



wwPDB EM Validation Summary Report ⓘ

Jun 10, 2024 – 08:26 PM EDT

PDB ID : 8UGL
EMDB ID : EMD-42229
Title : High resolution in-situ structure of complex IV in respiratory supercomplex
Authors : Zheng, W.; Zhu, J.; Zhang, K.
Deposited on : 2023-10-05
Resolution : 3.00 Å(reported)

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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.dev92
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

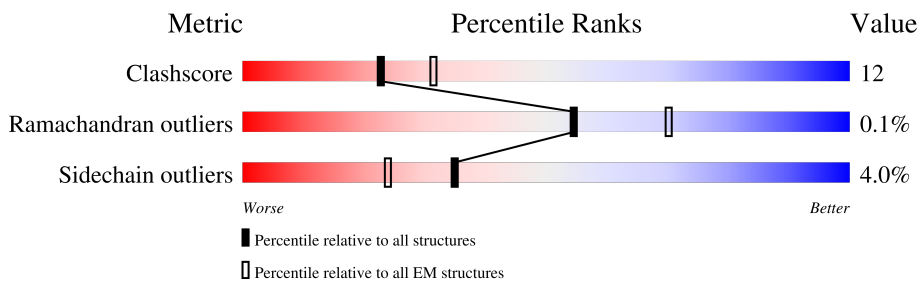
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	4A	514	
2	4B	229	
3	4C	261	
4	4D	169	
5	4E	152	
6	4F	129	
7	4G	97	
8	4H	86	

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Mol	Chain	Length	Quality of chain
9	4I	75	
10	4J	80	
11	4K	80	
12	4L	63	
13	4M	70	
14	4N	82	

2 Entry composition [i](#)

There are 26 unique types of molecules in this entry. The entry contains 16927 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	4A	513	4025	2692	625	677	31	1	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	4B	227	1828	1190	281	339	18	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	4C	259	2096	1399	336	351	10	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	4D	139	1163	757	190	212	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	4E	105	852	544	144	162	2	0	0

- Molecule 6 is a protein called Cytochrome c oxidase subunit 5B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	4F	97	734	455	130	143	6	0	0

- Molecule 7 is a protein called Cytochrome c oxidase subunit 6A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	4G	75	617	398	118	100	1	0	0

- Molecule 8 is a protein called Cytochrome c oxidase subunit 6B1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	4H	82	687	434	125	123	5	0	0

- Molecule 9 is a protein called Cytochrome c oxidase subunit 6C.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	4I	67	550	359	97	91	3	0	0

- Molecule 10 is a protein called Cytochrome c oxidase subunit 7A1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	4J	58	456	293	78	82	3	0	0

- Molecule 11 is a protein called Cytochrome c oxidase subunit 7B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	4K	49	383	249	65	68	1	0	0

- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	4L	46	381	254	64	61	2	0	0

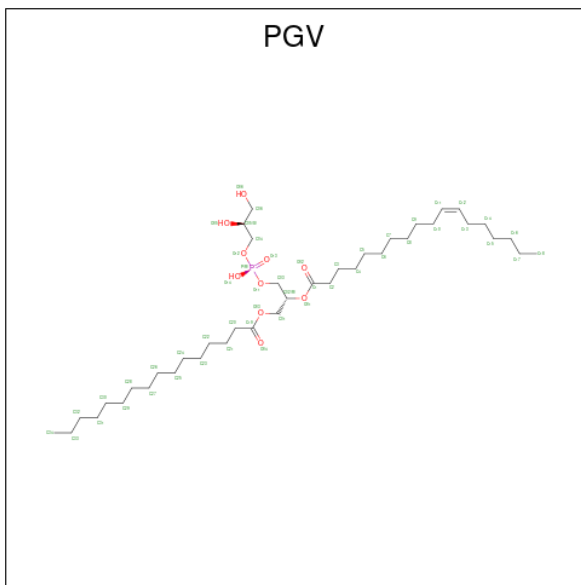
- Molecule 13 is a protein called Cytochrome c oxidase subunit 8.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
13	4M	43	338	222	57	59	0	0

- Molecule 14 is a protein called Cytochrome c oxidase subunit NDUFA4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	4N	82	660	432	112	114	2	0	0

- Molecule 15 is (1R)-2-{{[[[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: C₄₀H₇₇O₁₀P).



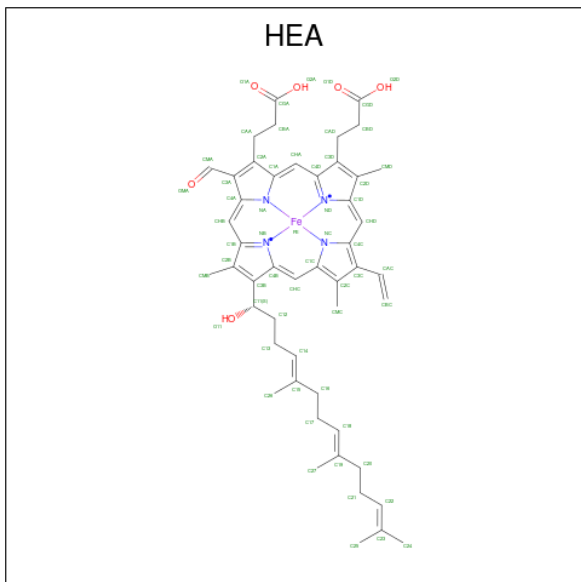
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
15	4A	1	51	40	10	1	0
15	4A	1	51	40	10	1	0
15	4A	1	51	40	10	1	0
15	4B	1	51	40	10	1	0
15	4C	1	51	40	10	1	0
15	4C	1	51	40	10	1	0
15	4C	1	51	40	10	1	0
15	4C	1	51	40	10	1	0
15	4C	1	51	40	10	1	0
15	4C	1	51	40	10	1	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
15	4G	1	Total 51	C 40	O 10	P 1	0
15	4J	1	Total 51	C 40	O 10	P 1	0
15	4K	1	Total 51	C 40	O 10	P 1	0
15	4L	1	Total 51	C 40	O 10	P 1	0
15	4M	1	Total 51	C 40	O 10	P 1	0

- Molecule 16 is HEME-A (three-letter code: HEA) (formula: $C_{49}H_{56}FeN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Fe	N	O	
16	4A	1	Total 60	C 49	Fe 1	N 4	O 6	0
16	4A	1	Total 60	C 49	Fe 1	N 4	O 6	0

- Molecule 17 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
			Total	Cu	
17	4A	1	Total 1	Cu 1	0

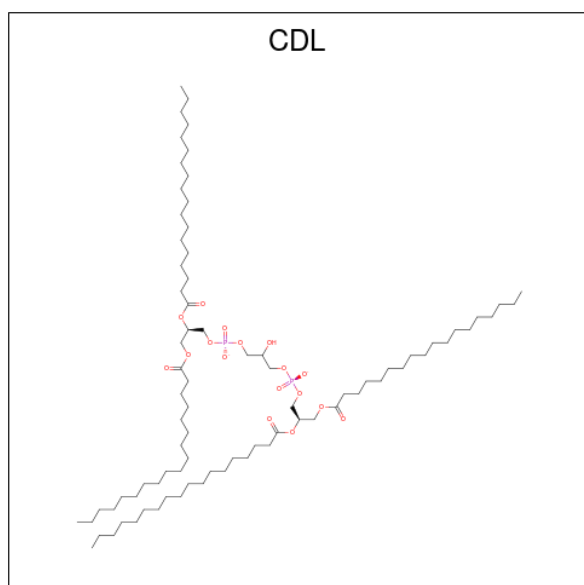
- Molecule 18 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
18	4A	1	Total	Mg	0
			1	1	

- Molecule 19 is SODIUM ION (three-letter code: NA) (formula: Na).

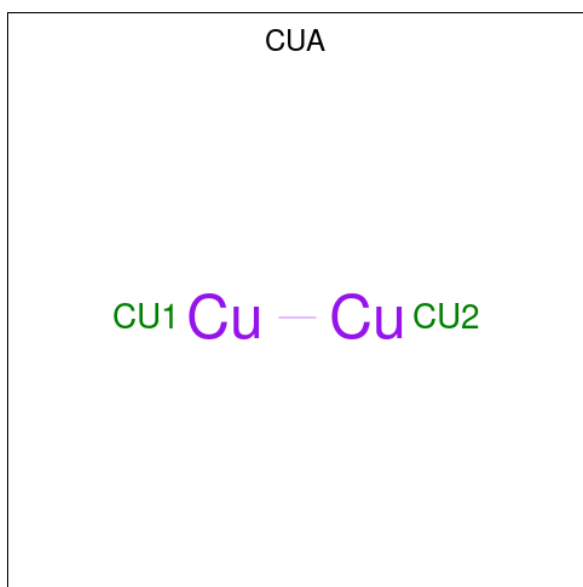
Mol	Chain	Residues	Atoms		AltConf
19	4A	1	Total	Na	0
			1	1	

- Molecule 20 is CARDIOLIPIN (three-letter code: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



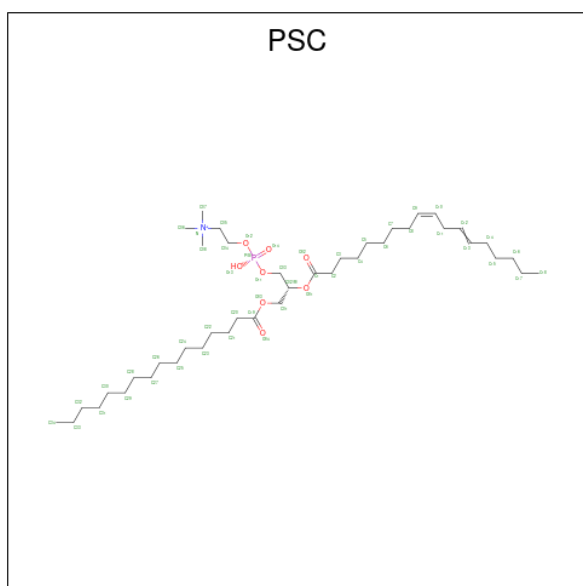
Mol	Chain	Residues	Atoms				AltConf
20	4B	1	Total	C	O	P	0
			100	81	17	2	
20	4C	1	Total	C	O	P	0
			100	81	17	2	
20	4D	1	Total	C	O	P	0
			100	81	17	2	

- Molecule 21 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu₂).



Mol	Chain	Residues	Atoms		AltConf
21	4B	1	Total	Cu	0
			2	2	

- Molecule 22 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (three-letter code: PSC) (formula: C₄₂H₈₁NO₈P).

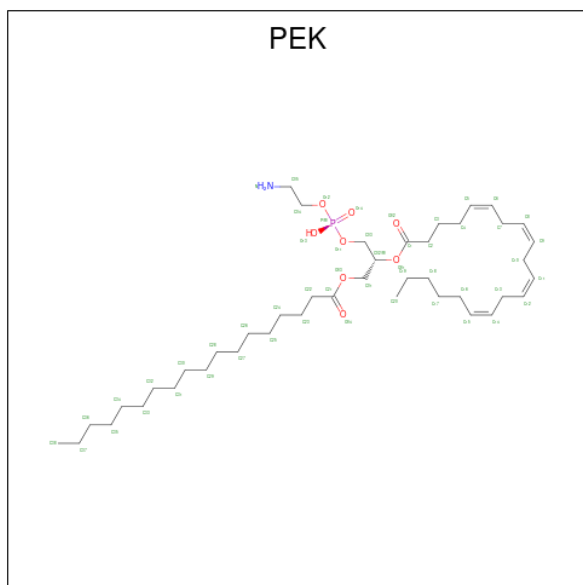


Mol	Chain	Residues	Atoms					AltConf
22	4B	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 23 is ZINC ION (three-letter code: ZN) (formula: Zn).

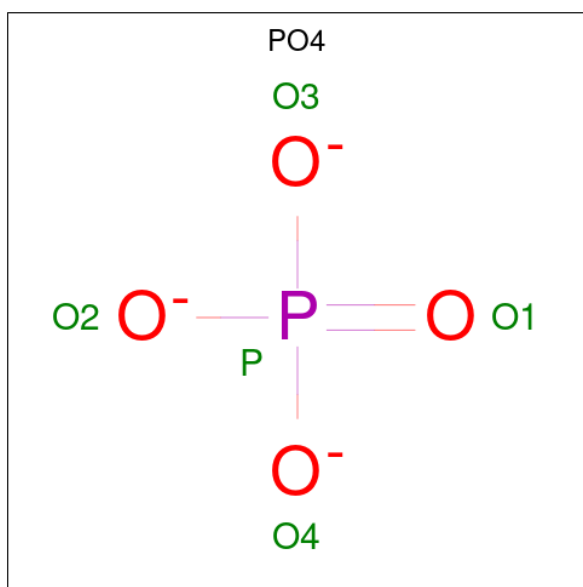
Mol	Chain	Residues	Atoms		AltConf
23	4F	1	Total	Zn	0
			1	1	

- Molecule 24 is (1S)-2-[[[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY]-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (three-letter code: PEK) (formula: C₄₃H₇₈NO₈P).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
24	4G	1	53	43	1	8	1	0
24	4G	1	52	42	1	8	1	0

- Molecule 25 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			AltConf
25	4H	1	Total	O	P	0
			5	4	1	

- Molecule 26 is water.

Mol	Chain	Residues	Atoms		AltConf
26	4A	108	Total	O	0
			108	108	
26	4B	115	Total	O	0
			115	115	
26	4C	103	Total	O	0
			103	103	
26	4D	81	Total	O	0
			81	81	
26	4E	55	Total	O	0
			55	55	
26	4F	65	Total	O	0
			65	65	
26	4G	40	Total	O	0
			40	40	
26	4H	43	Total	O	0
			43	43	
26	4I	25	Total	O	0
			25	25	
26	4J	38	Total	O	0
			38	38	
26	4K	27	Total	O	0
			27	27	

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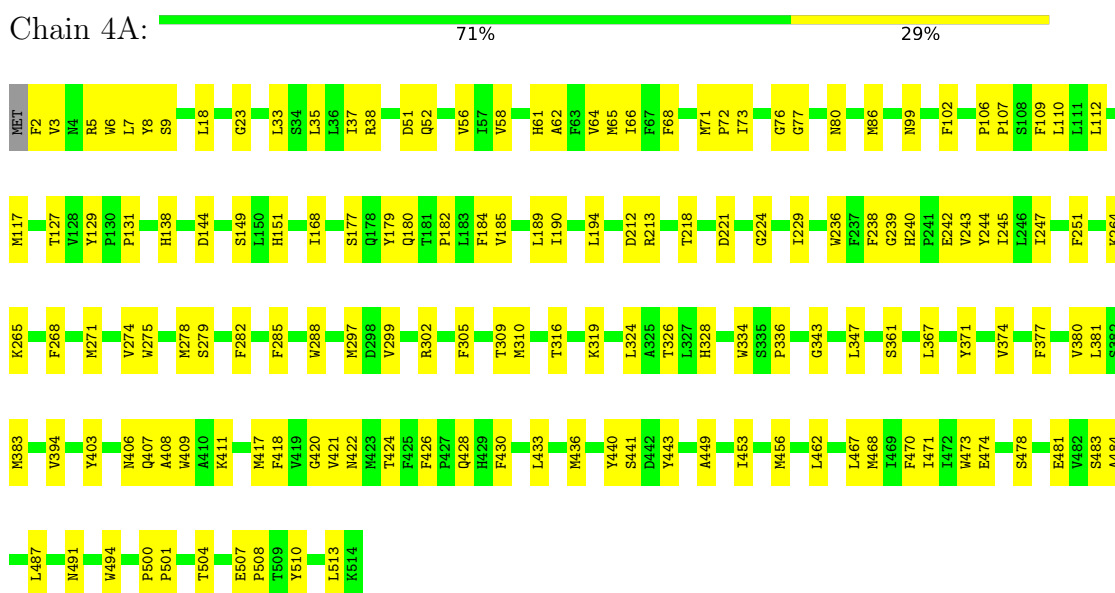
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Mol	Chain	Residues	Atoms		AltConf
26	4L	23	Total 23	O 23	0
26	4M	28	Total 28	O 28	0
26	4N	53	Total 53	O 53	0

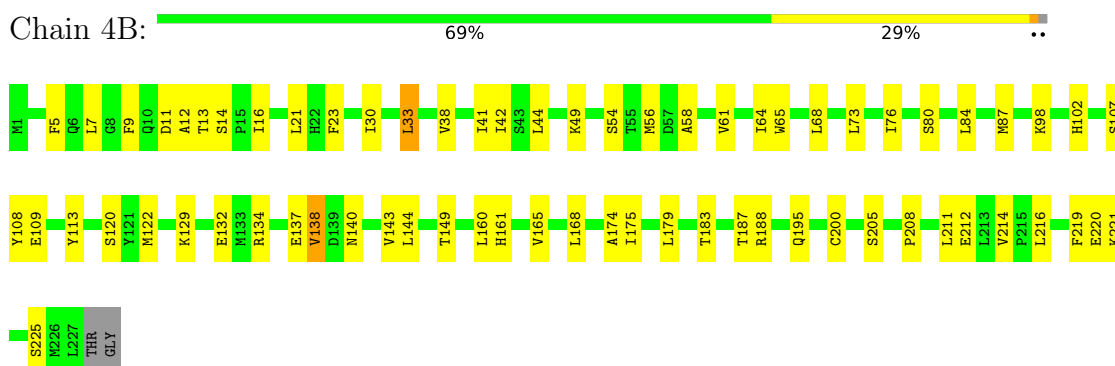
3 Residue-property plots [i](#)

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: Cytochrome c oxidase subunit 1

