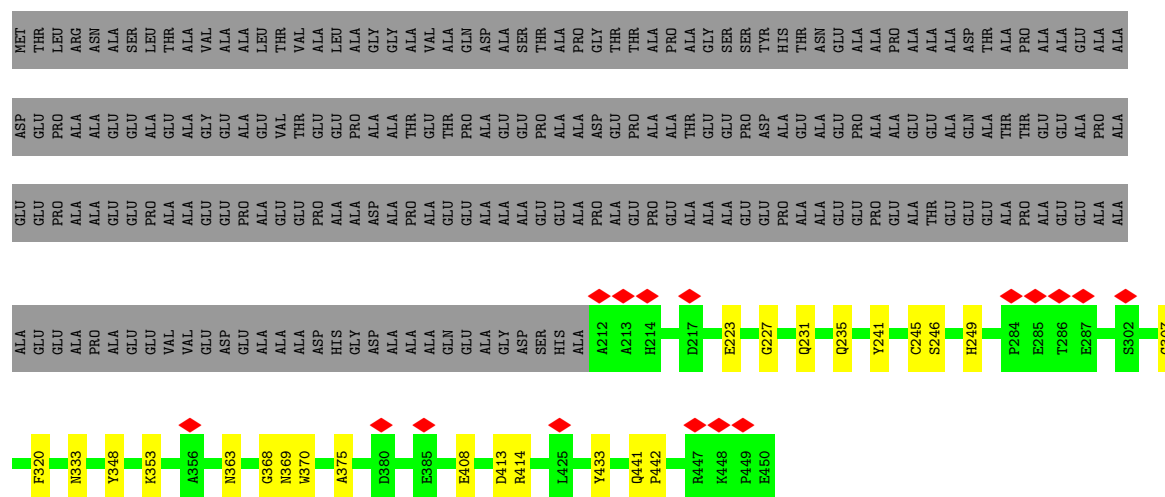
- Molecule 19: Cytochrome b



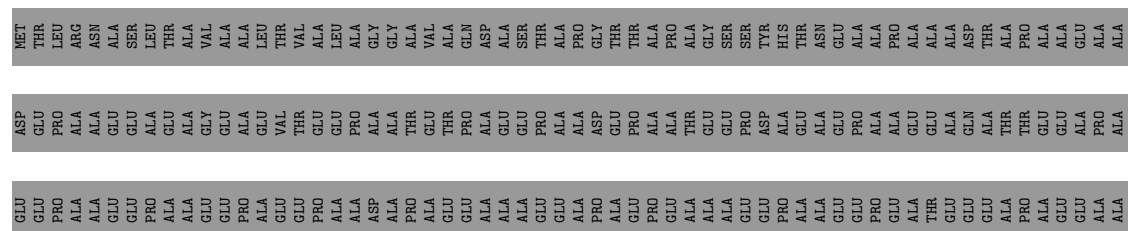
- Molecule 19: Cytochrome b

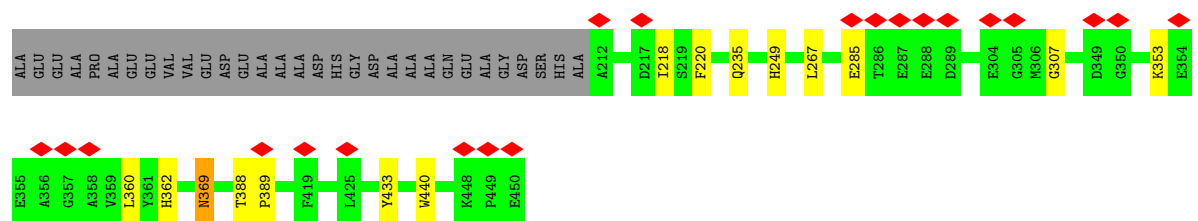


- Molecule 20: Cytochrome c1

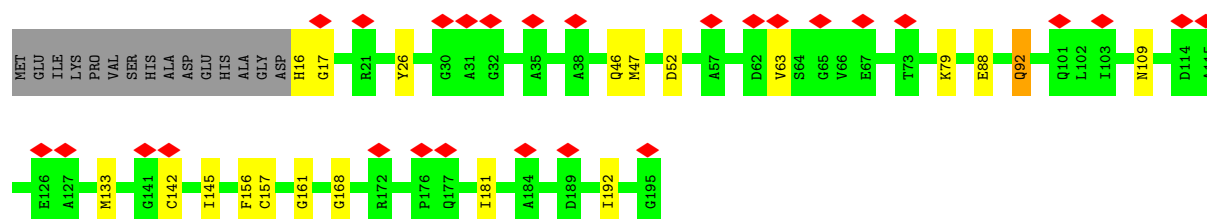
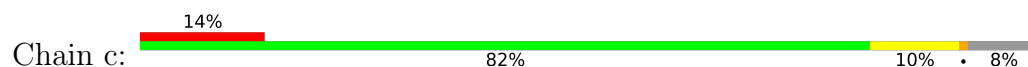


- Molecule 20: Cytochrome c1

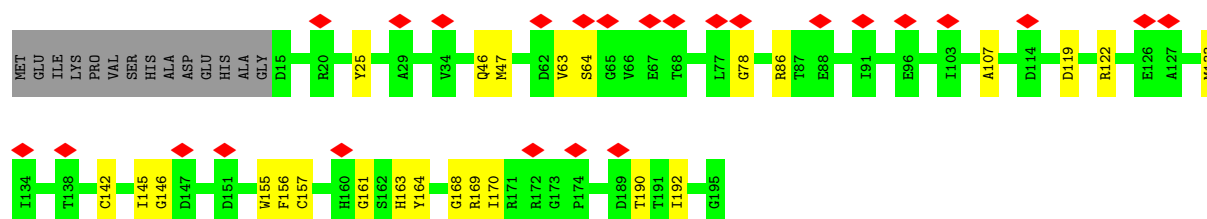
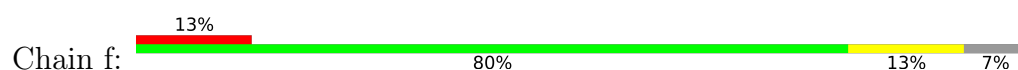




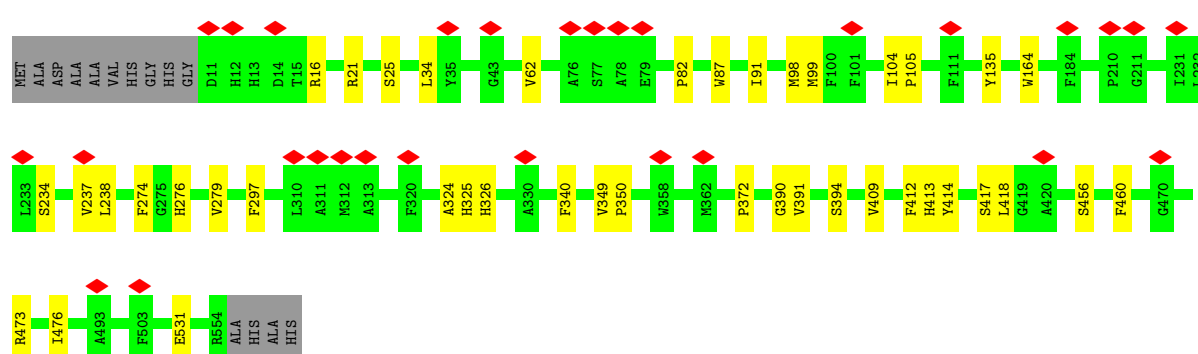
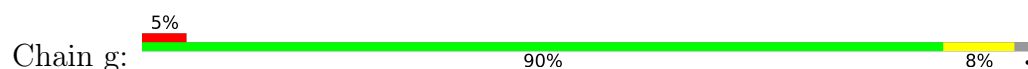
- Molecule 21: Ubiquinol-cytochrome c reductase iron-sulfur subunit



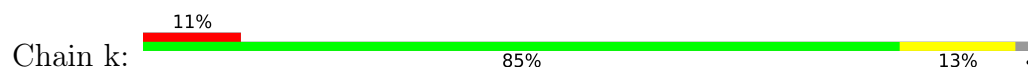
- Molecule 21: Ubiquinol-cytochrome c reductase iron-sulfur subunit

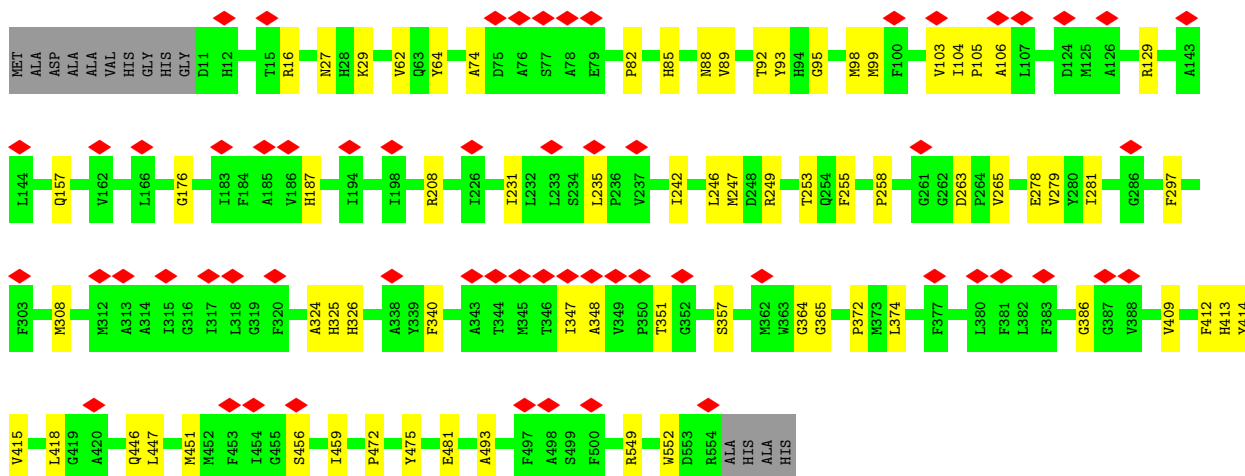


- Molecule 22: Cytochrome c oxidase subunit 1

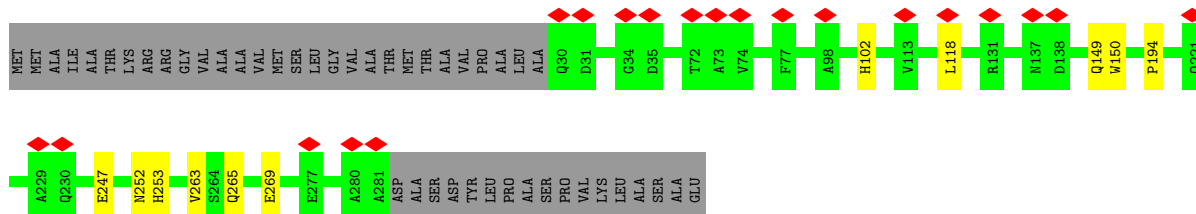
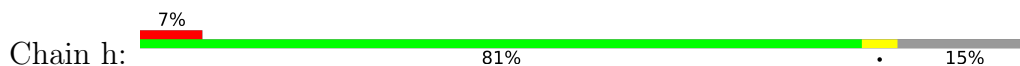


- Molecule 22: Cytochrome c oxidase subunit 1

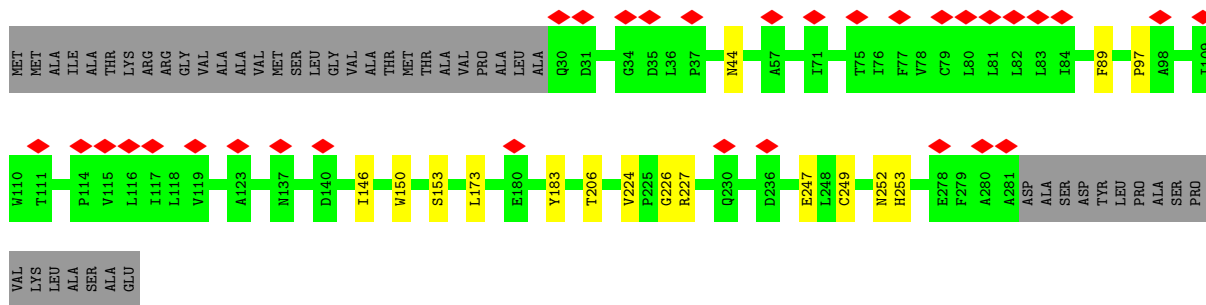
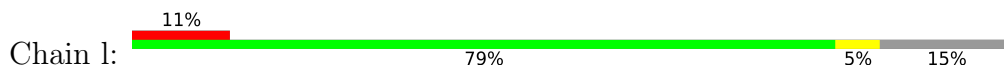




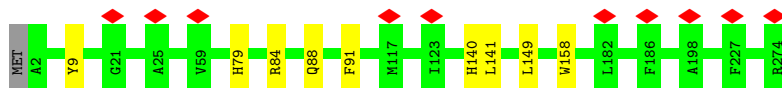
- Molecule 23: Cytochrome c oxidase subunit 2



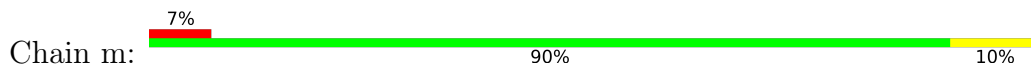
- Molecule 23: Cytochrome c oxidase subunit 2

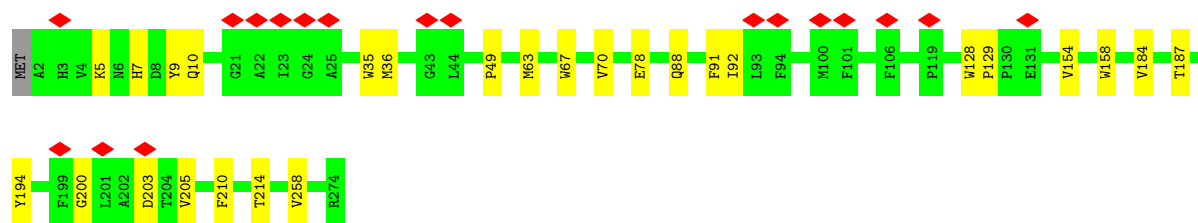


- Molecule 24: cytochrome-c oxidase

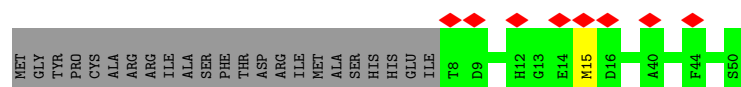


- Molecule 24: cytochrome-c oxidase

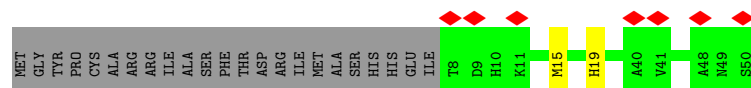




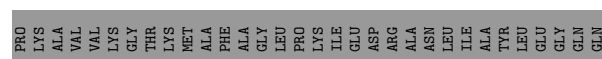
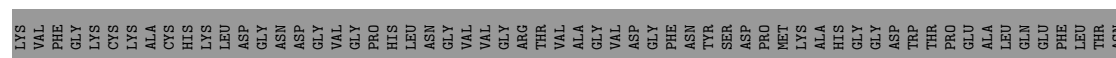
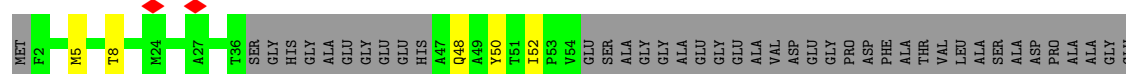
- Molecule 25: Aa3 type cytochrome c oxidase subunit IV



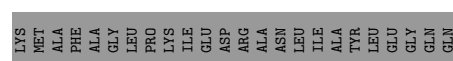
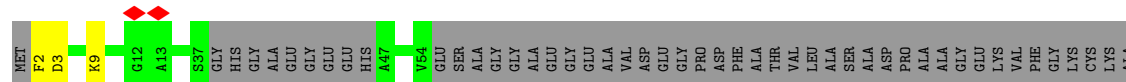
- Molecule 25: Aa3 type cytochrome c oxidase subunit IV



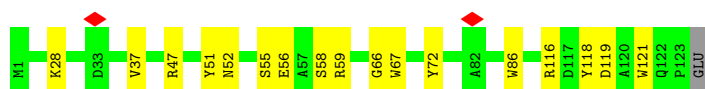
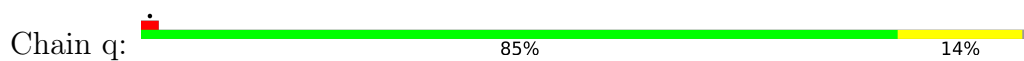
- Molecule 26: Cytochrome c, class I



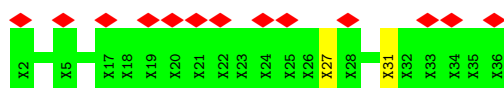
- Molecule 26: Cytochrome c, class I



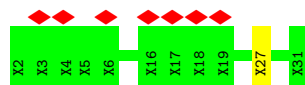
- Molecule 27: NADH:ubiquinone oxidoreductase 17.2 kD subunit



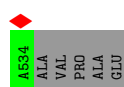
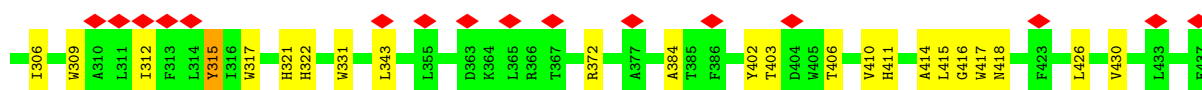
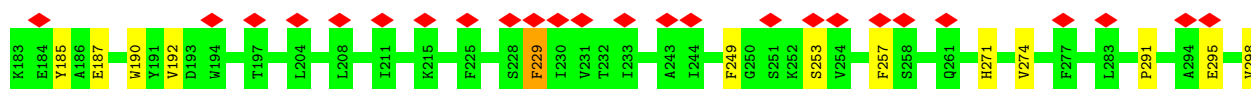
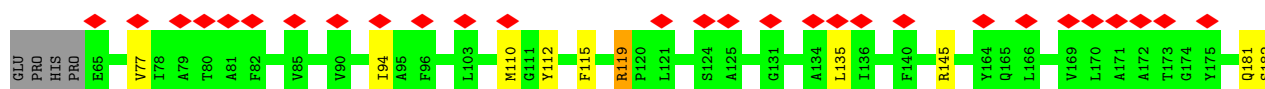
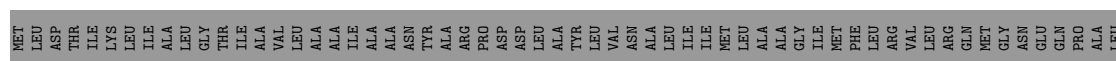
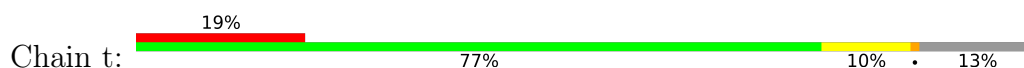
- Molecule 28: Transmembrane helix of unknown identity



- Molecule 29: Transmembrane helix of unknown identity



- Molecule 30: cytochrome-c oxidase



- Molecule 31: Cytochrome c oxidase, cbb3-type, subunit II





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	4238	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	55.2	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.068	Depositor
Minimum map value	-0.012	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0112	Depositor
Map size ($\text{\AA}$)	393.0, 393.0, 393.0	wwPDB
Map dimensions	375, 375, 375	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.048, 1.048, 1.048	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, HEC, NA, U10, DU0, CDL, MN, FME, FMN, CU, HEA, ZN, 2MR, SF4, FES, HEM, CUA

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	0/988	0.56	0/1345
2	B	0.32	0/1297	0.65	0/1758
3	C	0.32	0/1624	0.65	0/2208
4	D	0.32	0/3339	0.62	0/4520
5	E	0.25	0/1865	0.63	0/2537
6	F	0.28	0/3308	0.63	0/4456
7	G	0.28	0/5156	0.64	0/6982
8	H	0.32	0/2815	0.61	0/3837
9	I	0.33	0/1354	0.63	0/1828
10	J	0.31	0/1548	0.61	1/2104 (0.0%)
11	K	0.35	0/775	0.57	0/1050
12	L	0.25	0/5357	0.56	1/7293 (0.0%)
13	M	0.29	0/4010	0.58	0/5460
14	N	0.31	0/3634	0.56	0/4935
15	P	0.27	0/2511	0.65	1/3409 (0.0%)
16	Q	0.30	0/872	0.63	0/1181
17	R	0.23	0/503	0.67	0/685
18	Z	0.30	0/1669	0.62	0/2266
19	a	0.35	0/3641	0.60	0/4993
19	d	0.32	0/3650	0.62	0/5005
20	b	0.29	0/1906	0.54	0/2592
20	e	0.29	0/1906	0.63	0/2592
21	c	0.25	0/1382	0.55	0/1880
21	f	0.24	0/1390	0.55	0/1891
22	g	0.26	0/4483	0.62	0/6118
22	k	0.23	0/4483	0.60	0/6118
23	h	0.24	0/2033	0.60	0/2787
23	l	0.22	0/2033	0.60	0/2787
24	i	0.28	0/2270	0.52	0/3107
24	m	0.26	0/2270	0.56	0/3107
25	j	0.25	0/339	0.48	0/457
25	n	0.22	0/339	0.55	0/457

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
26	o	0.28	0/321	0.58	0/436
26	p	0.30	0/327	0.50	0/444
27	q	0.29	0/1049	0.63	0/1434
30	t	0.22	0/3863	0.62	0/5281
31	u	0.24	0/1551	0.59	0/2104
32	v	0.22	0/2154	0.60	0/2955
All	All	0.28	0/84015	0.60	3/114399 (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
2	B	0	1
3	C	0	1
6	F	0	3
7	G	0	2
8	H	0	1
12	L	0	1
13	M	0	1
14	N	0	2
15	P	0	2
16	Q	0	1
19	d	0	1
22	g	0	2
30	t	0	3
31	u	0	1
All	All	0	22

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	87	ARG	CA-CB-CG	-5.35	103.40	114.10
12	L	266	THR	N-CA-C	5.10	118.95	111.04
15	P	327	LEU	N-CA-C	5.10	116.92	111.36

There are no chirality outliers.

