



Full wwPDB EM Validation Report ⓘ

Apr 8, 2024 – 11:58 AM EDT

PDB ID : 8TO2
EMDB ID : EMD-41434
Title : Bottom cylinder of high-resolution phycobilisome quenched by OCP (local refinement)
Authors : Sauer, P.V.; Sutter, M.; Cupellini, L.
Deposited on : 2023-08-02
Resolution : 2.00 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

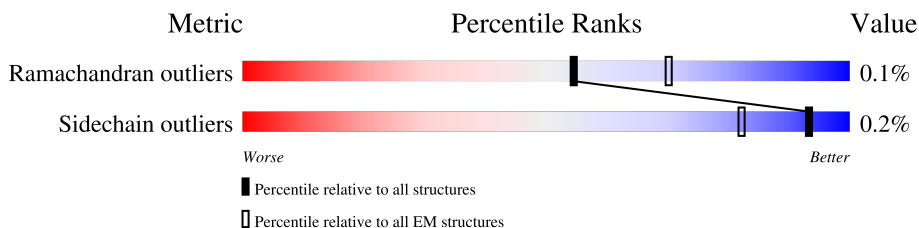
EMDB validation analysis : 0.0.1.dev92
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.1

1 Overall quality at a glance

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

The reported resolution of this entry is 2.00 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.



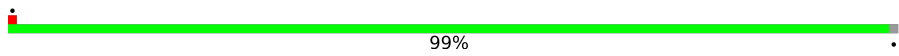
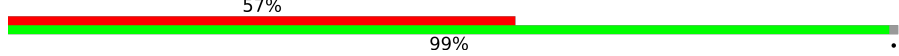
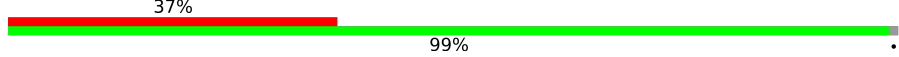
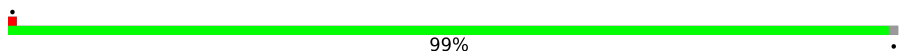
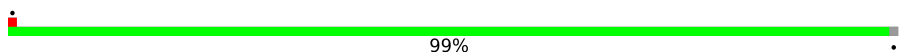
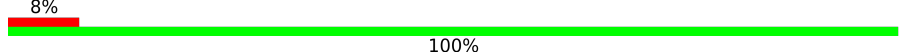
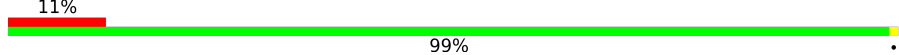
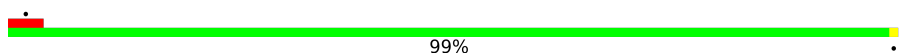



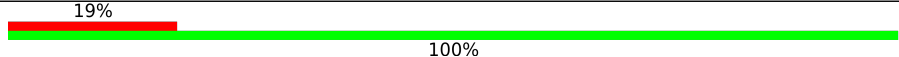
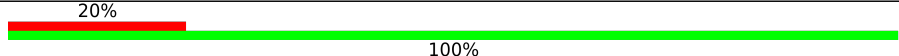
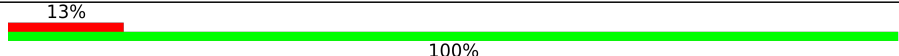
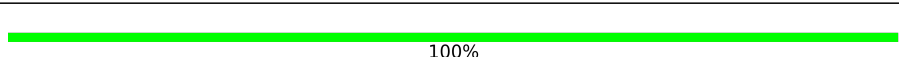


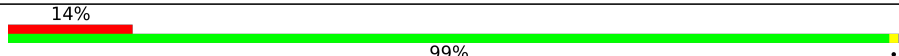
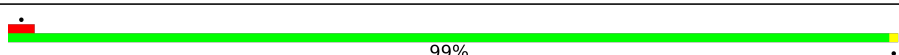

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	A	896	 9% 71% 28%
2	B	317	 9% 53% 47%
3	C	67	 24% 99%
3	c	67	 9% 100%
4	D	161	 11% 99%
4	F	161	 7% 99%
4	H	161	 8% 99%
4	J	161	 99%
4	L	161	 99%

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Mol	Chain	Length	Quality of chain
4	N	161	 99%
4	f	161	 57% 99%
4	h	161	 37% 99%
4	j	161	 99%
4	l	161	 99%
5	E	161	 8% 100%
5	G	161	 11% 99%
5	I	161	 99%
5	K	161	 100%
5	M	161	 100%
5	O	161	 100%
5	e	161	 19% 100%
5	g	161	 20% 100%
5	i	161	 13% 100%
5	k	161	 100%
5	m	161	 100%
6	P	249	 23% 77%
7	d	161	 14% 99%
8	o	169	 99%
9	p	121	 30% 70%

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 74379 atoms, of which 37194 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 Phycobiliprotein ApcE.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	641	10119	3225	5039	895	947	13	0	0

- Molecule 2 is a protein called Orange carotenoid-binding protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	B	169	2544	809	1275	215	237	8	0	0

- Molecule 3 is a protein called Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	C	67	1114	343	568	104	94	5	0	0
3	c	67	1114	343	568	104	94	5	0	0

- Molecule 4 is a protein called Allophycocyanin alpha chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	D	160	2420	754	1210	207	242	7	0	0
4	F	160	2420	754	1210	207	242	7	0	0
4	H	160	2420	754	1210	207	242	7	0	0
4	J	160	2420	754	1210	207	242	7	0	0
4	L	160	2420	754	1210	207	242	7	0	0
4	N	160	2420	754	1210	207	242	7	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace	
4	f	160	Total	C	H	N	O	S	0	0
			2420	754	1210	207	242	7		
4	h	160	Total	C	H	N	O	S	0	0
			2420	754	1210	207	242	7		
4	j	160	Total	C	H	N	O	S	0	0
			2420	754	1210	207	242	7		
4	l	160	Total	C	H	N	O	S	0	0
			2420	754	1210	207	242	7		

- Molecule 5 is a protein called Allophycocyanin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace	
5	E	161	Total	C	H	N	O	S	0	0
			2424	757	1218	202	240	7		
5	G	161	Total	C	H	N	O	S	0	0
			2424	757	1218	202	240	7		
5	I	161	Total	C	H	N	O	S	0	0
			2424	757	1218	202	240	7		
5	K	161	Total	C	H	N	O	S	0	0
			2424	757	1218	202	240	7		
5	M	161	Total	C	H	N	O	S	0	0
			2424	757	1218	202	240	7		
5	O	161	Total	C	H	N	O	S	0	0
			2424	757	1218	202	240	7		
5	e	161	Total	C	H	N	O	S	0	0
			2424	757	1218	202	240	7		
5	g	161	Total	C	H	N	O	S	0	0
			2424	757	1218	202	240	7		
5	i	161	Total	C	H	N	O	S	0	0
			2424	757	1218	202	240	7		
5	k	161	Total	C	H	N	O	S	0	0
			2424	757	1218	202	240	7		
5	m	161	Total	C	H	N	O	S	0	0
			2424	757	1218	202	240	7		

- Molecule 6 is a protein called Phycobilisome rod-core linker polypeptide CpcG.

Mol	Chain	Residues	Atoms					AltConf	Trace	
6	P	57	Total	C	H	N	O	S	0	0
			916	282	465	87	80	2		

- Molecule 7 is a protein called Allophycocyanin subunit alpha-B.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
7	d	160	2504	797	1250	212	241	4	0	0

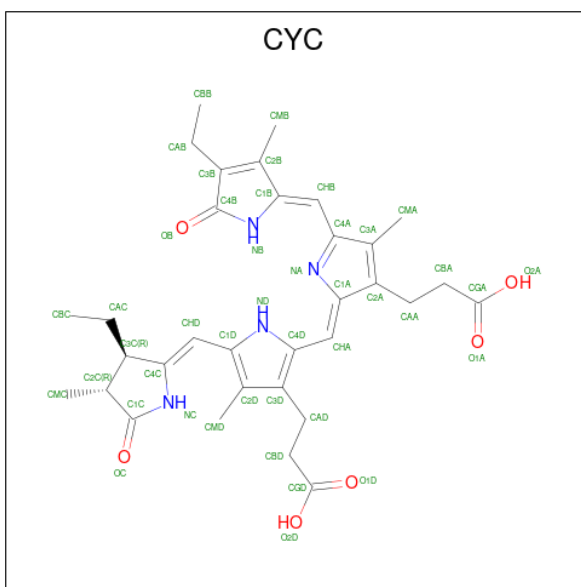
- Molecule 8 is a protein called Allophycocyanin subunit beta-18.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
8	o	169	2633	825	1311	229	259	9	0	0

- Molecule 9 is a protein called Translation initiation factor IF-2.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
9	p	36	560	172	283	55	49	1	0	0

- Molecule 10 is PHYCOCYANOBILIN (three-letter code: CYC) (formula: $C_{33}H_{40}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



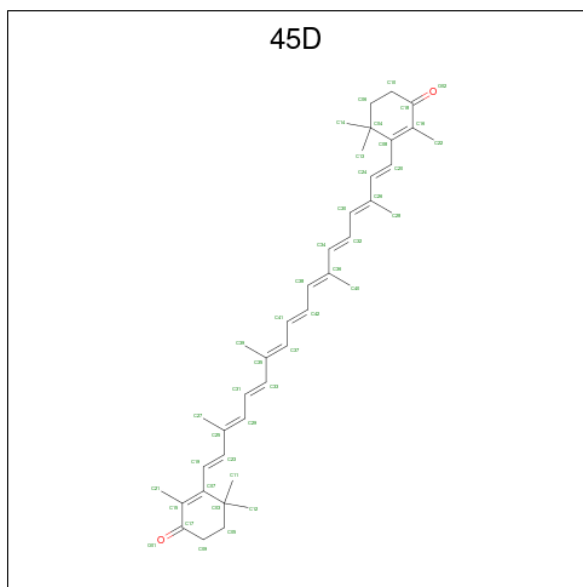
Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	N	O	
10	A	1	80	33	37	4	6	0
10	D	1	80	33	37	4	6	0
10	E	1	80	33	37	4	6	0
10	F	1	80	33	37	4	6	0

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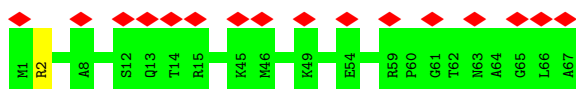
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Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	N	O	
10	G	1	Total 80	C 33	H 37	N 4	O 6	0
10	H	1	Total 80	C 33	H 37	N 4	O 6	0
10	I	1	Total 80	C 33	H 37	N 4	O 6	0
10	J	1	Total 80	C 33	H 37	N 4	O 6	0
10	K	1	Total 79	C 33	H 36	N 4	O 6	0
10	L	1	Total 80	C 33	H 37	N 4	O 6	0
10	M	1	Total 80	C 33	H 37	N 4	O 6	0
10	N	1	Total 80	C 33	H 37	N 4	O 6	0
10	O	1	Total 80	C 33	H 37	N 4	O 6	0
10	d	1	Total 80	C 33	H 37	N 4	O 6	0
10	e	1	Total 80	C 33	H 37	N 4	O 6	0
10	f	1	Total 80	C 33	H 37	N 4	O 6	0
10	g	1	Total 80	C 33	H 37	N 4	O 6	0
10	h	1	Total 80	C 33	H 37	N 4	O 6	0
10	i	1	Total 80	C 33	H 37	N 4	O 6	0
10	j	1	Total 80	C 33	H 37	N 4	O 6	0
10	k	1	Total 80	C 33	H 37	N 4	O 6	0
10	l	1	Total 79	C 33	H 36	N 4	O 6	0
10	m	1	Total 79	C 33	H 36	N 4	O 6	0
10	o	1	Total 80	C 33	H 37	N 4	O 6	0

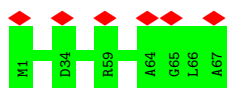
- Molecule 11 is beta,beta-carotene-4,4'-dione (three-letter code: 45D) (formula: C₄₀H₅₂O₂) (labeled as "Ligand of Interest" by depositor).



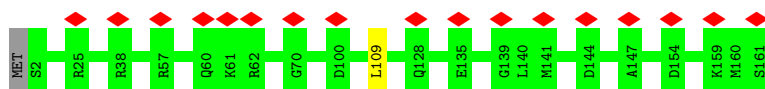
Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
11	B	1	94	40	52	2	0



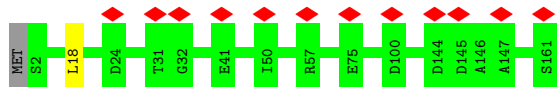
- Molecule 3: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core



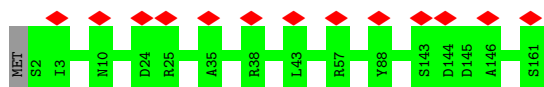
- Molecule 4: Allophycocyanin alpha chain



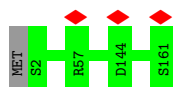
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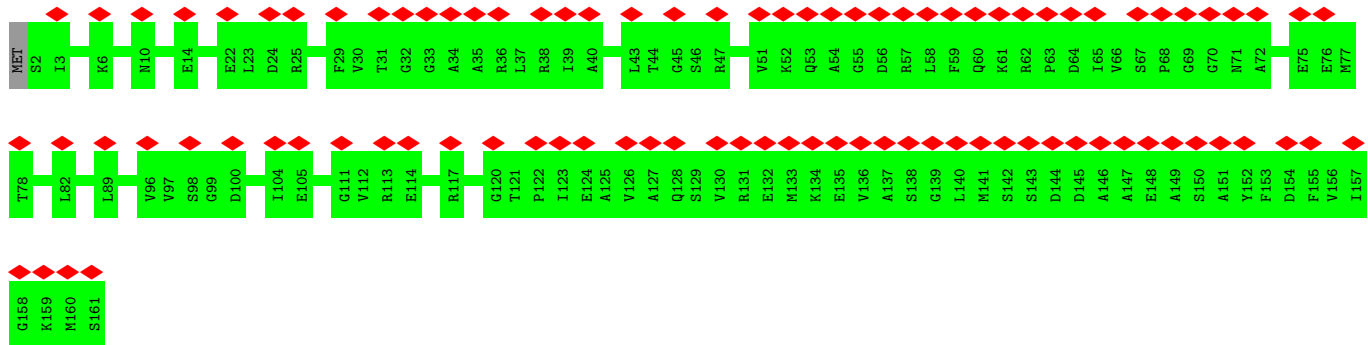
- Molecule 4: Allophycocyanin alpha chain



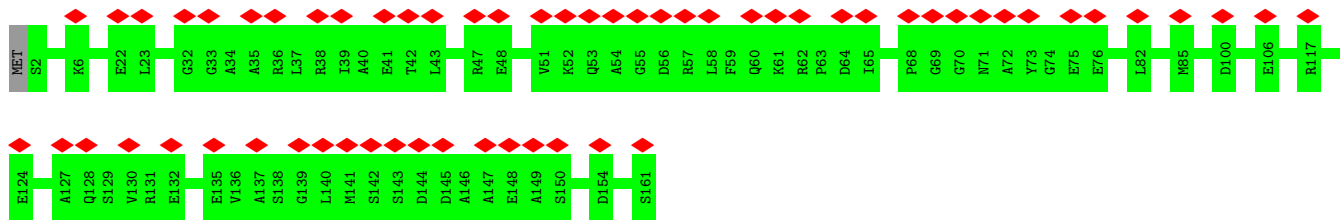
• Molecule 4: Allophycocyanin alpha chain



• Molecule 4: Allophycocyanin alpha chain



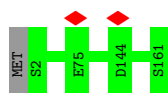
• Molecule 4: Allophycocyanin alpha chain



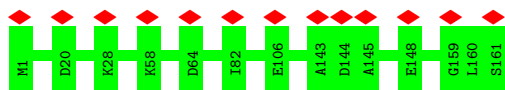
• Molecule 4: Allophycocyanin alpha chain



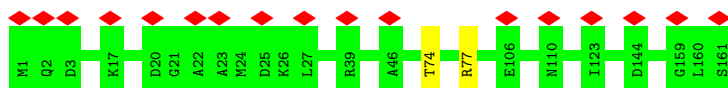
• Molecule 4: Allophycocyanin alpha chain



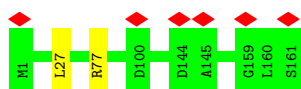
• Molecule 5: Allophycocyanin beta chain



- Molecule 5: Allophycocyanin beta chain



- Molecule 5: Allophycocyanin beta chain



- Molecule 5: Allophycocyanin beta chain



There are no outlier residues recorded for this chain.