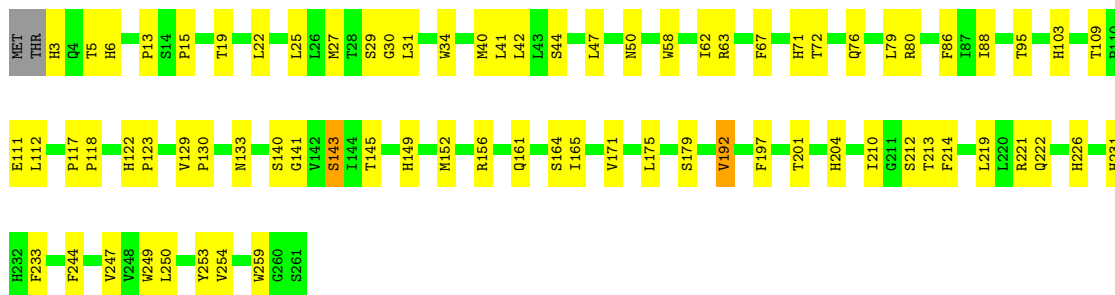


- Molecule 2: Cytochrome c oxidase subunit 2

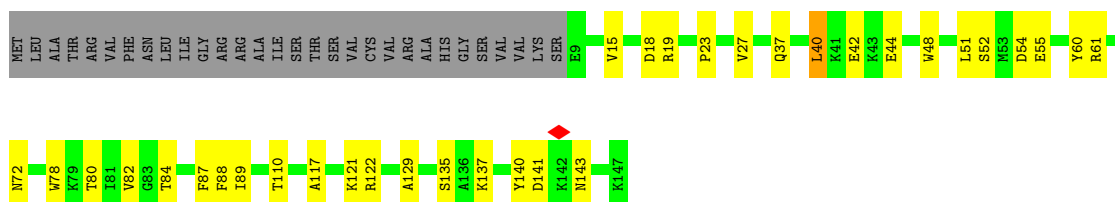


- Molecule 3: Cytochrome c oxidase subunit 3

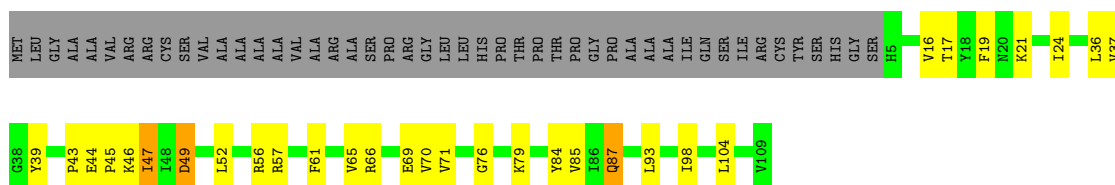




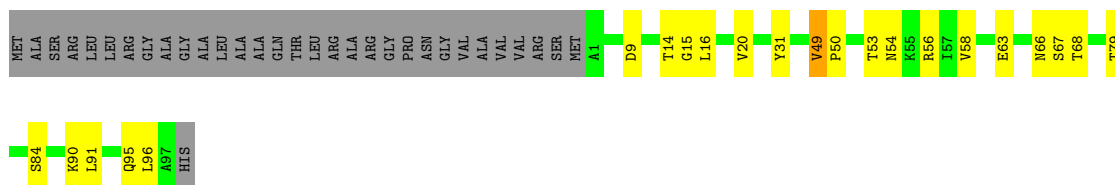
- Molecule 4: Cytochrome c oxidase subunit 4



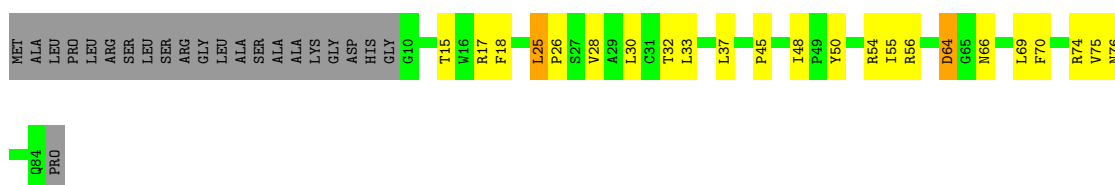
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

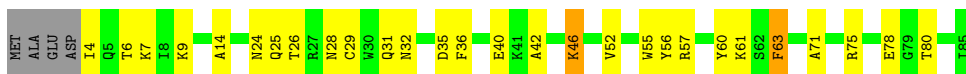


- Molecule 7: Cytochrome c oxidase subunit 6A2



- Molecule 8: Cytochrome c oxidase subunit 6B1

Chain 4H:  63% 30% 5%



- Molecule 9: Cytochrome c oxidase subunit 6C

Chain 4I:  69% 20% 11%



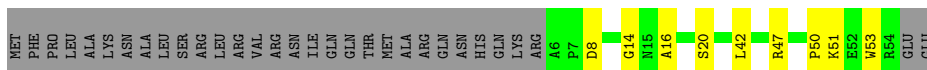
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial

Chain 4J:  55% 18% 28%



- Molecule 11: Cytochrome c oxidase subunit 7B

Chain 4K:  50% 11% 39%



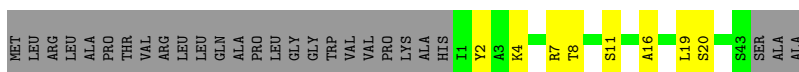
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

Chain 4L:  54% 19% 27%




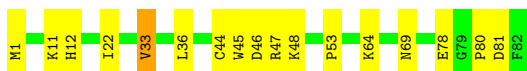
- Molecule 13: Cytochrome c oxidase subunit 8

Chain 4M:  50% 11% 39%



- Molecule 14: Cytochrome c oxidase subunit NDUFA4

Chain 4N:  79% 20% 1%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	56000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.697	Depositor
Minimum map value	-1.154	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.049	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	212.992, 212.992, 212.992	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.416, 0.416, 0.416	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PEK, HEA, CUA, PSC, CDL, PGV, FME, MG, NA, CU, ZN, PO4

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	4A	0.33	2/4165 (0.0%)	0.59	4/5691 (0.1%)
2	4B	0.24	0/1865	0.46	0/2544
3	4C	0.24	0/2179	0.39	0/2981
4	4D	0.25	0/1197	0.42	0/1617
5	4E	0.24	0/871	0.48	0/1182
6	4F	0.24	0/749	0.49	0/1016
7	4G	0.24	0/644	0.51	0/881
8	4H	0.25	0/708	0.48	0/956
9	4I	0.25	0/563	0.46	0/748
10	4J	0.23	0/466	0.42	0/631
11	4K	0.23	0/396	0.42	0/543
12	4L	0.25	0/394	0.41	0/528
13	4M	0.23	0/349	0.42	0/477
14	4N	0.25	0/680	0.43	0/921
All	All	0.27	2/15226 (0.0%)	0.49	4/20716 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	4A	501	PRO	CG-CD	-9.73	1.18	1.50
1	4A	501	PRO	CB-CG	-9.18	1.04	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4A	501	PRO	N-CD-CG	-19.90	73.35	103.20
1	4A	501	PRO	CA-CB-CG	-19.43	67.09	104.00
1	4A	501	PRO	CB-CG-CD	10.89	148.99	106.50
1	4A	501	PRO	CA-N-CD	-7.58	100.89	111.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	4A	4025	0	3999	118	0
2	4B	1828	0	1837	53	0
3	4C	2096	0	2027	60	0
4	4D	1163	0	1143	27	0
5	4E	852	0	845	20	0
6	4F	734	0	718	13	0
7	4G	617	0	585	16	0
8	4H	687	0	645	21	0
9	4I	550	0	560	8	0
10	4J	456	0	459	11	0
11	4K	383	0	366	9	0
12	4L	381	0	380	10	0
13	4M	338	0	345	9	0
14	4N	660	0	664	13	0
15	4A	153	0	228	21	0
15	4B	51	0	76	12	0
15	4C	306	0	456	40	0
15	4G	51	0	76	5	0
15	4J	51	0	76	3	0
15	4K	51	0	76	6	0
15	4L	51	0	76	10	0
15	4M	51	0	76	5	0
16	4A	120	0	108	8	0
17	4A	1	0	0	0	0
18	4A	1	0	0	0	0
19	4A	1	0	0	0	0
20	4B	100	0	156	9	0
20	4C	100	0	156	14	0
20	4D	100	0	156	20	0
21	4B	2	0	0	1	0
22	4B	52	0	80	9	0
23	4F	1	0	0	0	0
24	4G	105	0	149	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	4H	5	0	0	0	0
26	4A	108	0	0	6	0
26	4B	115	0	0	7	0
26	4C	103	0	0	3	0
26	4D	81	0	0	4	0
26	4E	55	0	0	1	0
26	4F	65	0	0	1	0
26	4G	40	0	0	1	0
26	4H	43	0	0	4	0
26	4I	25	0	0	0	0
26	4J	38	0	0	0	0
26	4K	27	0	0	0	0
26	4L	23	0	0	2	0
26	4M	28	0	0	0	0
26	4N	53	0	0	0	0
All	All	16927	0	16518	408	0

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

The worst 5 of 408 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)
2:4B:200:CYS:SG	21:4B:303:CUA:CU1	1.48	1.03
12:4L:18:LYS:NZ	26:4L:201:HOH:O	2.09	0.84
20:4D:201:CDL:H351	20:4D:201:CDL:H551	1.60	0.82
15:4M:101:PGV:H221	15:4M:101:PGV:H61	1.60	0.82
15:4C:303:PGV:H21	15:4C:303:PGV:H92	1.62	0.81

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	4A	512/514 (100%)	500 (98%)	12 (2%)	0	100	100
2	4B	225/229 (98%)	216 (96%)	9 (4%)	0	100	100
3	4C	257/261 (98%)	249 (97%)	8 (3%)	0	100	100
4	4D	137/169 (81%)	131 (96%)	6 (4%)	0	100	100
5	4E	103/152 (68%)	99 (96%)	4 (4%)	0	100	100
6	4F	95/129 (74%)	94 (99%)	1 (1%)	0	100	100
7	4G	73/97 (75%)	69 (94%)	4 (6%)	0	100	100
8	4H	80/86 (93%)	77 (96%)	3 (4%)	0	100	100
9	4I	65/75 (87%)	64 (98%)	1 (2%)	0	100	100
10	4J	56/80 (70%)	55 (98%)	1 (2%)	0	100	100
11	4K	47/80 (59%)	46 (98%)	1 (2%)	0	100	100
12	4L	44/63 (70%)	43 (98%)	1 (2%)	0	100	100
13	4M	41/70 (59%)	41 (100%)	0	0	100	100
14	4N	80/82 (98%)	72 (90%)	7 (9%)	1 (1%)	12	45
All	All	1815/2087 (87%)	1756 (97%)	58 (3%)	1 (0%)	54	85

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	4N	33	VAL

5.3.2 Protein sidechains [i](#)

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	4A	425/425 (100%)	418 (98%)	7 (2%)	62	86
2	4B	210/211 (100%)	202 (96%)	8 (4%)	33	69
3	4C	223/225 (99%)	216 (97%)	7 (3%)	40	75
4	4D	124/149 (83%)	116 (94%)	8 (6%)	17	50
5	4E	92/124 (74%)	87 (95%)	5 (5%)	22	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	4F	80/101 (79%)	76 (95%)	4 (5%)	24	60
7	4G	65/80 (81%)	56 (86%)	9 (14%)	3	17
8	4H	73/76 (96%)	70 (96%)	3 (4%)	30	67
9	4I	54/61 (88%)	51 (94%)	3 (6%)	21	56
10	4J	49/68 (72%)	47 (96%)	2 (4%)	30	67
11	4K	38/66 (58%)	38 (100%)	0	100	100
12	4L	39/55 (71%)	38 (97%)	1 (3%)	46	78
13	4M	37/57 (65%)	36 (97%)	1 (3%)	44	77
14	4N	70/70 (100%)	65 (93%)	5 (7%)	14	46
All	All	1579/1768 (89%)	1516 (96%)	63 (4%)	35	68

5 of 63 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	4D	87	PHE
10	4J	33	ARG
6	4F	9	ASP
10	4J	10	LYS
14	4N	33	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
3	4C	243	HIS
8	4H	22	ASN
13	4M	39	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](#)

1 non-standard protein/DNA/RNA residue is 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
2	FME	4B	1	2	8,9,10	0.92	0	7,9,11	0.93	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
2	FME	4B	1	2	-	4/7/9/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	4B	1	FME	O1-CN-N-CA
2	4B	1	FME	C-CA-CB-CG
2	4B	1	FME	N-CA-CB-CG
2	4B	1	FME	CB-CG-SD-CE

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 29 ligands modelled in this entry, 4 are monoatomic - leaving 25 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
15	PGV	4J	101	-	50,50,50	0.29	0	53,56,56	0.35	0
15	PGV	4L	101	-	50,50,50	0.30	0	53,56,56	0.38	0
15	PGV	4M	101	-	50,50,50	0.29	0	53,56,56	0.31	0
15	PGV	4A	602	-	50,50,50	0.28	0	53,56,56	0.36	0
15	PGV	4B	301	-	50,50,50	0.28	0	53,56,56	0.33	0
15	PGV	4G	101	-	50,50,50	0.29	0	53,56,56	0.46	1 (1%)
15	PGV	4C	307	-	50,50,50	0.29	0	53,56,56	0.35	0
21	CUA	4B	303	2	0,1,1	-	-	-	-	-
15	PGV	4C	302	-	50,50,50	0.30	0	53,56,56	0.67	1 (1%)
15	PGV	4C	301	-	50,50,50	0.28	0	53,56,56	0.32	0
16	HEA	4A	605	1	57,67,67	2.10	16 (28%)	61,103,103	2.44	28 (45%)
20	CDL	4C	306	-	99,99,99	0.27	0	105,111,111	0.40	1 (0%)
15	PGV	4C	305	-	50,50,50	0.30	0	53,56,56	0.56	1 (1%)
24	PEK	4G	103	-	51,51,52	0.47	0	54,56,57	0.46	0
15	PGV	4K	101	-	50,50,50	0.29	0	53,56,56	0.32	0
20	CDL	4D	201	-	99,99,99	0.27	0	105,111,111	0.37	0
16	HEA	4A	604	1	57,67,67	2.10	18 (31%)	61,103,103	2.51	26 (42%)
22	PSC	4B	304	-	51,51,51	0.47	0	57,59,59	0.43	0
25	PO4	4H	101	-	4,4,4	0.93	0	6,6,6	0.41	0
15	PGV	4C	304	-	50,50,50	0.30	0	53,56,56	0.39	0
24	PEK	4G	102	-	52,52,52	0.46	0	55,57,57	0.45	0
15	PGV	4A	603	-	50,50,50	0.30	0	53,56,56	0.34	0
15	PGV	4A	601	-	50,50,50	0.28	0	53,56,56	0.32	0
15	PGV	4C	303	-	50,50,50	0.29	0	53,56,56	0.33	0
20	CDL	4B	302	-	99,99,99	0.26	0	105,111,111	0.30	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
15	PGV	4J	101	-	-	12/55/55/55	-
15	PGV	4L	101	-	-	8/55/55/55	-
15	PGV	4M	101	-	-	8/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	PGV	4A	602	-	-	9/55/55/55	-
15	PGV	4B	301	-	-	11/55/55/55	-
15	PGV	4G	101	-	-	10/55/55/55	-
15	PGV	4C	307	-	-	4/55/55/55	-
15	PGV	4C	302	-	-	7/55/55/55	-
15	PGV	4C	301	-	-	1/55/55/55	-
16	HEA	4A	605	1	-	7/32/76/76	-
20	CDL	4C	306	-	-	27/110/110/110	-
15	PGV	4C	305	-	-	16/55/55/55	-
24	PEK	4G	103	-	-	9/55/55/56	-
15	PGV	4K	101	-	-	15/55/55/55	-
20	CDL	4D	201	-	-	19/110/110/110	-
16	HEA	4A	604	1	-	9/32/76/76	-
22	PSC	4B	304	-	-	18/55/55/55	-
15	PGV	4C	304	-	-	15/55/55/55	-
24	PEK	4G	102	-	-	10/56/56/56	-
15	PGV	4A	603	-	-	11/55/55/55	-
15	PGV	4A	601	-	-	10/55/55/55	-
15	PGV	4C	303	-	-	10/55/55/55	-
20	CDL	4B	302	-	-	16/110/110/110	-

The worst 5 of 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	4A	604	HEA	C3B-C2B	5.54	1.47	1.34
16	4A	605	HEA	C3B-C2B	5.54	1.47	1.34
16	4A	604	HEA	C3A-C2A	5.32	1.47	1.40
16	4A	605	HEA	C3A-C2A	5.28	1.47	1.40
16	4A	605	HEA	C3D-C2D	5.03	1.47	1.36

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	4A	605	HEA	C3D-C4D-ND	6.68	116.83	110.36
16	4A	604	HEA	C3D-C4D-ND	6.48	116.64	110.36
16	4A	605	HEA	C2B-C1B-NB	5.63	116.63	109.88
16	4A	604	HEA	C2B-C1B-NB	5.53	116.51	109.88
16	4A	604	HEA	C3B-C4B-NB	5.48	116.33	109.84

There are no chirality outliers.