5 of 22 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	134	ARG	Sidechain
3	C	93	ARG	Sidechain
6	F	234	ARG	Sidechain
6	F	26	ARG	Sidechain
6	F	275	ARG	Sidechain

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	969	0	970	9	0
2	B	1270	0	1268	21	0
3	C	1586	0	1562	11	0
4	D	3277	0	3217	27	0
5	E	1822	0	1796	21	0
6	F	3241	0	3188	47	0
7	G	5068	0	5037	42	0
8	H	2722	0	2744	25	0
9	I	1319	0	1259	14	0
10	J	1528	0	1612	14	0
11	K	764	0	817	6	0
12	L	5193	0	5152	32	0
13	M	3915	0	4024	30	0
14	N	3556	0	3656	24	0
15	P	2468	0	2498	13	0
16	Q	849	0	812	7	0
17	R	488	0	450	6	0
18	Z	1642	0	1643	13	0
19	a	3504	0	3483	48	0
19	d	3513	0	3489	33	0
20	b	1855	0	1773	16	0
20	e	1855	0	1773	9	0
21	c	1353	0	1295	14	0
21	f	1361	0	1299	14	0
22	g	4322	0	4225	24	0
22	k	4322	0	4226	49	0
23	h	1976	0	1960	6	0
23	l	1976	0	1960	14	0
24	i	2183	0	2144	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	m	2183	0	2144	17	0
25	j	332	0	331	1	0
25	n	332	0	331	2	0
26	o	315	0	324	4	0
26	p	321	0	329	4	0
27	q	1018	0	942	10	0
28	r	175	0	38	1	0
29	s	150	0	33	1	0
30	t	3732	0	3692	32	0
31	u	1517	0	1507	21	0
32	v	2095	0	1968	17	0
33	B	8	0	0	3	0
33	F	8	0	0	2	0
33	G	16	0	0	1	0
33	I	16	0	0	0	0
34	D	1	0	0	0	0
35	E	4	0	0	1	0
35	G	4	0	0	0	0
35	c	4	0	0	0	0
35	f	4	0	0	0	0
36	F	31	0	19	6	0
37	H	37	0	0	0	0
37	N	37	0	0	0	0
37	f	37	0	0	0	0
38	H	63	0	90	8	0
38	a	126	0	180	12	0
38	d	126	0	180	9	0
39	R	1	0	0	0	0
40	a	100	0	156	3	0
41	a	86	0	60	11	0
41	d	86	0	60	11	0
41	t	86	0	60	5	0
42	b	1	0	0	0	0
42	e	1	0	0	0	0
42	g	1	0	0	0	0
42	k	1	0	0	0	0
42	t	2	0	0	0	0
43	b	43	0	30	1	0
43	e	43	0	30	1	0
43	u	43	0	30	4	0
43	v	86	0	60	6	0
44	g	120	0	108	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	k	120	0	108	9	0
45	g	1	0	0	0	0
45	k	1	0	0	0	0
45	t	1	0	0	0	0
46	g	1	0	0	0	0
47	h	2	0	0	0	0
47	l	2	0	0	0	0
All	All	83417	0	82142	645	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 4.

The worst 5 of 645 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)
31:u:210:ARG:H	31:u:211:PRO:HD2	1.51	0.75
22:k:308:MET:HE3	22:k:357:SER:HB2	1.69	0.74
5:E:204:HIS:O	6:F:18:ARG:NH2	2.20	0.74
1:A:21:LEU:HD13	38:H:402:U10:H561	1.72	0.71
22:k:98:MET:HB3	44:k:601:HEA:CAC	2.24	0.68

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	119/121 (98%)	114 (96%)	5 (4%)	0	100	100
2	B	160/175 (91%)	155 (97%)	4 (2%)	1 (1%)	21	59
3	C	192/208 (92%)	185 (96%)	7 (4%)	0	100	100
4	D	408/412 (99%)	394 (97%)	14 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	235/239 (98%)	226 (96%)	8 (3%)	1 (0%)	30	67
6	F	420/431 (97%)	402 (96%)	18 (4%)	0	100	100
7	G	663/674 (98%)	635 (96%)	27 (4%)	1 (0%)	43	78
8	H	339/345 (98%)	328 (97%)	11 (3%)	0	100	100
9	I	160/163 (98%)	157 (98%)	3 (2%)	0	100	100
10	J	197/199 (99%)	194 (98%)	3 (2%)	0	100	100
11	K	99/101 (98%)	98 (99%)	1 (1%)	0	100	100
12	L	654/703 (93%)	625 (96%)	28 (4%)	1 (0%)	43	78
13	M	501/513 (98%)	494 (99%)	6 (1%)	1 (0%)	43	78
14	N	478/499 (96%)	468 (98%)	10 (2%)	0	100	100
15	P	326/330 (99%)	317 (97%)	8 (2%)	1 (0%)	36	72
16	Q	101/103 (98%)	101 (100%)	0	0	100	100
17	R	59/62 (95%)	54 (92%)	5 (8%)	0	100	100
18	Z	214/217 (99%)	206 (96%)	8 (4%)	0	100	100
19	a	431/440 (98%)	422 (98%)	9 (2%)	0	100	100
19	d	432/440 (98%)	425 (98%)	7 (2%)	0	100	100
20	b	237/450 (53%)	231 (98%)	6 (2%)	0	100	100
20	e	237/450 (53%)	234 (99%)	2 (1%)	1 (0%)	30	67
21	c	178/195 (91%)	171 (96%)	7 (4%)	0	100	100
21	f	179/195 (92%)	174 (97%)	5 (3%)	0	100	100
22	g	542/558 (97%)	528 (97%)	14 (3%)	0	100	100
22	k	542/558 (97%)	526 (97%)	16 (3%)	0	100	100
23	h	250/298 (84%)	240 (96%)	10 (4%)	0	100	100
23	l	250/298 (84%)	240 (96%)	10 (4%)	0	100	100
24	i	271/274 (99%)	263 (97%)	8 (3%)	0	100	100
24	m	271/274 (99%)	262 (97%)	9 (3%)	0	100	100
25	j	41/66 (62%)	40 (98%)	1 (2%)	0	100	100
25	n	41/66 (62%)	40 (98%)	1 (2%)	0	100	100
26	o	39/176 (22%)	39 (100%)	0	0	100	100
26	p	40/176 (23%)	40 (100%)	0	0	100	100
27	q	121/124 (98%)	116 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	t	468/539 (87%)	439 (94%)	27 (6%)	2 (0%)	30	67
31	u	187/241 (78%)	177 (95%)	8 (4%)	2 (1%)	11	46
32	v	274/349 (78%)	245 (89%)	25 (9%)	4 (2%)	8	40
All	All	10356/11662 (89%)	10005 (97%)	336 (3%)	15 (0%)	49	83

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
31	u	210	ARG
13	M	238	VAL
32	v	283	ALA
5	E	137	CYS
20	e	369	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	97/97 (100%)	97 (100%)	0	100	100
2	B	136/145 (94%)	134 (98%)	2 (2%)	57	72
3	C	172/183 (94%)	172 (100%)	0	100	100
4	D	341/342 (100%)	341 (100%)	0	100	100
5	E	189/190 (100%)	189 (100%)	0	100	100
6	F	331/335 (99%)	330 (100%)	1 (0%)	86	86
7	G	530/535 (99%)	529 (100%)	1 (0%)	87	87
8	H	277/279 (99%)	276 (100%)	1 (0%)	84	84
9	I	136/137 (99%)	136 (100%)	0	100	100
10	J	158/158 (100%)	158 (100%)	0	100	100
11	K	81/81 (100%)	80 (99%)	1 (1%)	63	75
12	L	518/543 (95%)	518 (100%)	0	100	100
13	M	410/416 (99%)	408 (100%)	2 (0%)	81	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	N	357/369 (97%)	355 (99%)	2 (1%)	78	83
15	P	248/250 (99%)	248 (100%)	0	100	100
16	Q	87/87 (100%)	87 (100%)	0	100	100
17	R	51/52 (98%)	51 (100%)	0	100	100
18	Z	167/168 (99%)	167 (100%)	0	100	100
19	a	360/366 (98%)	360 (100%)	0	100	100
19	d	361/366 (99%)	361 (100%)	0	100	100
20	b	192/319 (60%)	192 (100%)	0	100	100
20	e	192/319 (60%)	192 (100%)	0	100	100
21	c	139/151 (92%)	138 (99%)	1 (1%)	76	81
21	f	140/151 (93%)	140 (100%)	0	100	100
22	g	447/454 (98%)	447 (100%)	0	100	100
22	k	447/454 (98%)	445 (100%)	2 (0%)	84	84
23	h	211/243 (87%)	210 (100%)	1 (0%)	81	83
23	l	211/243 (87%)	211 (100%)	0	100	100
24	i	220/221 (100%)	220 (100%)	0	100	100
24	m	220/221 (100%)	219 (100%)	1 (0%)	81	83
25	j	34/53 (64%)	34 (100%)	0	100	100
25	n	34/53 (64%)	34 (100%)	0	100	100
26	o	32/126 (25%)	31 (97%)	1 (3%)	35	56
26	p	33/126 (26%)	33 (100%)	0	100	100
27	q	103/104 (99%)	103 (100%)	0	100	100
30	t	376/428 (88%)	369 (98%)	7 (2%)	50	67
31	u	163/205 (80%)	159 (98%)	4 (2%)	42	63
32	v	211/269 (78%)	206 (98%)	5 (2%)	43	64
All	All	8412/9239 (91%)	8380 (100%)	32 (0%)	81	84

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
32	v	117	VAL
32	v	162	ASP
22	k	279	VAL

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Mol	Chain	Res	Type
23	h	102	HIS
32	v	256	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 58 such sidechains are listed below:

Mol	Chain	Res	Type
20	b	394	GLN
30	t	322	HIS
20	e	372	GLN
30	t	155	ASN
22	k	526	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
10	FME	J	1	10	8,9,10	0.97	0	7,9,11	0.81	0
4	2MR	D	65	4	10,12,13	2.41	2 (20%)	5,13,15	1.19	1 (20%)
27	FME	q	1	27	8,9,10	0.97	0	7,9,11	0.90	0
12	FME	L	1	12	8,9,10	0.89	0	7,9,11	1.42	1 (14%)
13	FME	M	1	13	8,9,10	0.99	0	7,9,11	1.12	1 (14%)
1	FME	A	1	1	8,9,10	0.88	0	7,9,11	0.97	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
10	FME	J	1	10	-	1/7/9/11	-
4	2MR	D	65	4	-	1/10/13/15	-
27	FME	q	1	27	-	1/7/9/11	-
12	FME	L	1	12	-	0/7/9/11	-
13	FME	M	1	13	-	4/7/9/11	-
1	FME	A	1	1	-	1/7/9/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	65	2MR	CZ-NH2	5.20	1.44	1.33
4	D	65	2MR	CZ-NE	4.80	1.44	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	1	FME	C-CA-N	2.89	114.94	109.73
4	D	65	2MR	NE-CZ-NH2	-2.63	117.07	119.48
13	M	1	FME	C-CA-N	2.31	113.91	109.73

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	65	2MR	O-C-CA-CB
10	J	1	FME	O-C-CA-CB
13	M	1	FME	O-C-CA-CB
13	M	1	FME	N-CA-CB-CG
13	M	1	FME	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 49 ligands modelled in this entry, 12 are monoatomic - leaving 37 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	SF4	I	1002	9	0,12,12	-	-	-		
47	CUA	l	301	23	0,1,1	-	-	-		
47	CUA	h	301	23	0,1,1	-	-	-		
38	U10	a	504	-	63,63,63	0.69	0	76,79,79	1.00	3 (3%)
33	SF4	I	1001	9	0,12,12	-	-	-		
41	HEM	t	603	42,30	50,50,50	1.36	5 (10%)	66,82,82	1.04	2 (3%)
41	HEM	d	502	19	50,50,50	1.36	6 (12%)	66,82,82	1.16	6 (9%)
37	DU0	f	201	-	42,42,42	0.64	0	66,66,66	0.84	4 (6%)
35	FES	c	1000	21	0,4,4	-	-	-		
43	HEC	v	1001	32	50,50,50	1.77	6 (12%)	68,82,82	1.78	14 (20%)
44	HEA	k	602	22	66,67,67	1.70	10 (15%)	78,103,103	2.34	29 (37%)
41	HEM	t	602	42,45,30	50,50,50	1.47	7 (14%)	66,82,82	1.10	4 (6%)
33	SF4	F	501	6	0,12,12	-	-	-		
44	HEA	k	601	22	66,67,67	1.46	6 (9%)	78,103,103	2.49	27 (34%)
33	SF4	B	1001	2	0,12,12	-	-	-		
37	DU0	H	401	-	42,42,42	0.58	0	66,66,66	0.86	0
43	HEC	b	502	20	50,50,50	1.58	2 (4%)	68,82,82	1.54	10 (14%)
44	HEA	g	602	22	66,67,67	1.40	8 (12%)	78,103,103	2.29	26 (33%)
38	U10	d	501	-	63,63,63	0.68	0	76,79,79	1.15	5 (6%)
33	SF4	G	702	7	0,12,12	-	-	-		
43	HEC	e	502	20	50,50,50	1.56	2 (4%)	68,82,82	1.72	12 (17%)
33	SF4	G	701	7	0,12,12	-	-	-		
41	HEM	a	505	19	50,50,50	1.46	8 (16%)	66,82,82	1.21	6 (9%)
38	U10	H	402	-	63,63,63	0.67	0	76,79,79	1.31	9 (11%)
35	FES	E	401	5	0,4,4	-	-	-		
35	FES	f	202	21	0,4,4	-	-	-		
41	HEM	d	503	19	50,50,50	1.37	5 (10%)	66,82,82	1.05	4 (6%)
37	DU0	N	501	-	42,42,42	0.63	0	66,66,66	0.82	1 (1%)
43	HEC	v	1002	32	50,50,50	1.69	6 (12%)	68,82,82	1.65	11 (16%)
36	FMN	F	502	-	33,33,33	1.05	2 (6%)	48,50,50	1.29	9 (18%)
41	HEM	a	503	19	50,50,50	1.42	6 (12%)	66,82,82	1.04	3 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
44	HEA	g	603	22	66,67,67	1.41	8 (12%)	78,103,103	2.44	29 (37%)
43	HEC	u	1000	31	50,50,50	1.67	5 (10%)	68,82,82	1.53	9 (13%)
35	FES	G	703	7	0,4,4	-	-	-	-	-
38	U10	d	504	-	63,63,63	0.70	0	76,79,79	1.07	5 (6%)
40	CDL	a	501	-	99,99,99	0.91	6 (6%)	105,111,111	0.92	4 (3%)
38	U10	a	502	-	63,63,63	0.68	0	76,79,79	1.03	5 (6%)

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	SF4	I	1002	9	-	-	0/6/5/5
38	U10	a	504	-	-	8/63/87/87	0/1/1/1
33	SF4	I	1001	9	-	-	0/6/5/5
41	HEM	t	603	42,30	-	7/14/54/54	-
41	HEM	d	502	19	-	8/14/54/54	-
37	DU0	f	201	-	-	2/10/98/98	0/6/6/6
35	FES	c	1000	21	-	-	0/1/1/1
43	HEC	v	1001	32	1/1/3/7	4/14/54/54	-
44	HEA	k	602	22	-	11/36/76/76	-
41	HEM	t	602	42,45,30	-	5/14/54/54	-
33	SF4	F	501	6	-	-	0/6/5/5
44	HEA	k	601	22	-	5/36/76/76	-
37	DU0	H	401	-	-	0/10/98/98	0/6/6/6
43	HEC	b	502	20	-	6/14/54/54	-
44	HEA	g	602	22	-	11/36/76/76	-
33	SF4	B	1001	2	-	-	0/6/5/5
38	U10	d	501	-	-	18/63/87/87	0/1/1/1
33	SF4	G	702	7	-	-	0/6/5/5
43	HEC	e	502	20	1/1/3/7	8/14/54/54	-
41	HEM	a	505	19	-	5/14/54/54	-
33	SF4	G	701	7	-	-	0/6/5/5
38	U10	H	402	-	-	22/63/87/87	0/1/1/1
35	FES	E	401	5	-	-	0/1/1/1
35	FES	f	202	21	-	-	0/1/1/1
41	HEM	d	503	19	-	8/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	DU0	N	501	-	-	0/10/98/98	0/6/6/6
43	HEC	v	1002	32	1/1/3/7	4/14/54/54	-
36	FMN	F	502	-	-	2/18/18/18	0/3/3/3
41	HEM	a	503	19	-	6/14/54/54	-
44	HEA	g	603	22	-	5/36/76/76	-
43	HEC	u	1000	31	1/1/3/7	8/14/54/54	-
35	FES	G	703	7	-	-	0/1/1/1
38	U10	d	504	-	-	8/63/87/87	0/1/1/1
40	CDL	a	501	-	-	24/110/110/110	-
38	U10	a	502	-	-	13/63/87/87	0/1/1/1