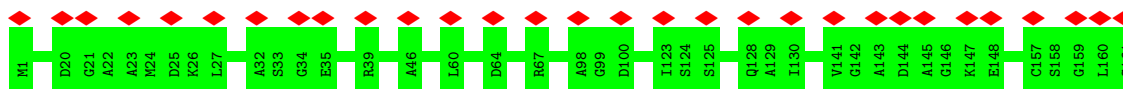
- Molecule 5: Allophycocyanin beta chain



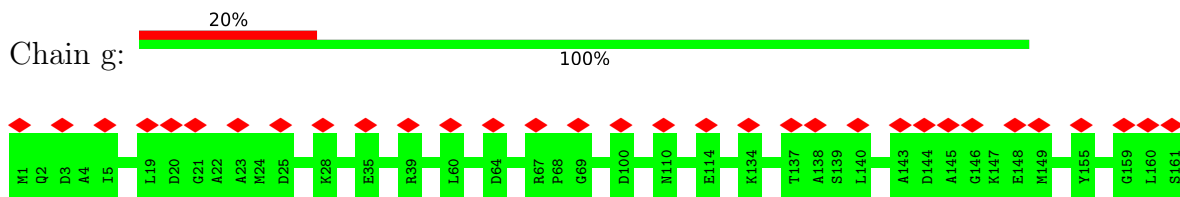
- Molecule 5: Allophycocyanin beta chain



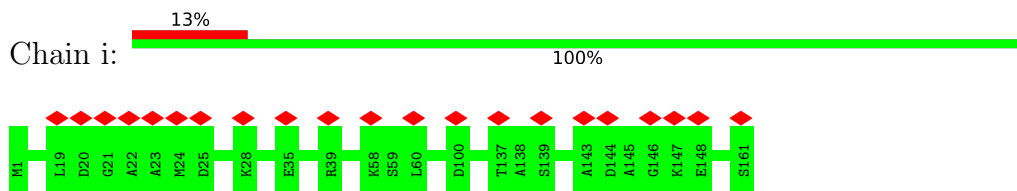
- Molecule 5: Allophycocyanin beta chain



- Molecule 5: Allophycocyanin beta chain



• Molecule 5: Allophycocyanin beta chain



• Molecule 5: Allophycocyanin beta chain



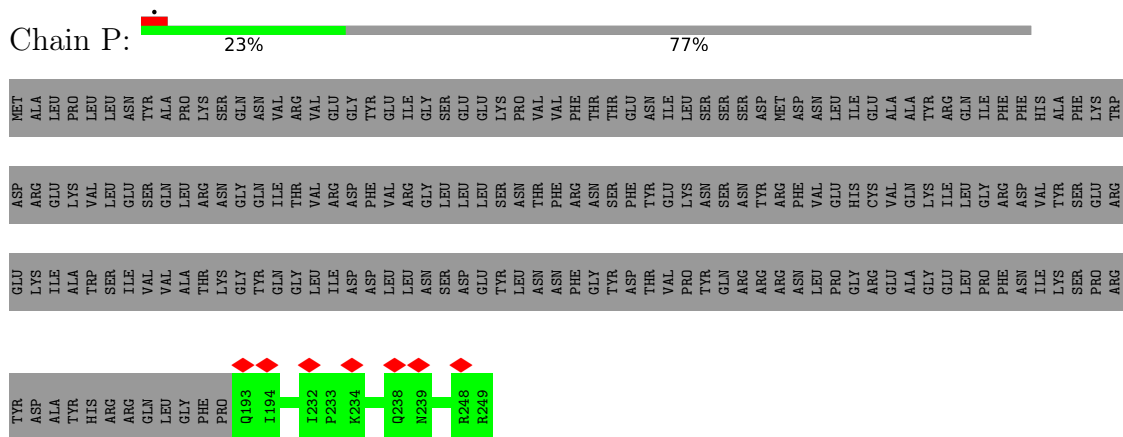
There are no outlier residues recorded for this chain.

• Molecule 5: Allophycocyanin beta chain

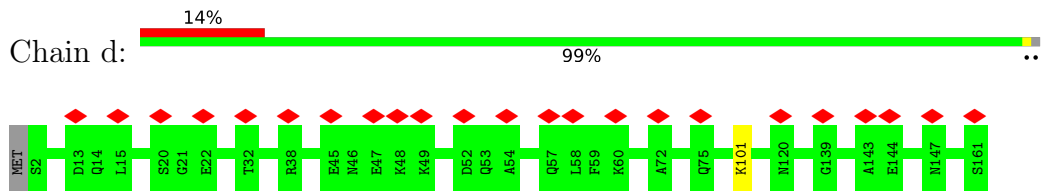


There are no outlier residues recorded for this chain.

• Molecule 6: Phycobilisome rod-core linker polypeptide CpcG

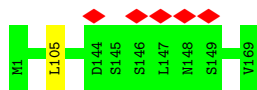


• Molecule 7: Allophycocyanin subunit alpha-B



• Molecule 8: Allophycocyanin subunit beta-18

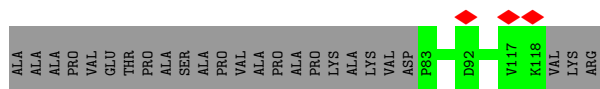




- Molecule 9: Translation initiation factor IF-2



MET LEU LYS LYS PHE LEU GLY ALA LYS LYS PHE LEU TYR VAL GLN LEU ASP GLU SER GLN ALA PRO ALA VAL GLU ALA ASP VAL ALA ILE VAL LYS SER GLU VAL ALA PRO VAL GLU LYS PRO ALA PRO THR SER LYS THR LYS THR SER ALA THR LYS



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	153576	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.296	Depositor
Minimum map value	-0.490	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.037	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	372.224, 372.224, 372.224	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.727, 0.727, 0.727	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: 45D, CYC

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	0/5191	0.55	2/7015 (0.0%)
2	B	0.28	0/1294	0.48	0/1763
3	C	0.28	0/555	0.63	0/743
3	c	0.27	0/555	0.58	0/743
4	D	0.27	0/1225	0.56	2/1652 (0.1%)
4	F	0.27	0/1225	0.55	0/1652
4	H	0.27	0/1225	0.54	0/1652
4	J	0.28	0/1225	0.54	0/1652
4	L	0.28	0/1225	0.54	0/1652
4	N	0.27	0/1225	0.53	0/1652
4	f	0.26	0/1225	0.53	0/1652
4	h	0.26	0/1225	0.52	0/1652
4	j	0.28	0/1225	0.54	0/1652
4	l	0.28	0/1225	0.55	0/1652
5	E	0.28	0/1220	0.50	0/1650
5	G	0.28	0/1220	0.53	0/1650
5	I	0.29	0/1220	0.54	2/1650 (0.1%)
5	K	0.32	0/1220	0.53	0/1650
5	M	0.30	0/1220	0.50	0/1650
5	O	0.29	0/1220	0.51	0/1650
5	e	0.27	0/1220	0.51	0/1650
5	g	0.26	0/1220	0.49	0/1650
5	i	0.28	0/1220	0.48	0/1650
5	k	0.30	0/1220	0.50	0/1650
5	m	0.29	0/1220	0.50	0/1650
6	P	0.25	0/459	0.53	0/620
7	d	0.28	0/1277	0.49	0/1730
8	o	0.28	0/1341	0.57	2/1813 (0.1%)
9	p	0.25	0/283	0.54	0/381
All	All	0.28	0/36625	0.53	8/49478 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	591	LEU	CB-CG-CD2	6.15	121.45	111.00
4	D	109	LEU	CB-CG-CD1	5.92	121.06	111.00
8	o	105	LEU	CB-CG-CD2	5.87	120.98	111.00
5	I	27	LEU	CB-CG-CD1	5.62	120.56	111.00
5	I	27	LEU	CB-CG-CD2	5.33	120.07	111.00
8	o	105	LEU	CB-CG-CD1	5.30	120.01	111.00
4	D	109	LEU	CB-CG-CD2	5.26	119.95	111.00
1	A	591	LEU	CB-CG-CD1	5.08	119.63	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	635/896 (71%)	623 (98%)	11 (2%)	1 (0%)	47	44
2	B	167/317 (53%)	158 (95%)	8 (5%)	1 (1%)	25	19
3	C	65/67 (97%)	64 (98%)	1 (2%)	0	100	100
3	c	65/67 (97%)	65 (100%)	0	0	100	100
4	D	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
4	F	158/161 (98%)	155 (98%)	2 (1%)	1 (1%)	25	19
4	H	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
4	J	158/161 (98%)	153 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	L	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
4	N	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
4	f	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
4	h	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
4	j	158/161 (98%)	158 (100%)	0	0	100	100
4	l	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
5	E	159/161 (99%)	151 (95%)	8 (5%)	0	100	100
5	G	159/161 (99%)	153 (96%)	5 (3%)	1 (1%)	25	19
5	I	159/161 (99%)	153 (96%)	6 (4%)	0	100	100
5	K	159/161 (99%)	156 (98%)	3 (2%)	0	100	100
5	M	159/161 (99%)	156 (98%)	3 (2%)	0	100	100
5	O	159/161 (99%)	158 (99%)	1 (1%)	0	100	100
5	e	159/161 (99%)	155 (98%)	4 (2%)	0	100	100
5	g	159/161 (99%)	156 (98%)	3 (2%)	0	100	100
5	i	159/161 (99%)	156 (98%)	3 (2%)	0	100	100
5	k	159/161 (99%)	155 (98%)	4 (2%)	0	100	100
5	m	159/161 (99%)	157 (99%)	2 (1%)	0	100	100
6	P	55/249 (22%)	54 (98%)	1 (2%)	0	100	100
7	d	158/161 (98%)	158 (100%)	0	0	100	100
8	o	167/169 (99%)	165 (99%)	2 (1%)	0	100	100
9	p	34/121 (28%)	34 (100%)	0	0	100	100
All	All	4675/5428 (86%)	4588 (98%)	83 (2%)	4 (0%)	54	49

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	G	74	THR
4	F	18	LEU
1	A	530	THR
2	B	175	PRO

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	A	536/753 (71%)	533 (99%)	3 (1%)	86	90
2	B	129/257 (50%)	129 (100%)	0	100	100
3	C	58/58 (100%)	57 (98%)	1 (2%)	60	65
3	c	58/58 (100%)	58 (100%)	0	100	100
4	D	128/129 (99%)	128 (100%)	0	100	100
4	F	128/129 (99%)	128 (100%)	0	100	100
4	H	128/129 (99%)	128 (100%)	0	100	100
4	J	128/129 (99%)	128 (100%)	0	100	100
4	L	128/129 (99%)	127 (99%)	1 (1%)	81	86
4	N	128/129 (99%)	128 (100%)	0	100	100
4	f	128/129 (99%)	128 (100%)	0	100	100
4	h	128/129 (99%)	128 (100%)	0	100	100
4	j	128/129 (99%)	128 (100%)	0	100	100
4	l	128/129 (99%)	128 (100%)	0	100	100
5	E	125/125 (100%)	125 (100%)	0	100	100
5	G	125/125 (100%)	124 (99%)	1 (1%)	81	86
5	I	125/125 (100%)	124 (99%)	1 (1%)	81	86
5	K	125/125 (100%)	125 (100%)	0	100	100
5	M	125/125 (100%)	125 (100%)	0	100	100
5	O	125/125 (100%)	125 (100%)	0	100	100
5	e	125/125 (100%)	125 (100%)	0	100	100
5	g	125/125 (100%)	125 (100%)	0	100	100
5	i	125/125 (100%)	125 (100%)	0	100	100
5	k	125/125 (100%)	125 (100%)	0	100	100
5	m	125/125 (100%)	125 (100%)	0	100	100
6	P	49/221 (22%)	49 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	d	132/133 (99%)	131 (99%)	1 (1%)	81	86
8	o	140/140 (100%)	140 (100%)	0	100	100
9	p	30/98 (31%)	30 (100%)	0	100	100
All	All	3787/4383 (86%)	3779 (100%)	8 (0%)	93	95

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	211	ARG
1	A	292	ARG
1	A	553	ARG
3	C	2	ARG
5	G	77	ARG
5	I	77	ARG
4	L	71	ASN
7	d	101	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
4	D	71	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

25 ligands 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	CYC	I	200	5	42,46,46	0.71	1 (2%)	50,67,67	0.67	1 (2%)
10	CYC	E	200	5	42,46,46	0.74	1 (2%)	50,67,67	0.79	2 (4%)
10	CYC	f	200	4	42,46,46	0.62	1 (2%)	50,67,67	0.63	1 (2%)
10	CYC	e	200	5	42,46,46	0.72	1 (2%)	50,67,67	0.86	2 (4%)
10	CYC	i	200	5	42,46,46	0.66	1 (2%)	50,67,67	0.80	3 (6%)
10	CYC	m	200	5	42,46,46	0.70	1 (2%)	50,67,67	0.75	3 (6%)
10	CYC	L	200	4	42,46,46	0.65	1 (2%)	50,67,67	0.87	2 (4%)
10	CYC	l	200	4	42,46,46	0.58	1 (2%)	50,67,67	0.84	3 (6%)
10	CYC	d	200	7	42,46,46	0.79	1 (2%)	50,67,67	1.12	3 (6%)
10	CYC	j	200	4	42,46,46	0.70	1 (2%)	50,67,67	0.90	3 (6%)
10	CYC	N	200	4	42,46,46	0.59	1 (2%)	50,67,67	0.81	2 (4%)
10	CYC	A	1000	1	42,46,46	0.71	1 (2%)	50,67,67	1.04	3 (6%)
10	CYC	H	200	4	42,46,46	0.64	1 (2%)	50,67,67	0.71	2 (4%)
10	CYC	h	200	4	42,46,46	0.63	1 (2%)	50,67,67	0.64	1 (2%)
10	CYC	g	200	5	42,46,46	0.72	1 (2%)	50,67,67	0.61	1 (2%)
10	CYC	O	200	5	42,46,46	0.57	1 (2%)	50,67,67	0.69	2 (4%)
10	CYC	D	200	4	42,46,46	0.61	1 (2%)	50,67,67	0.69	3 (6%)
10	CYC	k	200	5	42,46,46	0.52	1 (2%)	50,67,67	1.06	3 (6%)
10	CYC	G	200	5	42,46,46	0.78	1 (2%)	50,67,67	0.86	3 (6%)
10	CYC	o	200	8	42,46,46	0.62	1 (2%)	50,67,67	0.78	3 (6%)
11	45D	B	400	-	43,43,43	1.01	3 (6%)	54,60,60	1.42	10 (18%)
10	CYC	M	200	5	42,46,46	0.59	1 (2%)	50,67,67	0.95	3 (6%)
10	CYC	F	200	4	42,46,46	0.54	1 (2%)	50,67,67	0.85	3 (6%)
10	CYC	J	200	4	42,46,46	0.48	1 (2%)	50,67,67	0.80	3 (6%)
10	CYC	K	200	5	42,46,46	0.63	1 (2%)	50,67,67	1.10	3 (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
10	CYC	I	200	5	-	9/25/74/74	0/4/4/4
10	CYC	E	200	5	-	8/25/74/74	0/4/4/4
10	CYC	f	200	4	-	8/25/74/74	0/4/4/4
10	CYC	e	200	5	-	4/25/74/74	0/4/4/4
10	CYC	i	200	5	-	6/25/74/74	0/4/4/4
10	CYC	m	200	5	-	11/25/74/74	0/4/4/4
10	CYC	L	200	4	-	8/25/74/74	0/4/4/4
10	CYC	l	200	4	-	9/25/74/74	0/4/4/4
10	CYC	d	200	7	-	7/25/74/74	0/4/4/4
10	CYC	j	200	4	-	4/25/74/74	0/4/4/4
10	CYC	N	200	4	-	8/25/74/74	0/4/4/4
10	CYC	A	1000	1	-	7/25/74/74	0/4/4/4
10	CYC	H	200	4	-	6/25/74/74	0/4/4/4
10	CYC	h	200	4	-	5/25/74/74	0/4/4/4
10	CYC	g	200	5	-	5/25/74/74	0/4/4/4
10	CYC	O	200	5	-	8/25/74/74	0/4/4/4
10	CYC	D	200	4	-	8/25/74/74	0/4/4/4
10	CYC	k	200	5	-	6/25/74/74	0/4/4/4
10	CYC	G	200	5	-	6/25/74/74	0/4/4/4
10	CYC	o	200	8	-	8/25/74/74	0/4/4/4
11	45D	B	400	-	-	13/29/69/69	0/2/2/2
10	CYC	M	200	5	-	8/25/74/74	0/4/4/4
10	CYC	F	200	4	-	7/25/74/74	0/4/4/4
10	CYC	J	200	4	-	8/25/74/74	0/4/4/4
10	CYC	K	200	5	-	8/25/74/74	0/4/4/4

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	d	200	CYC	CHA-C1A	4.41	1.38	1.35
10	G	200	CYC	CHA-C1A	4.33	1.38	1.35
10	E	200	CYC	CHA-C1A	4.20	1.38	1.35
10	g	200	CYC	CHA-C1A	4.13	1.38	1.35
10	I	200	CYC	CHA-C1A	4.10	1.38	1.35
10	e	200	CYC	CHA-C1A	4.00	1.38	1.35
10	m	200	CYC	CHA-C1A	3.90	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	1000	CYC	CHA-C1A	3.86	1.38	1.35
10	i	200	CYC	CHA-C1A	3.65	1.38	1.35
11	B	400	45D	C34-C36	3.63	1.53	1.45
10	j	200	CYC	CHA-C1A	3.62	1.38	1.35
10	h	200	CYC	CHA-C1A	3.51	1.38	1.35
10	o	200	CYC	CHA-C1A	3.46	1.38	1.35
10	L	200	CYC	CHA-C1A	3.46	1.38	1.35
10	f	200	CYC	CHA-C1A	3.45	1.38	1.35
10	H	200	CYC	CHA-C1A	3.40	1.38	1.35
10	D	200	CYC	CHA-C1A	3.37	1.37	1.35
10	K	200	CYC	CHA-C1A	3.19	1.37	1.35
10	N	200	CYC	CHA-C1A	3.14	1.37	1.35
10	l	200	CYC	CHA-C1A	3.06	1.37	1.35
10	M	200	CYC	CHA-C1A	3.05	1.37	1.35
10	O	200	CYC	CHA-C1A	2.85	1.37	1.35
10	F	200	CYC	CHA-C1A	2.83	1.37	1.35
10	k	200	CYC	CHA-C1A	2.33	1.37	1.35
10	J	200	CYC	CHA-C1A	2.29	1.37	1.35
11	B	400	45D	C04-C08	2.12	1.56	1.53
11	B	400	45D	C24-C20	2.03	1.39	1.33