5 of 262 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	4A	601	PGV	C03-O11-P-O13
15	4A	601	PGV	O04-C19-O03-C01
15	4A	601	PGV	C20-C19-O03-C01
15	4A	602	PGV	C02-C03-O11-P
15	4A	603	PGV	O03-C01-C02-O01

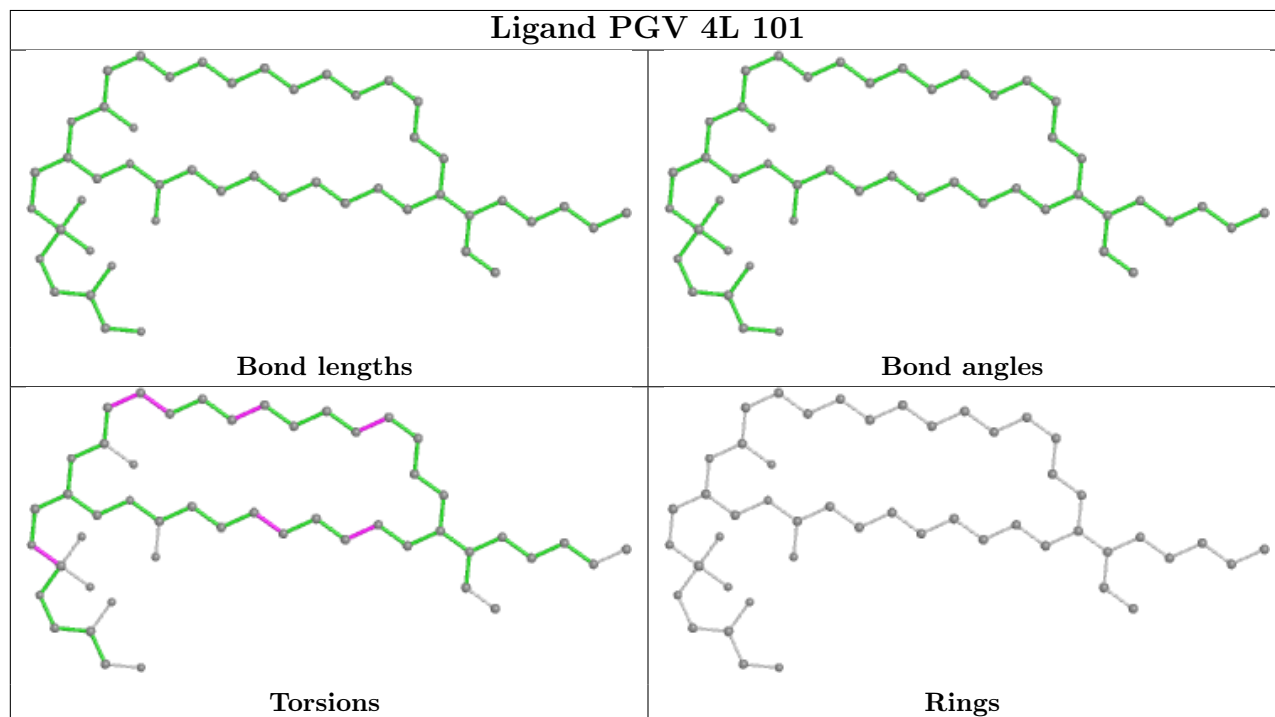
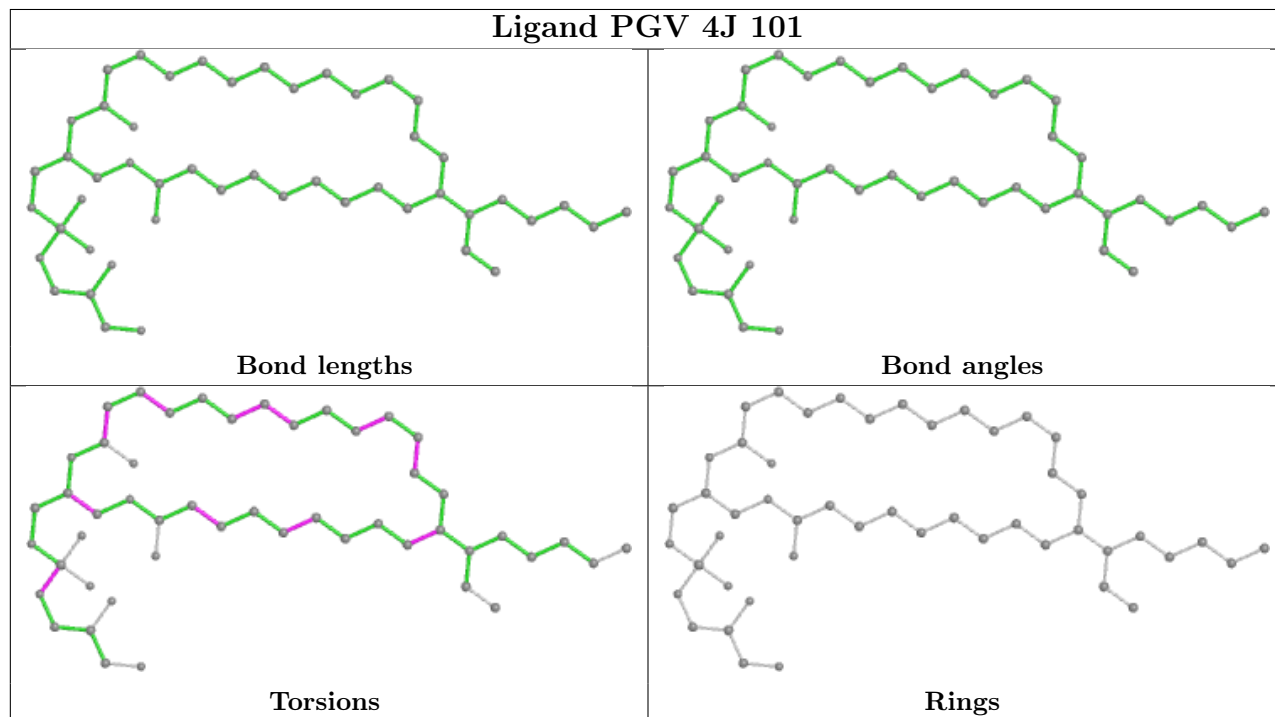
There are no ring outliers.

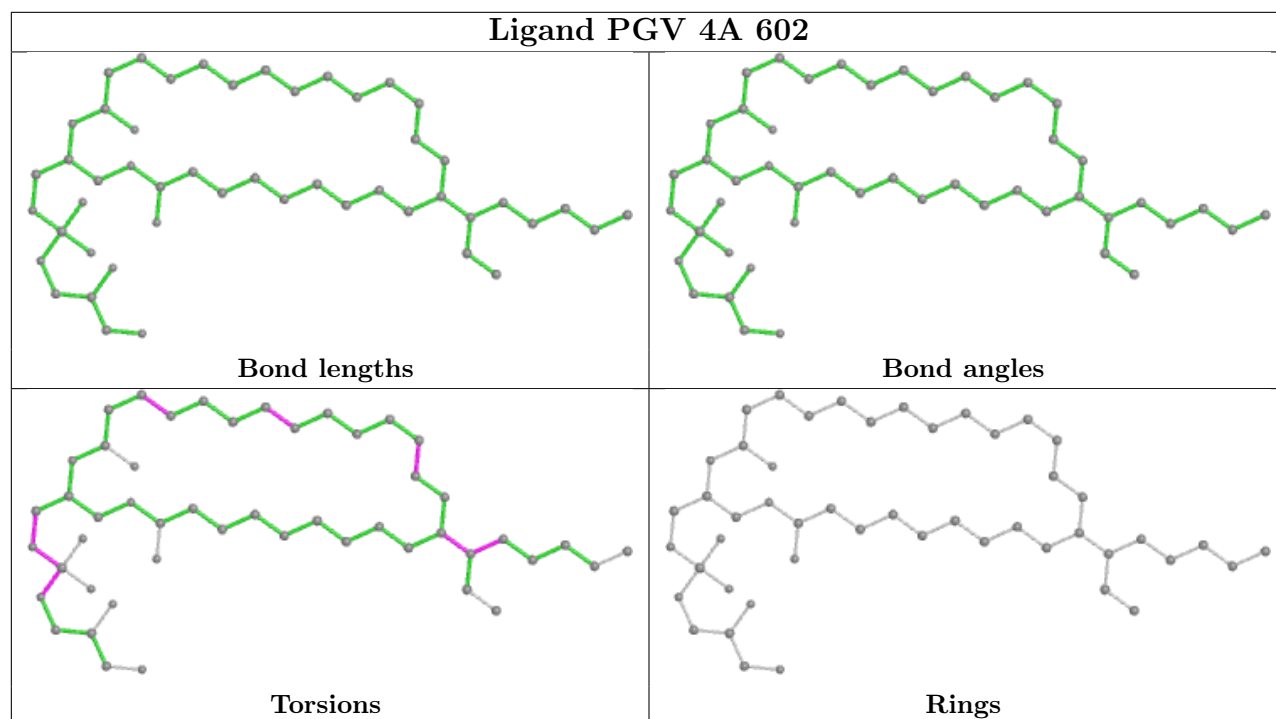
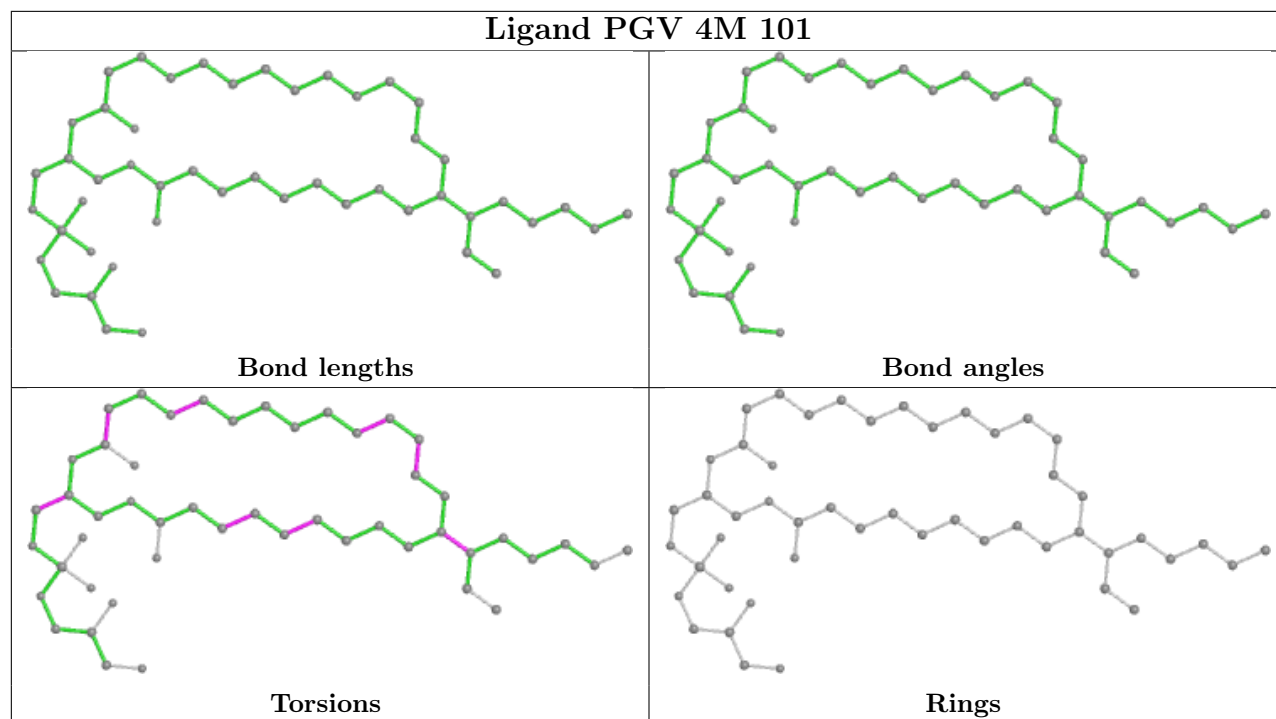
24 monomers are involved in 157 short contacts:

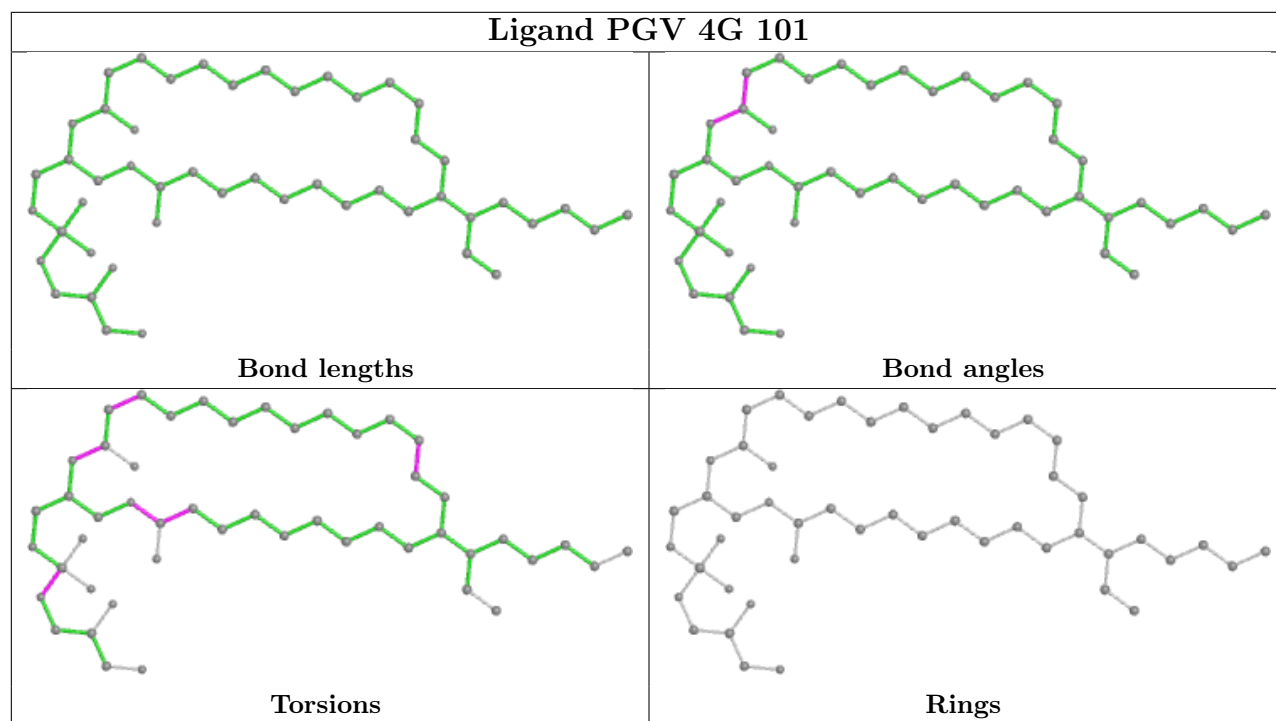
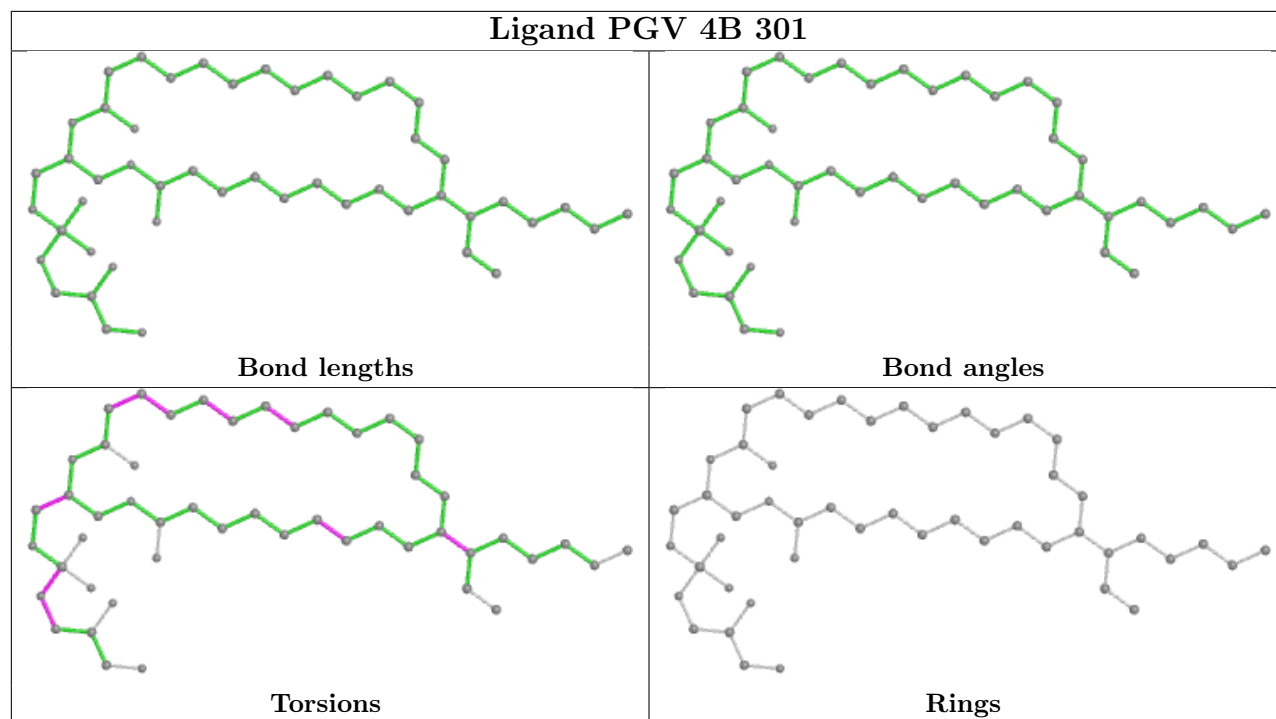
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	4J	101	PGV	3	0
15	4L	101	PGV	10	0
15	4M	101	PGV	5	0
15	4A	602	PGV	6	0
15	4B	301	PGV	12	0
15	4G	101	PGV	5	0
15	4C	307	PGV	10	0
21	4B	303	CUA	1	0
15	4C	302	PGV	6	0
15	4C	301	PGV	4	0
16	4A	605	HEA	1	0
20	4C	306	CDL	14	0
15	4C	305	PGV	4	0
24	4G	103	PEK	5	0
15	4K	101	PGV	6	0
20	4D	201	CDL	20	0
16	4A	604	HEA	7	0
22	4B	304	PSC	9	0
15	4C	304	PGV	11	0
24	4G	102	PEK	4	0
15	4A	603	PGV	6	0
15	4A	601	PGV	9	0
15	4C	303	PGV	7	0
20	4B	302	CDL	9	0