The worst 5 of 98 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	v	1001	HEC	C3D-C2D	7.78	1.53	1.36
43	v	1002	HEC	C3D-C2D	7.70	1.53	1.36
43	u	1000	HEC	C3D-C2D	7.37	1.52	1.36
43	b	502	HEC	C3D-C2D	7.00	1.51	1.36
43	e	502	HEC	C3D-C2D	6.80	1.51	1.36

The worst 5 of 237 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	k	602	HEA	C4B-NB-C1B	6.49	111.78	105.07
44	k	601	HEA	CAA-CBA-CGA	-6.42	99.79	113.60
44	k	601	HEA	C3A-C2A-C1A	-6.42	100.95	107.08
44	k	602	HEA	C4A-NA-C1A	6.31	111.53	105.35
44	g	602	HEA	C3A-C2A-C1A	-6.27	101.09	107.08

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
43	e	502	HEC	NA
43	u	1000	HEC	NA
43	v	1001	HEC	NA
43	v	1002	HEC	NA

5 of 198 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
38	H	402	U10	C23-C24-C26-C27
38	H	402	U10	C25-C24-C26-C27
38	d	501	U10	C4-C3-O3-C3M
38	d	501	U10	C6-C7-C8-C9
38	d	504	U10	C3-C4-O4-C4M

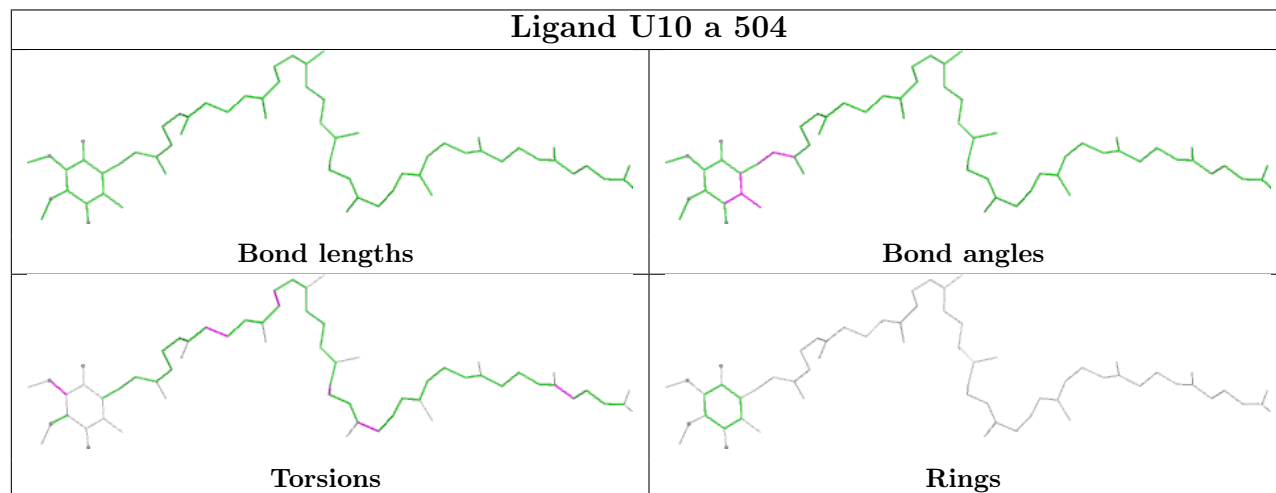
There are no ring outliers.

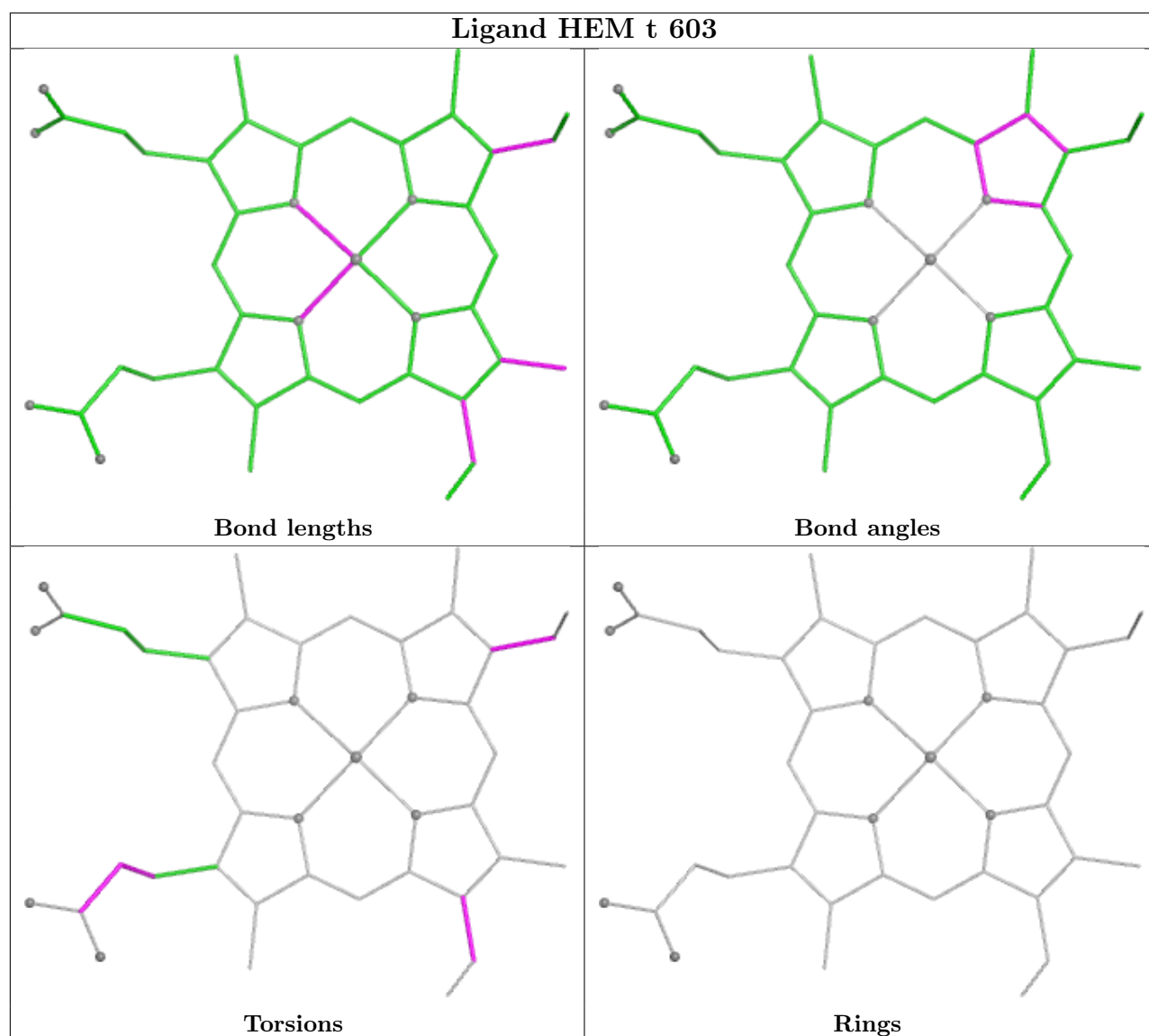
26 monomers are involved in 98 short contacts:

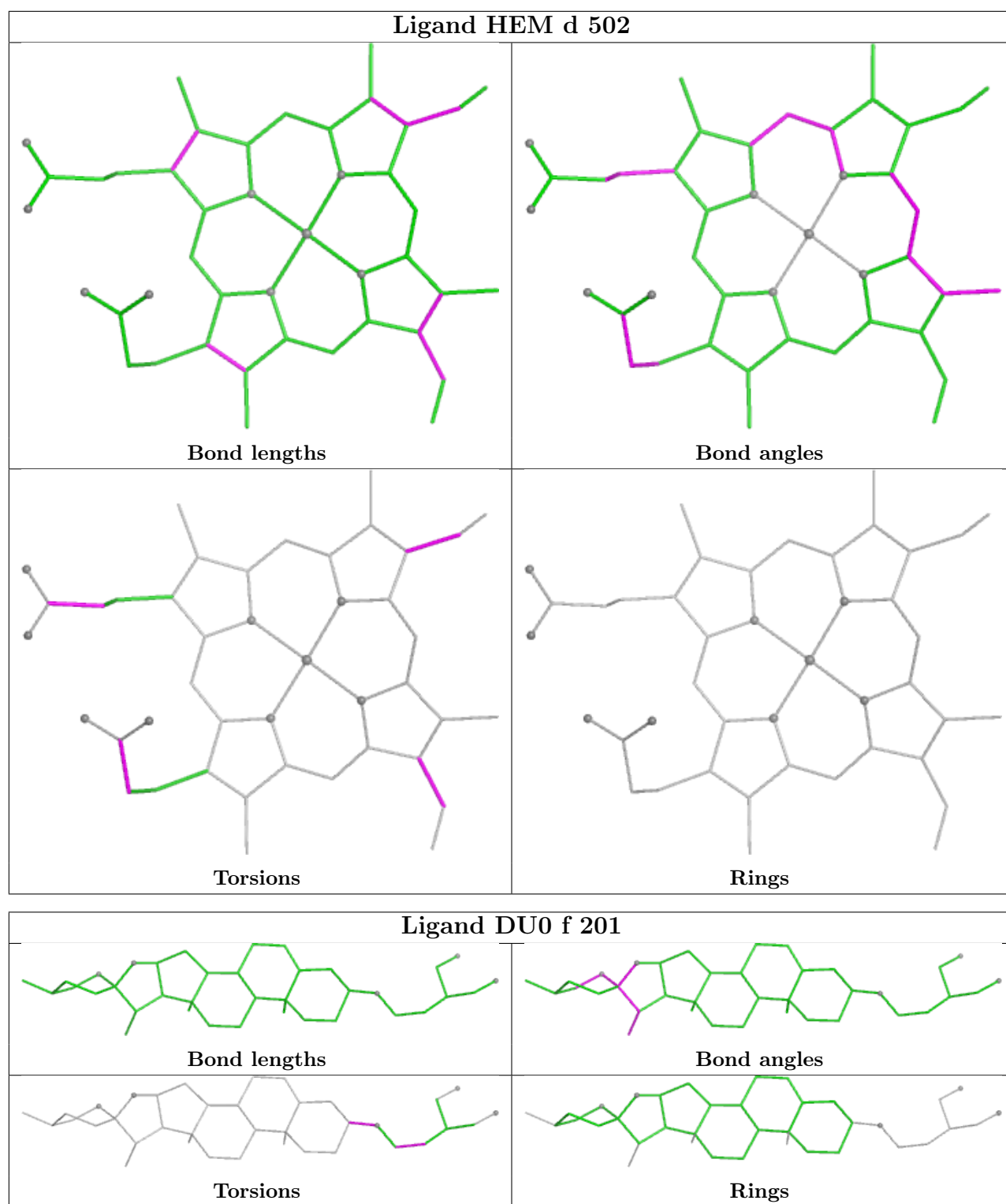
Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	a	504	U10	6	0
41	t	603	HEM	1	0
41	d	502	HEM	7	0
43	v	1001	HEC	3	0
44	k	602	HEA	2	0
41	t	602	HEM	4	0
33	F	501	SF4	2	0
44	k	601	HEA	7	0
33	B	1001	SF4	3	0
43	b	502	HEC	1	0
44	g	602	HEA	4	0
38	d	501	U10	8	0
43	e	502	HEC	1	0
33	G	701	SF4	1	0
41	a	505	HEM	7	0
38	H	402	U10	8	0
35	E	401	FES	1	0
41	d	503	HEM	4	0
43	v	1002	HEC	3	0
36	F	502	FMN	6	0
41	a	503	HEM	4	0
44	g	603	HEA	3	0
43	u	1000	HEC	4	0
38	d	504	U10	1	0
40	a	501	CDL	3	0
38	a	502	U10	6	0

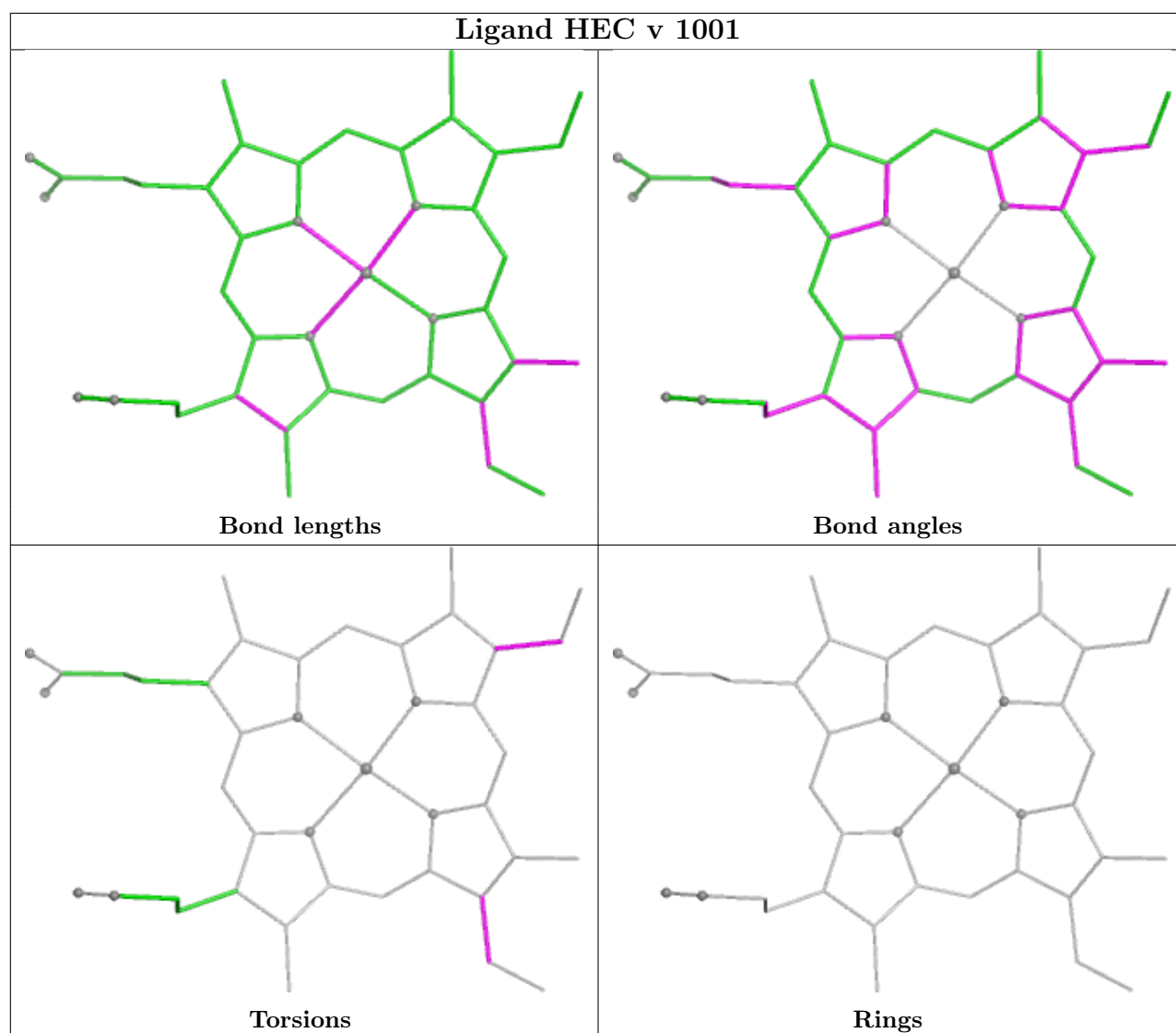
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

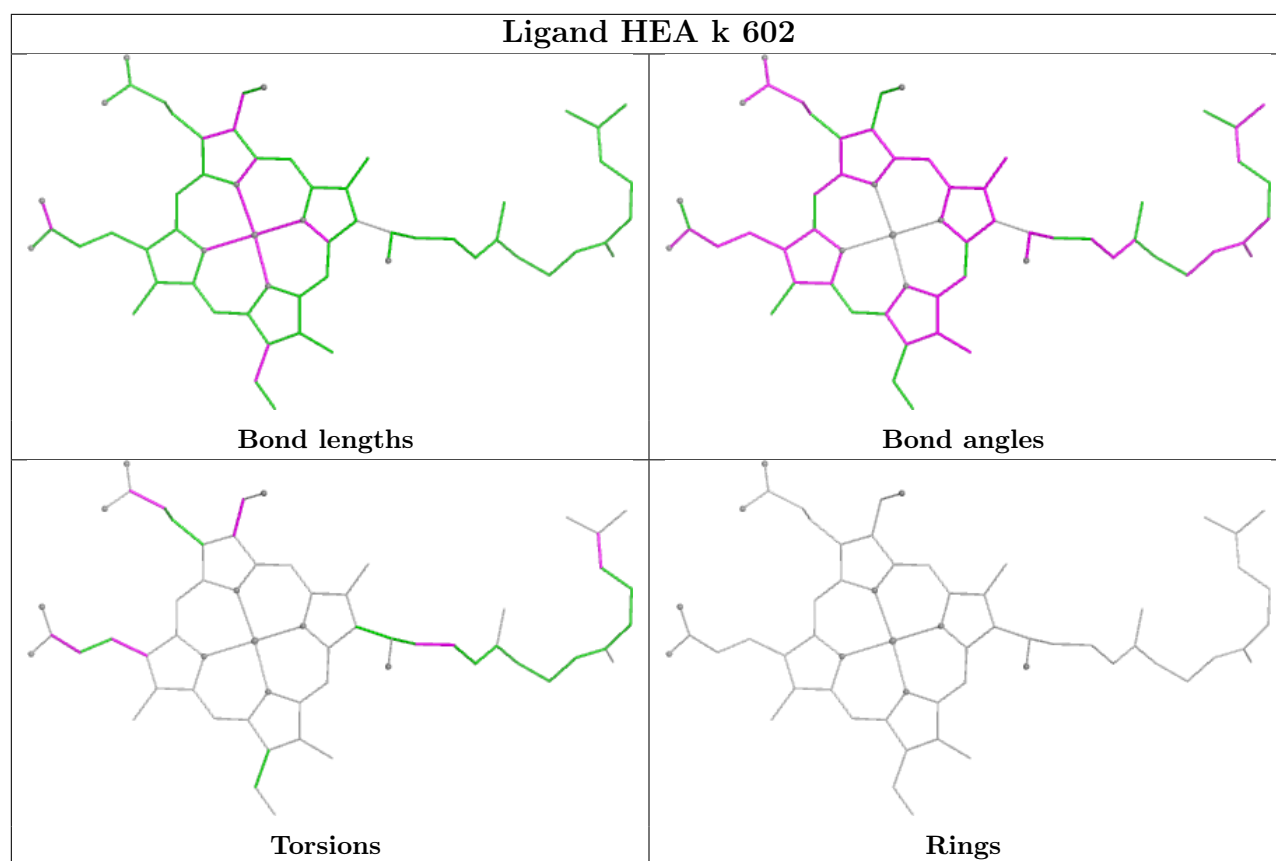
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.