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	d	200	CYC	C1B-CHB-C4A	5.66	141.92	128.08
10	k	200	CYC	C1B-CHB-C4A	5.53	141.58	128.08
10	K	200	CYC	C1B-CHB-C4A	5.50	141.51	128.08
10	A	1000	CYC	C1B-CHB-C4A	5.32	141.09	128.08
10	j	200	CYC	C1B-CHB-C4A	4.59	139.29	128.08
10	M	200	CYC	C1B-CHB-C4A	4.32	138.65	128.08
10	L	200	CYC	C1B-CHB-C4A	4.32	138.63	128.08
10	N	200	CYC	C1B-CHB-C4A	3.64	136.97	128.08
10	E	200	CYC	CHA-C1A-NA	-3.53	123.93	128.83
10	e	200	CYC	C1B-CHB-C4A	3.51	136.67	128.08
10	F	200	CYC	C1B-CHB-C4A	3.44	136.49	128.08
10	G	200	CYC	C1B-CHB-C4A	3.43	136.46	128.08
10	e	200	CYC	CHA-C1A-NA	-3.37	124.15	128.83
10	i	200	CYC	C1B-CHB-C4A	3.36	136.28	128.08
10	o	200	CYC	CHA-C1A-NA	-3.28	124.28	128.83
10	F	200	CYC	CHA-C1A-NA	-3.27	124.29	128.83
10	l	200	CYC	C1B-CHB-C4A	3.24	135.99	128.08
10	G	200	CYC	CHA-C1A-NA	-3.19	124.40	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	200	CYC	C1B-CHB-C4A	3.17	135.82	128.08
10	d	200	CYC	CHA-C1A-NA	-3.06	124.59	128.83
10	I	200	CYC	CHA-C1A-NA	-3.04	124.61	128.83
10	h	200	CYC	CHA-C1A-NA	-3.03	124.63	128.83
10	N	200	CYC	CHA-C1A-NA	-2.95	124.73	128.83
10	J	200	CYC	CHA-C1A-NA	-2.95	124.73	128.83
10	D	200	CYC	CHA-C1A-NA	-2.79	124.96	128.83
10	H	200	CYC	C1B-CHB-C4A	2.79	134.89	128.08
10	f	200	CYC	CHA-C1A-NA	-2.77	124.98	128.83
10	M	200	CYC	CHA-C1A-NA	-2.75	125.02	128.83
10	i	200	CYC	CHA-C1A-NA	-2.73	125.04	128.83
11	B	400	45D	C23-C19-C07	-2.69	119.66	127.20
11	B	400	45D	C05-C03-C07	2.68	114.61	110.48
10	g	200	CYC	CHA-C1A-NA	-2.66	125.14	128.83
10	H	200	CYC	CHA-C1A-NA	-2.63	125.17	128.83
11	B	400	45D	C40-C36-C34	2.61	122.19	118.08
11	B	400	45D	C22-C16-C08	-2.60	119.93	124.11
10	L	200	CYC	CHA-C1A-NA	-2.60	125.22	128.83
10	l	200	CYC	CHA-C1A-NA	-2.60	125.22	128.83
10	O	200	CYC	CHA-C1A-NA	-2.59	125.24	128.83
10	K	200	CYC	CHA-C1A-NA	-2.58	125.24	128.83
10	D	200	CYC	C1B-CHB-C4A	2.53	134.27	128.08
10	A	1000	CYC	CHA-C1A-NA	-2.52	125.33	128.83
10	m	200	CYC	CHA-C1A-NA	-2.51	125.34	128.83
11	B	400	45D	C21-C15-C07	-2.49	120.11	124.11
10	E	200	CYC	C1B-CHB-C4A	2.36	133.84	128.08
10	O	200	CYC	C1B-CHB-C4A	2.31	133.73	128.08
10	A	1000	CYC	C2C-C3C-C4C	2.30	104.79	101.34
10	k	200	CYC	CHA-C1A-NA	-2.30	125.64	128.83
10	m	200	CYC	C2C-C3C-C4C	2.29	104.77	101.34
10	M	200	CYC	C2C-C3C-C4C	2.27	104.74	101.34
10	d	200	CYC	C2C-C3C-C4C	2.27	104.73	101.34
10	o	200	CYC	C1B-CHB-C4A	2.27	133.62	128.08
10	l	200	CYC	C2C-C3C-C4C	2.27	104.73	101.34
11	B	400	45D	C06-C04-C08	2.26	113.95	110.48
10	o	200	CYC	C2C-C3C-C4C	2.22	104.66	101.34
10	J	200	CYC	C2C-C3C-C4C	2.21	104.64	101.34
10	j	200	CYC	CHA-C1A-NA	-2.20	125.77	128.83
10	m	200	CYC	C1B-CHB-C4A	2.20	133.45	128.08
10	K	200	CYC	C2C-C3C-C4C	2.18	104.60	101.34
11	B	400	45D	C34-C36-C38	-2.17	115.61	118.94
11	B	400	45D	C03-C07-C19	2.16	121.90	115.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	400	45D	C28-C26-C24	2.16	121.48	118.08
10	G	200	CYC	C2C-C3C-C4C	2.13	104.53	101.34
11	B	400	45D	C29-C31-C33	-2.11	116.64	123.22
10	k	200	CYC	C2C-C3C-C4C	2.05	104.42	101.34
10	D	200	CYC	C2C-C3C-C4C	2.05	104.41	101.34
10	i	200	CYC	C2C-C3C-C4C	2.04	104.40	101.34
10	j	200	CYC	C2C-C3C-C4C	2.04	104.39	101.34
10	F	200	CYC	C2C-C3C-C4C	2.01	104.35	101.34

There are no chirality outliers.

All (185) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	1000	CYC	NC-C4C-CHD-C1D
10	A	1000	CYC	ND-C1D-CHD-C4C
10	A	1000	CYC	C2D-C1D-CHD-C4C
10	D	200	CYC	NA-C4A-CHB-C1B
10	D	200	CYC	C3A-C4A-CHB-C1B
10	E	200	CYC	NA-C4A-CHB-C1B
10	E	200	CYC	C3A-C4A-CHB-C1B
10	E	200	CYC	ND-C1D-CHD-C4C
10	F	200	CYC	NA-C4A-CHB-C1B
10	F	200	CYC	C3A-C4A-CHB-C1B
10	G	200	CYC	NA-C4A-CHB-C1B
10	G	200	CYC	C3A-C4A-CHB-C1B
10	H	200	CYC	NA-C4A-CHB-C1B
10	H	200	CYC	C3A-C4A-CHB-C1B
10	H	200	CYC	ND-C1D-CHD-C4C
10	H	200	CYC	C2D-C1D-CHD-C4C
10	I	200	CYC	NA-C4A-CHB-C1B
10	I	200	CYC	C3A-C4A-CHB-C1B
10	I	200	CYC	ND-C1D-CHD-C4C
10	I	200	CYC	C2D-C1D-CHD-C4C
10	J	200	CYC	NA-C4A-CHB-C1B
10	J	200	CYC	C3A-C4A-CHB-C1B
10	J	200	CYC	ND-C1D-CHD-C4C
10	J	200	CYC	C2D-C1D-CHD-C4C
10	K	200	CYC	NA-C4A-CHB-C1B
10	K	200	CYC	C3A-C4A-CHB-C1B
10	K	200	CYC	C2C-C3C-CAC-CBC
10	K	200	CYC	C4C-C3C-CAC-CBC
10	K	200	CYC	ND-C1D-CHD-C4C

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Mol	Chain	Res	Type	Atoms
10	K	200	CYC	C2D-C1D-CHD-C4C
10	L	200	CYC	C4B-C3B-CAB-CBB
10	M	200	CYC	NA-C4A-CHB-C1B
10	M	200	CYC	ND-C1D-CHD-C4C
10	M	200	CYC	C2D-C1D-CHD-C4C
10	N	200	CYC	NA-C4A-CHB-C1B
10	N	200	CYC	C3A-C4A-CHB-C1B
10	O	200	CYC	NA-C4A-CHB-C1B
10	O	200	CYC	C3A-C4A-CHB-C1B
10	O	200	CYC	ND-C1D-CHD-C4C
10	O	200	CYC	C2D-C1D-CHD-C4C
10	d	200	CYC	ND-C1D-CHD-C4C
10	d	200	CYC	C2D-C1D-CHD-C4C
10	e	200	CYC	NA-C4A-CHB-C1B
10	e	200	CYC	C3A-C4A-CHB-C1B
10	f	200	CYC	NA-C4A-CHB-C1B
10	f	200	CYC	C3A-C4A-CHB-C1B
10	g	200	CYC	NA-C4A-CHB-C1B
10	g	200	CYC	C3A-C4A-CHB-C1B
10	h	200	CYC	NA-C4A-CHB-C1B
10	h	200	CYC	C3A-C4A-CHB-C1B
10	i	200	CYC	NA-C4A-CHB-C1B
10	i	200	CYC	C3A-C4A-CHB-C1B
10	i	200	CYC	C4B-C3B-CAB-CBB
10	i	200	CYC	ND-C1D-CHD-C4C
10	k	200	CYC	C3A-C4A-CHB-C1B
10	k	200	CYC	ND-C1D-CHD-C4C
10	l	200	CYC	NA-C4A-CHB-C1B
10	l	200	CYC	C3A-C4A-CHB-C1B
10	l	200	CYC	C2C-C3C-CAC-CBC
10	l	200	CYC	C4C-C3C-CAC-CBC
10	m	200	CYC	C3A-C2A-CAA-CBA
10	m	200	CYC	NA-C4A-CHB-C1B
10	m	200	CYC	C3A-C4A-CHB-C1B
10	m	200	CYC	C2C-C3C-CAC-CBC
10	m	200	CYC	C4C-C3C-CAC-CBC
10	m	200	CYC	ND-C1D-CHD-C4C
10	m	200	CYC	C2D-C1D-CHD-C4C
10	o	200	CYC	NA-C4A-CHB-C1B
10	o	200	CYC	C3A-C4A-CHB-C1B
10	o	200	CYC	ND-C1D-CHD-C4C
11	B	400	45D	C03-C07-C19-C23

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Mol	Chain	Res	Type	Atoms
11	B	400	45D	C15-C07-C19-C23
11	B	400	45D	C19-C23-C25-C27
11	B	400	45D	C19-C23-C25-C29
11	B	400	45D	C20-C24-C26-C28
11	B	400	45D	C20-C24-C26-C30
11	B	400	45D	C31-C33-C35-C37
11	B	400	45D	C31-C33-C35-C39
11	B	400	45D	C32-C34-C36-C38
11	B	400	45D	C32-C34-C36-C40
10	E	200	CYC	C2B-C3B-CAB-CBB
10	N	200	CYC	C2B-C3B-CAB-CBB
10	m	200	CYC	C1A-C2A-CAA-CBA
10	G	200	CYC	C2B-C3B-CAB-CBB
10	I	200	CYC	C2B-C3B-CAB-CBB
10	F	200	CYC	C4B-C3B-CAB-CBB
10	N	200	CYC	C4B-C3B-CAB-CBB
10	d	200	CYC	C2A-CAA-CBA-CGA
10	A	1000	CYC	C3A-C4A-CHB-C1B
10	A	1000	CYC	NA-C4A-CHB-C1B
10	L	200	CYC	NA-C4A-CHB-C1B
10	d	200	CYC	NA-C4A-CHB-C1B
10	j	200	CYC	NA-C4A-CHB-C1B
10	k	200	CYC	NA-C4A-CHB-C1B
10	L	200	CYC	C3A-C4A-CHB-C1B
10	M	200	CYC	C3A-C4A-CHB-C1B
10	d	200	CYC	C3A-C4A-CHB-C1B
10	j	200	CYC	C3A-C4A-CHB-C1B
11	B	400	45D	C04-C08-C20-C24
11	B	400	45D	C16-C08-C20-C24
10	D	200	CYC	C2B-C3B-CAB-CBB
10	L	200	CYC	C2B-C3B-CAB-CBB
10	f	200	CYC	C3D-CAD-CBD-CGD
10	E	200	CYC	C1A-C2A-CAA-CBA
10	d	200	CYC	C1A-C2A-CAA-CBA
10	d	200	CYC	C3A-C2A-CAA-CBA
10	G	200	CYC	C2A-CAA-CBA-CGA
10	h	200	CYC	C2A-CAA-CBA-CGA
10	l	200	CYC	C2A-CAA-CBA-CGA
10	E	200	CYC	C4B-C3B-CAB-CBB
10	E	200	CYC	C2A-CAA-CBA-CGA
10	E	200	CYC	C3A-C2A-CAA-CBA
10	I	200	CYC	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
10	f	200	CYC	C4D-C3D-CAD-CBD
10	D	200	CYC	C2A-CAA-CBA-CGA
11	B	400	45D	C25-C29-C31-C33
10	m	200	CYC	C2A-CAA-CBA-CGA
10	F	200	CYC	CAD-CBD-CGD-O2D
10	k	200	CYC	CAA-CBA-CGA-O1A
10	D	200	CYC	CAD-CBD-CGD-O1D
10	g	200	CYC	CAA-CBA-CGA-O1A
10	K	200	CYC	CAA-CBA-CGA-O2A
10	H	200	CYC	CAA-CBA-CGA-O1A
10	m	200	CYC	CAA-CBA-CGA-O1A
10	D	200	CYC	CAA-CBA-CGA-O1A
10	H	200	CYC	CAA-CBA-CGA-O2A
10	k	200	CYC	CAA-CBA-CGA-O2A
10	M	200	CYC	C4B-C3B-CAB-CBB
10	J	200	CYC	CAD-CBD-CGD-O1D
10	g	200	CYC	CAA-CBA-CGA-O2A
10	j	200	CYC	CAA-CBA-CGA-O1A
10	M	200	CYC	CAD-CBD-CGD-O1D
10	M	200	CYC	CAD-CBD-CGD-O2D
10	j	200	CYC	CAA-CBA-CGA-O2A
10	D	200	CYC	CAA-CBA-CGA-O2A
10	D	200	CYC	CAD-CBD-CGD-O2D
10	h	200	CYC	CAA-CBA-CGA-O1A
10	m	200	CYC	CAA-CBA-CGA-O2A
10	h	200	CYC	CAA-CBA-CGA-O2A
10	l	200	CYC	CAA-CBA-CGA-O1A
10	G	200	CYC	CAA-CBA-CGA-O1A
10	f	200	CYC	CAD-CBD-CGD-O2D
10	G	200	CYC	CAA-CBA-CGA-O2A
10	J	200	CYC	CAD-CBD-CGD-O2D
10	K	200	CYC	CAA-CBA-CGA-O1A
10	L	200	CYC	CAA-CBA-CGA-O2A
10	A	1000	CYC	CAA-CBA-CGA-O1A
10	A	1000	CYC	CAA-CBA-CGA-O2A
10	F	200	CYC	CAD-CBD-CGD-O1D
10	o	200	CYC	CAD-CBD-CGD-O1D
10	o	200	CYC	CAD-CBD-CGD-O2D
10	f	200	CYC	CAD-CBD-CGD-O1D
10	l	200	CYC	CAA-CBA-CGA-O2A
10	J	200	CYC	CAA-CBA-CGA-O2A
10	g	200	CYC	C2A-CAA-CBA-CGA

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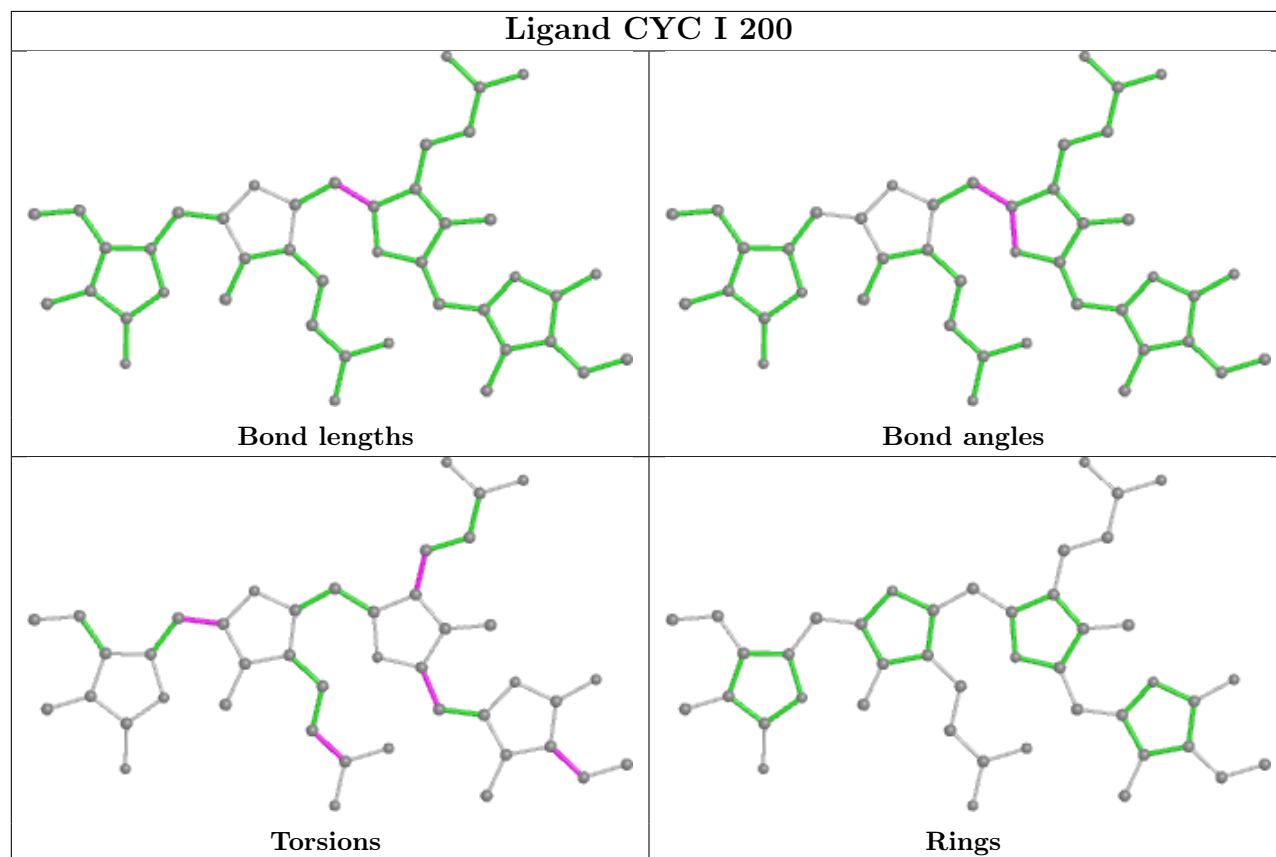
Mol	Chain	Res	Type	Atoms
10	N	200	CYC	CAA-CBA-CGA-O2A
10	F	200	CYC	CAA-CBA-CGA-O2A
10	I	200	CYC	CAD-CBD-CGD-O1D
10	L	200	CYC	CAA-CBA-CGA-O1A
10	J	200	CYC	CAA-CBA-CGA-O1A
10	O	200	CYC	CAA-CBA-CGA-O2A
10	I	200	CYC	C1A-C2A-CAA-CBA
10	l	200	CYC	CAD-CBD-CGD-O1D
10	o	200	CYC	CAA-CBA-CGA-O2A
10	N	200	CYC	CAA-CBA-CGA-O1A
10	O	200	CYC	CAA-CBA-CGA-O1A
10	L	200	CYC	CAD-CBD-CGD-O1D
10	i	200	CYC	CAA-CBA-CGA-O1A
10	i	200	CYC	CAA-CBA-CGA-O2A
10	o	200	CYC	CAA-CBA-CGA-O1A
10	F	200	CYC	CAA-CBA-CGA-O1A
10	l	200	CYC	CAD-CBD-CGD-O2D
10	L	200	CYC	CAD-CBD-CGD-O2D
10	o	200	CYC	C3A-C2A-CAA-CBA
10	I	200	CYC	CAD-CBD-CGD-O2D
10	f	200	CYC	CAA-CBA-CGA-O2A
10	N	200	CYC	CAD-CBD-CGD-O2D
10	O	200	CYC	CAD-CBD-CGD-O2D
10	e	200	CYC	CAD-CBD-CGD-O2D
10	O	200	CYC	CAD-CBD-CGD-O1D
10	f	200	CYC	CAA-CBA-CGA-O1A
10	M	200	CYC	CAA-CBA-CGA-O2A
10	e	200	CYC	CAD-CBD-CGD-O1D
10	N	200	CYC	CAD-CBD-CGD-O1D
10	k	200	CYC	CAD-CBD-CGD-O2D