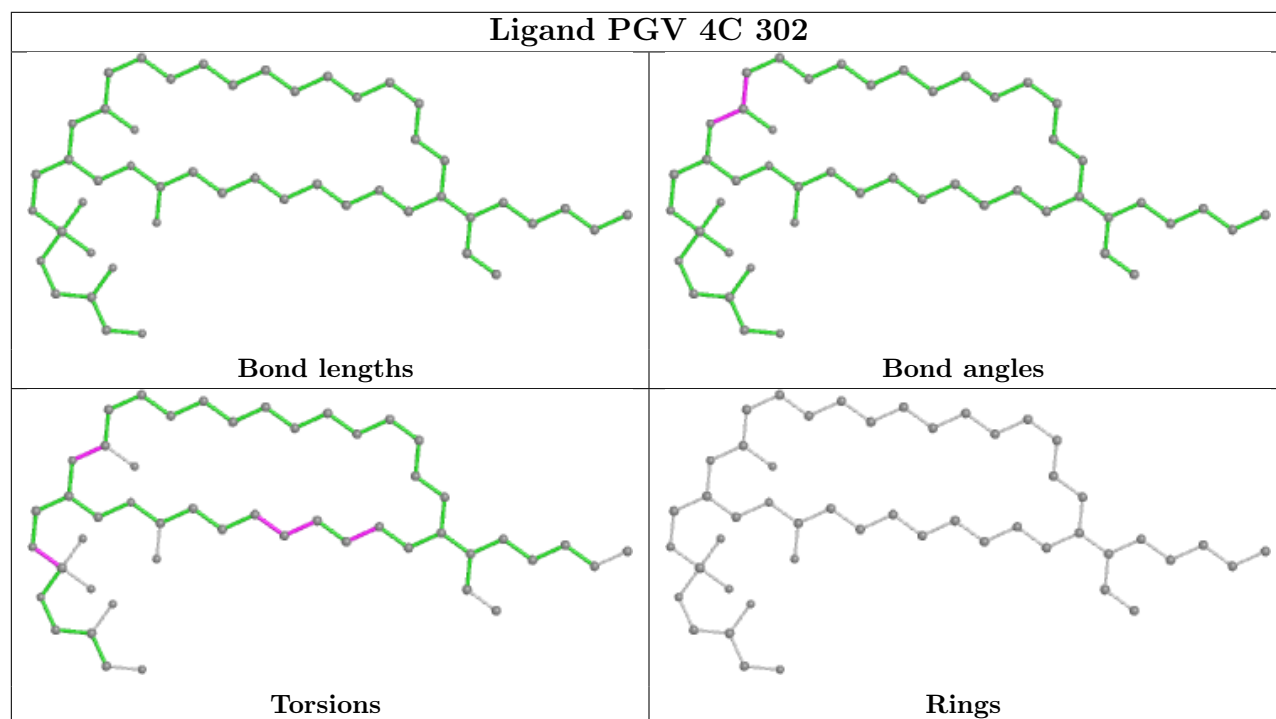
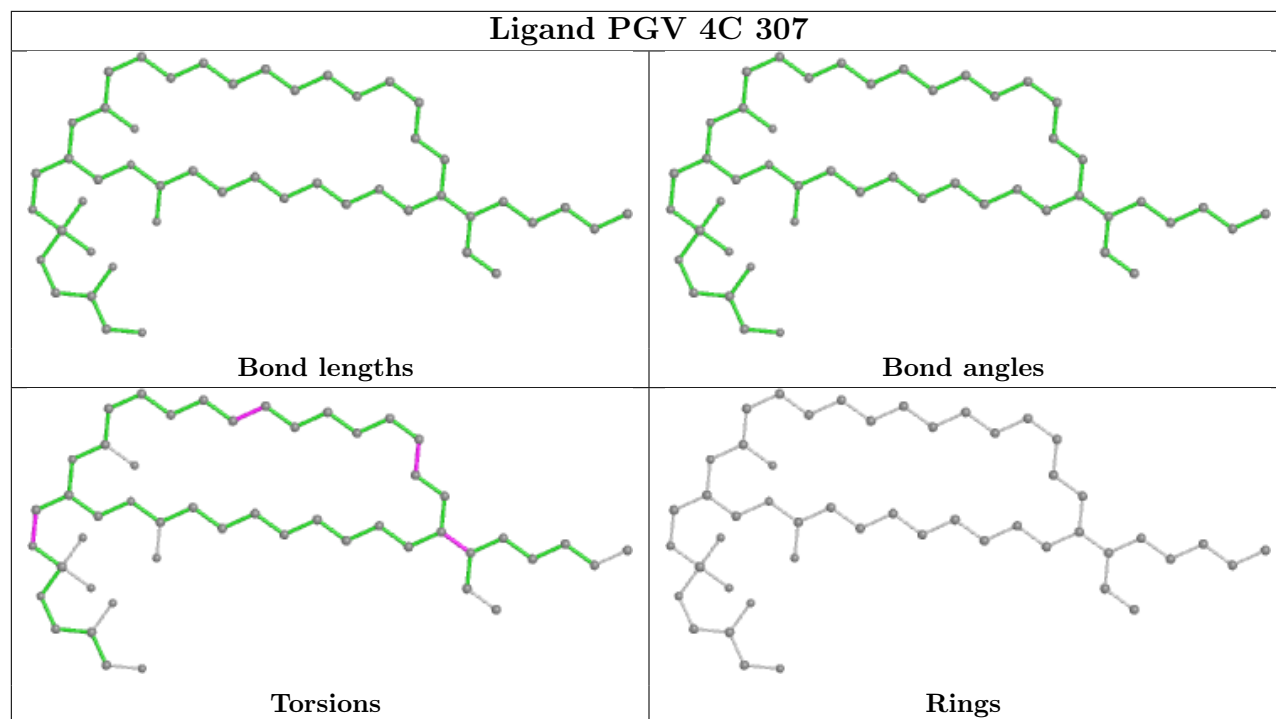
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

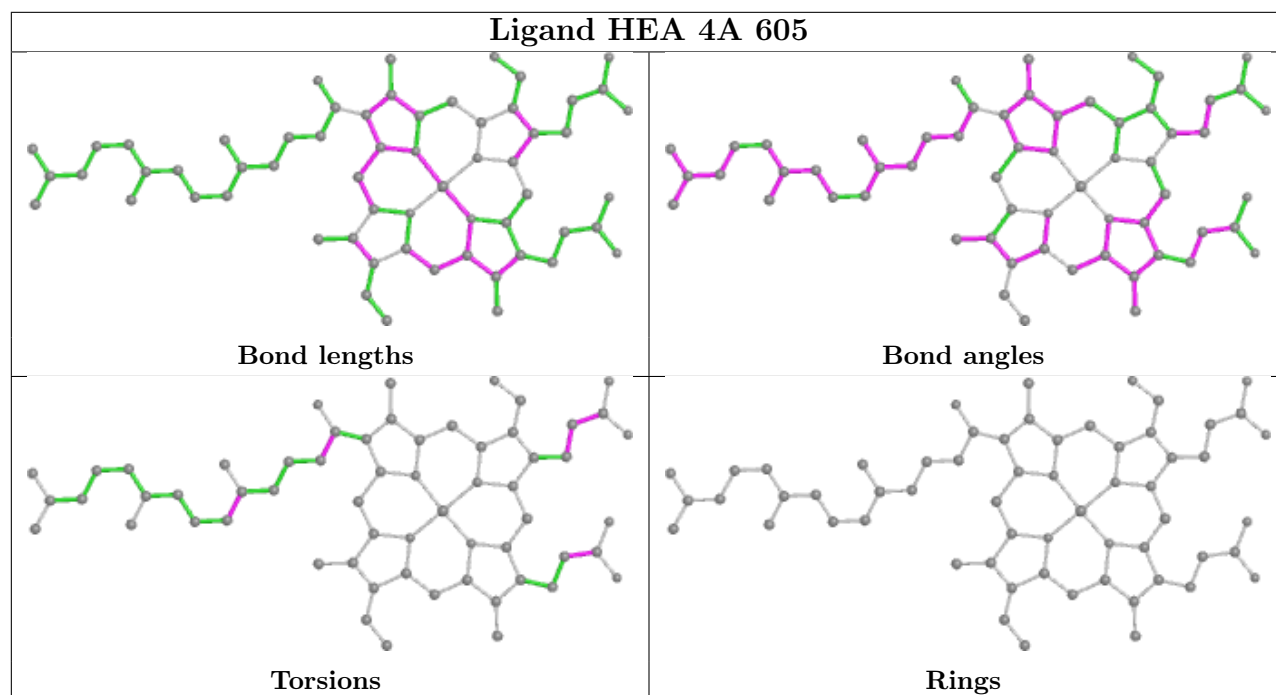
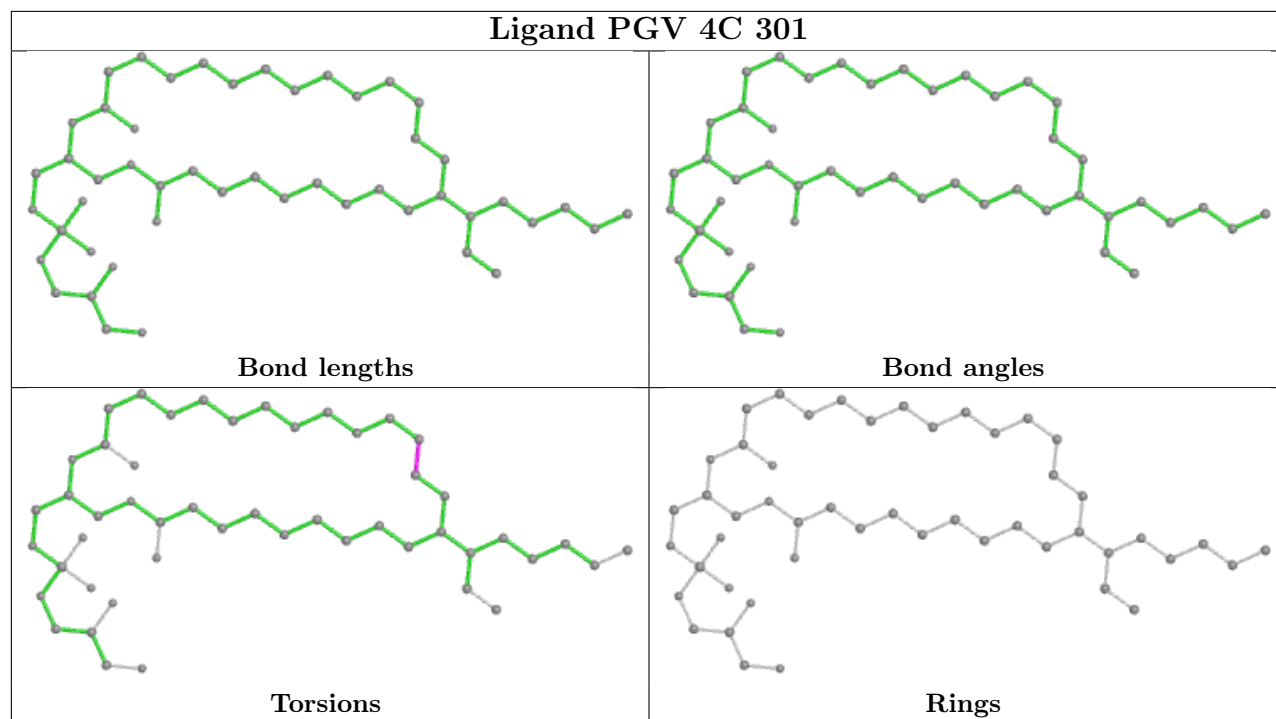
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.

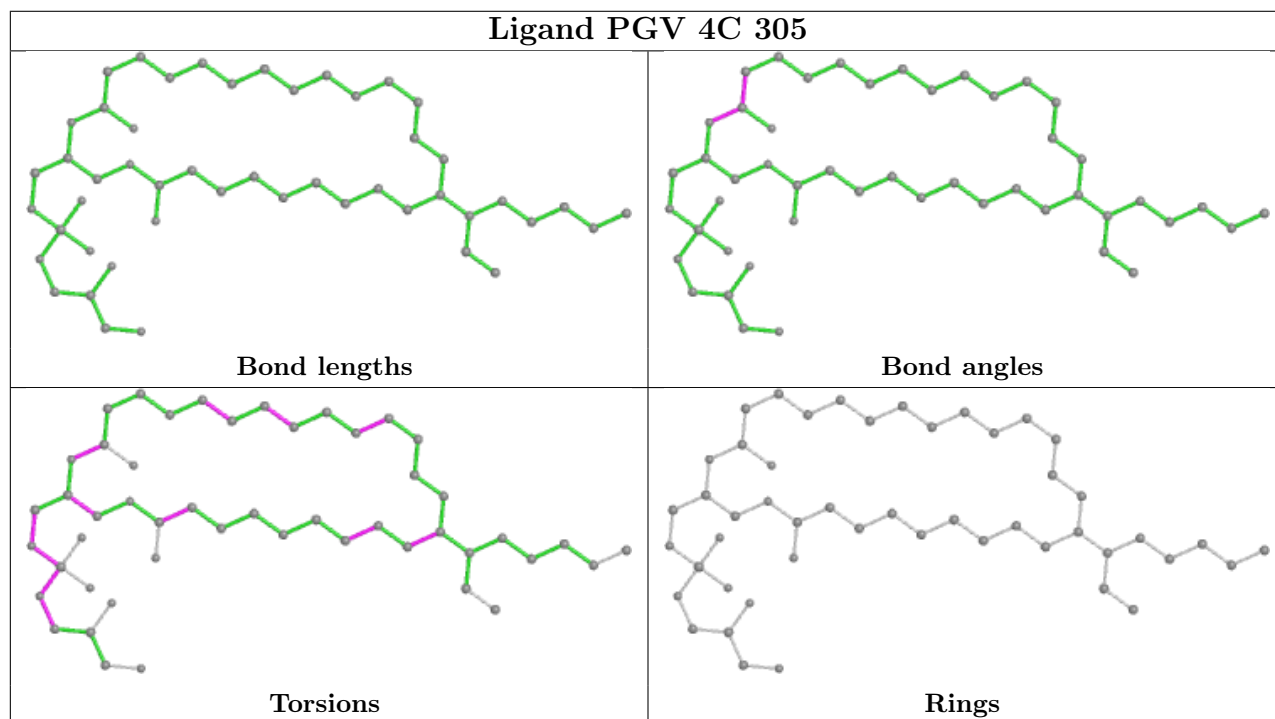
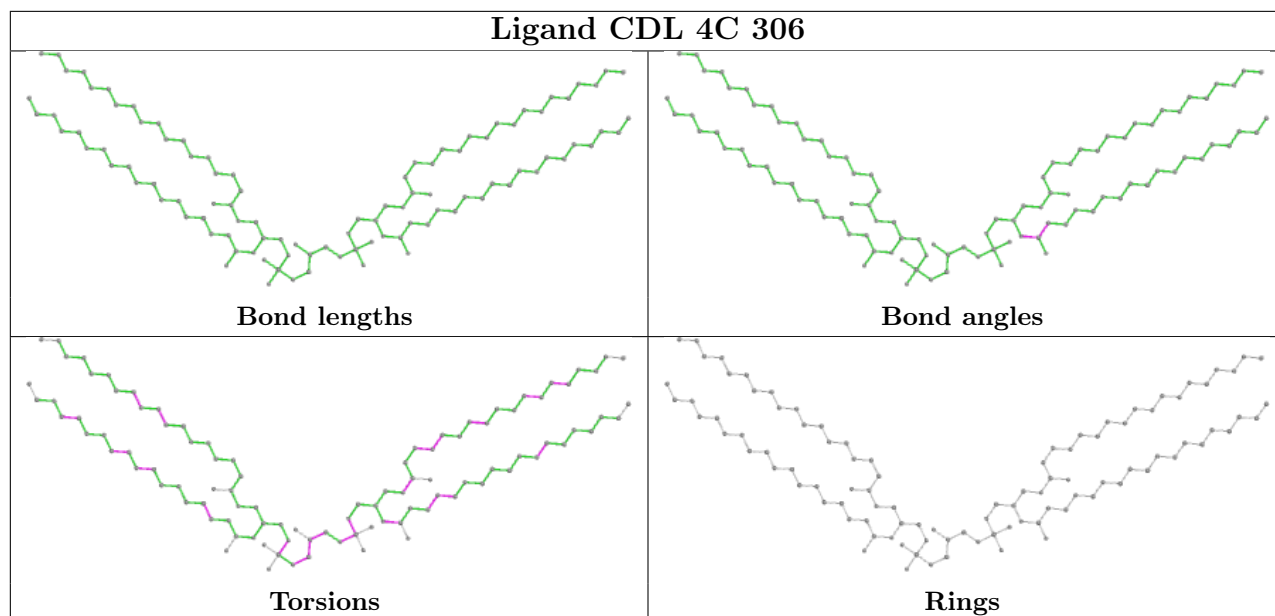