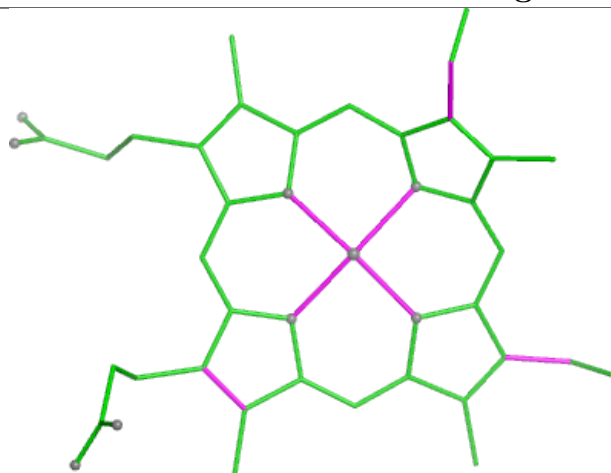




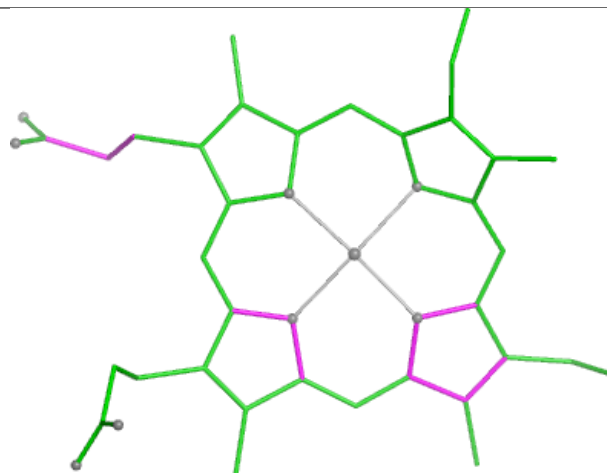




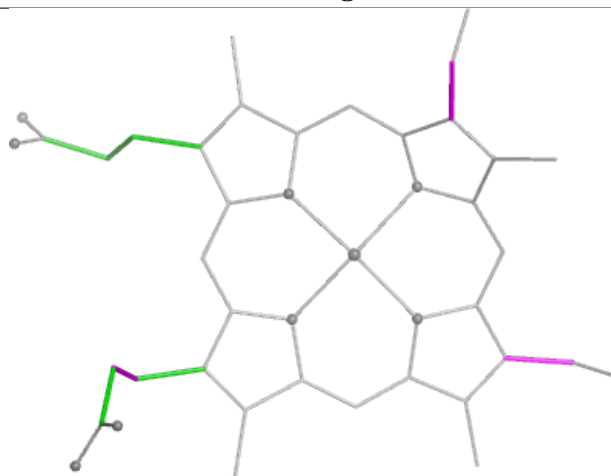
Ligand HEM t 602



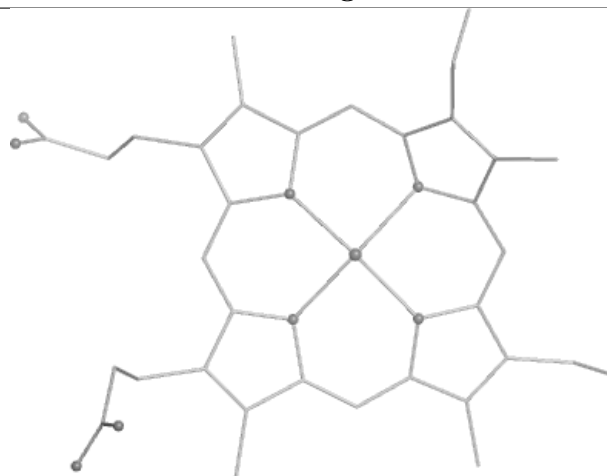
Bond lengths



Bond angles

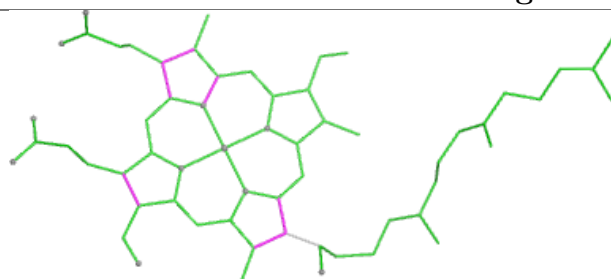


Torsions

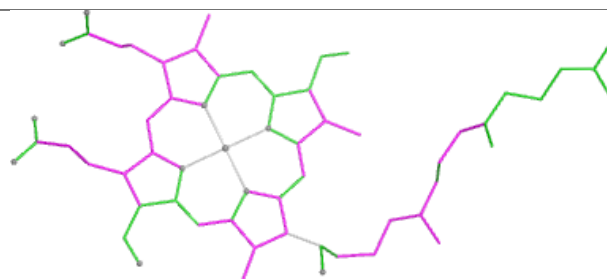


Rings

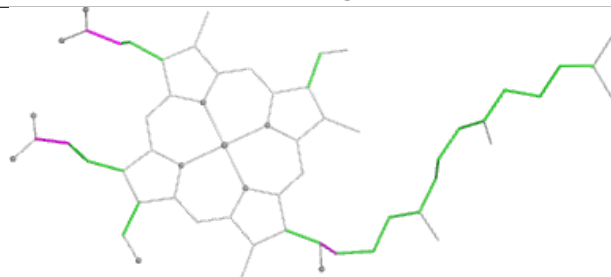
Ligand HEA k 601



Bond lengths



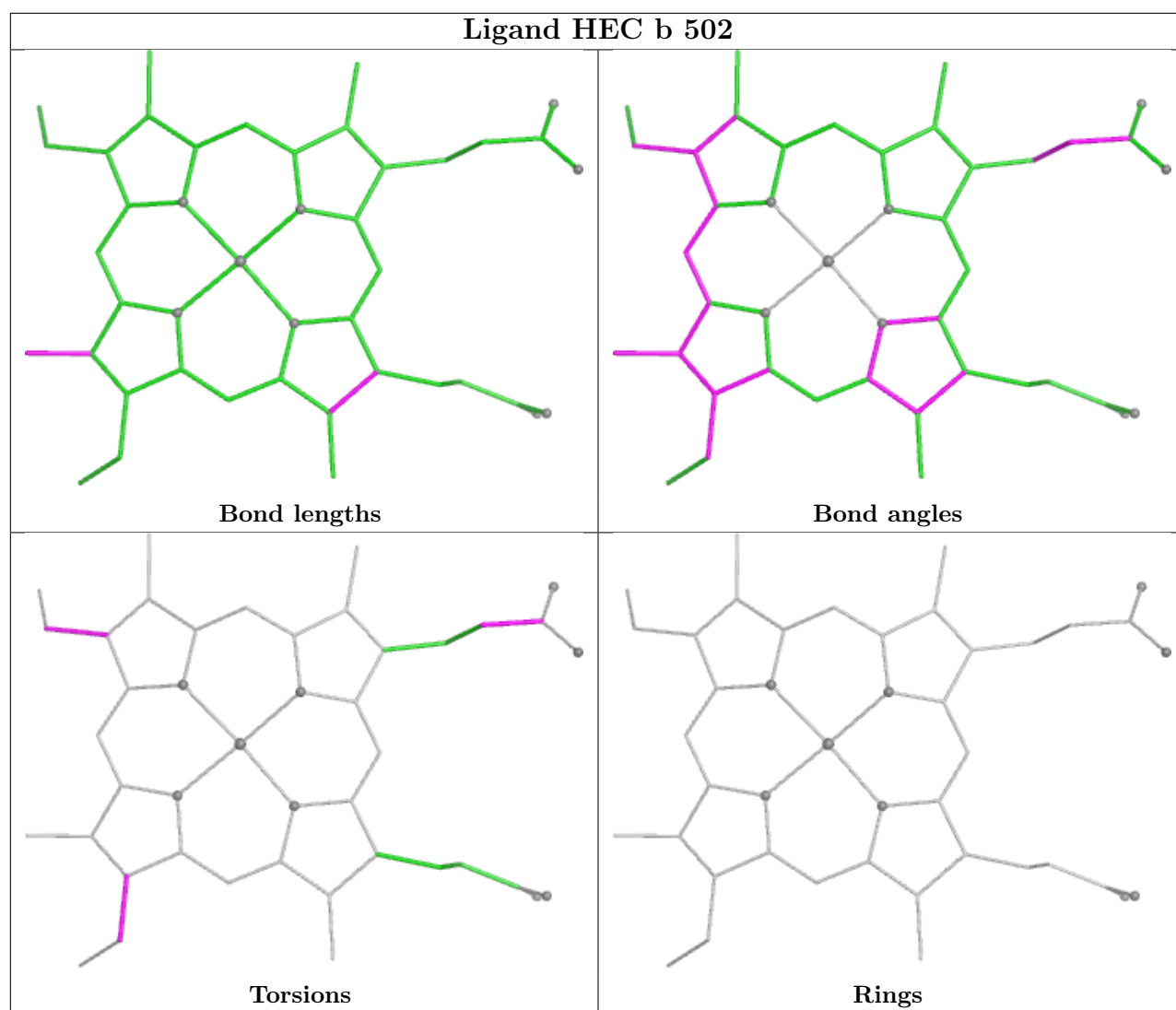
Bond angles

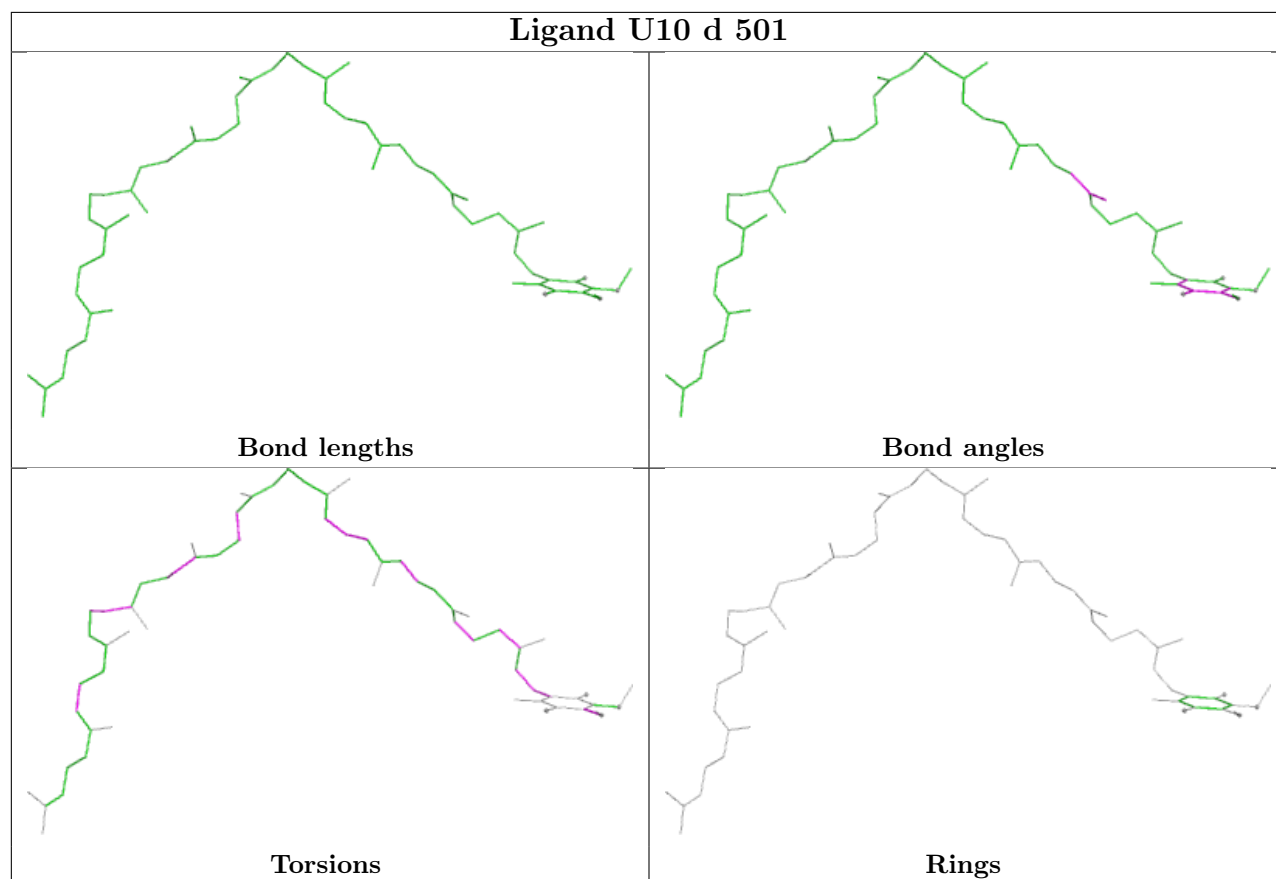
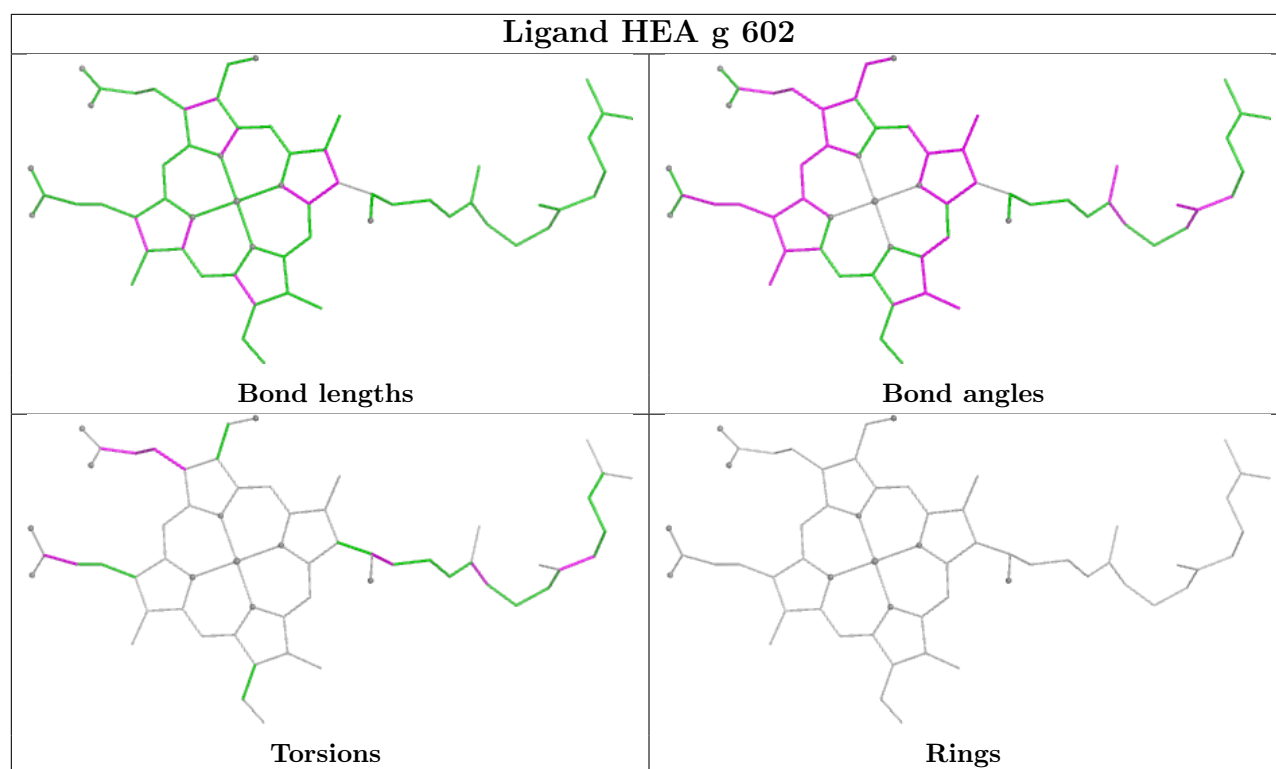