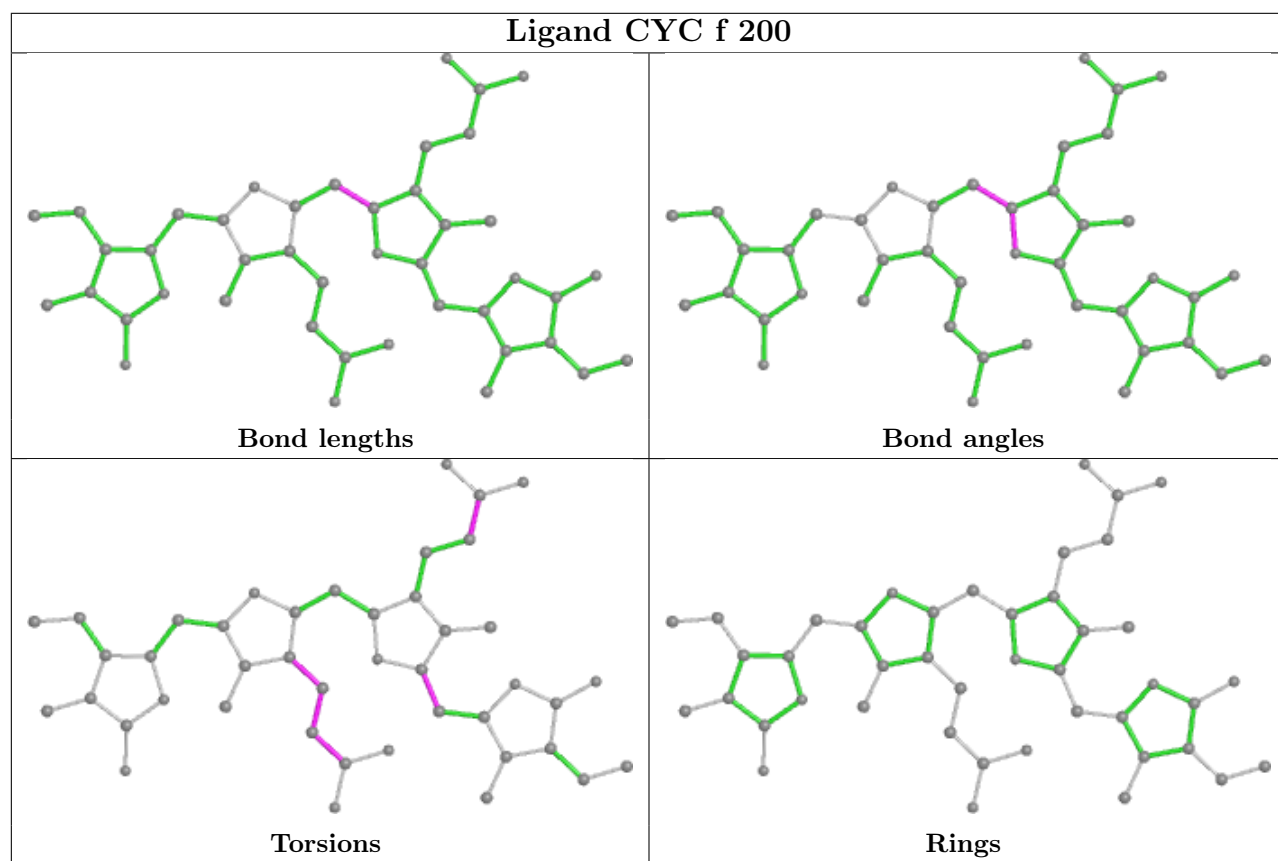
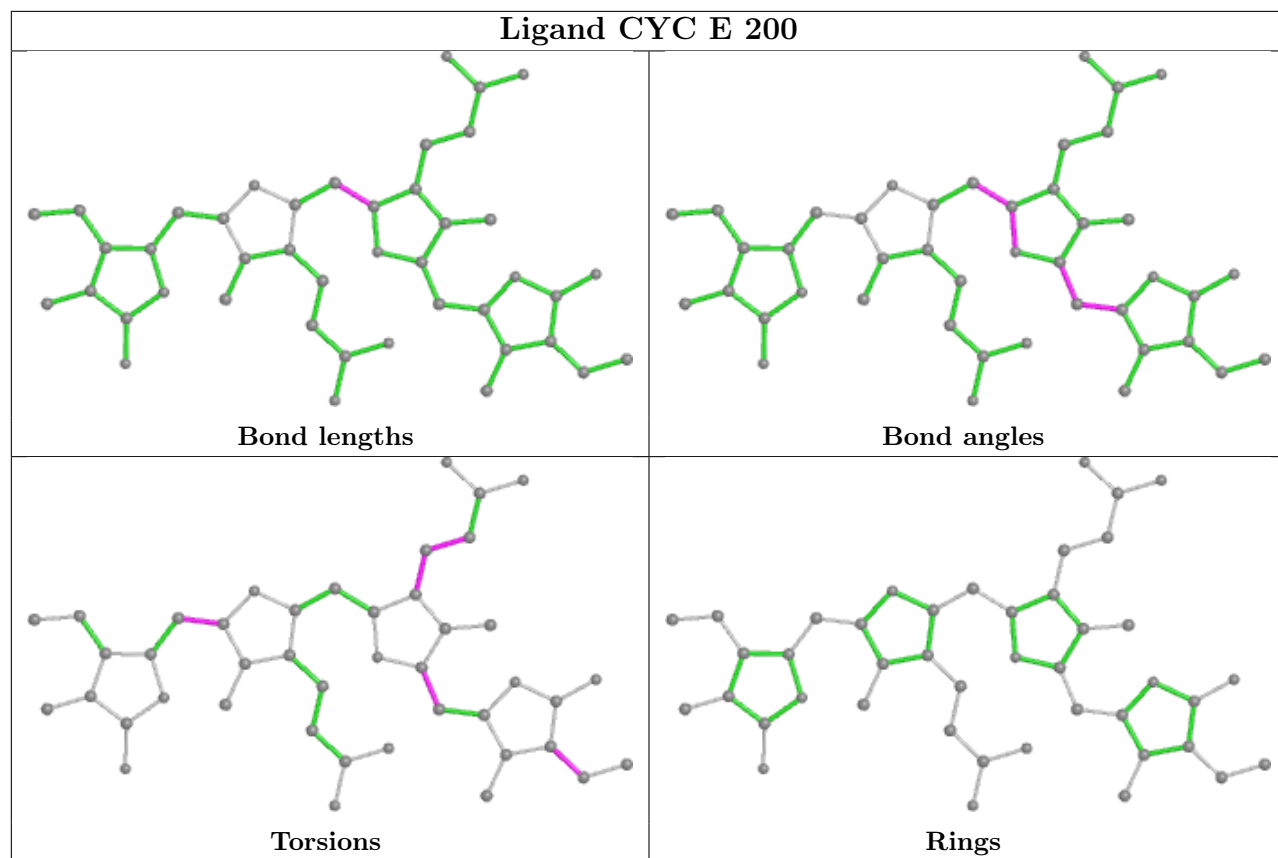
There are no ring outliers.

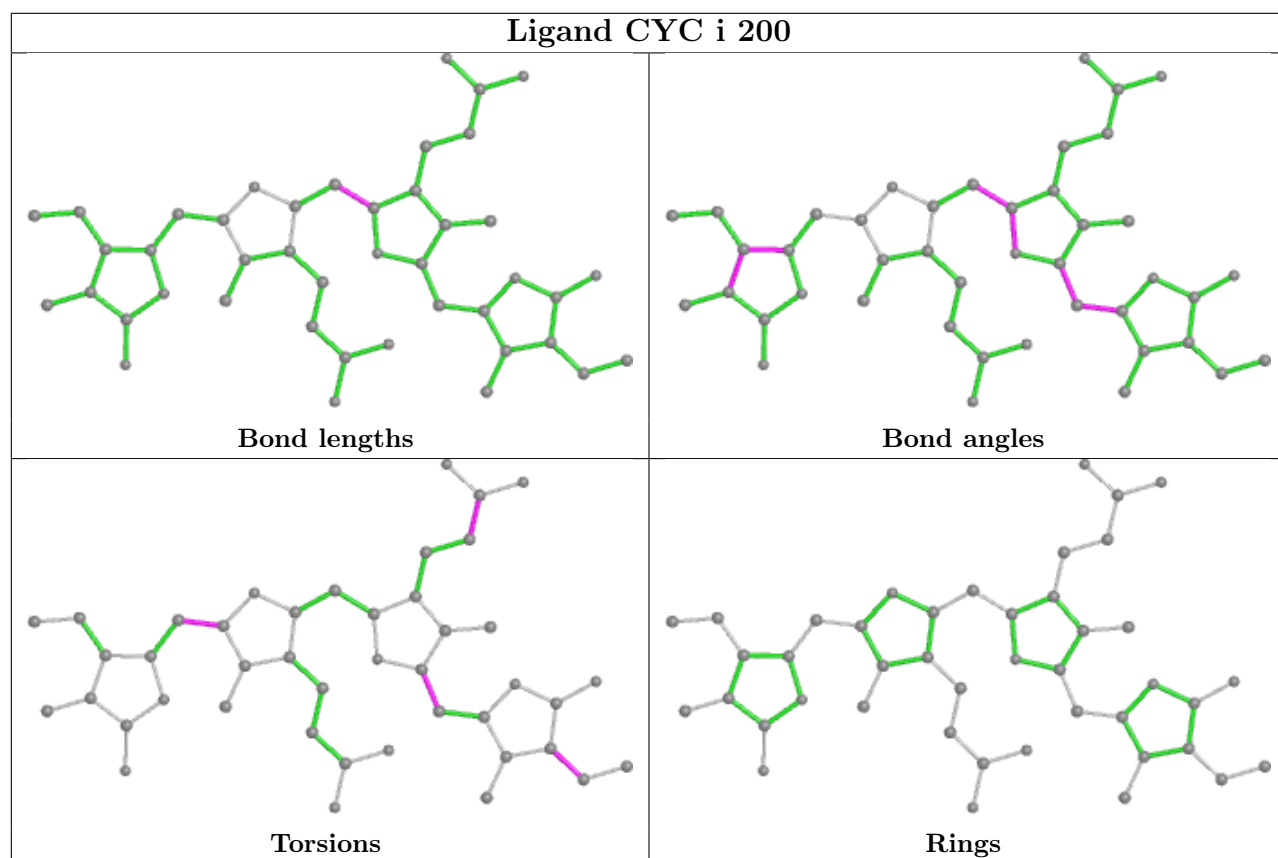
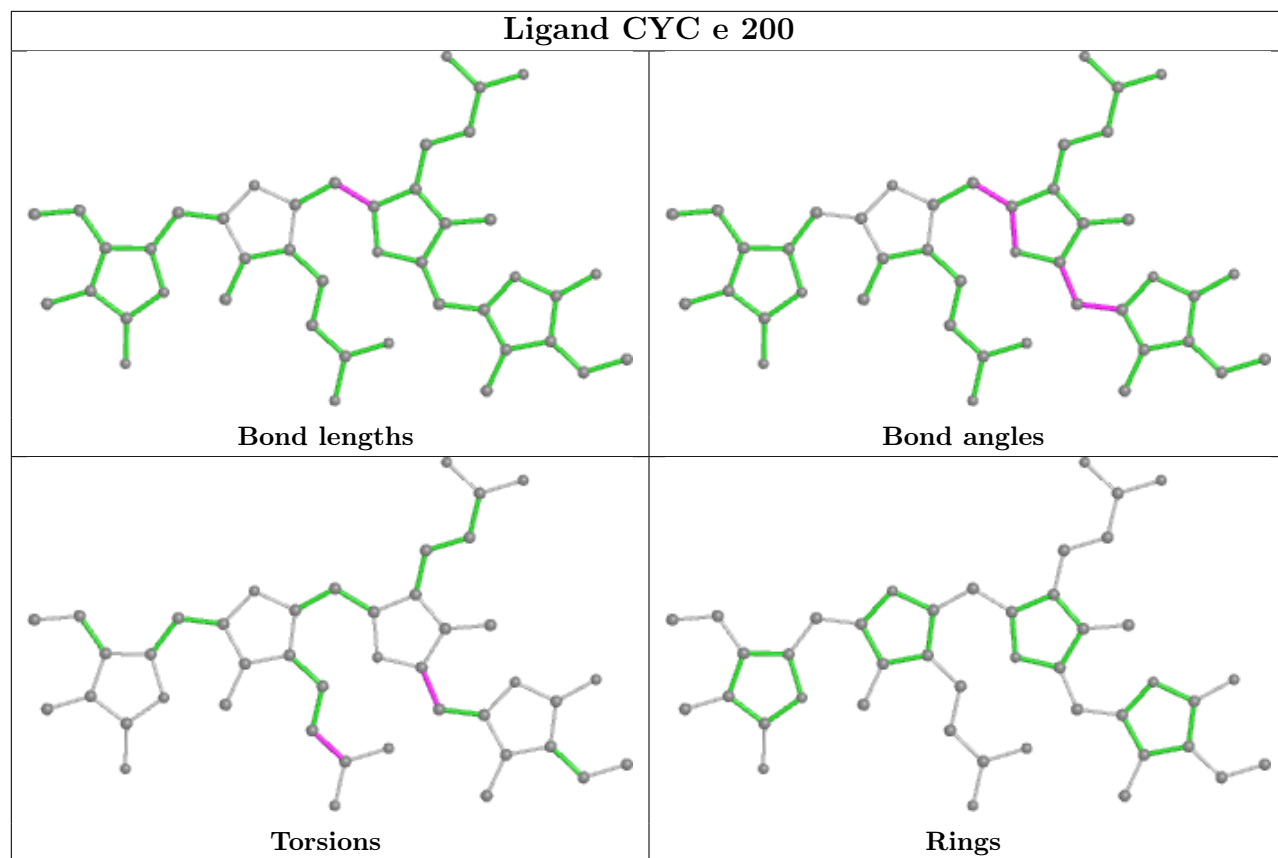
No monomer is involved in short contacts.