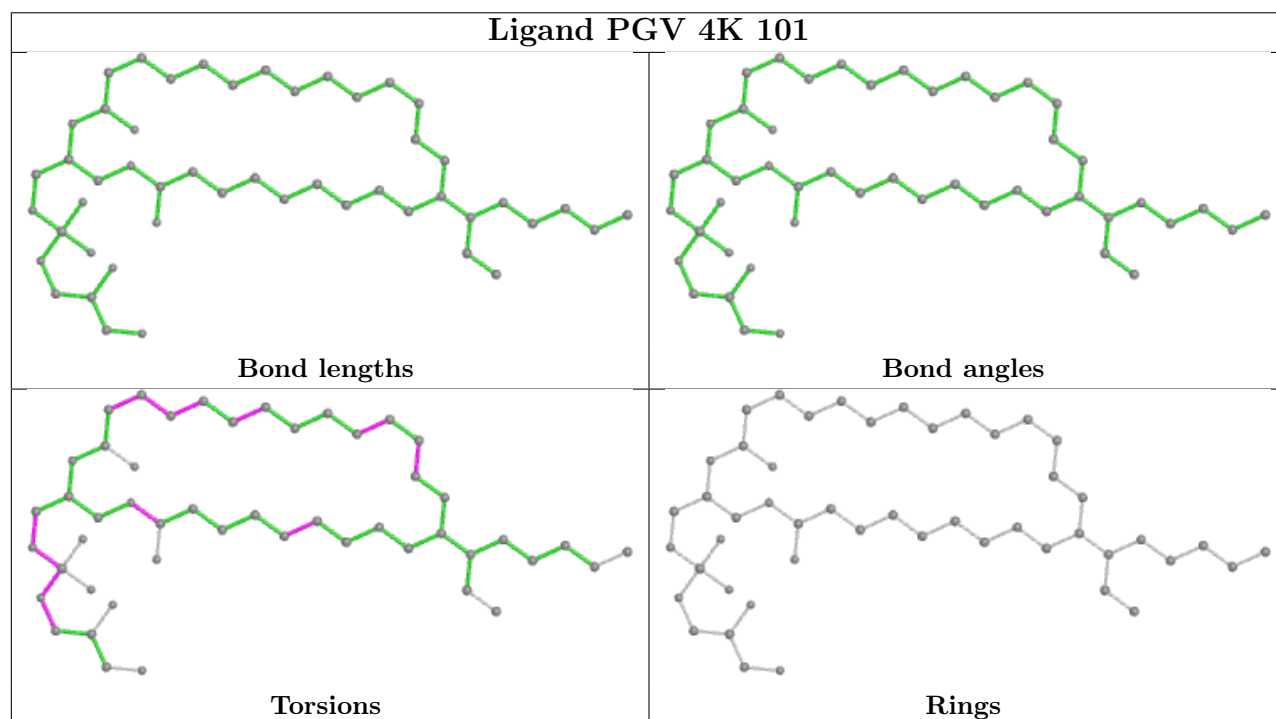
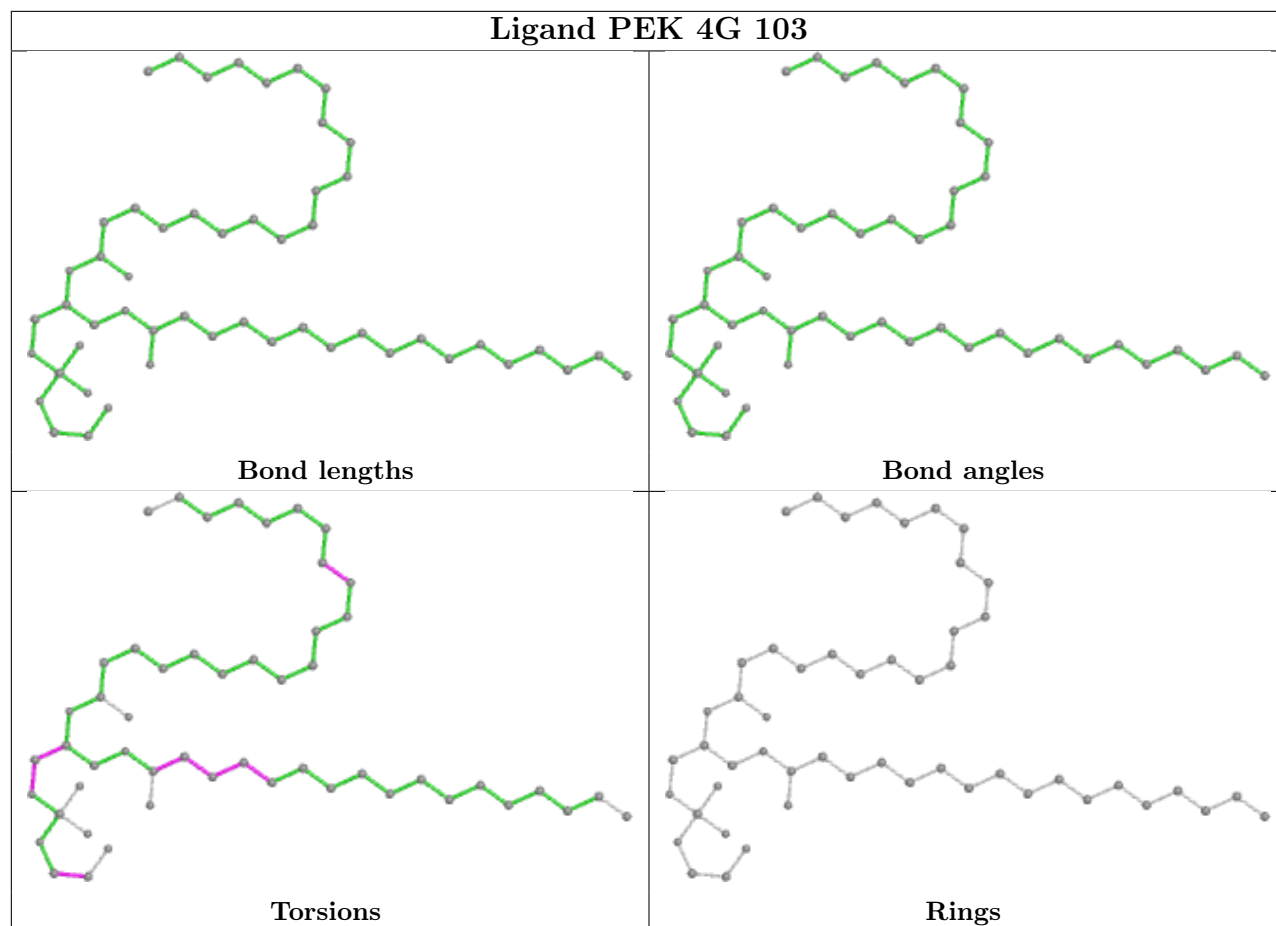


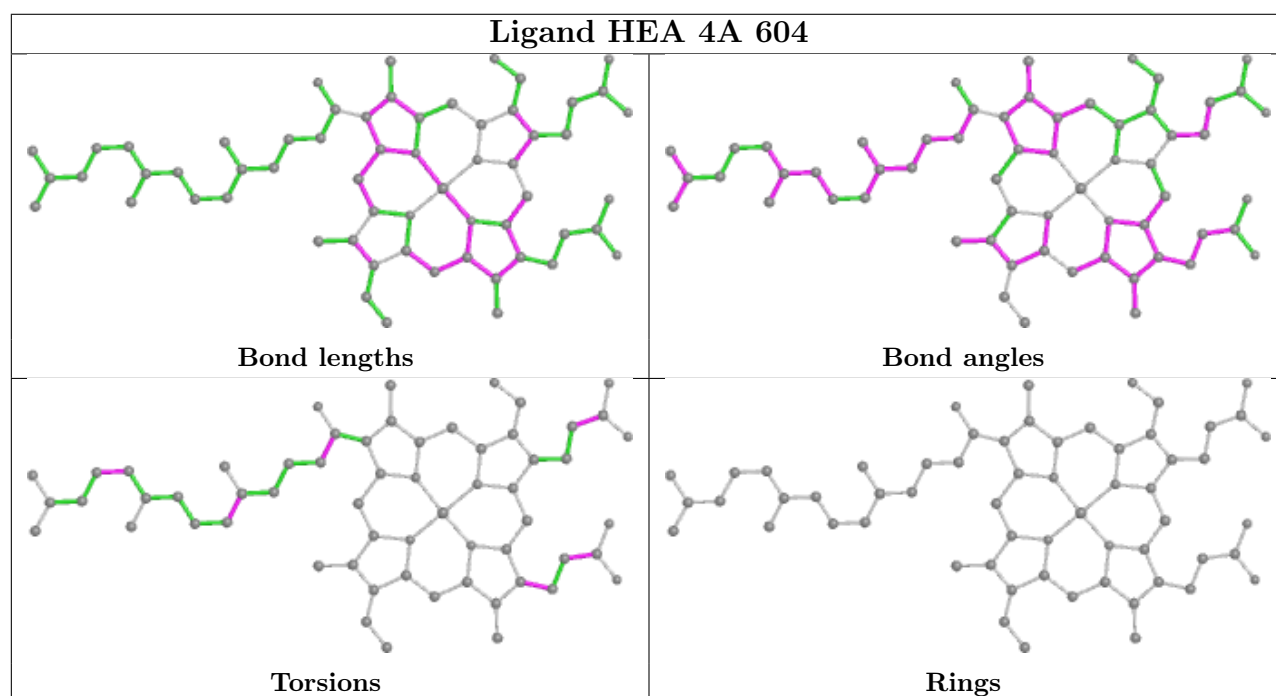
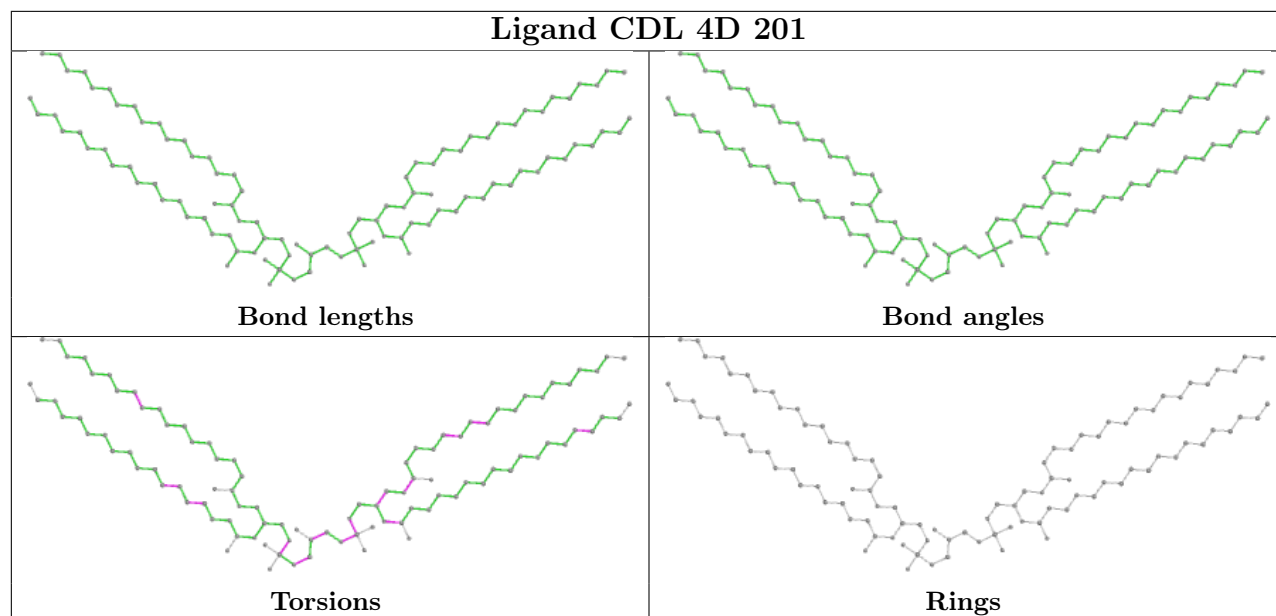


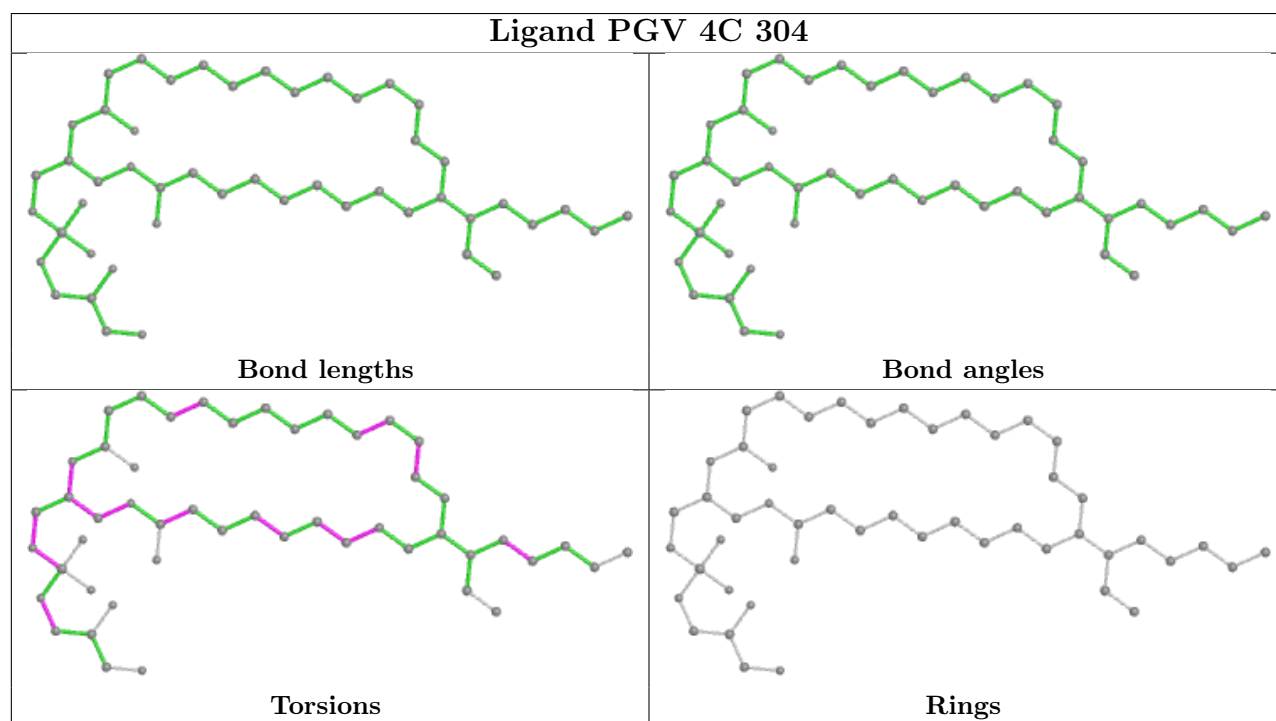
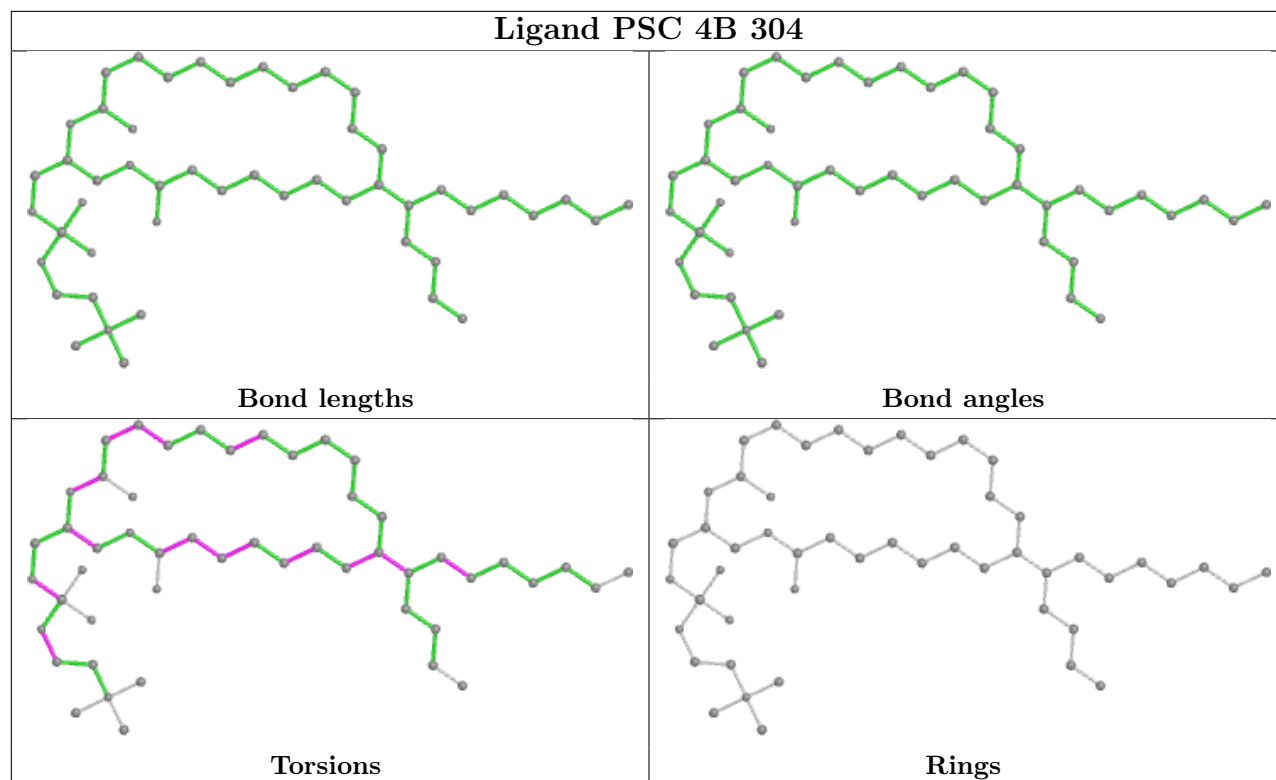