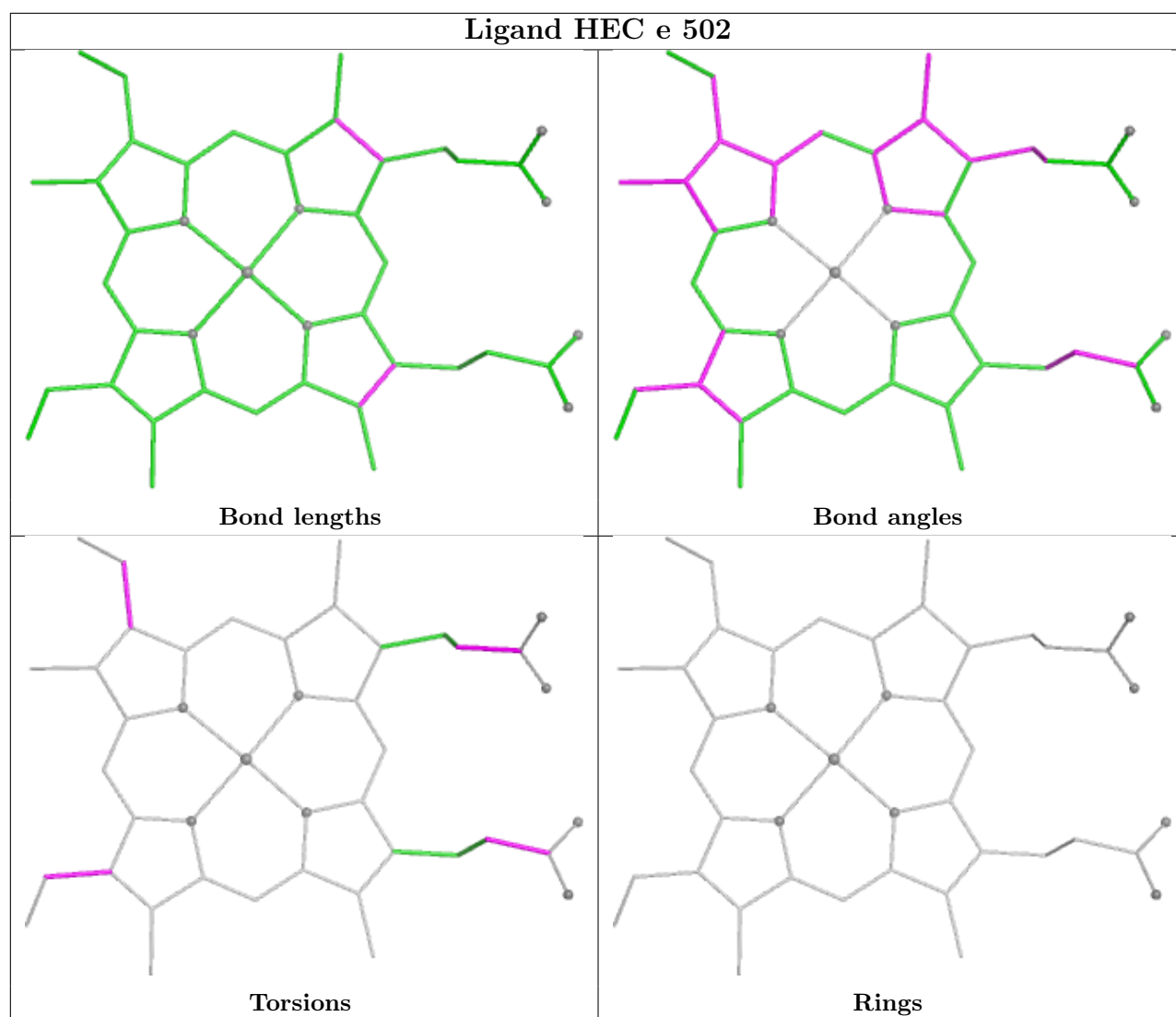
Torsions

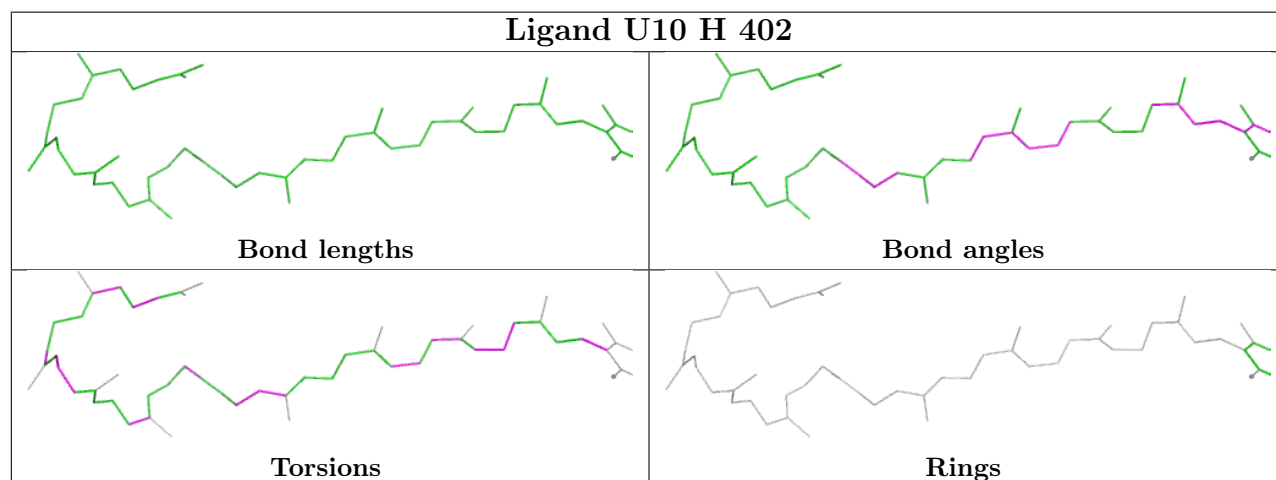
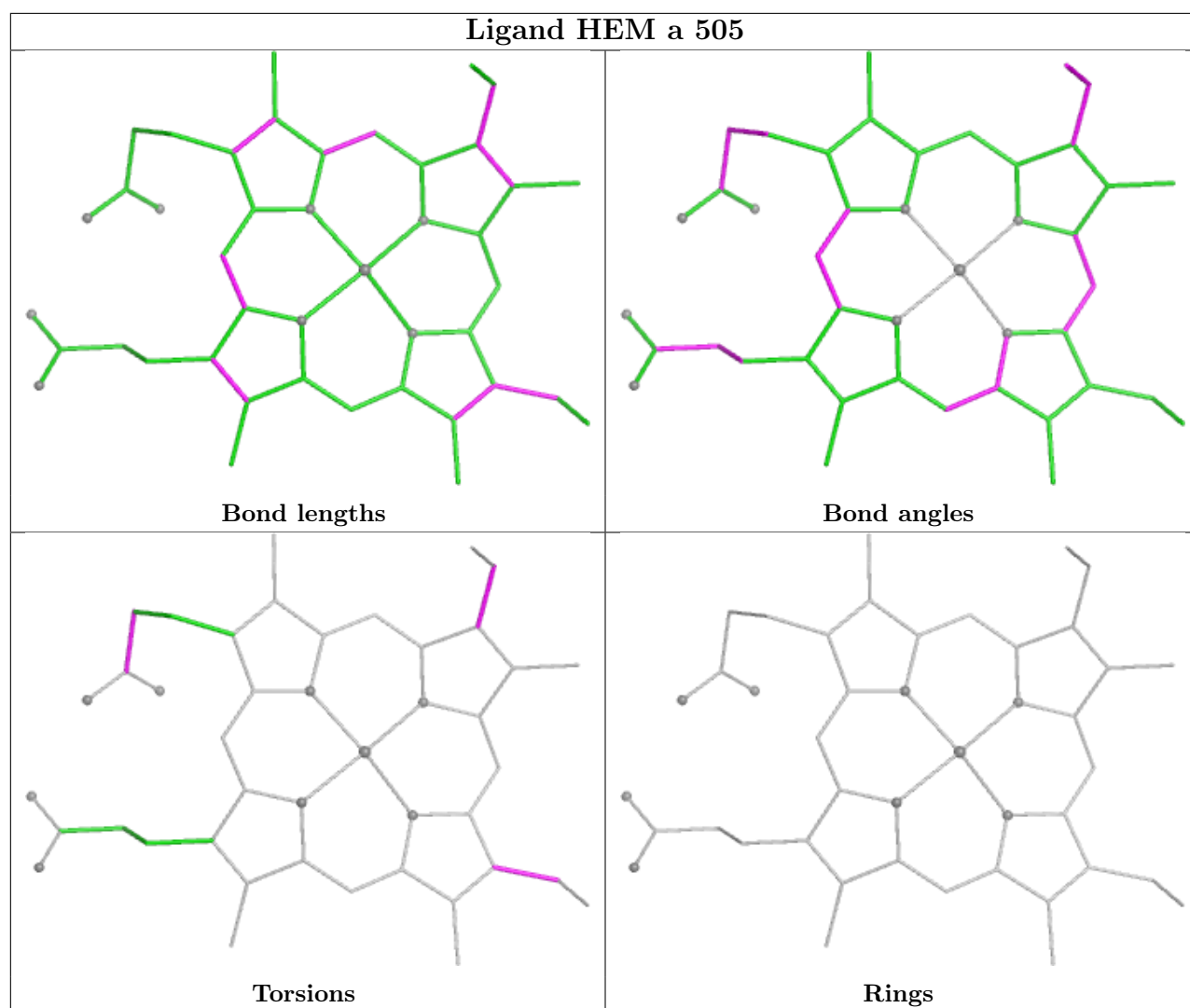