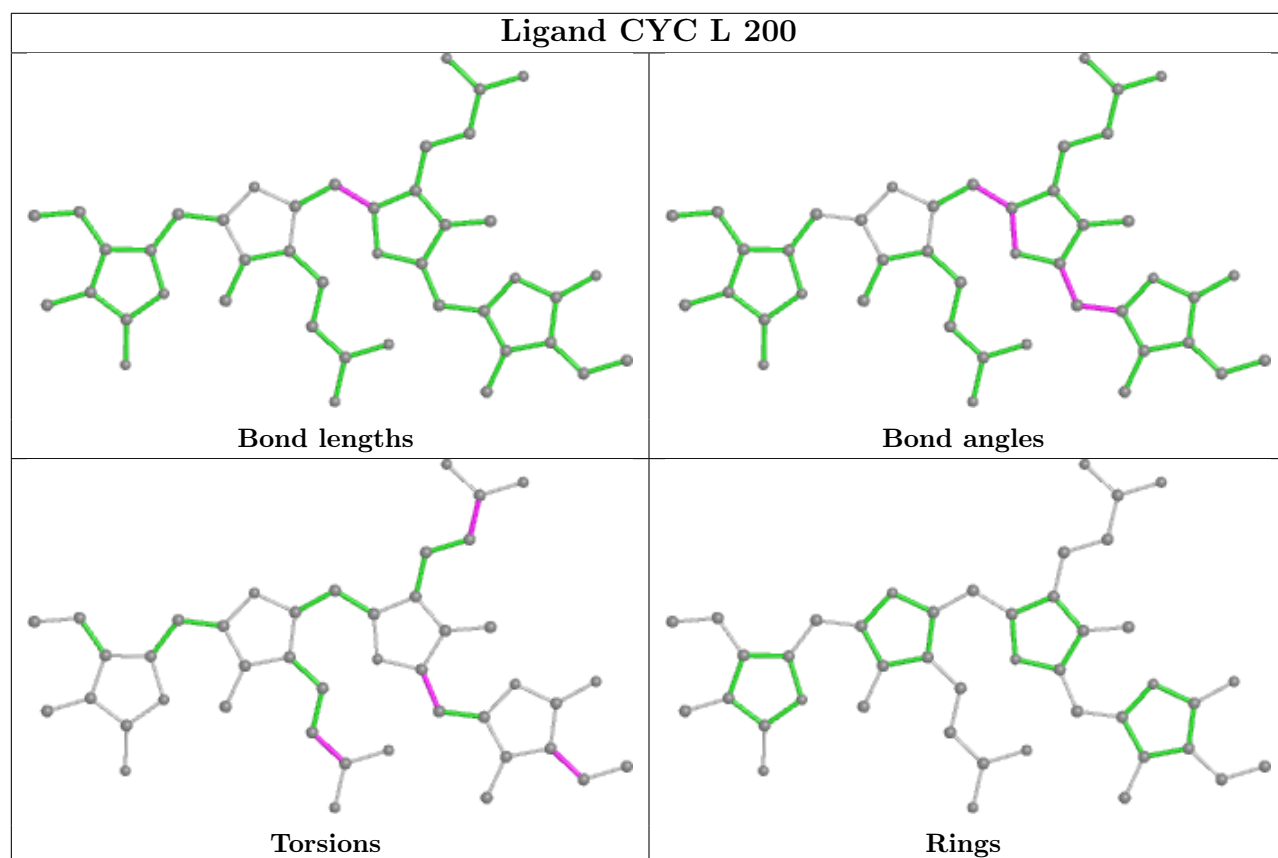
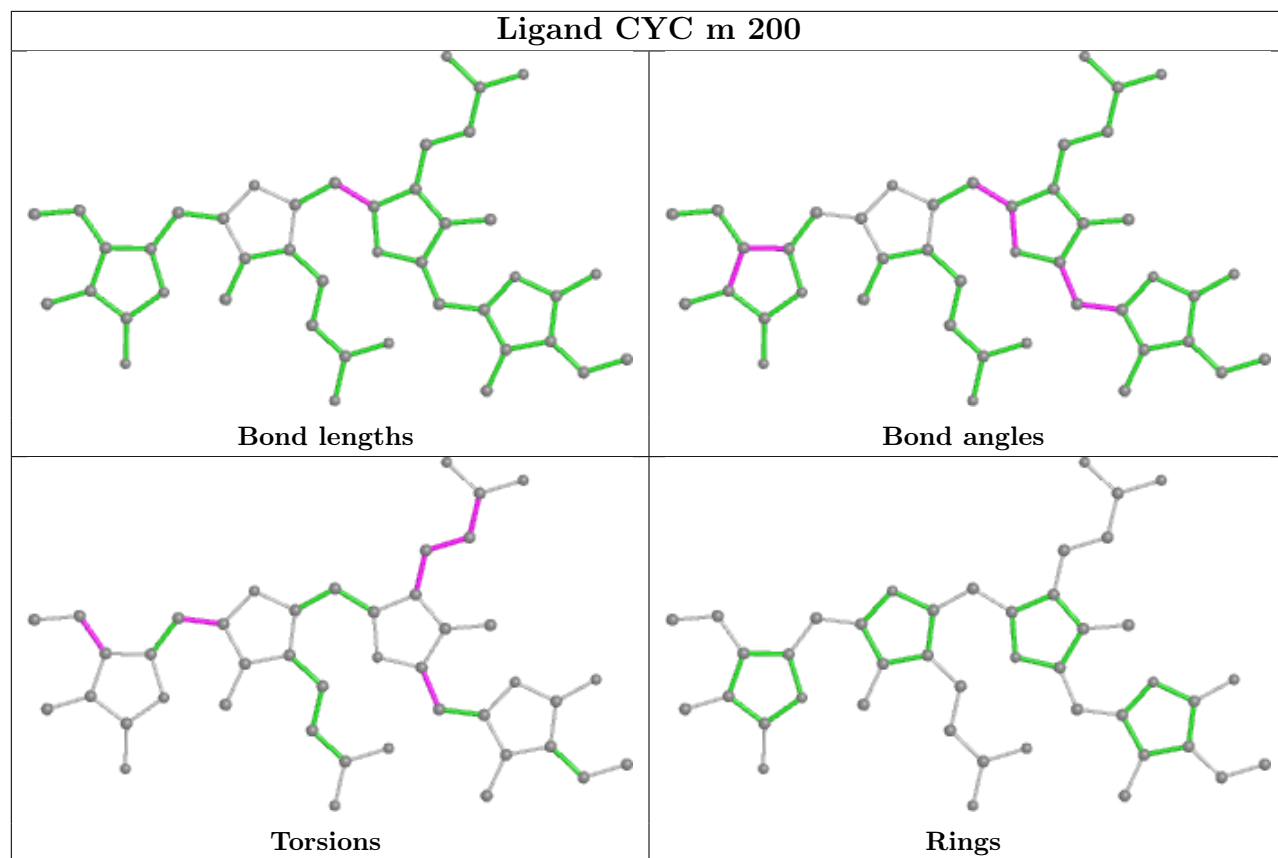
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

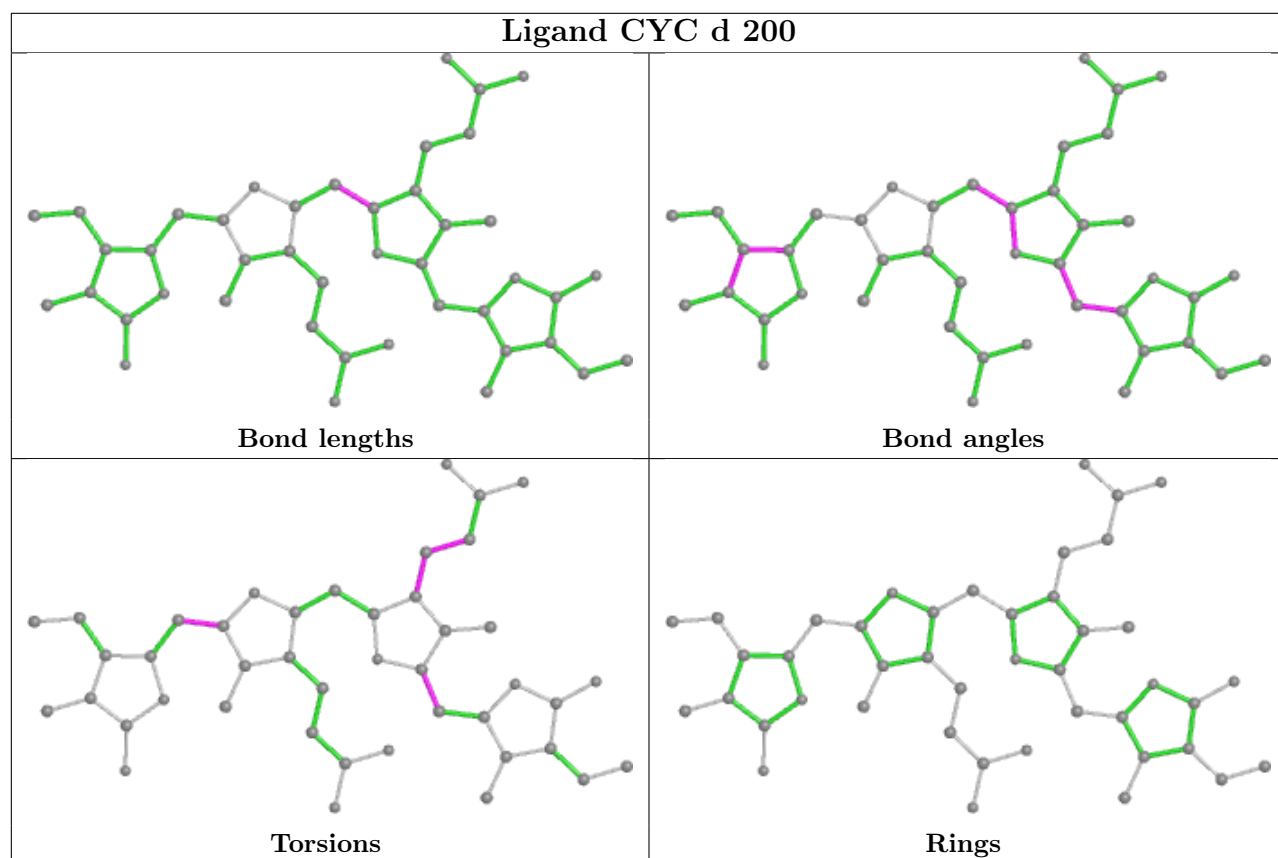
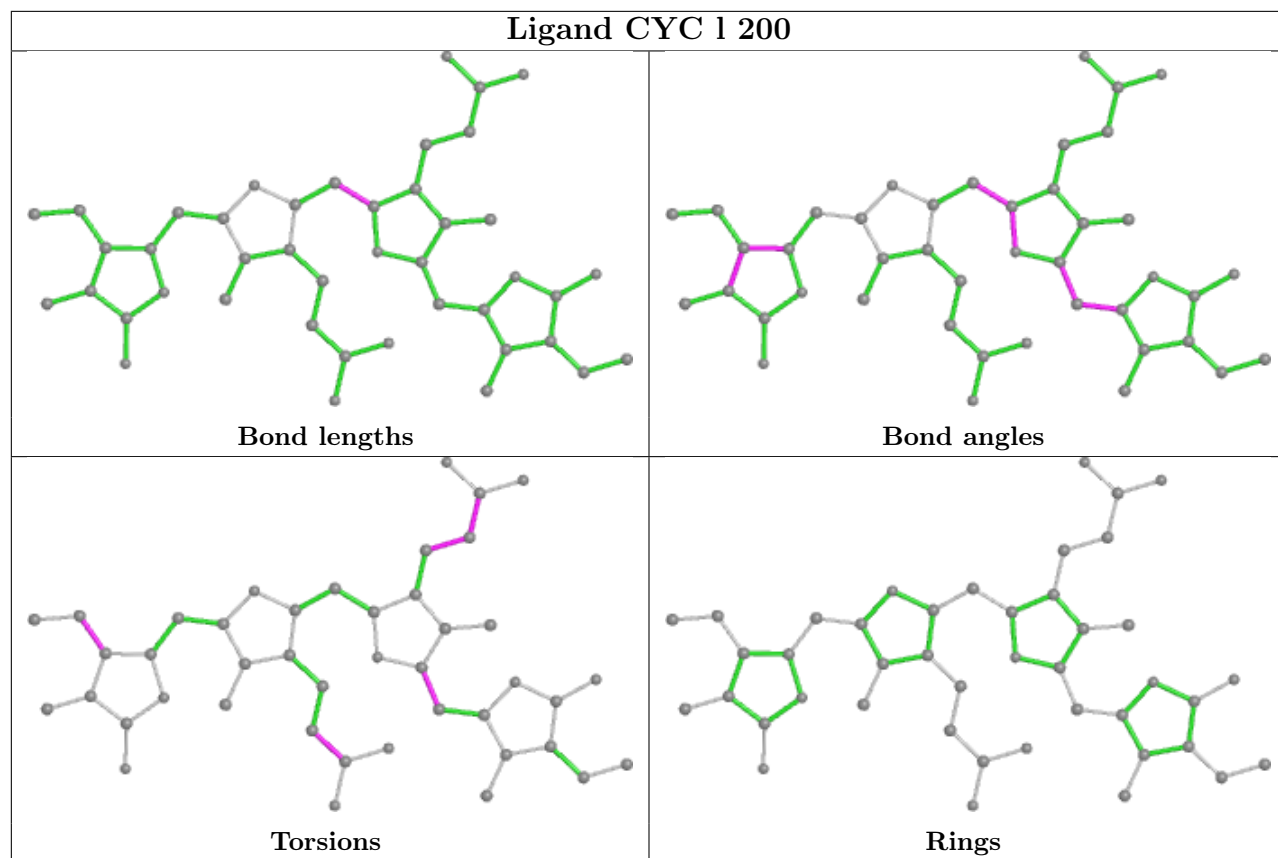
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

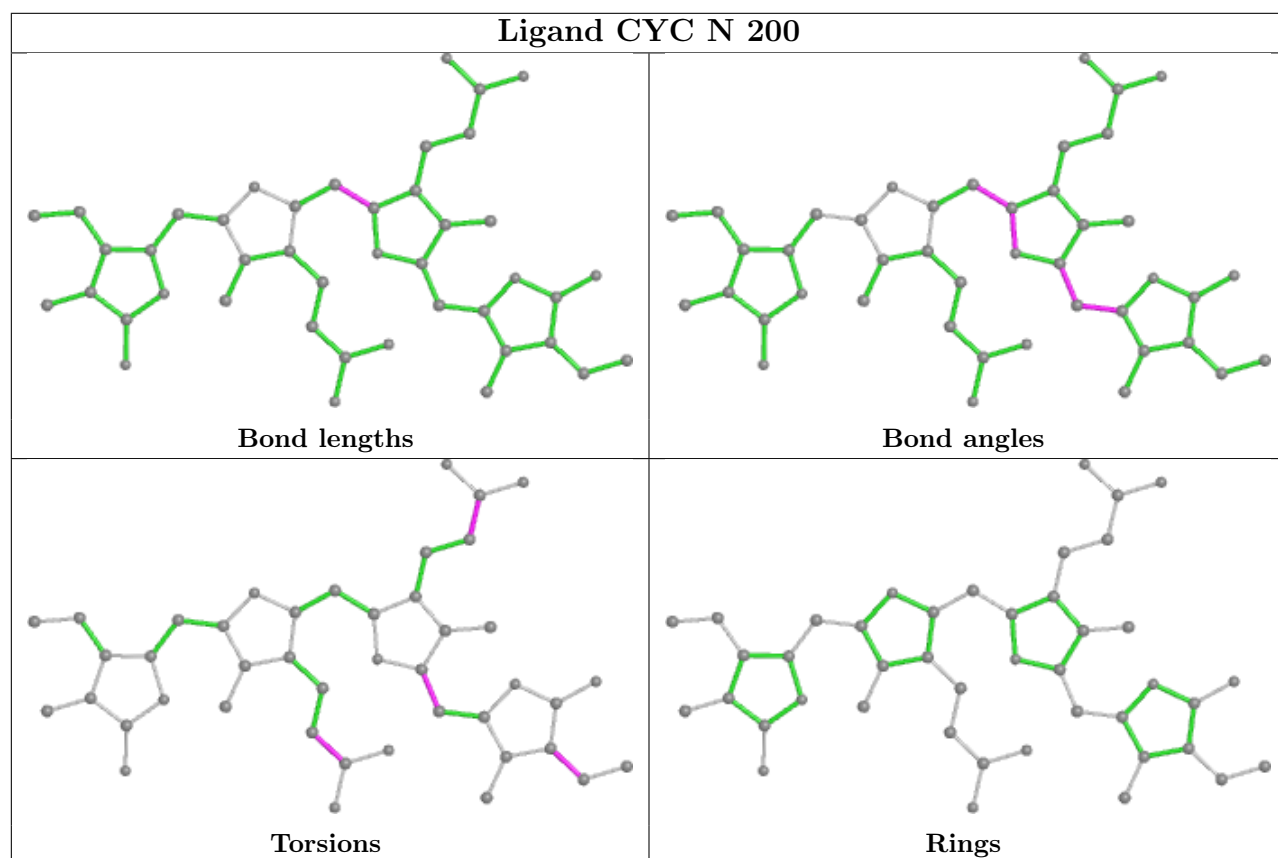
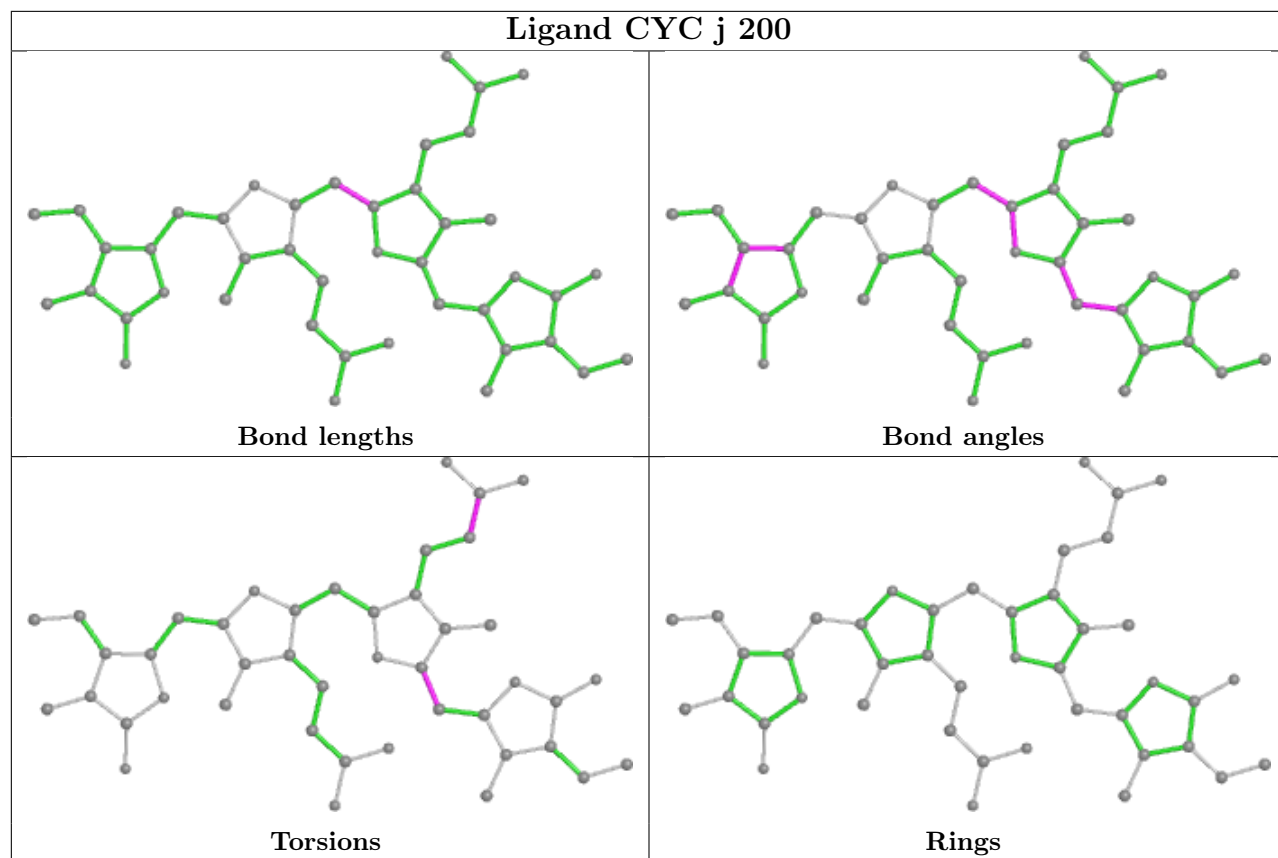