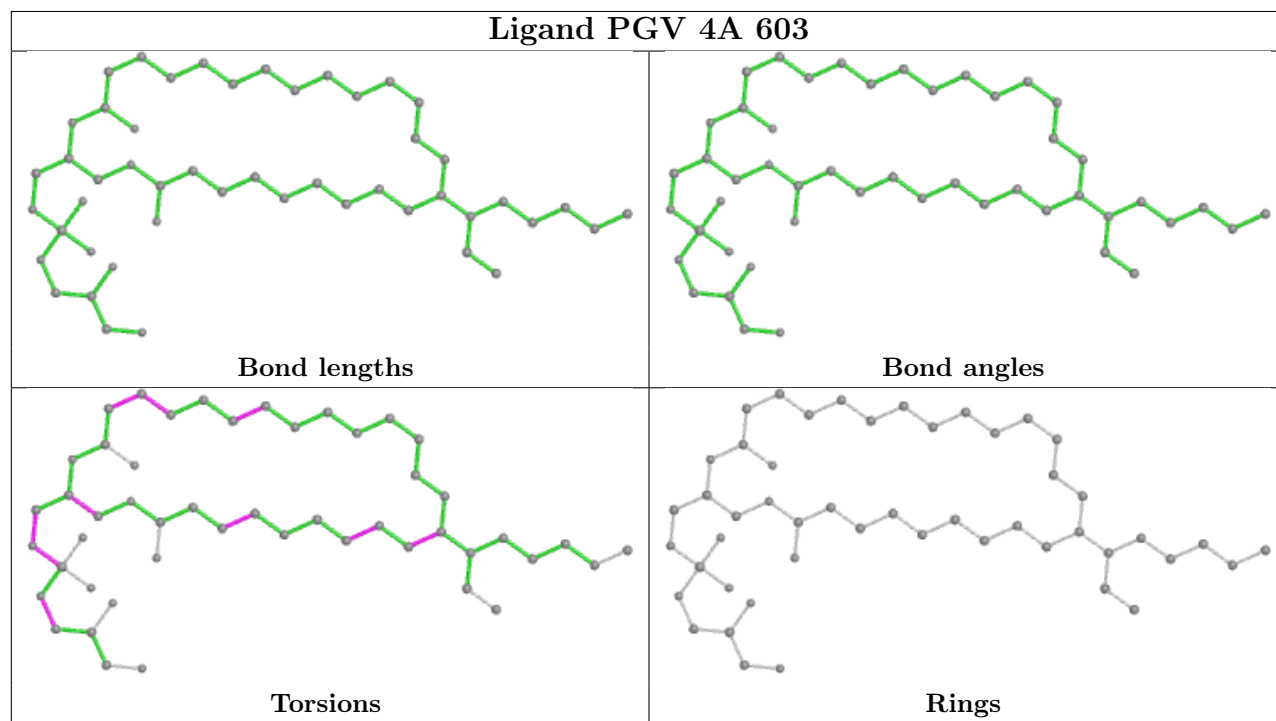
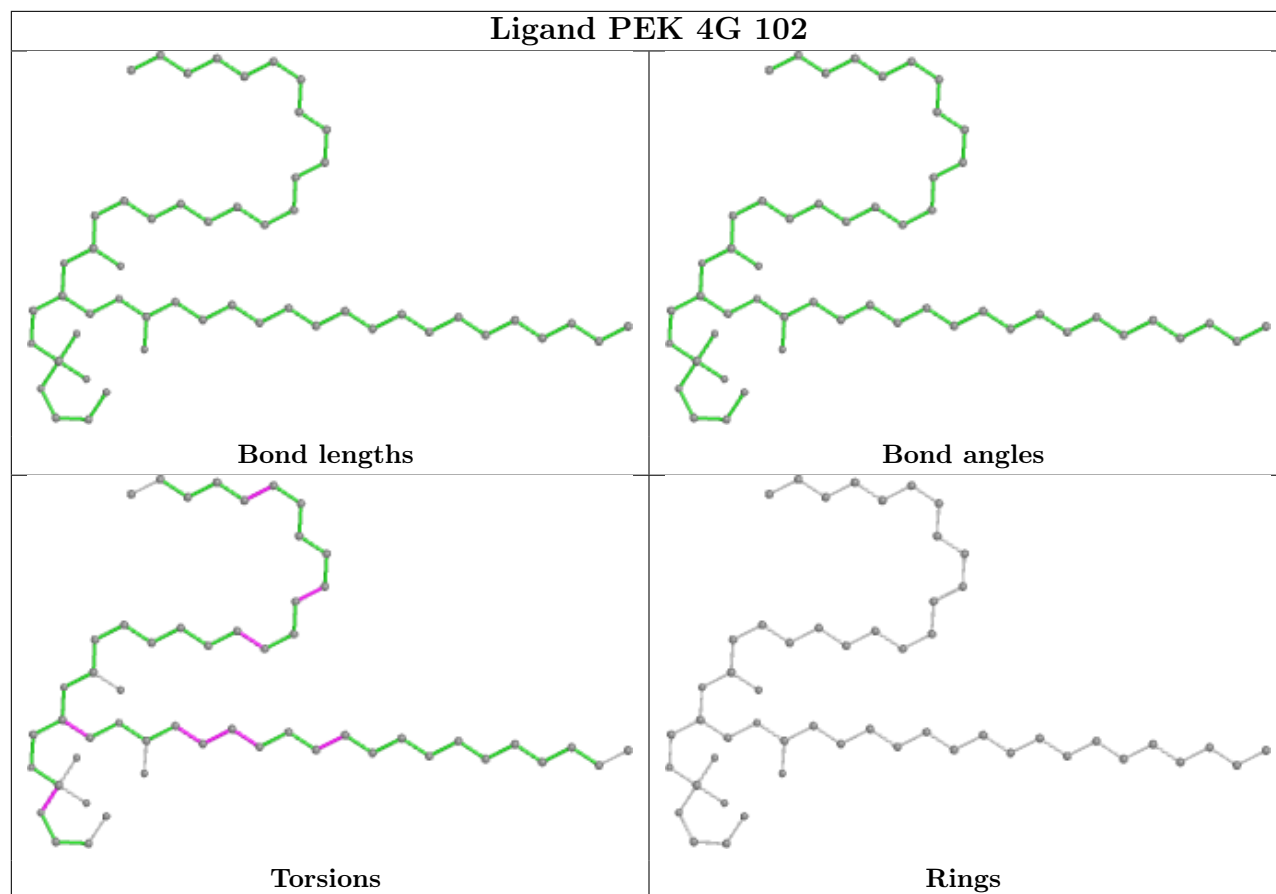


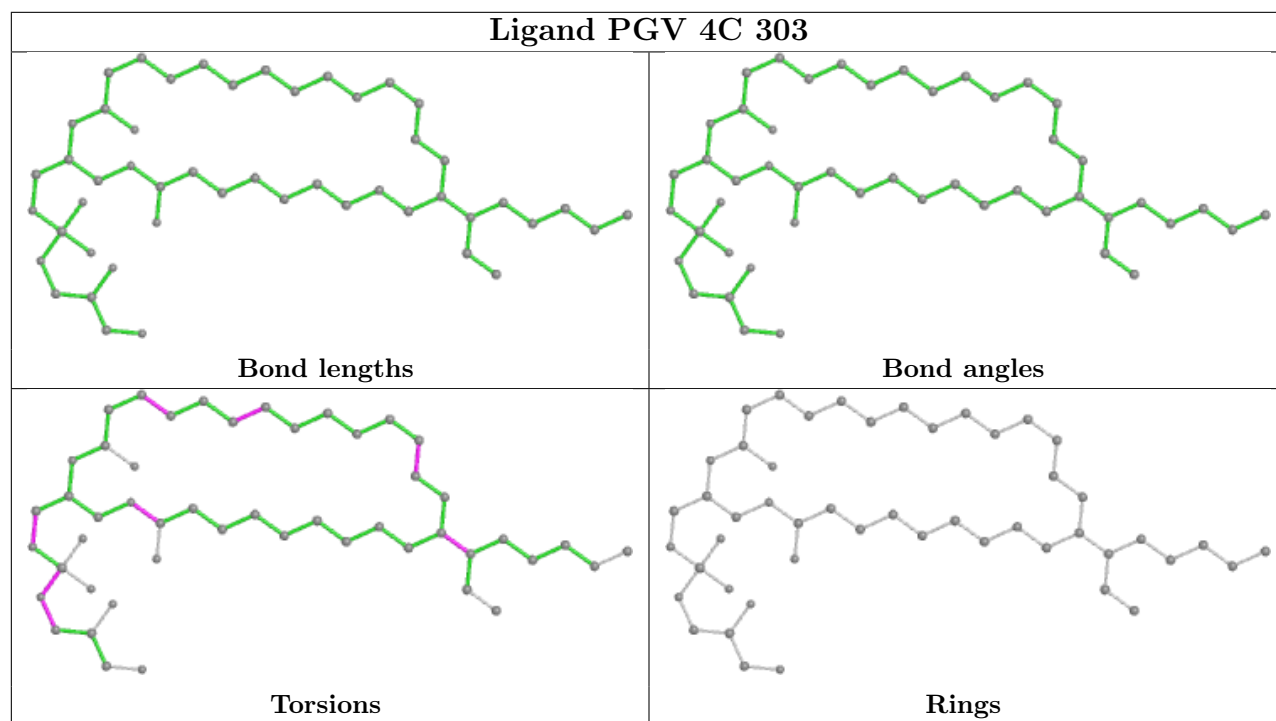
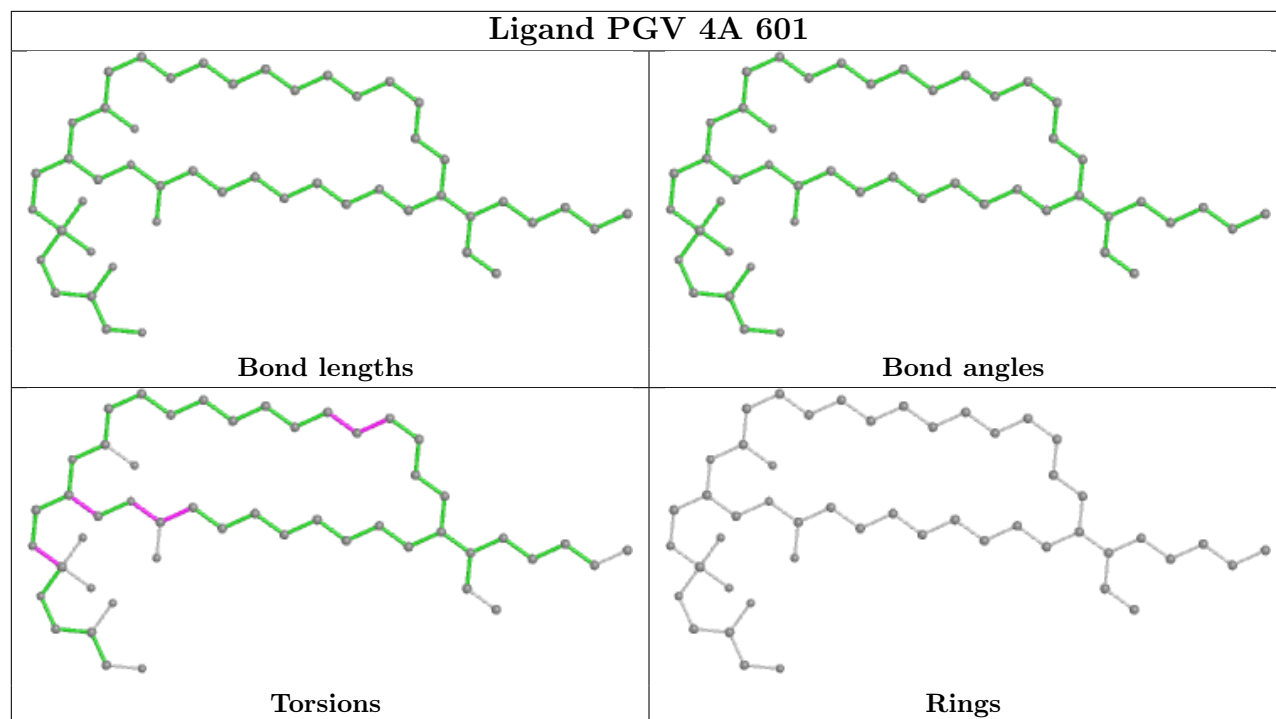


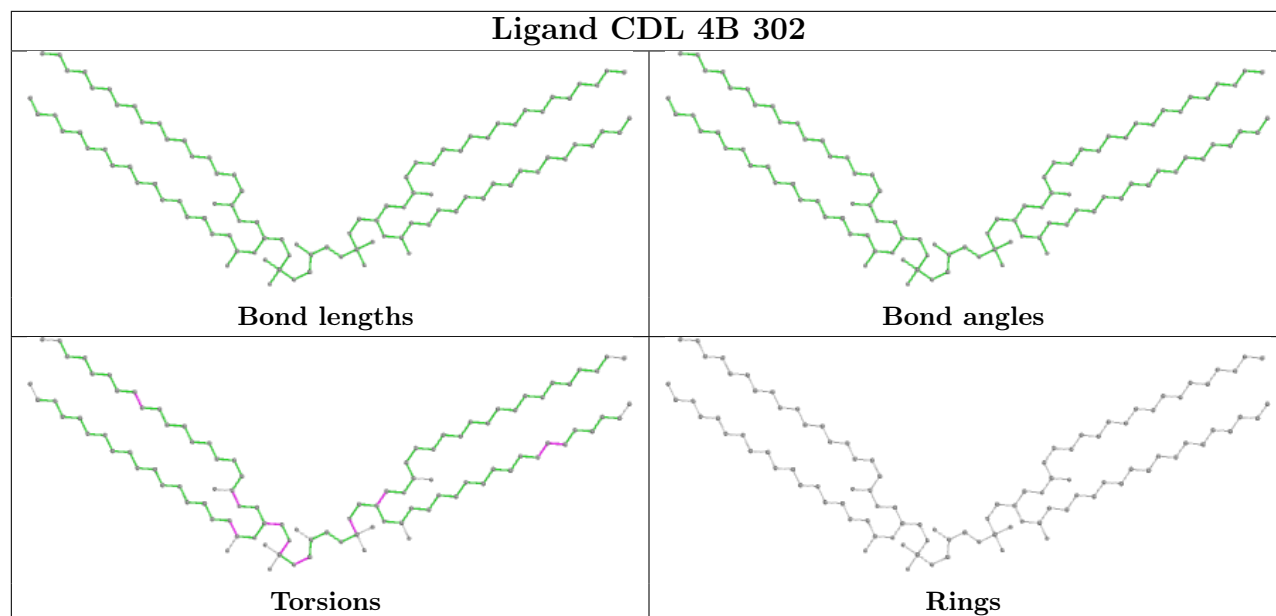












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

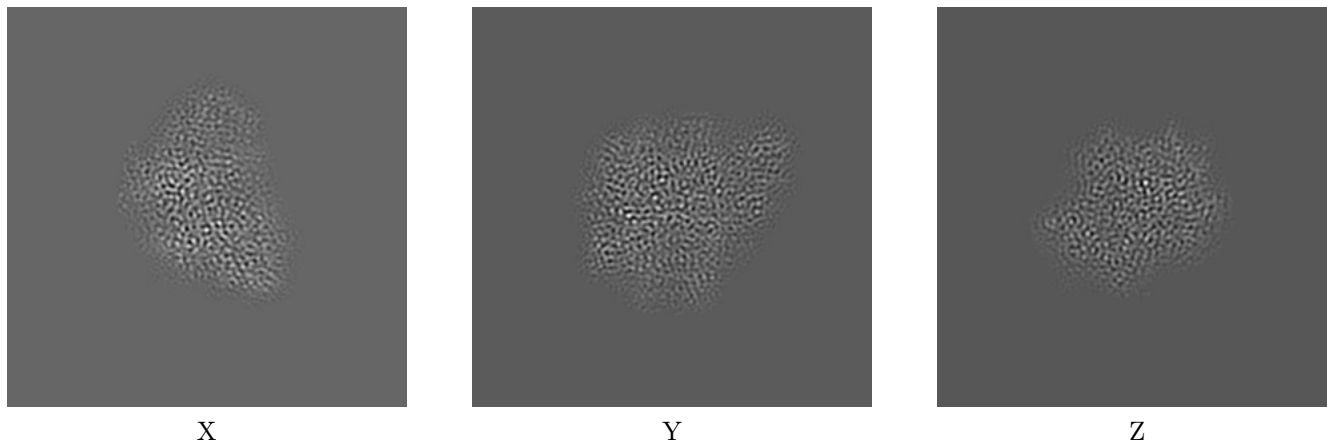
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42229. These allow visual inspection of the internal detail of the map and identification of artifacts.

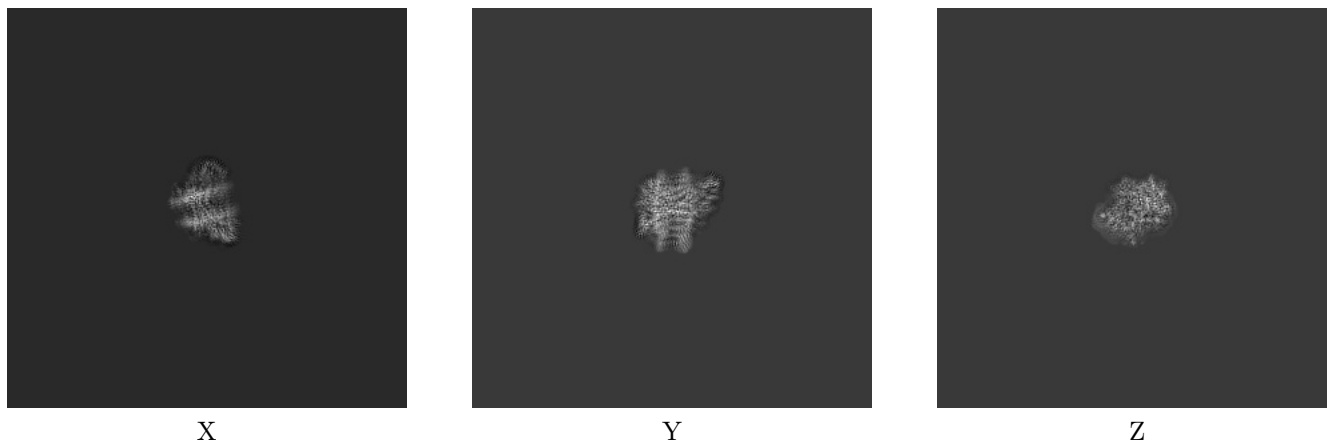
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



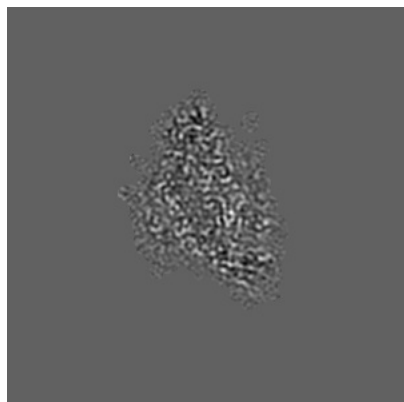
6.1.2 Raw map



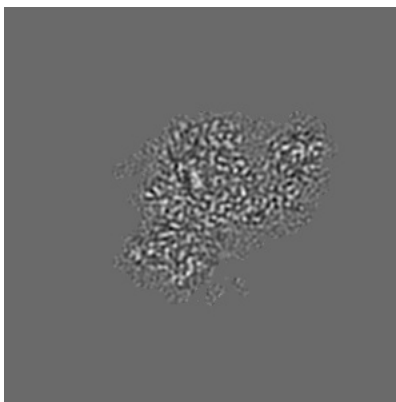
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