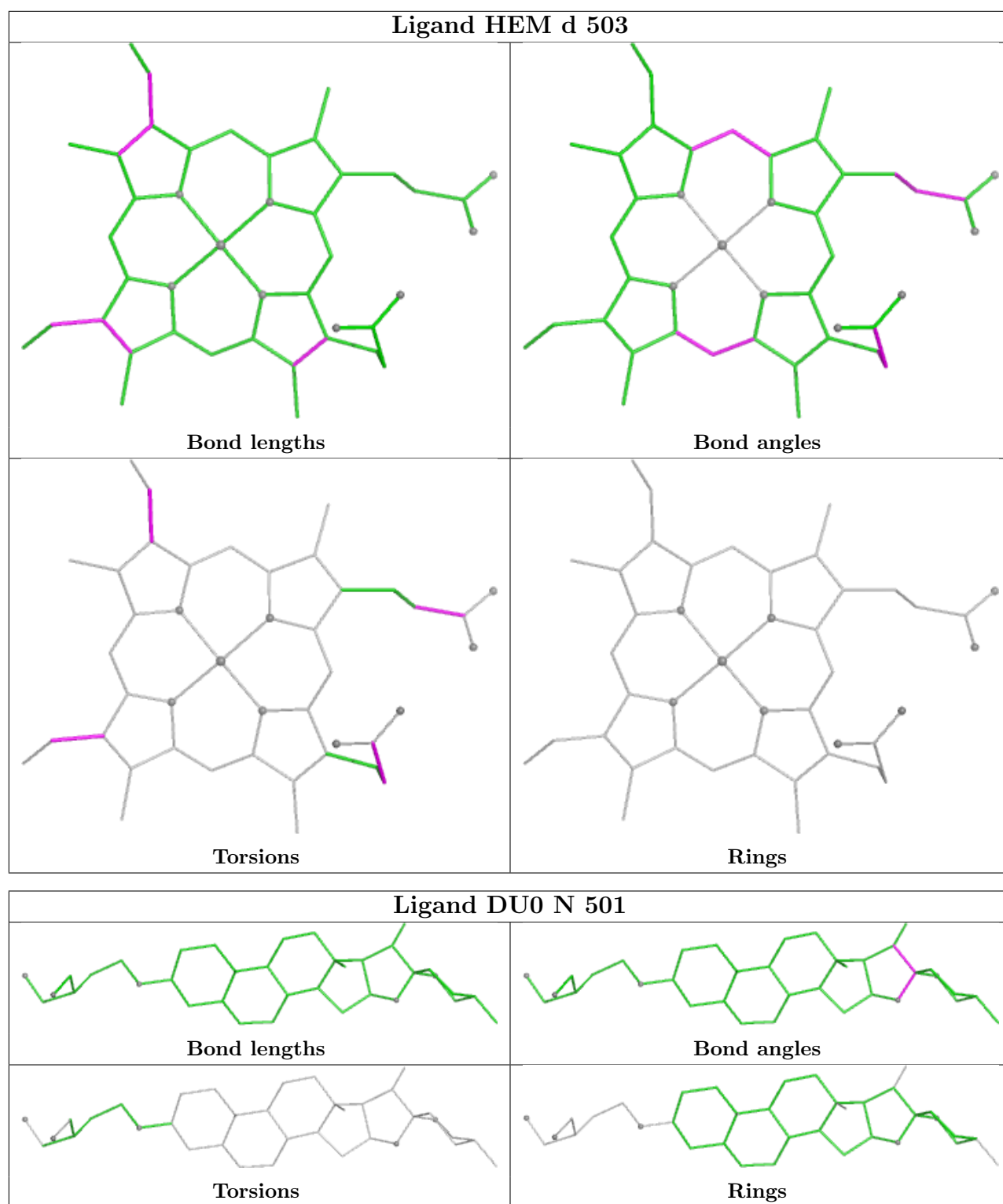
Rings

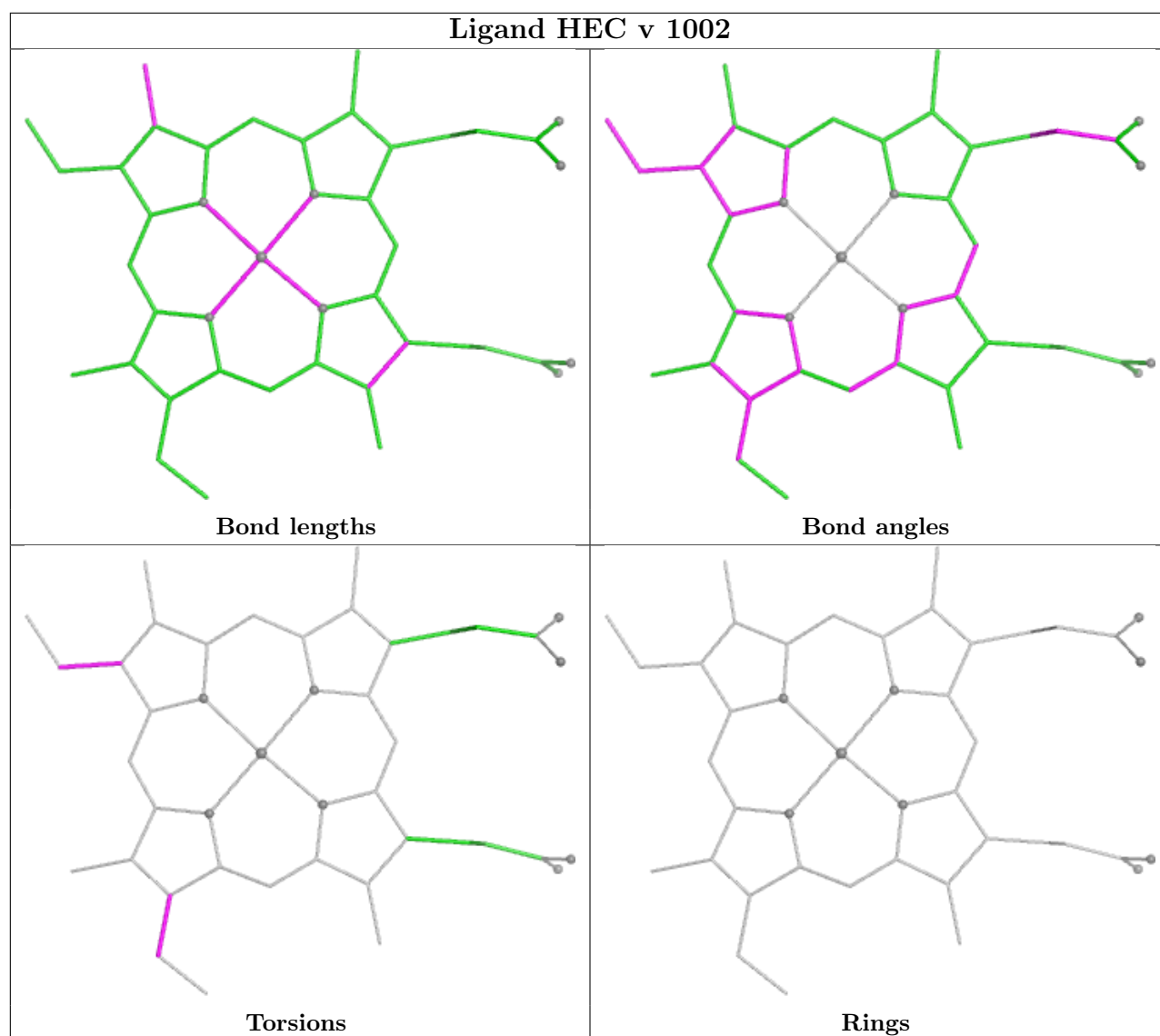


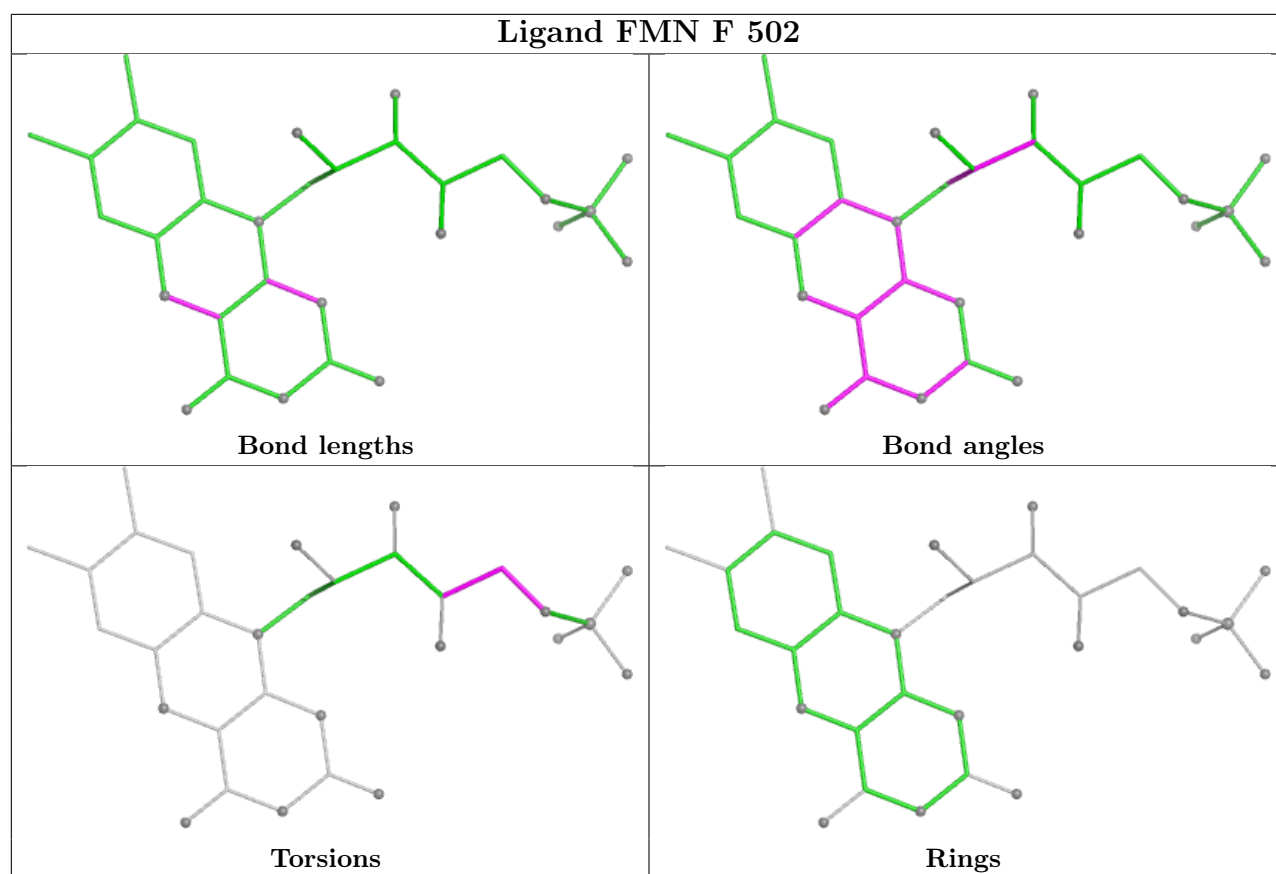


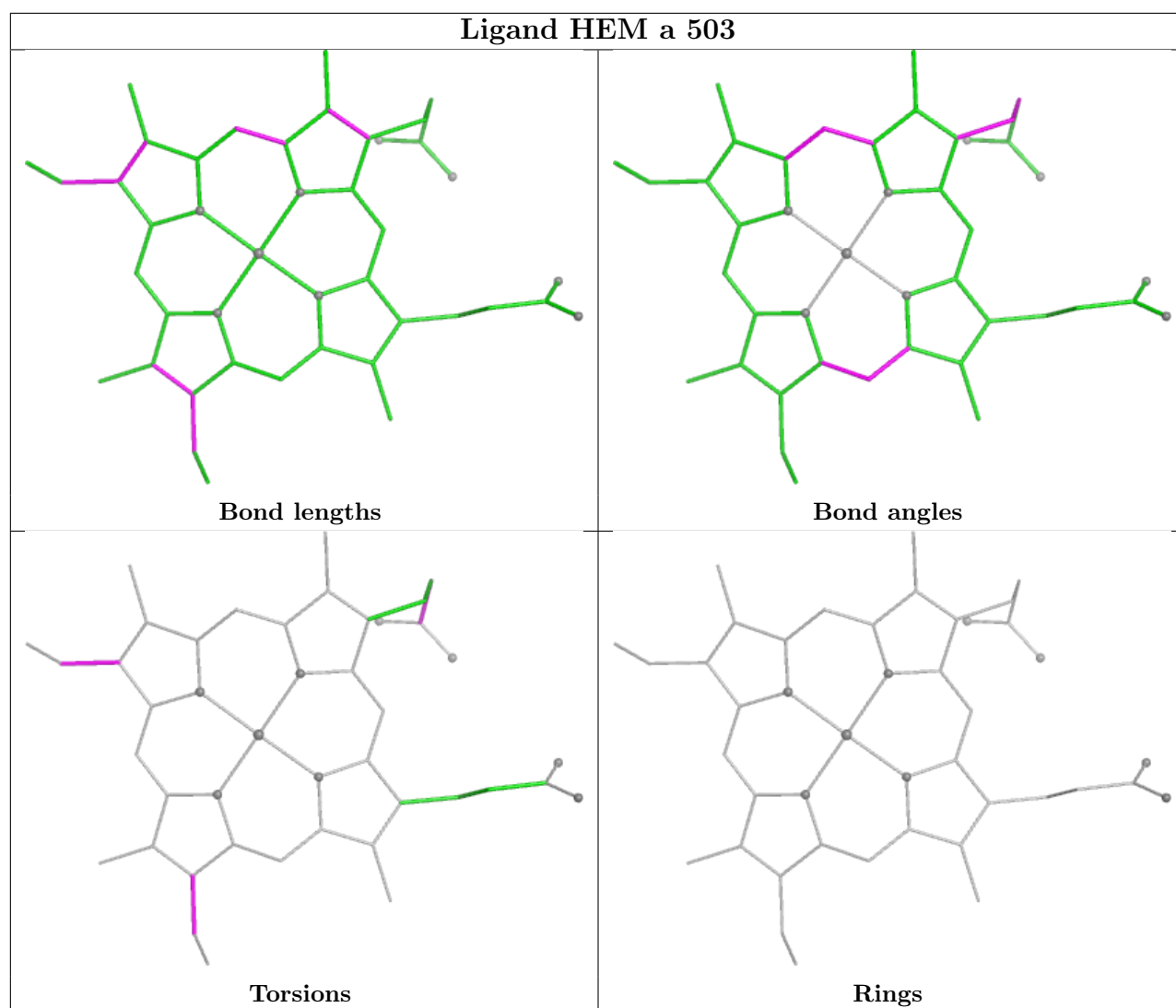


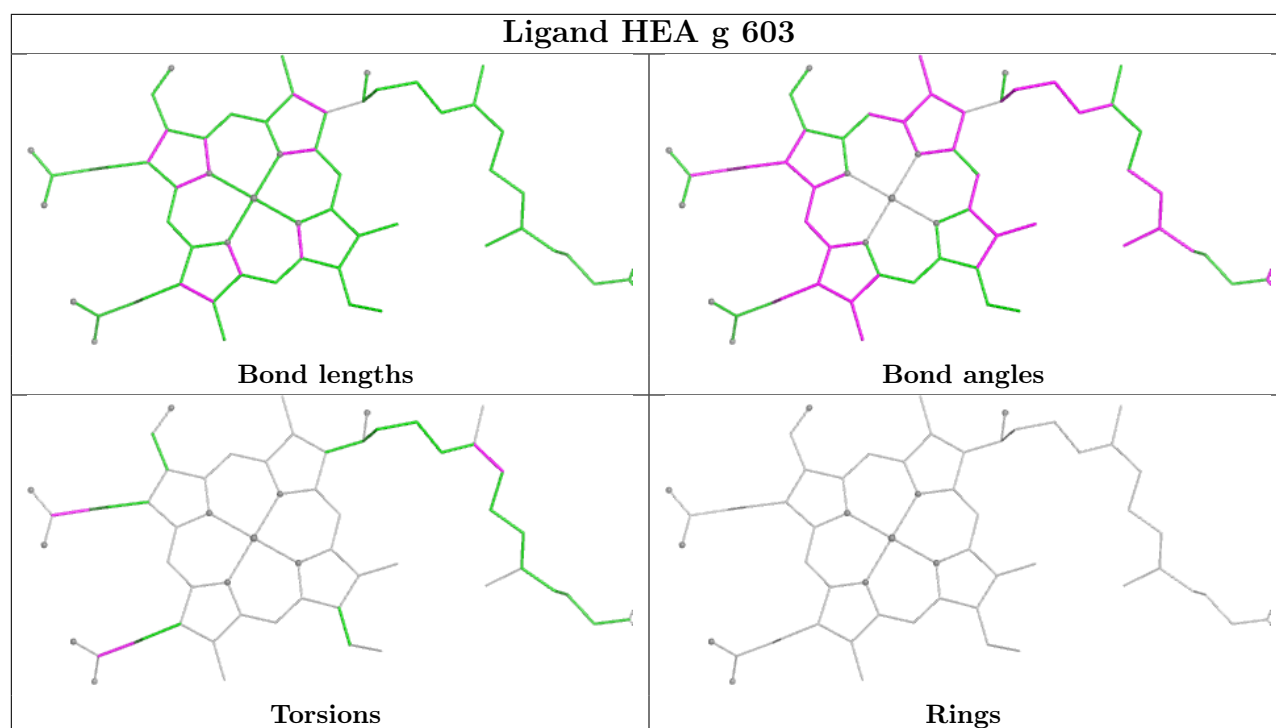


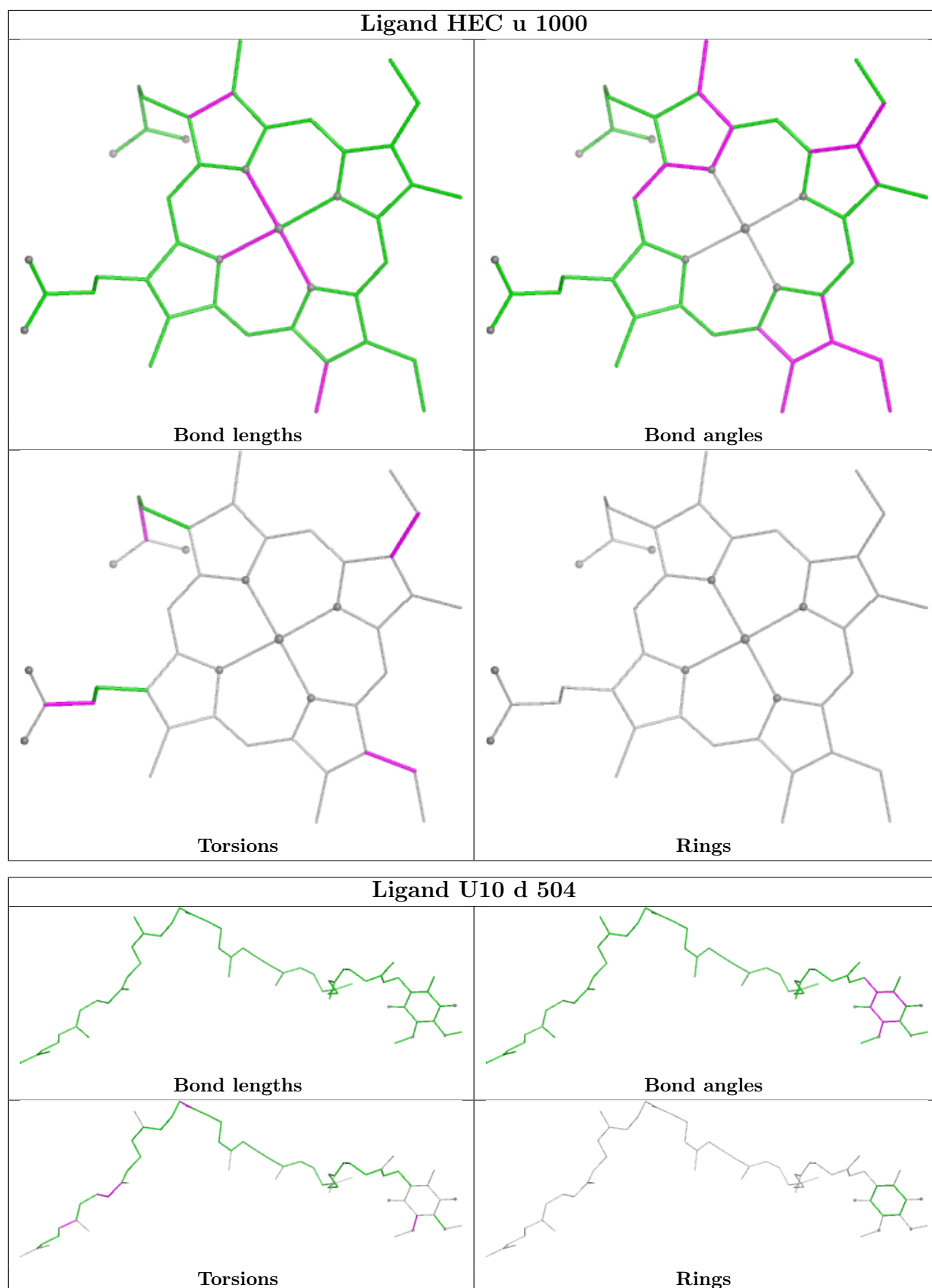


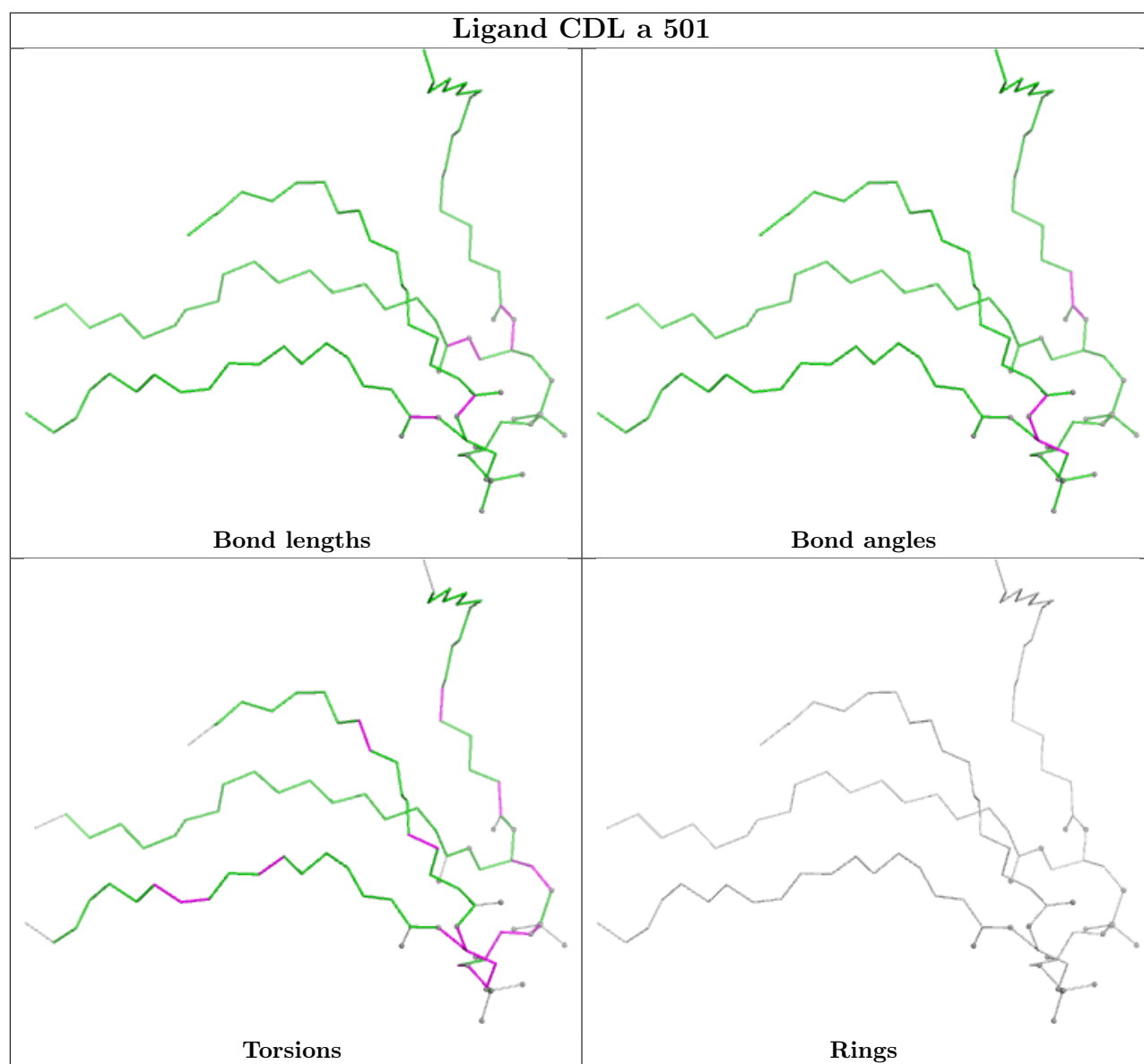


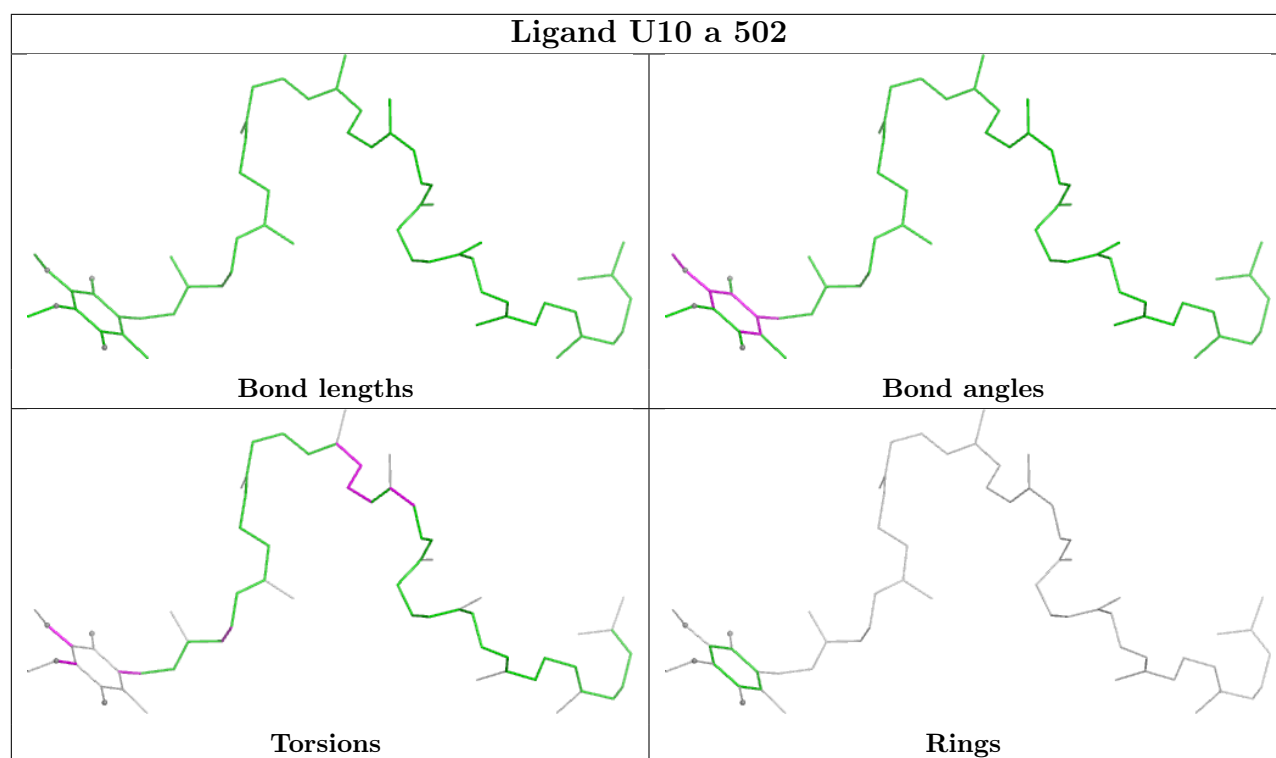












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

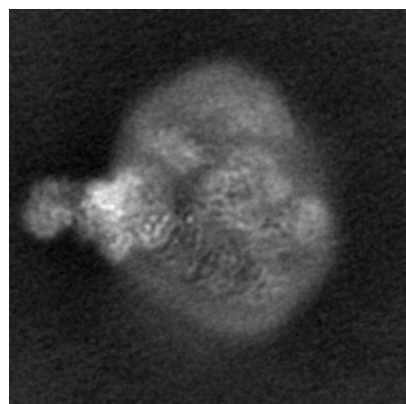
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51125. These allow visual inspection of the internal detail of the map and identification of artifacts.

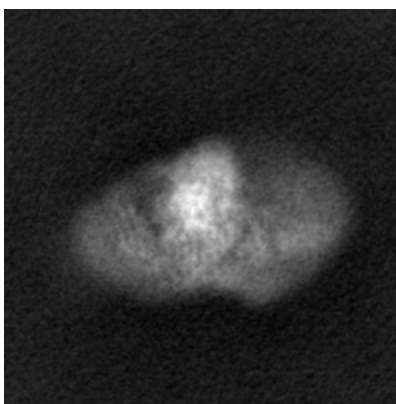
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

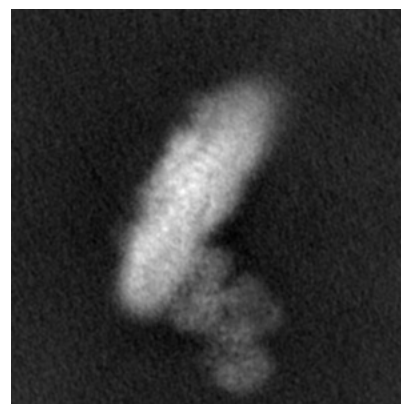
6.1.1 Primary map



X

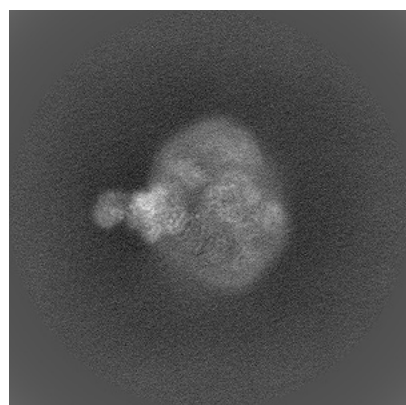


Y

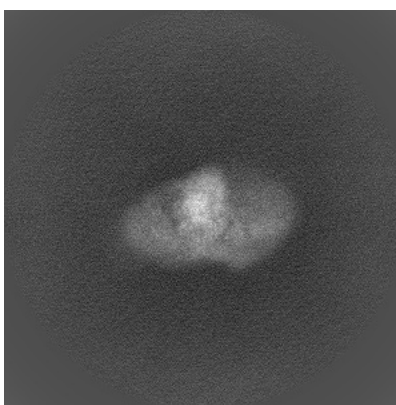


Z

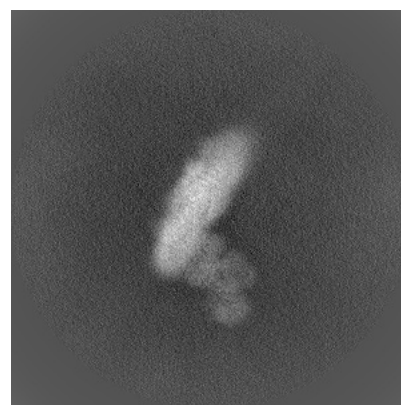
6.1.2 Raw map



X



Y

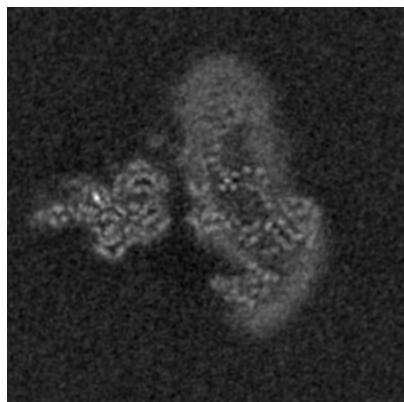


Z

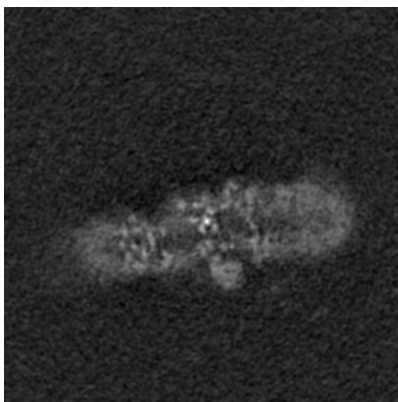
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