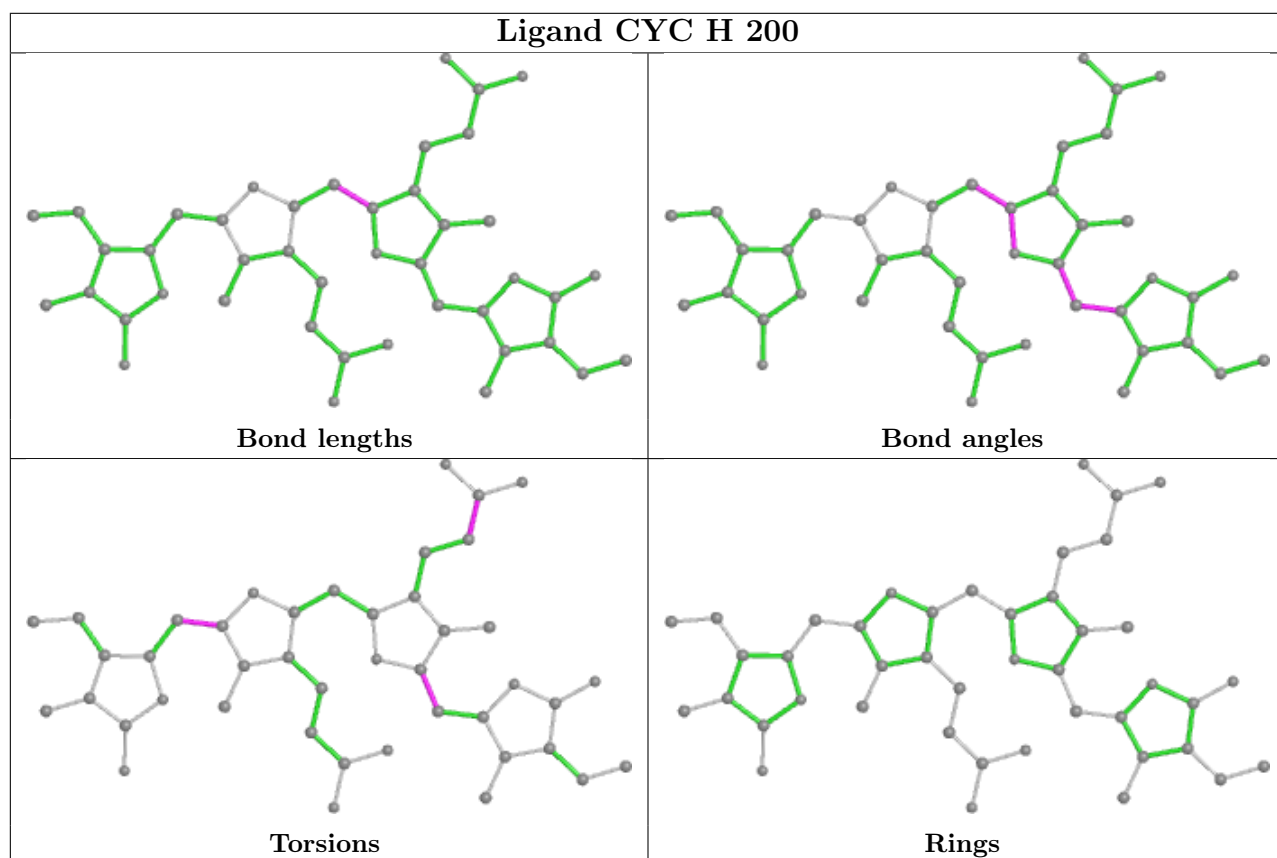
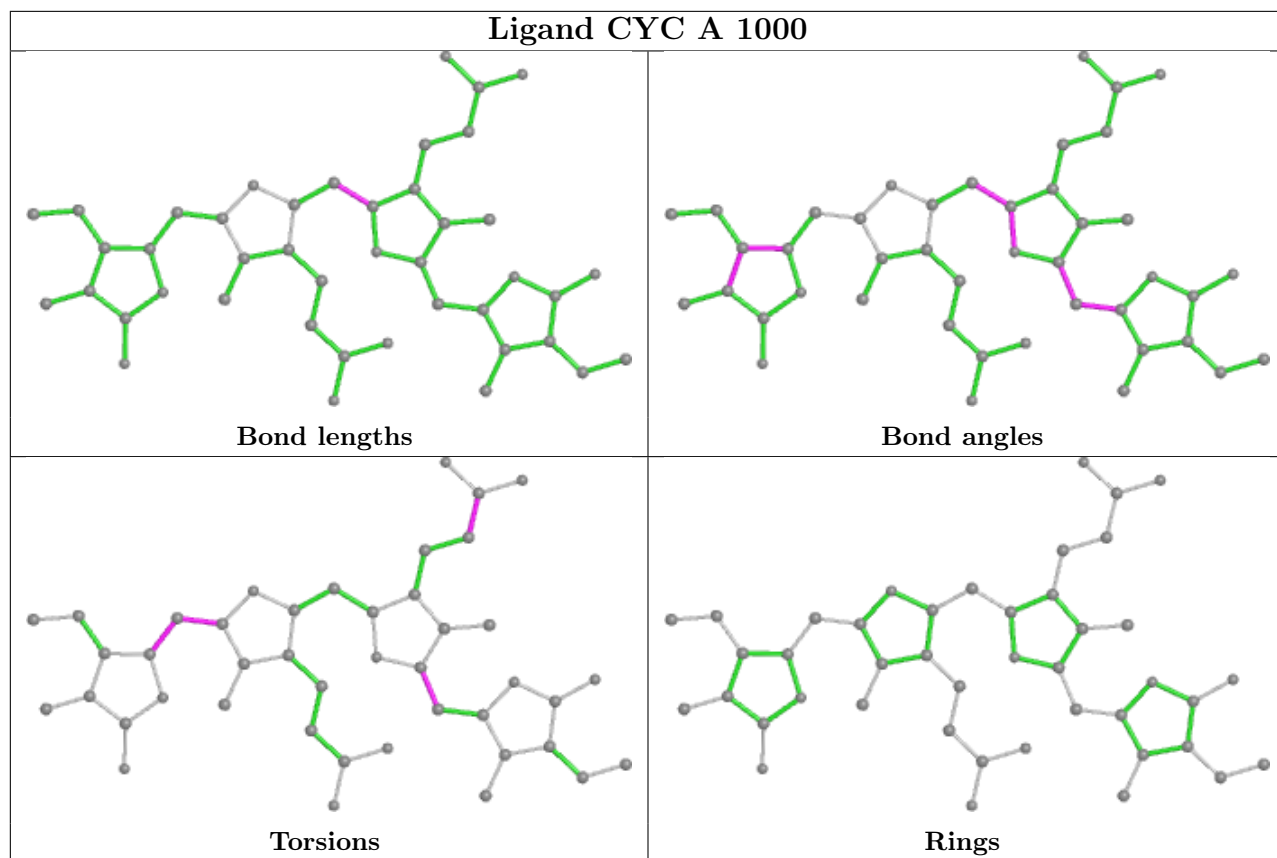


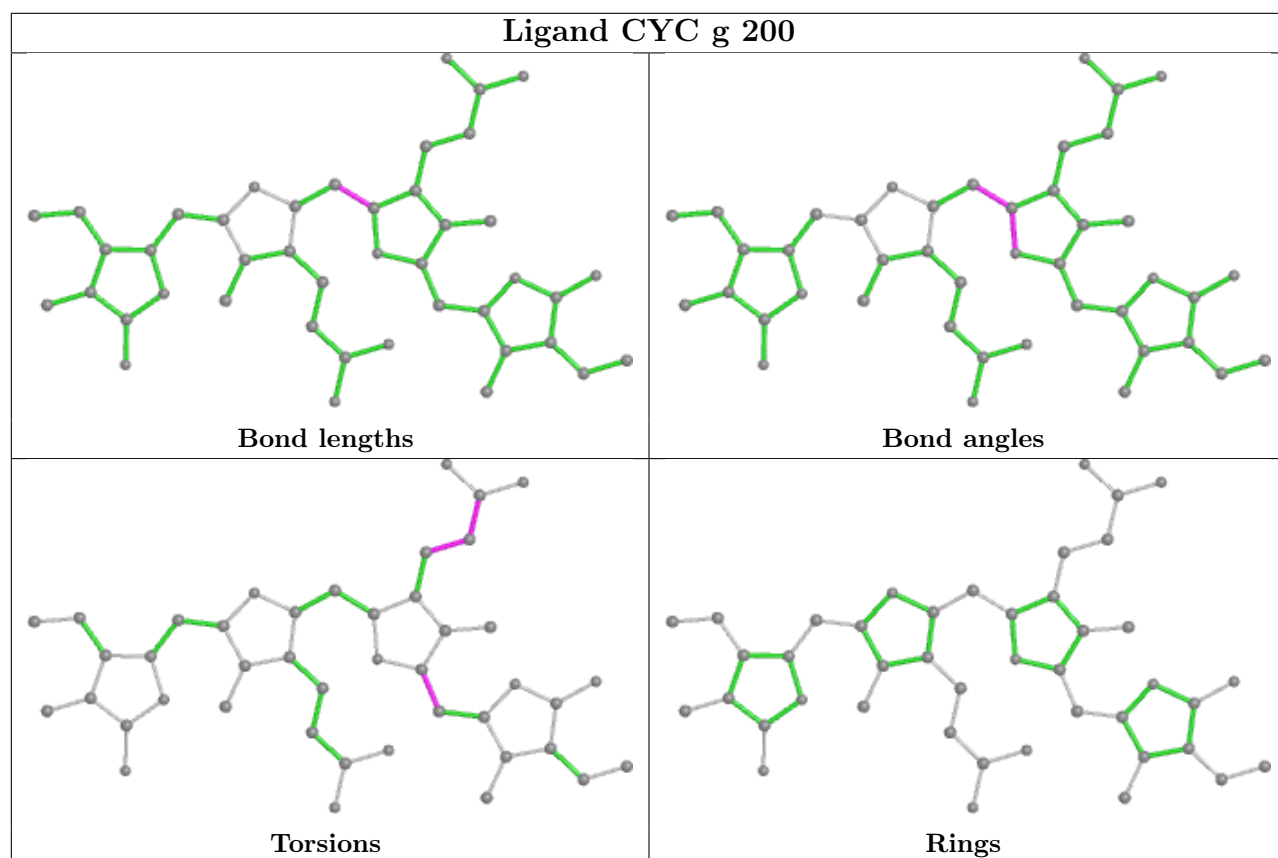
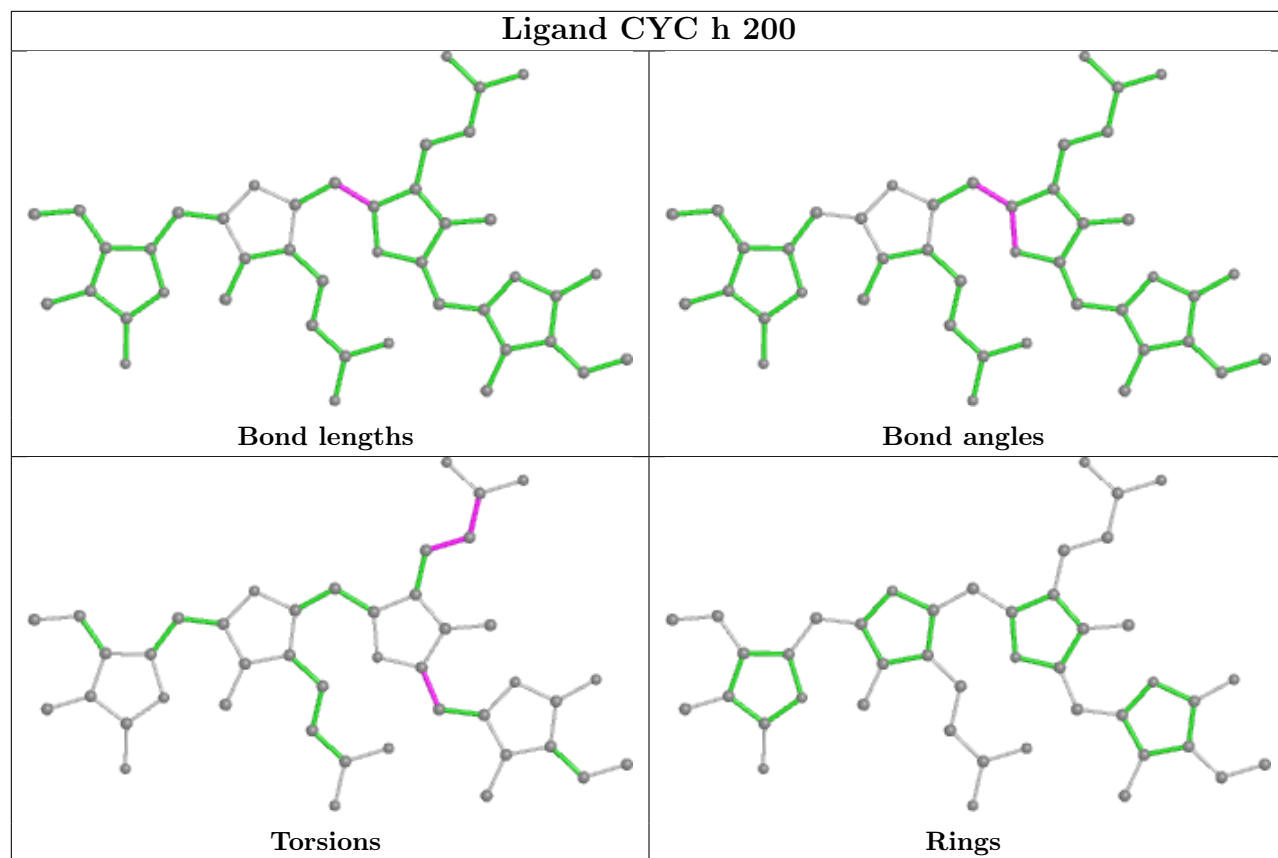


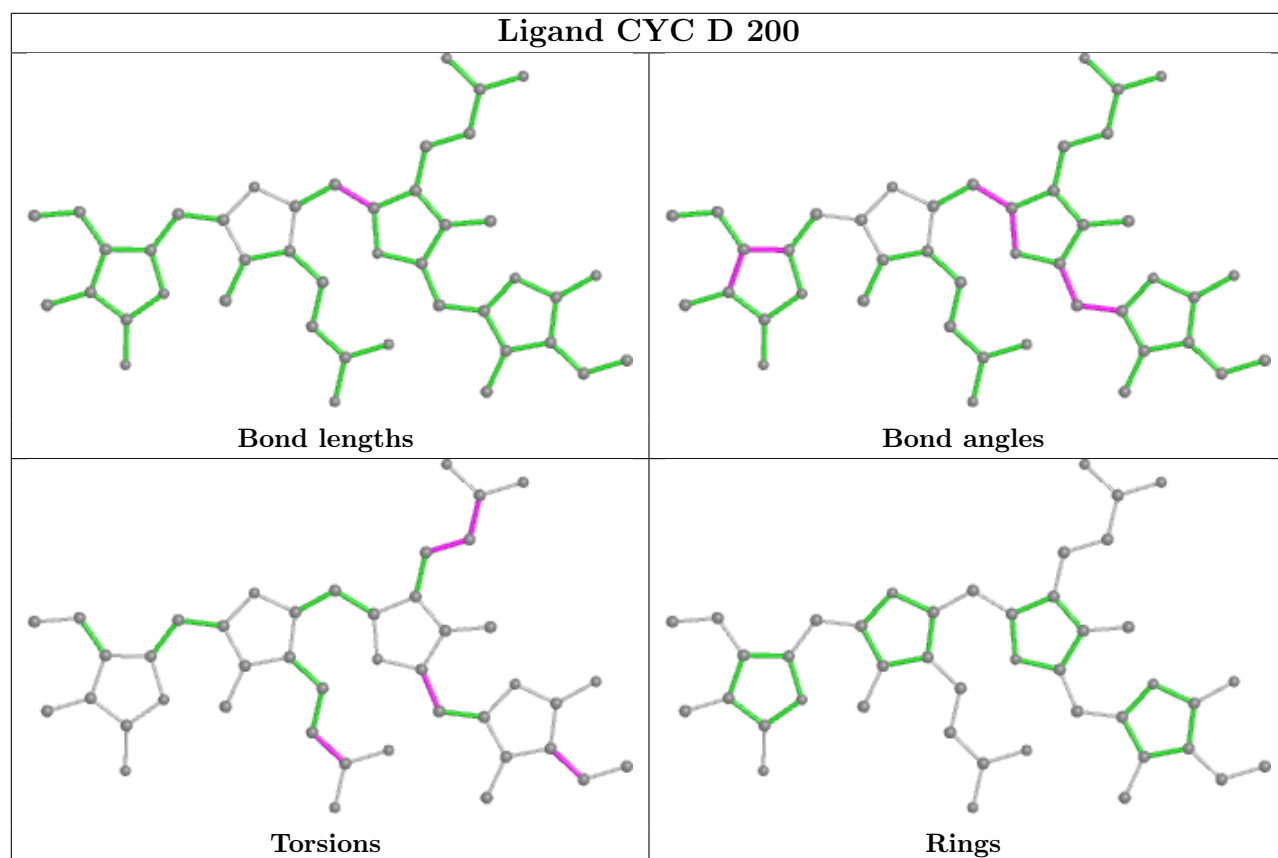
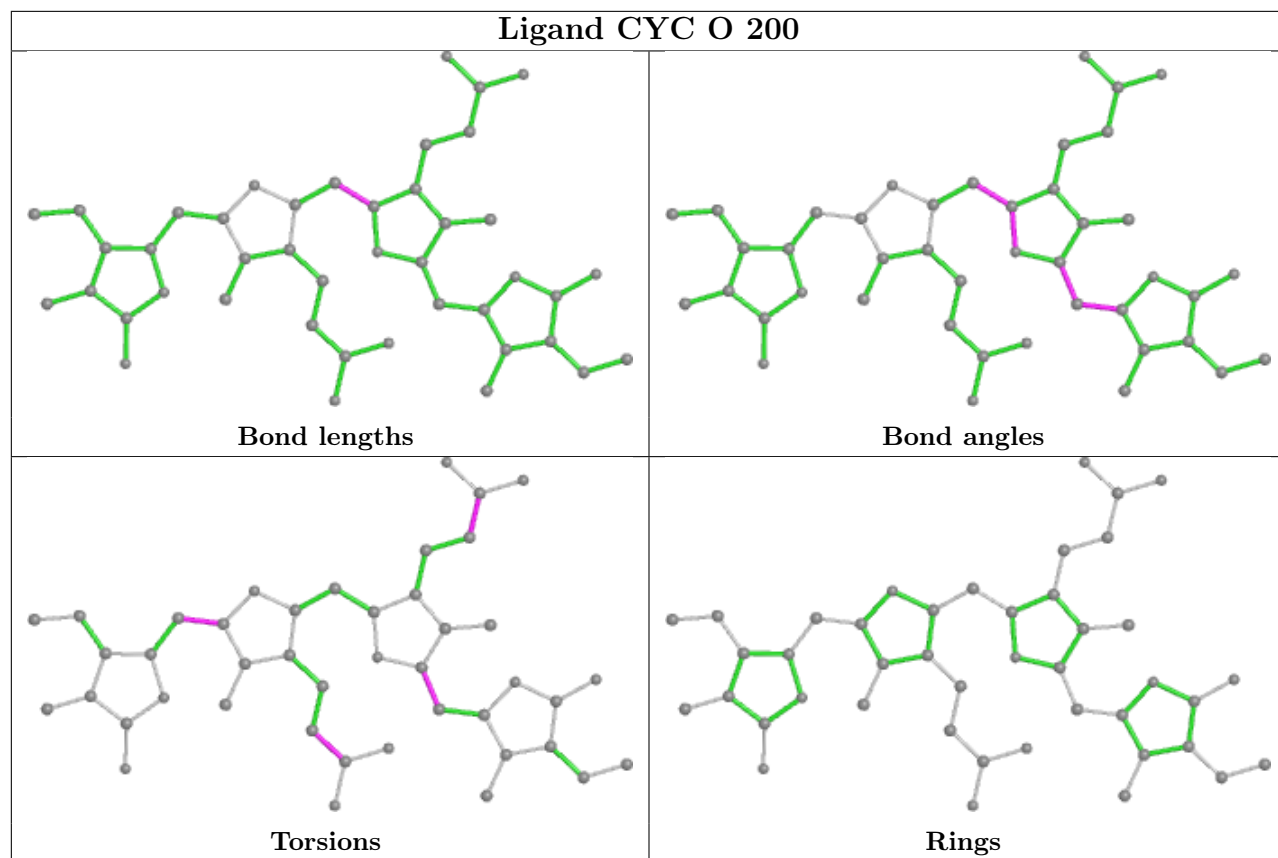