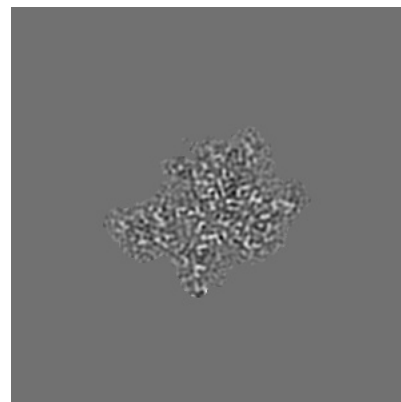
6.2.1 Primary map



X Index: 256

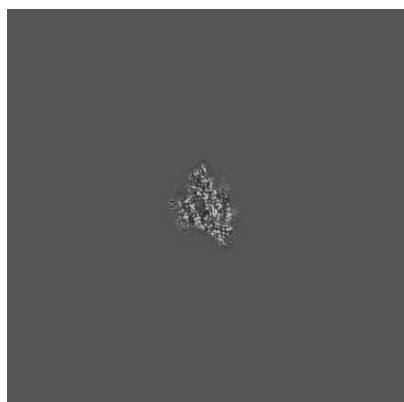


Y Index: 256

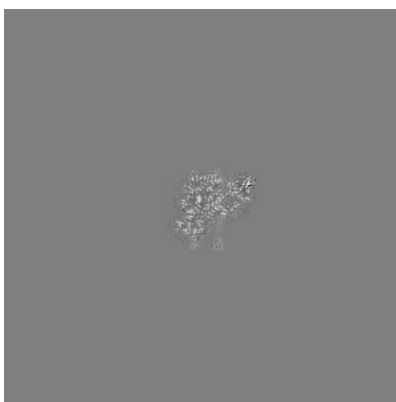


Z Index: 256

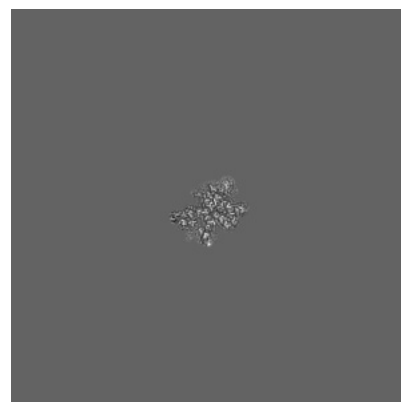
6.2.2 Raw map



X Index: 256



Y Index: 256

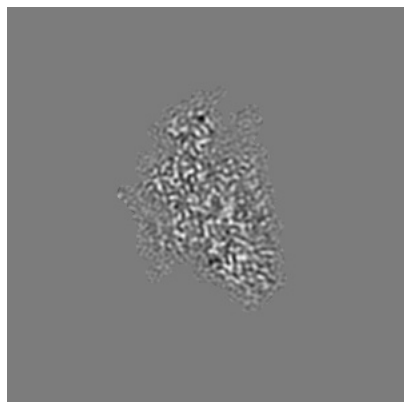


Z Index: 256

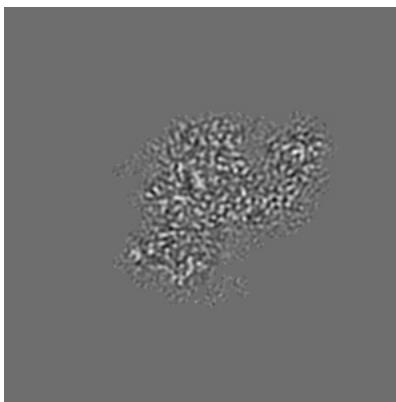
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

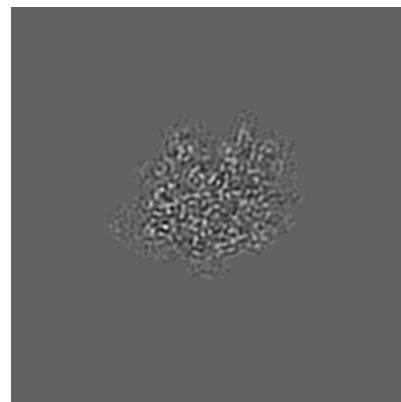
6.3.1 Primary map



X Index: 268

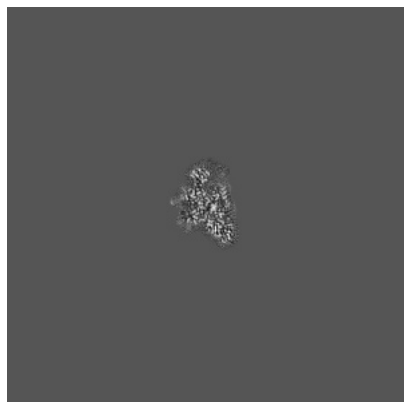


Y Index: 255

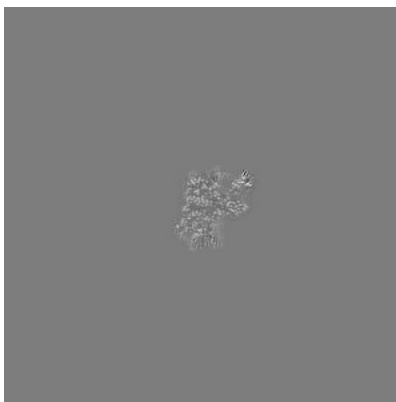


Z Index: 207

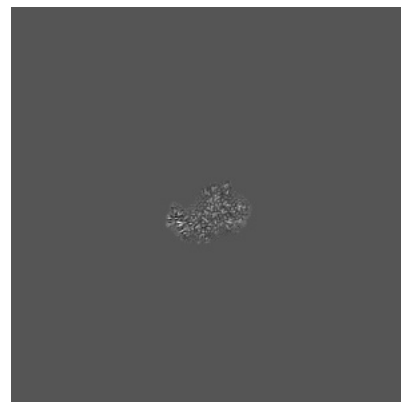
6.3.2 Raw map



X Index: 261



Y Index: 250

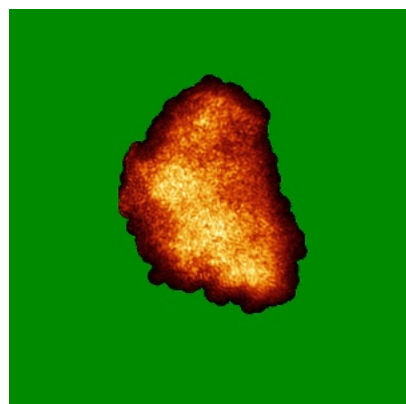


Z Index: 270

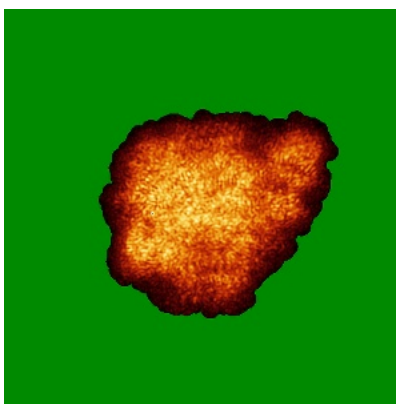
The images above show the largest variance slices of the map in three orthogonal directions.

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

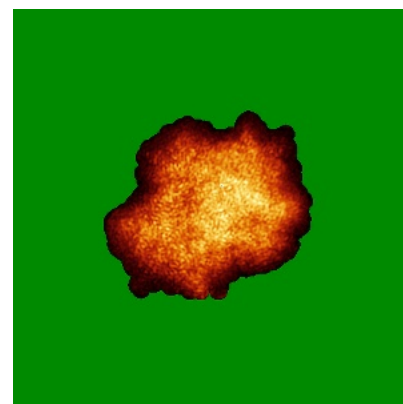
6.4.1 Primary map



X

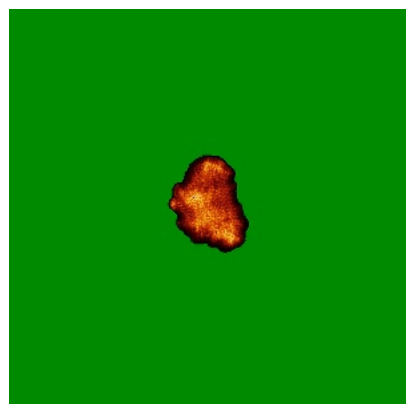


Y

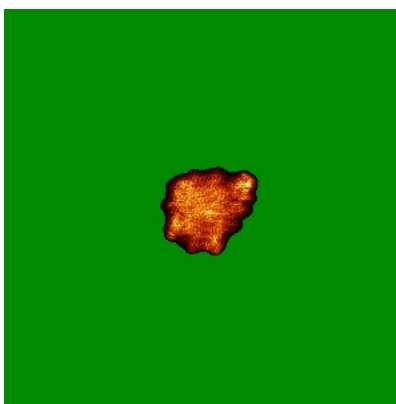


Z

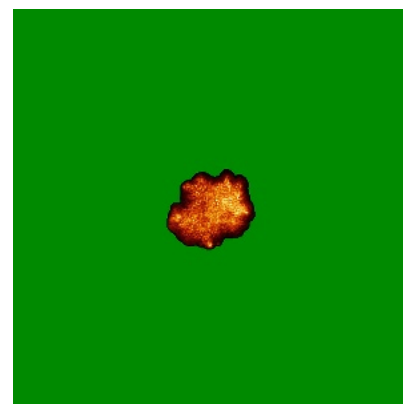
6.4.2 Raw map



X



Y

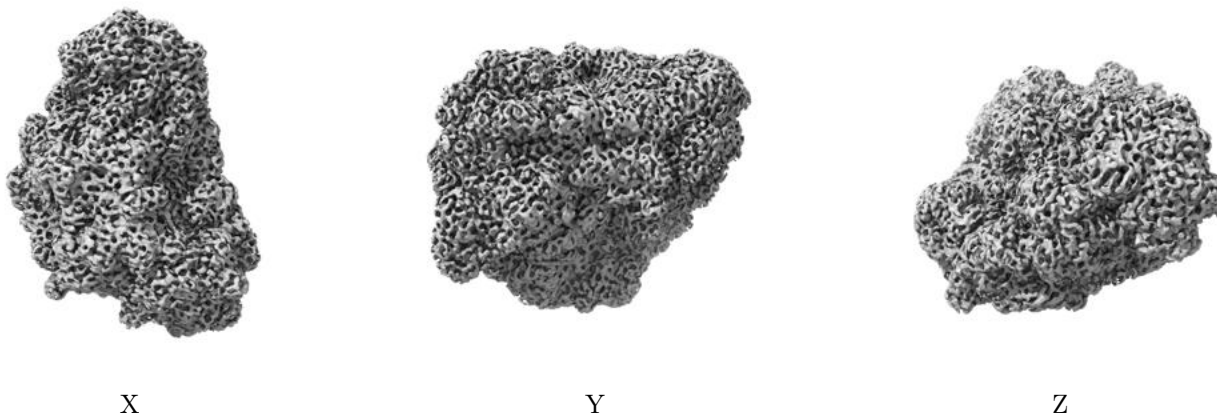


Z

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.

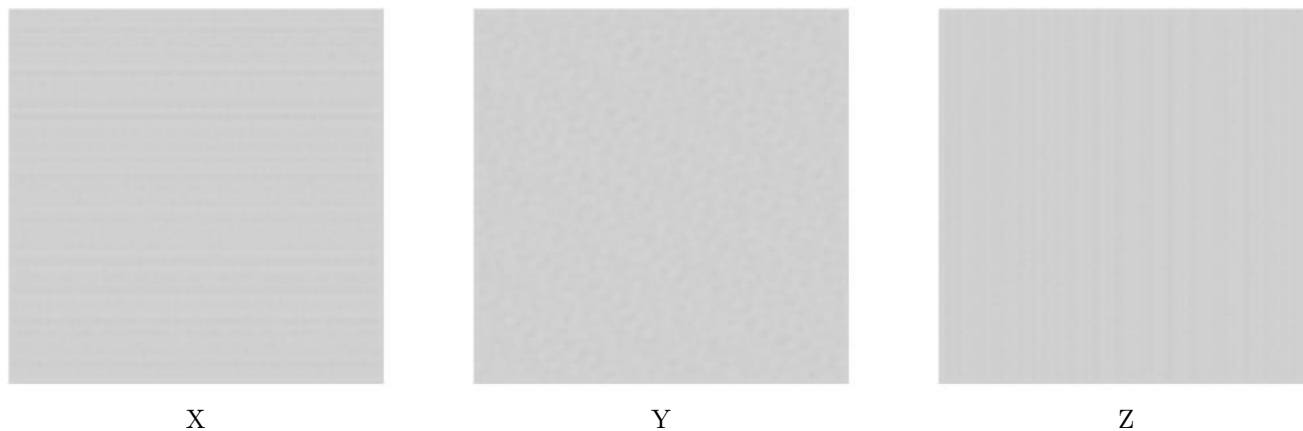
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

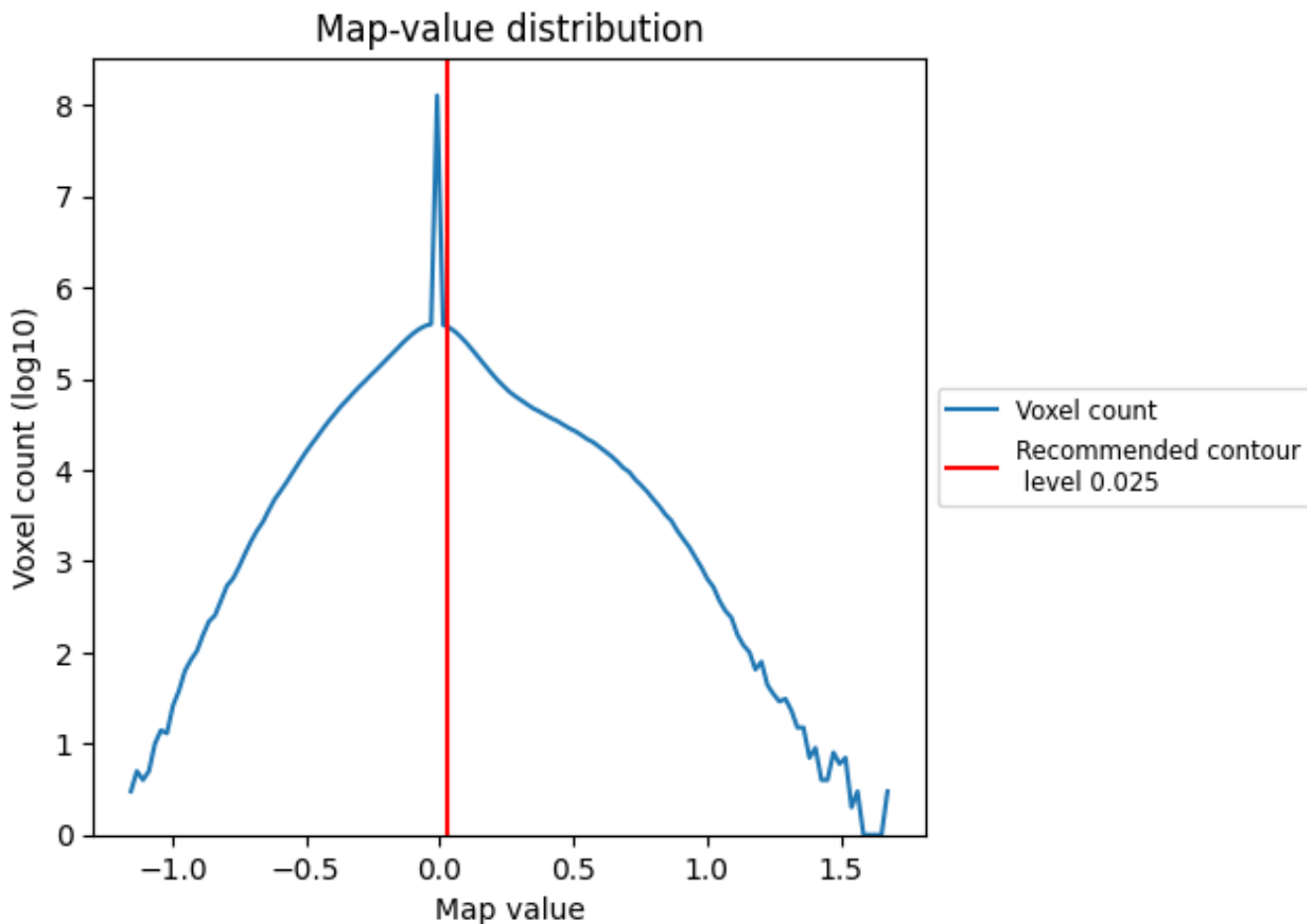
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

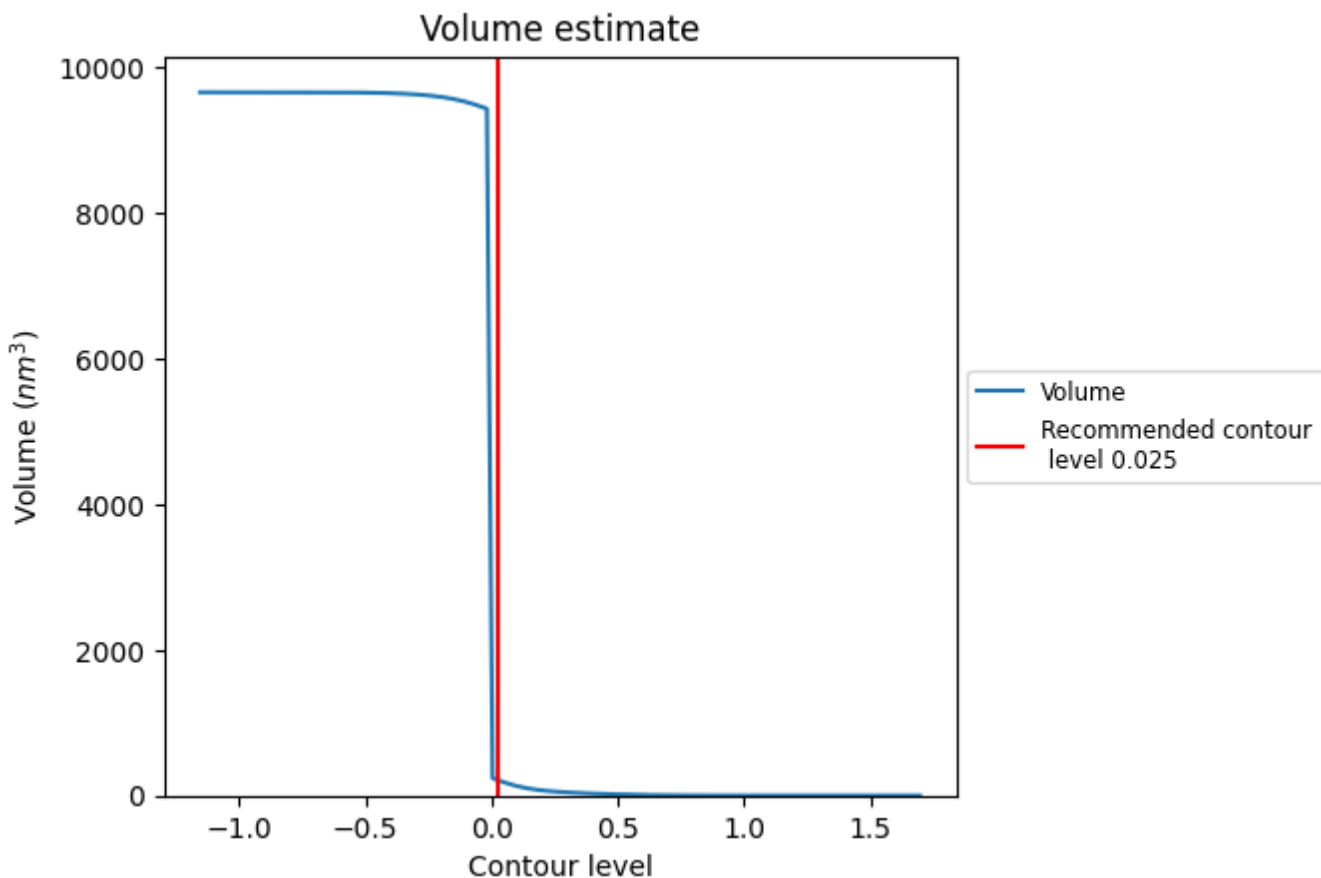
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