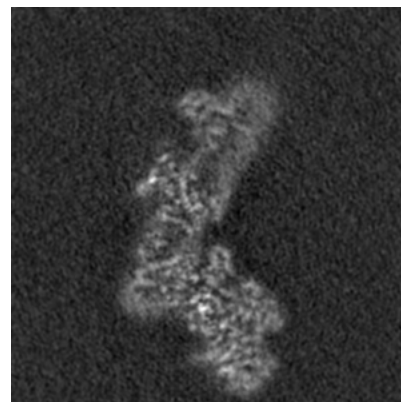
6.2.1 Primary map



X Index: 187

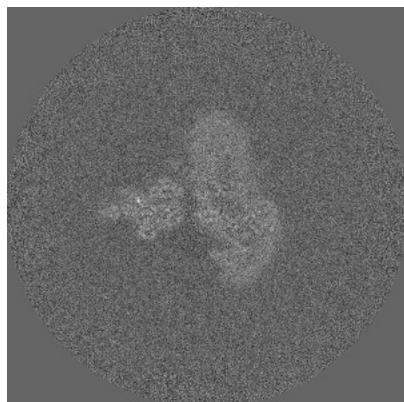


Y Index: 187

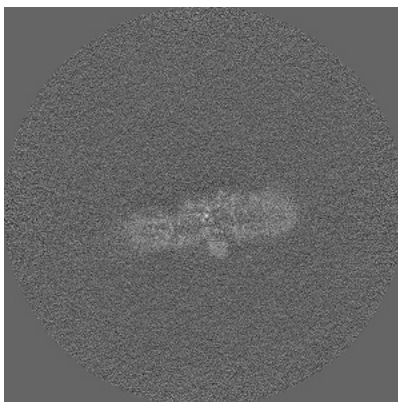


Z Index: 187

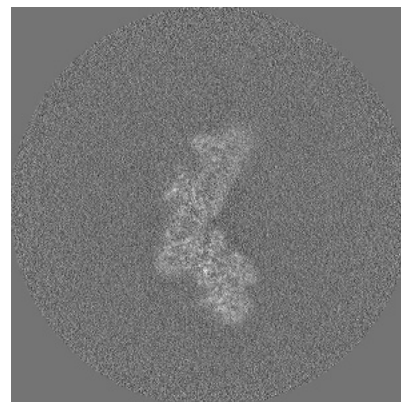
6.2.2 Raw map



X Index: 300



Y Index: 300

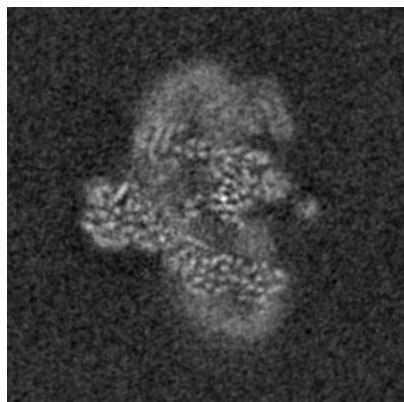


Z Index: 300

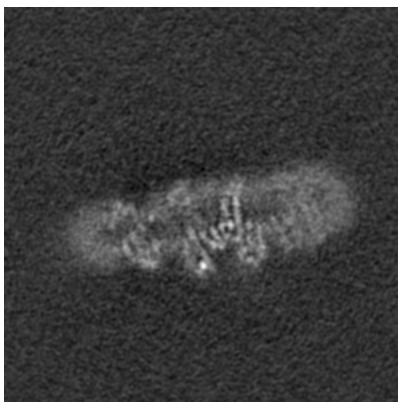
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

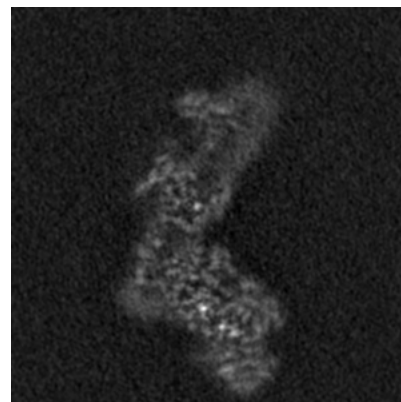
6.3.1 Primary map



X Index: 161

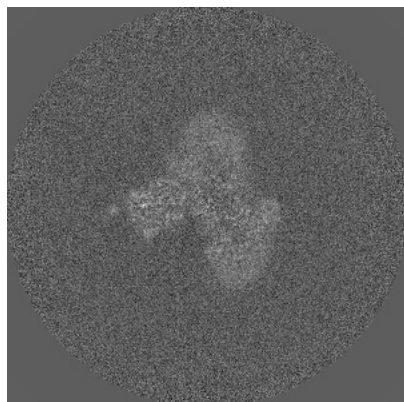


Y Index: 212

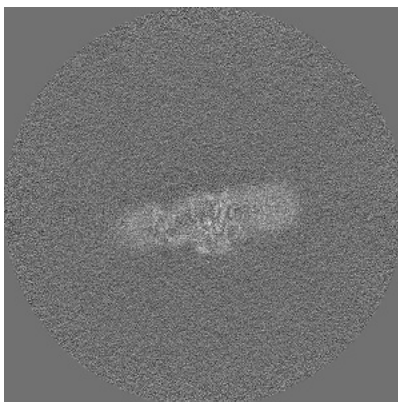


Z Index: 189

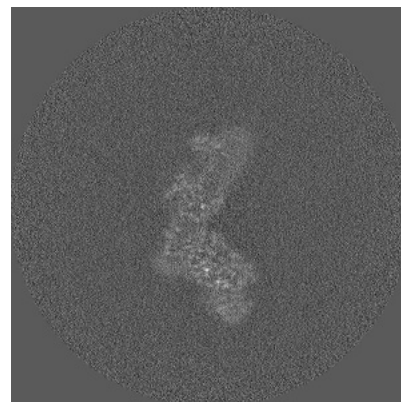
6.3.2 Raw map



X Index: 291



Y Index: 317

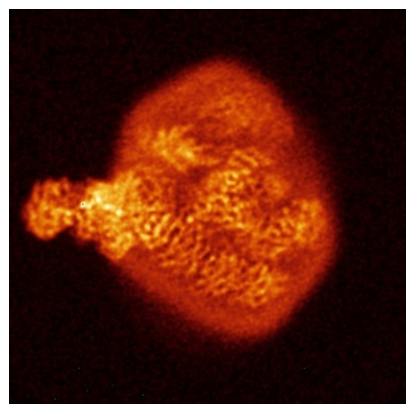


Z Index: 302

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

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

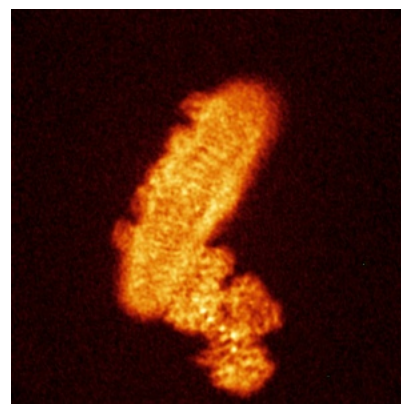
6.4.1 Primary map



X

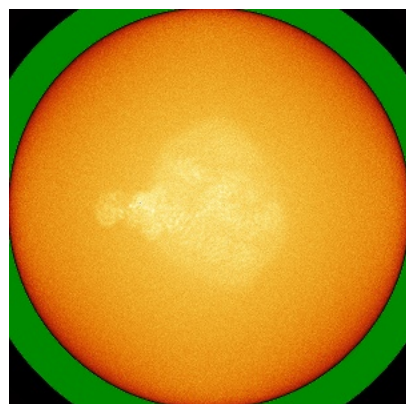


Y

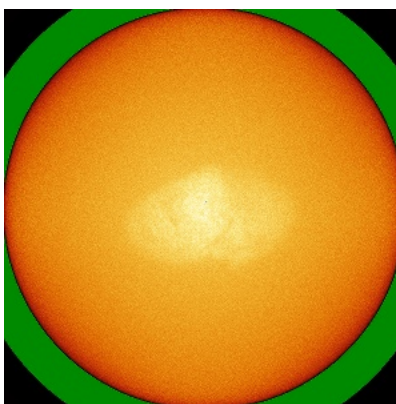


Z

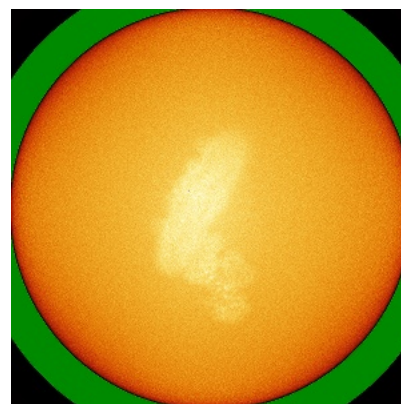
6.4.2 Raw map



X



Y

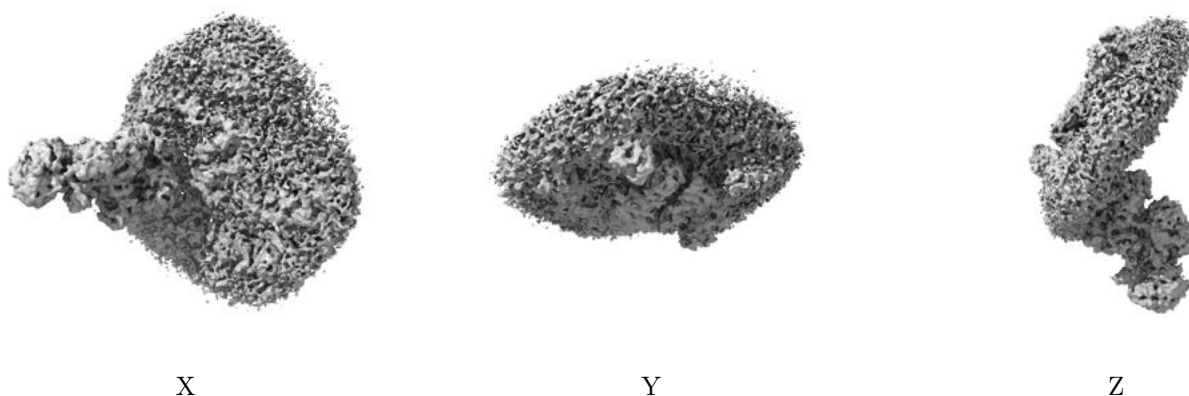


Z

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.

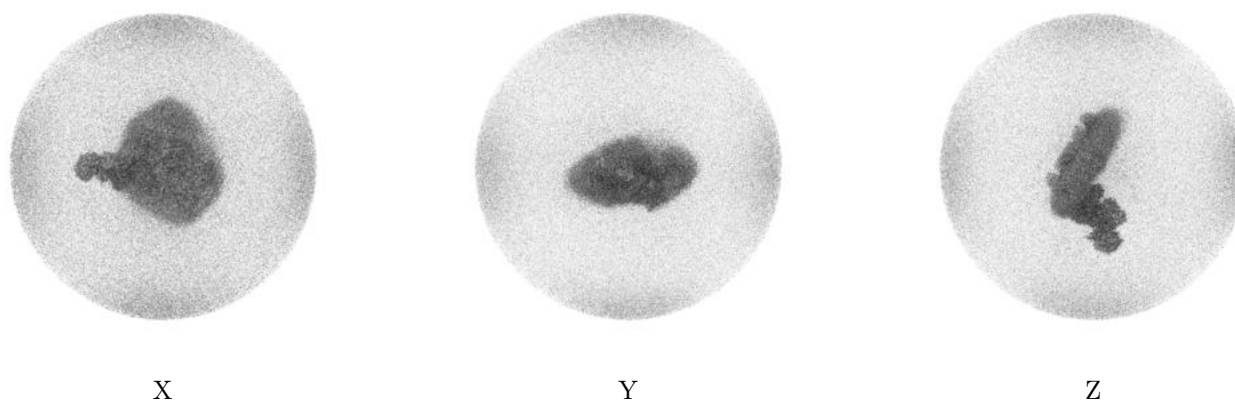
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0112. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

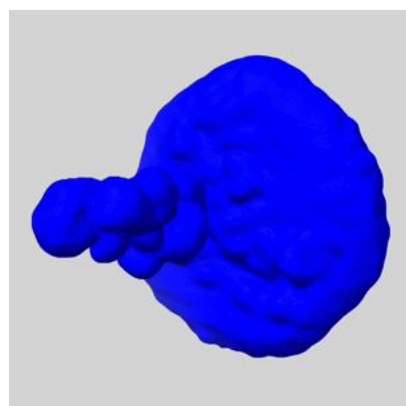
6.6 Mask visualisation [i](#)

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

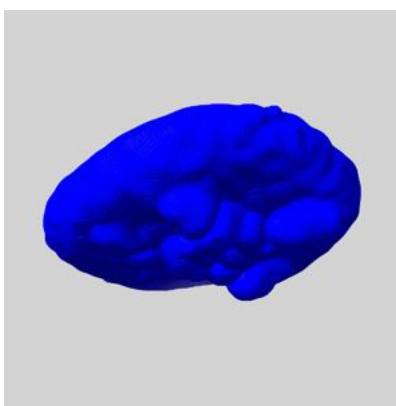
A mask typically either:

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

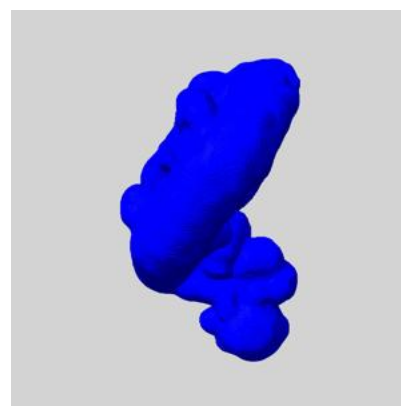
6.6.1 emd_51125_msk_1.map [i](#)



X



Y

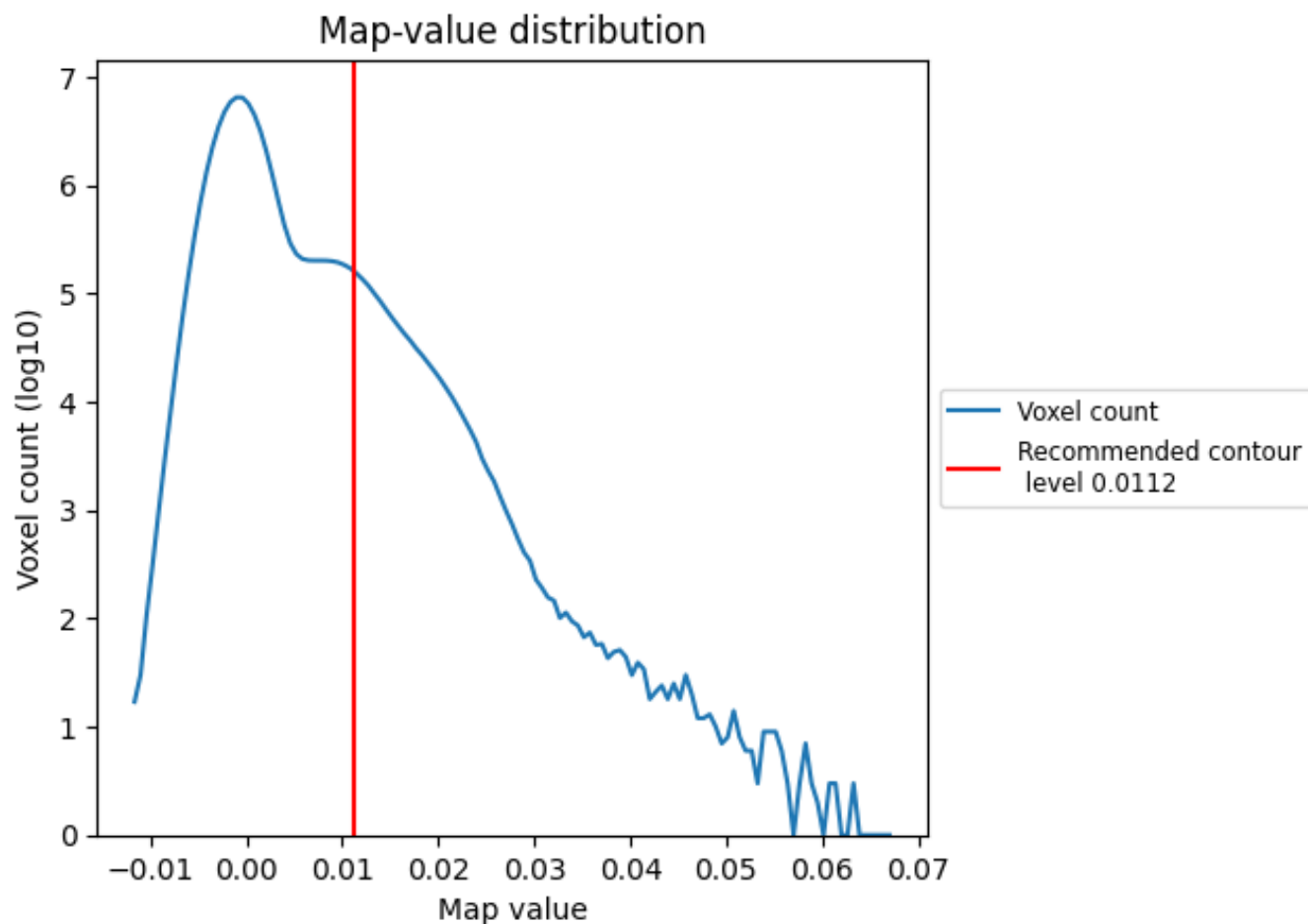


Z

7 Map analysis [i](#)

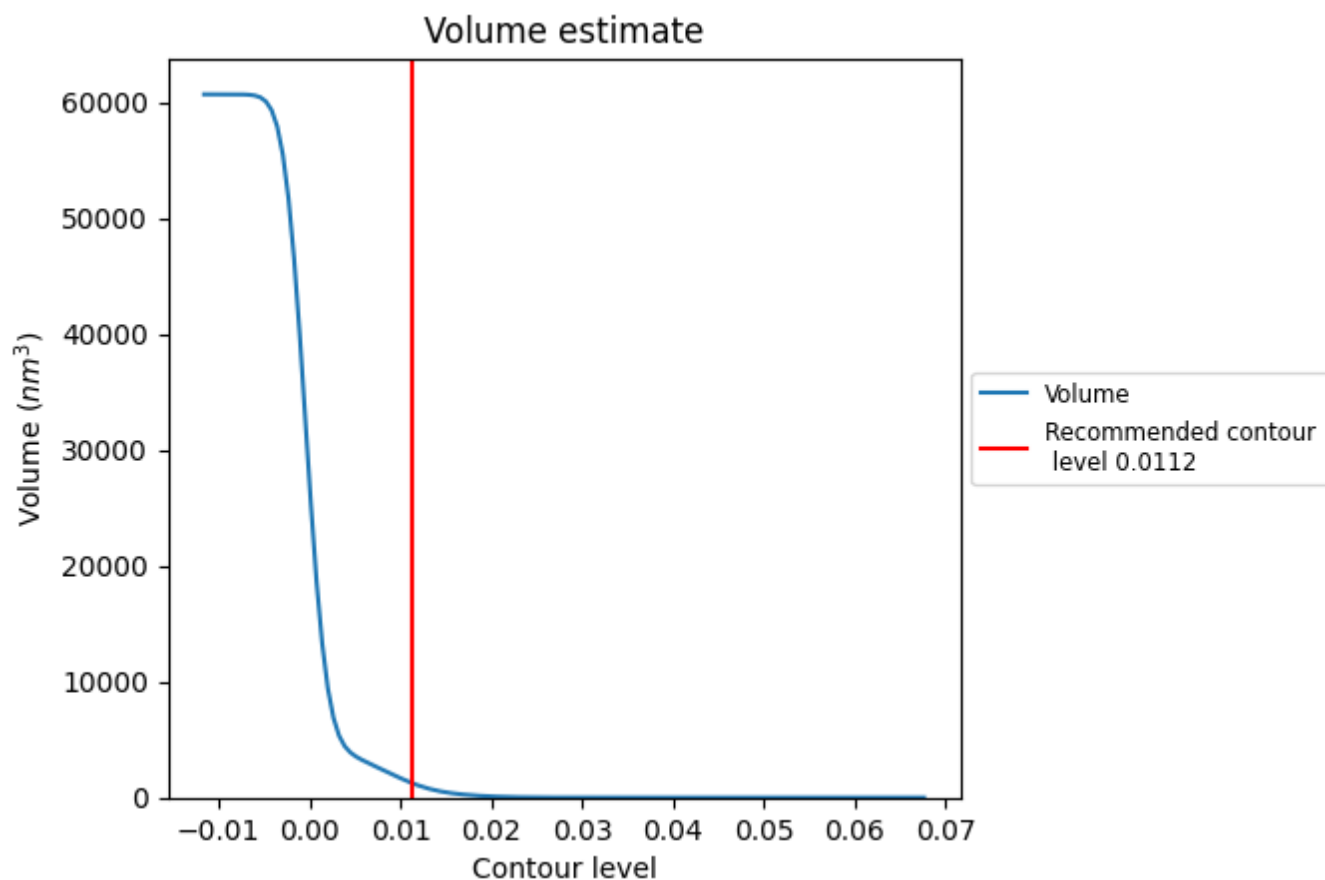
This section contains the results of statistical analysis of the map.