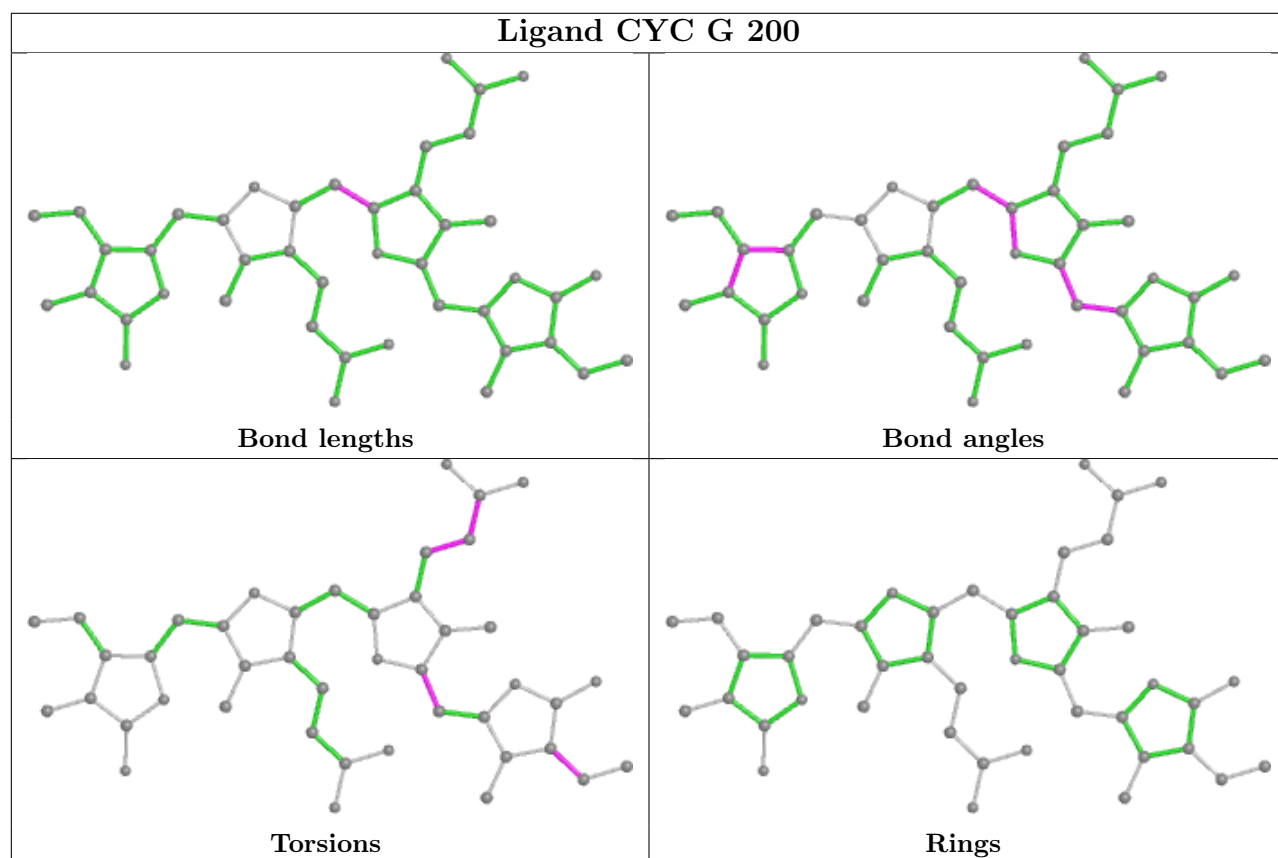
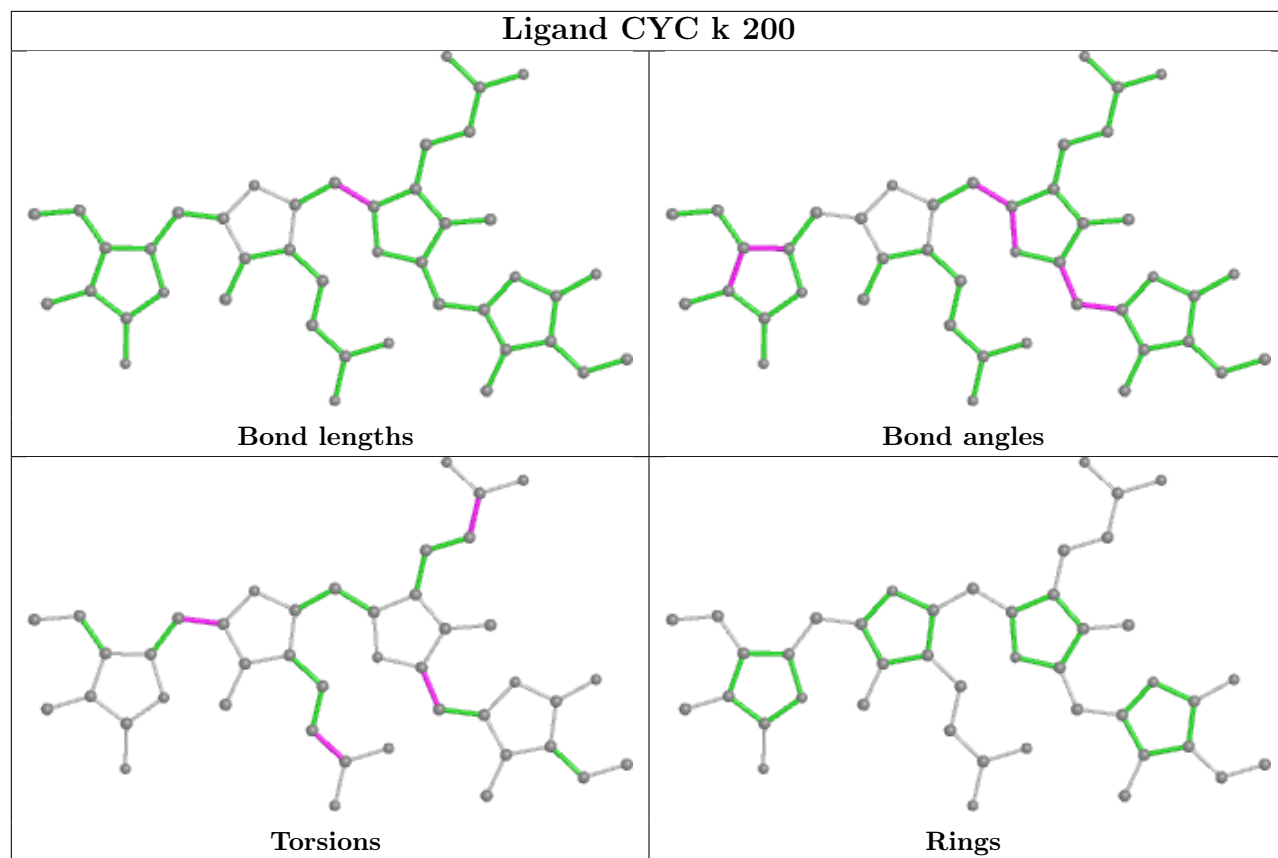


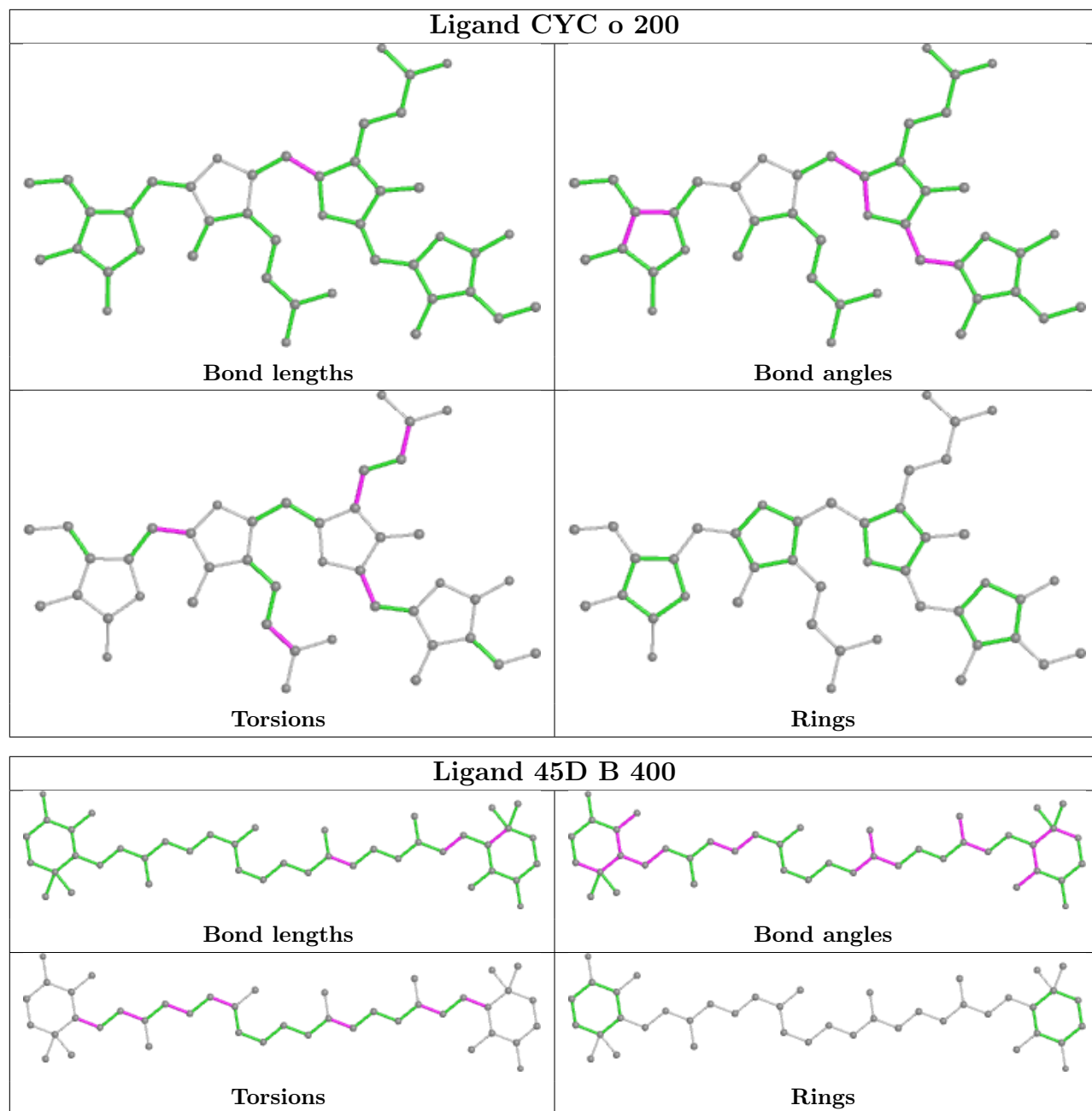


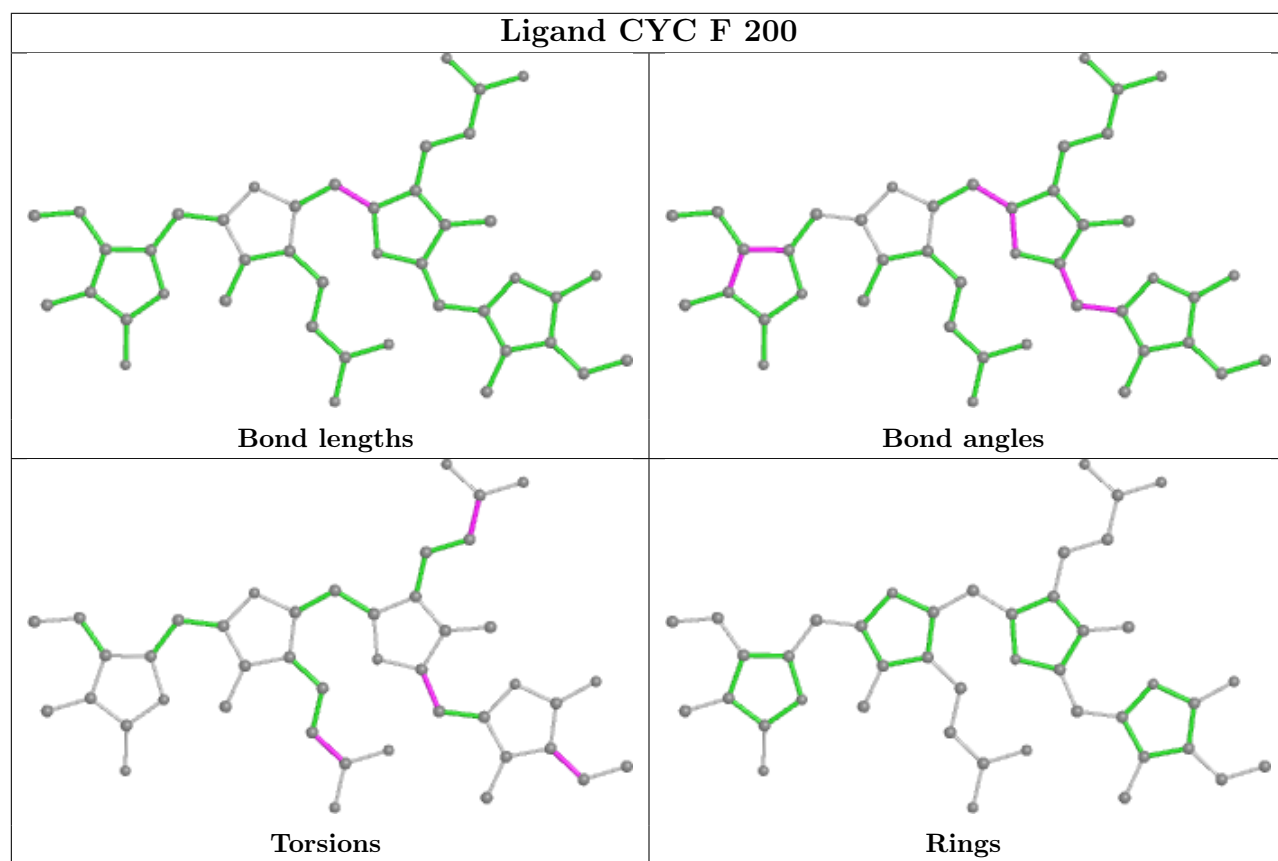
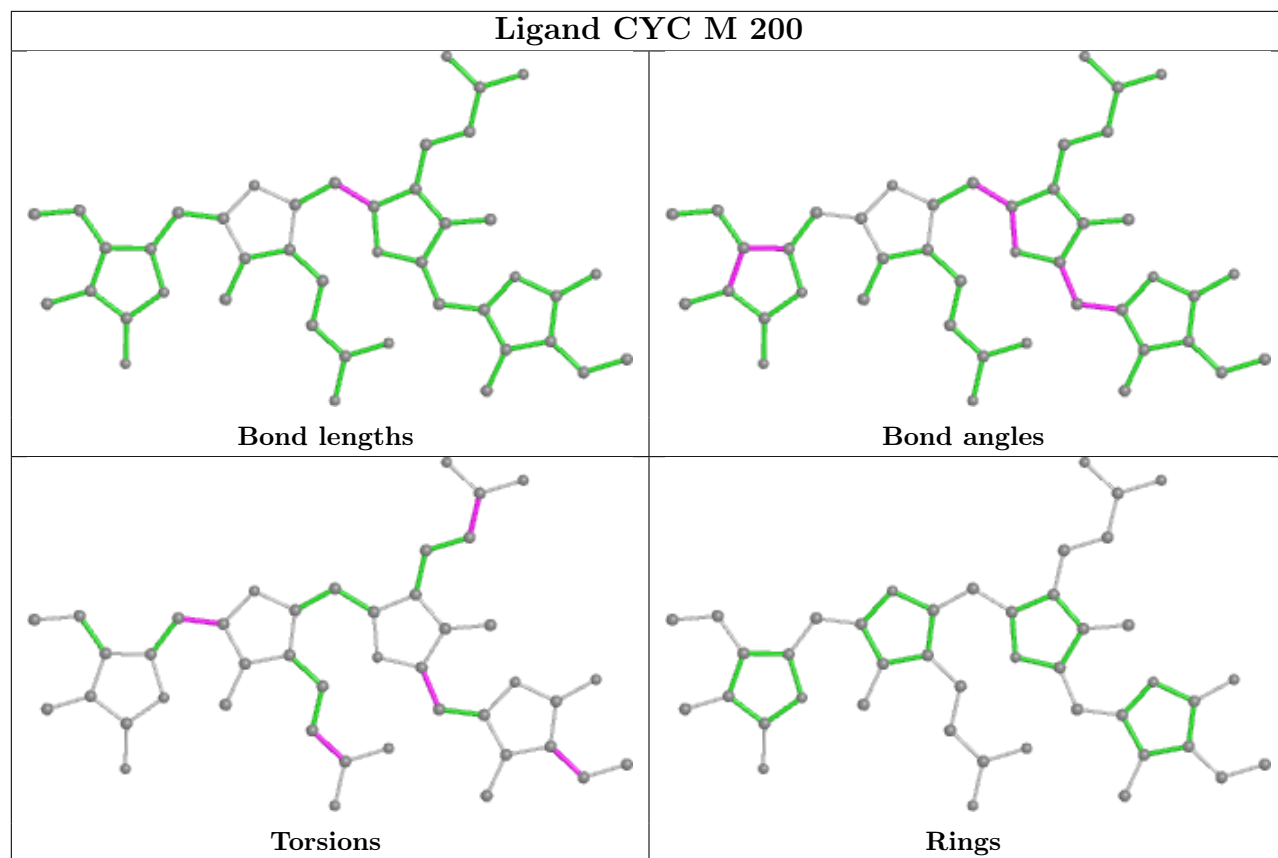