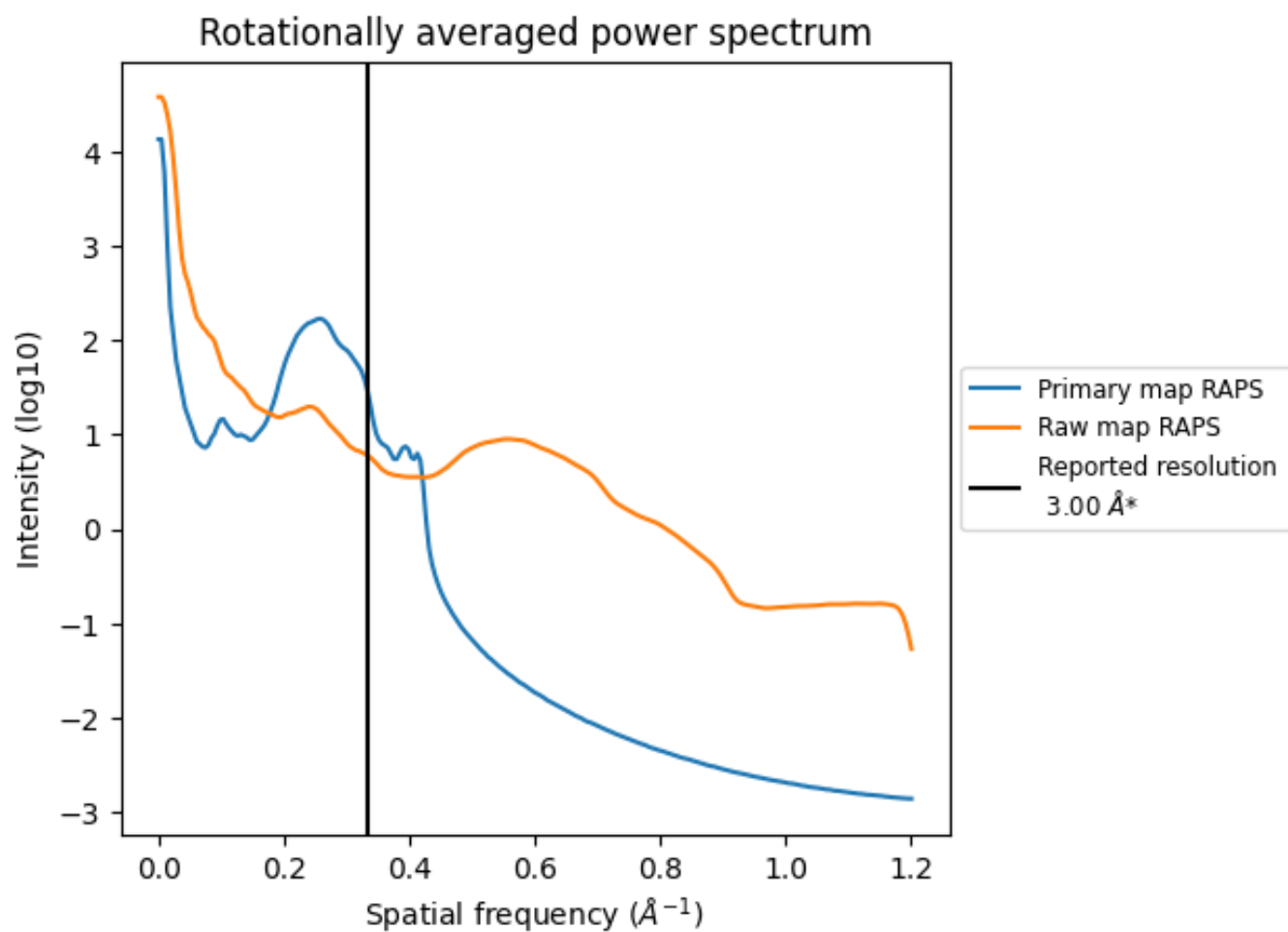
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 212 nm³; this corresponds to an approximate mass of 191 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

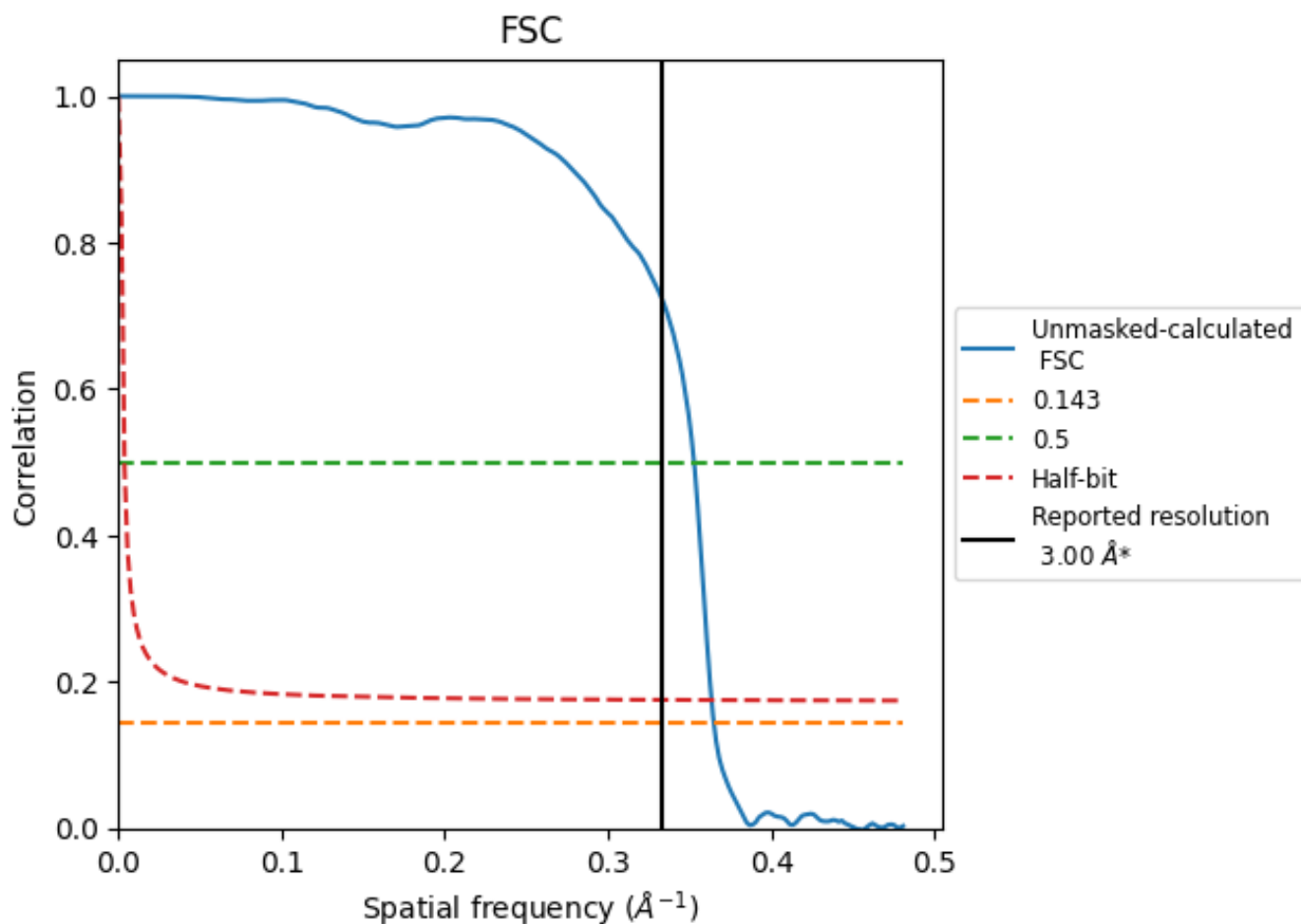


*Reported resolution corresponds to spatial frequency of 0.333 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.333\AA^{-1}

8.2 Resolution estimates [i](#)

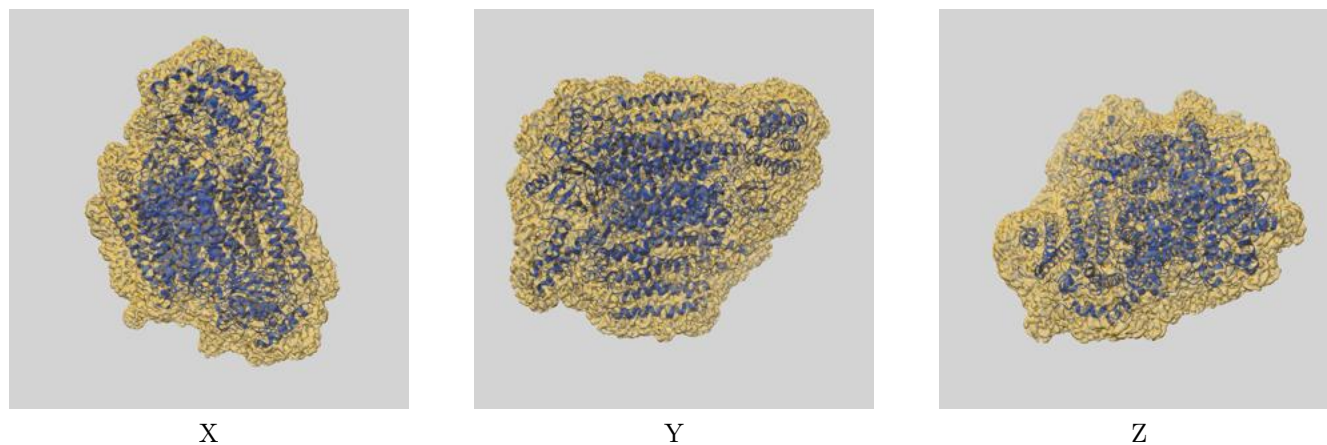
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.74	2.84	2.75

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

9 Map-model fit [i](#)

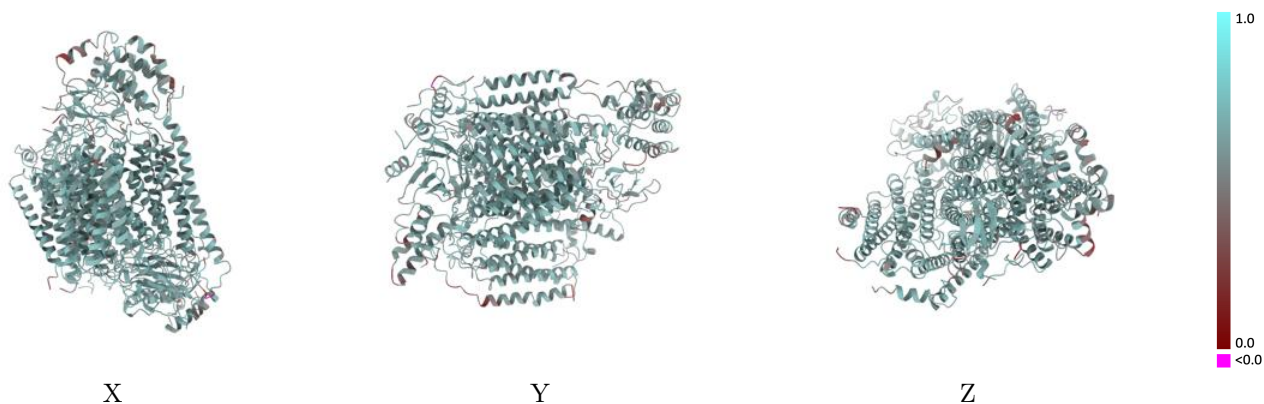
This section contains information regarding the fit between EMDB map EMD-42229 and PDB model 8UGL. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)



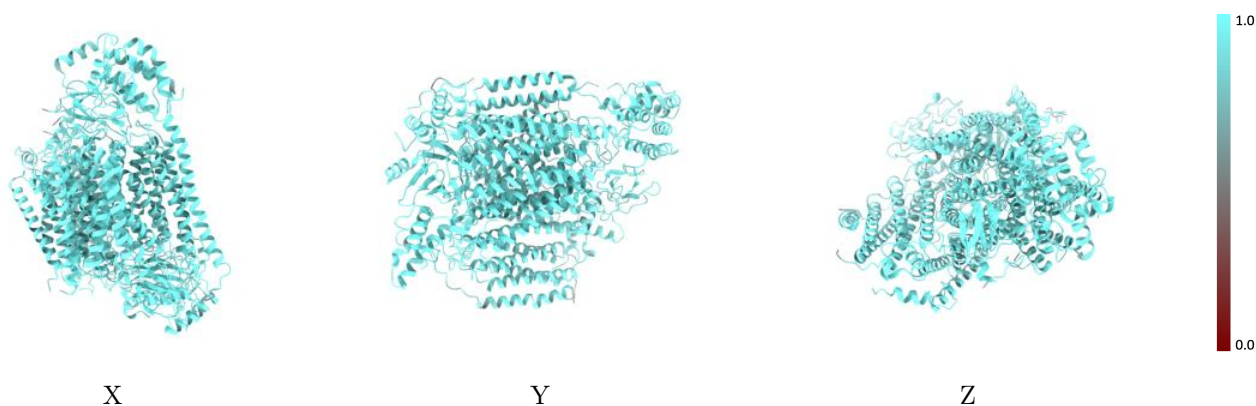
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



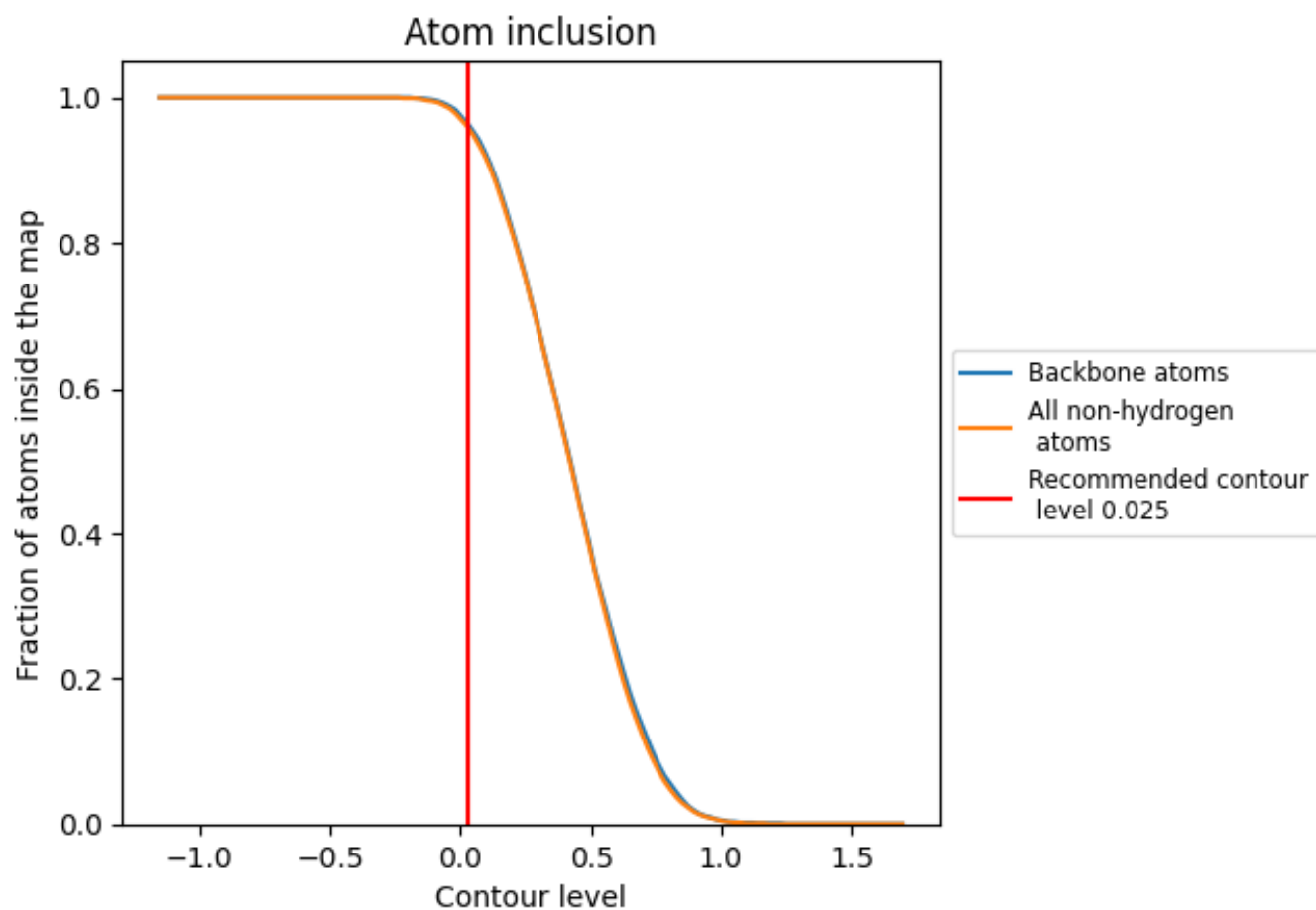
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.025).































9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 96% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9610	 0.5920
4A	 0.9900	 0.6430
4B	 0.9590	 0.5920
4C	 0.9700	 0.6010
4D	 0.9270	 0.5440
4E	 0.9340	 0.5440
4F	 0.9460	 0.5720
4G	 0.9230	 0.5300
4H	 0.9390	 0.5660
4I	 0.9700	 0.5910
4J	 0.9580	 0.5780
4K	 0.9320	 0.5430
4L	 0.9460	 0.5810
4M	 0.9400	 0.5690
4N	 0.9460	 0.5580