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.

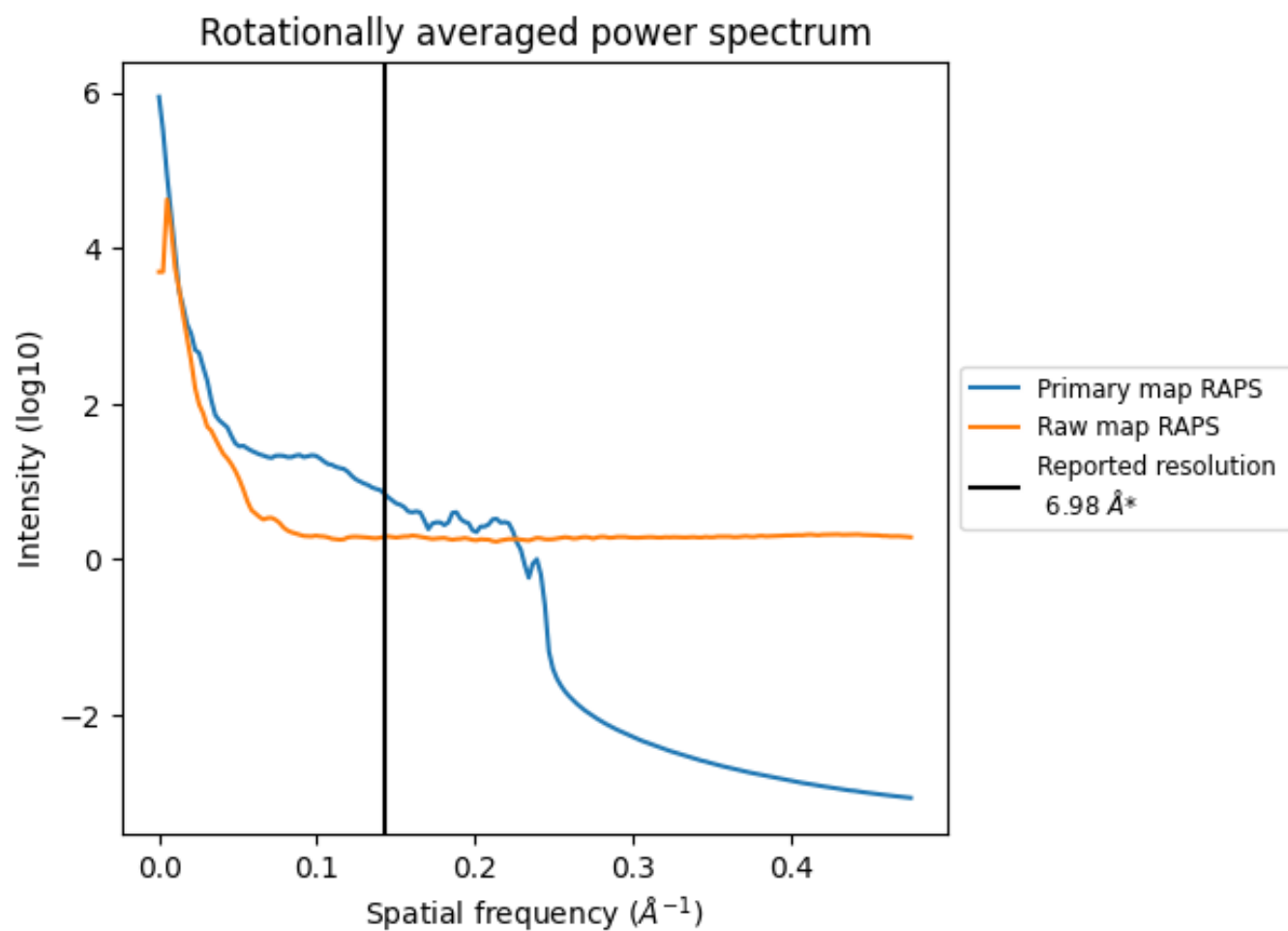
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1272 nm³; this corresponds to an approximate mass of 1149 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 ⓘ

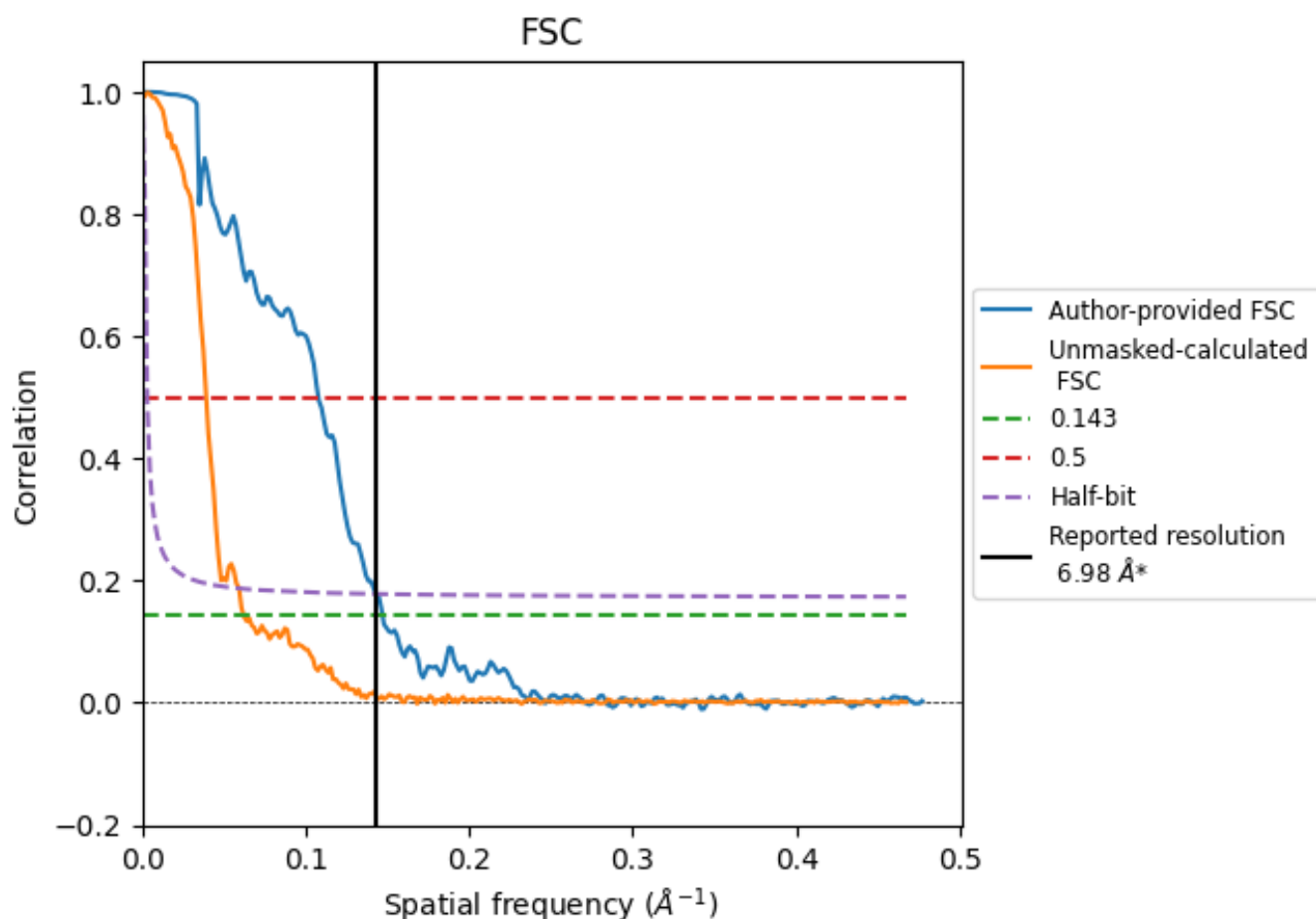


*Reported resolution corresponds to spatial frequency of 0.143 Å⁻¹

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 0.143 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

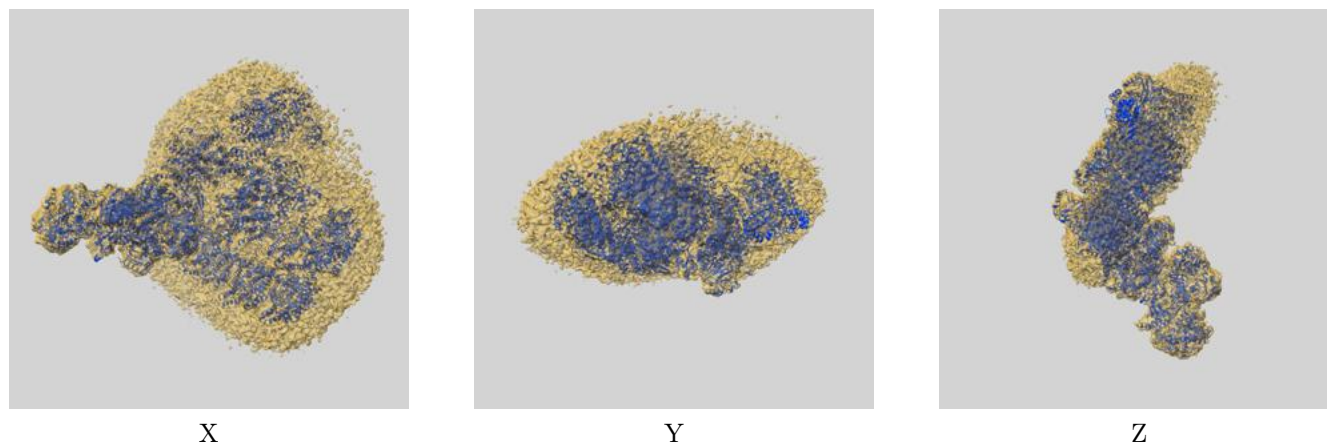
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.98	-	-
Author-provided FSC curve	6.80	9.28	7.00
Unmasked-calculated*	16.10	25.51	16.89

*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 16.10 differs from the reported value 6.98 by more than 10 %

9 Map-model fit [i](#)

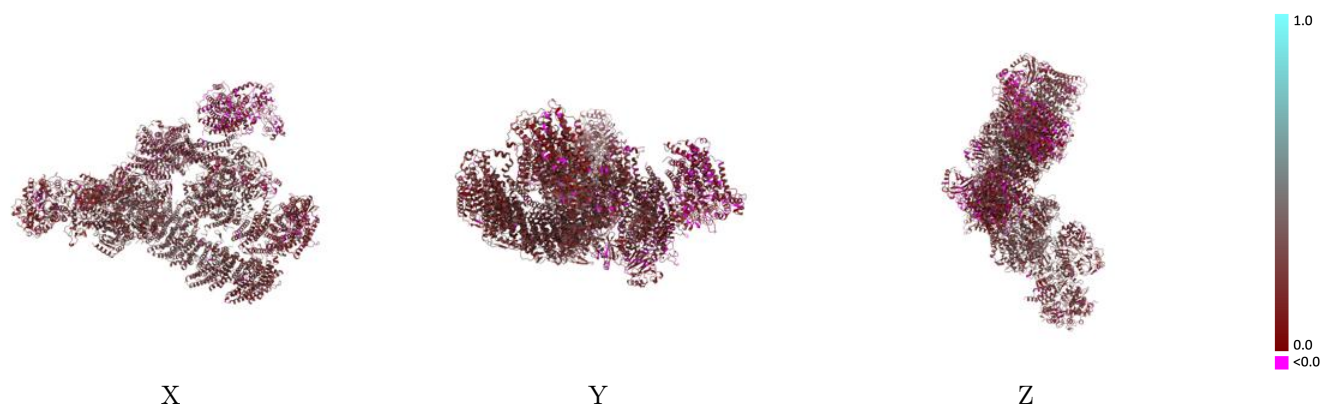
This section contains information regarding the fit between EMDB map EMD-51125 and PDB model 9G83. Per-residue inclusion information can be found in [section 3](#) on [page 18](#).

9.1 Map-model overlay [i](#)



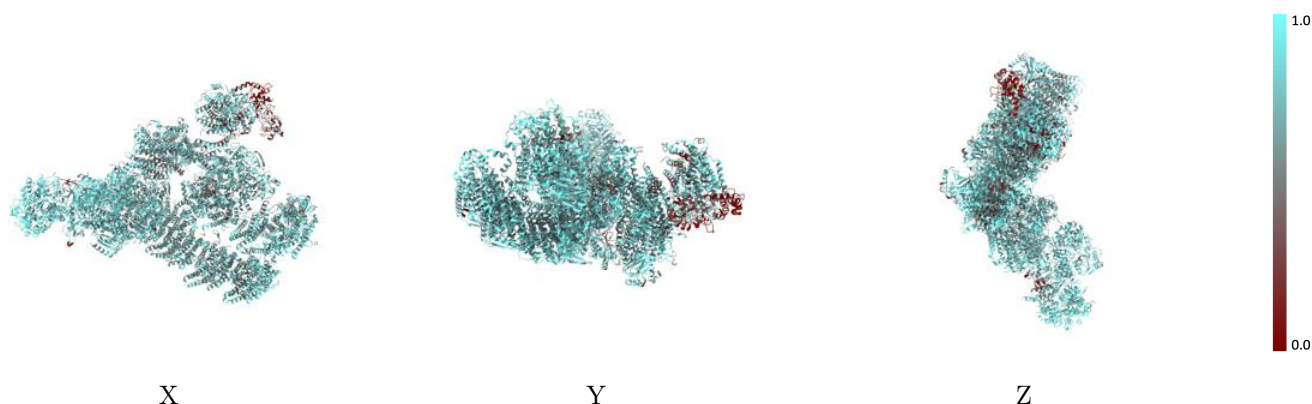
The images above show the 3D surface view of the map at the recommended contour level 0.0112 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



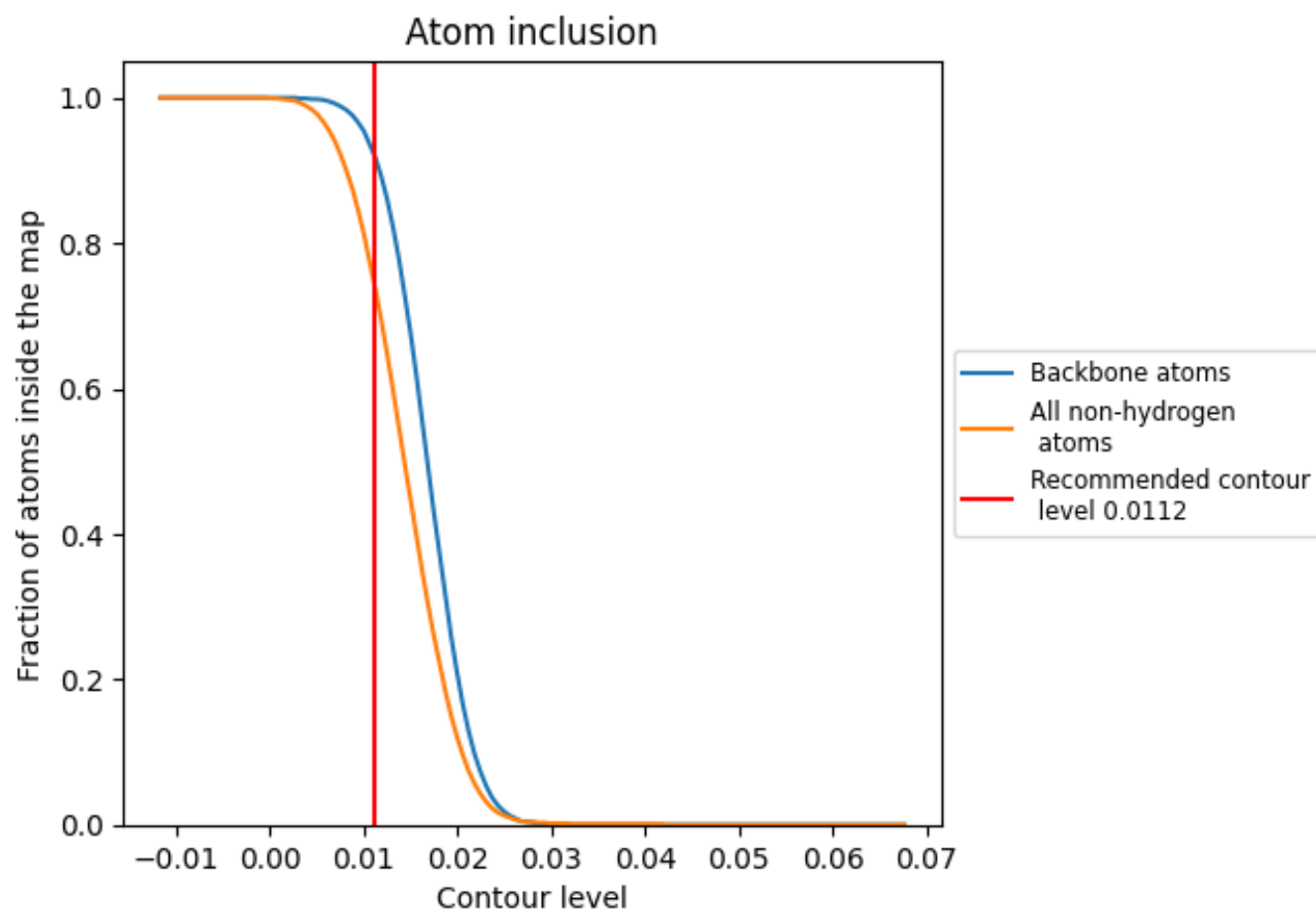
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0112).

9.4 Atom inclusion ⓘ



At the recommended contour level, 92% of all backbone atoms, 74% 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 (0.0112) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7400	 0.2190
A	 0.7070	 0.2590
B	 0.7640	 0.2810
C	 0.7940	 0.2760
D	 0.7920	 0.2700
E	 0.8590	 0.2200
F	 0.8530	 0.2020
G	 0.8140	 0.2320
H	 0.7300	 0.2420
I	 0.8550	 0.2580
J	 0.7270	 0.2570
K	 0.7030	 0.2550
L	 0.7610	 0.2170
M	 0.7420	 0.2310
N	 0.7380	 0.2480
P	 0.7200	 0.2360
Q	 0.8440	 0.2770
R	 0.2860	 0.1840
Z	 0.7790	 0.2680
a	 0.7260	 0.2660
b	 0.7850	 0.2630
c	 0.7350	 0.1860
d	 0.7230	 0.2330
e	 0.7540	 0.2350
f	 0.7440	 0.1820
g	 0.7550	 0.1920
h	 0.7760	 0.1950
i	 0.7430	 0.2300
j	 0.6380	 0.2070
k	 0.7330	 0.1500
l	 0.7490	 0.1600
m	 0.7420	 0.1970
n	 0.6050	 0.2350
o	 0.7600	 0.2460
p	 0.8210	 0.2660



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
q	 0.8700	 0.2690
r	 0.6110	 0.2760
s	 0.6670	 0.2530
t	 0.6650	 0.1390
u	 0.5620	 0.1420
v	 0.3370	 0.1440