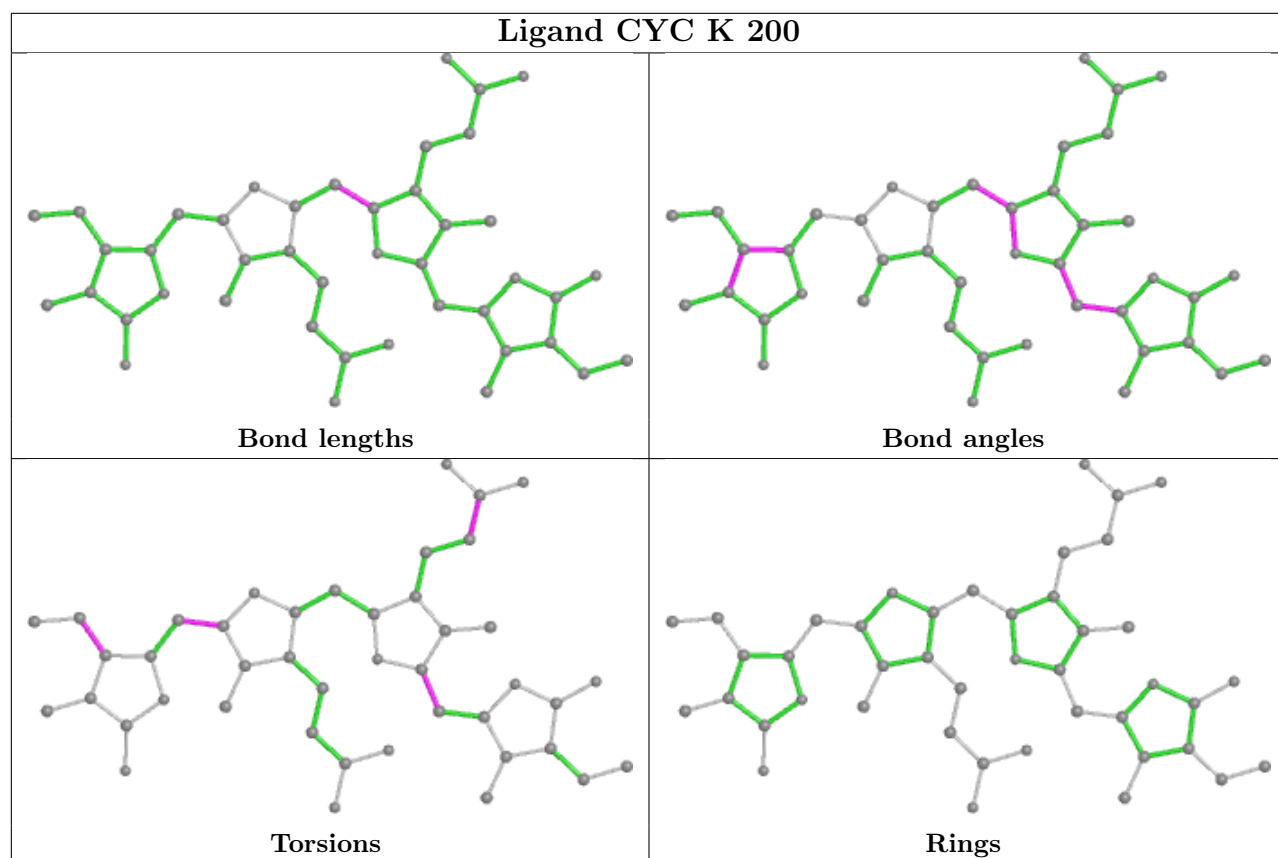
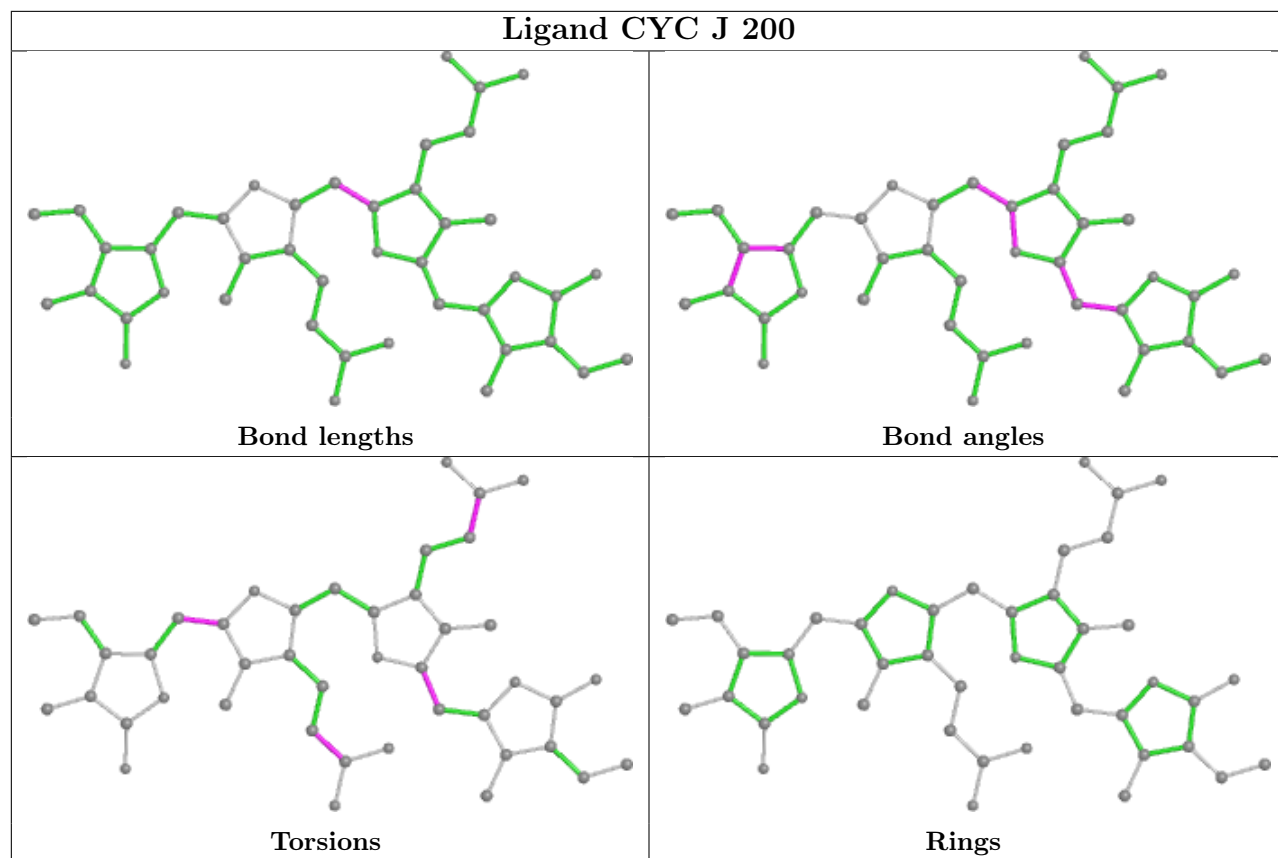












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

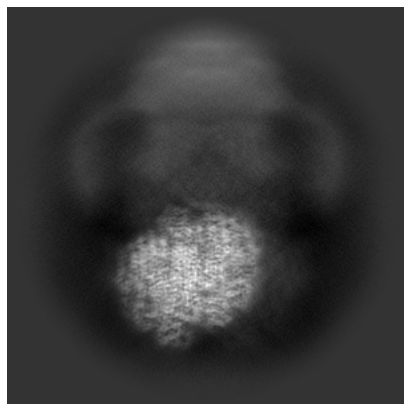
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41434. These allow visual inspection of the internal detail of the map and identification of artifacts.

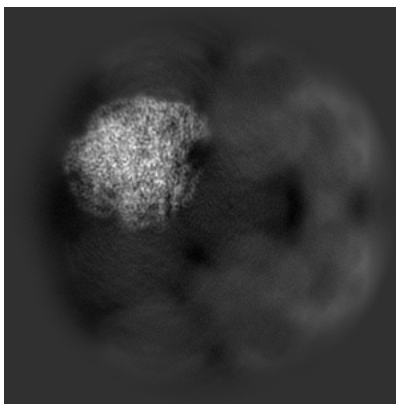
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

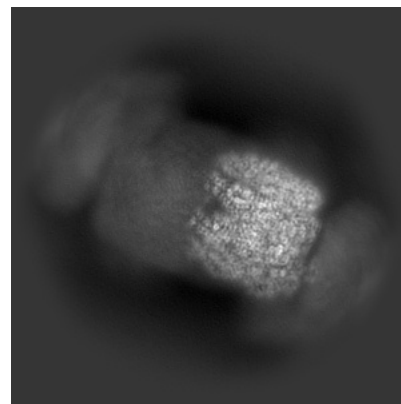
6.1.1 Primary map



X

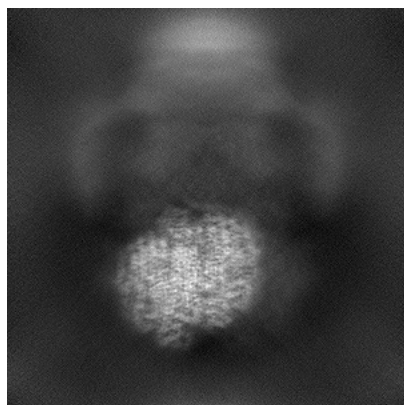


Y

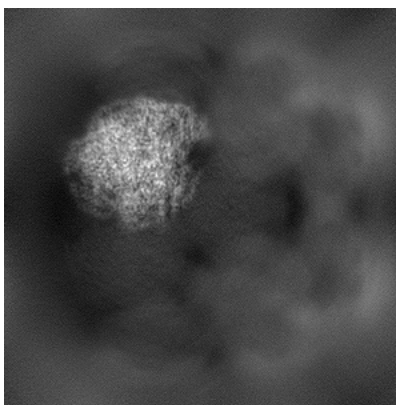


Z

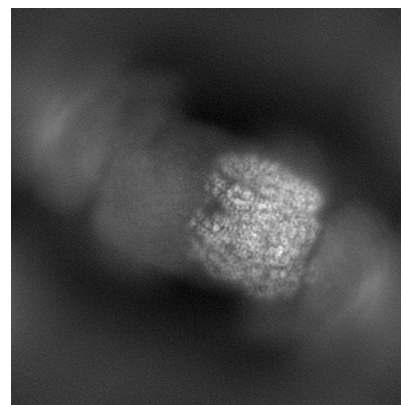
6.1.2 Raw map



X



Y

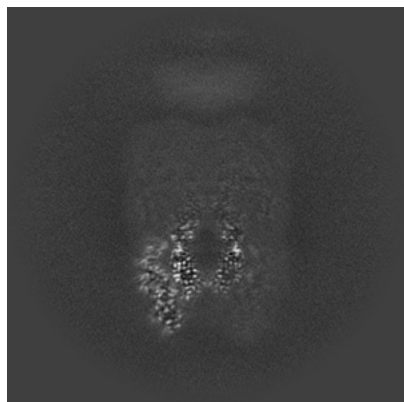


Z

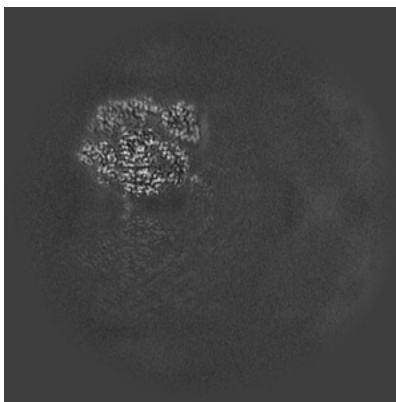
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

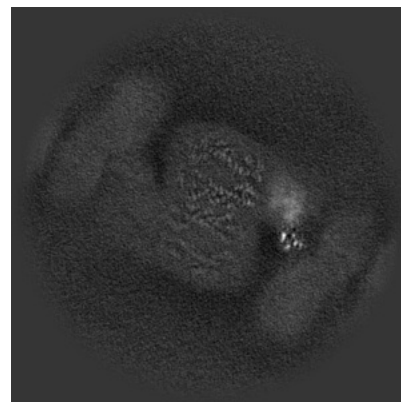
6.2.1 Primary map



X Index: 256

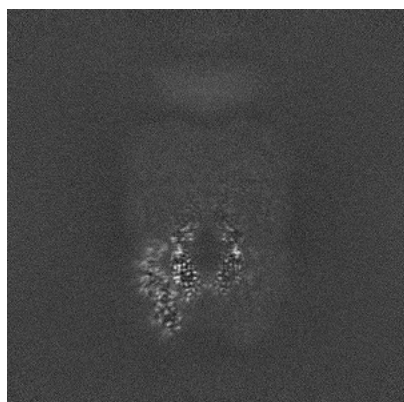


Y Index: 256

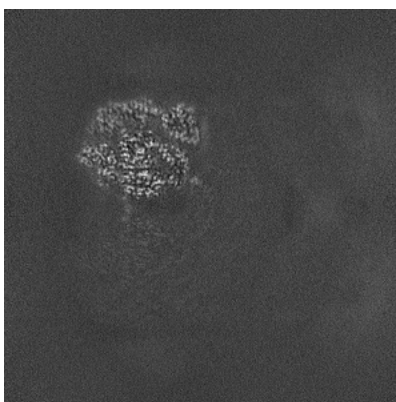


Z Index: 256

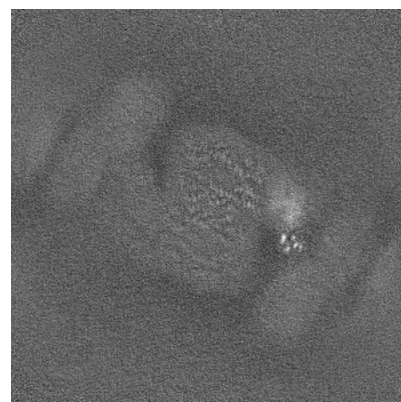
6.2.2 Raw map



X Index: 256



Y Index: 256

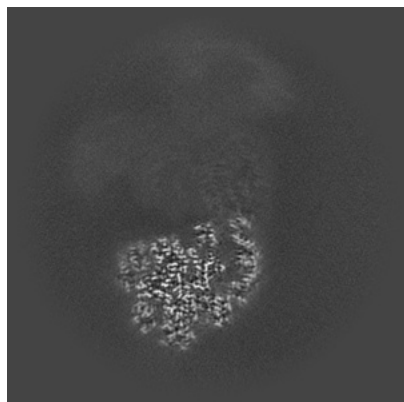


Z Index: 256

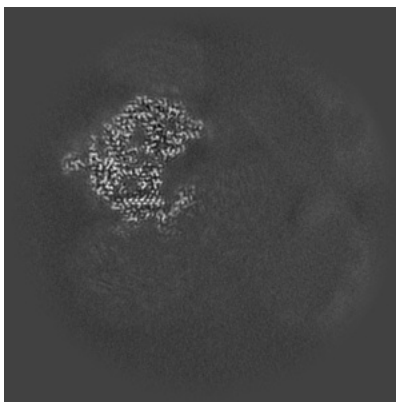
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

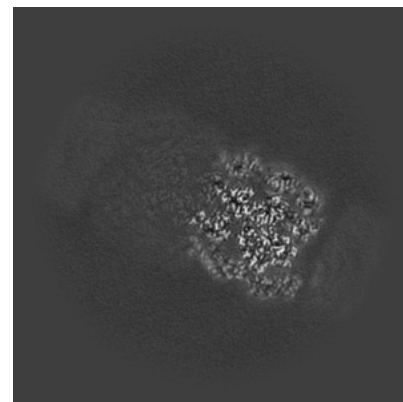
6.3.1 Primary map



X Index: 310

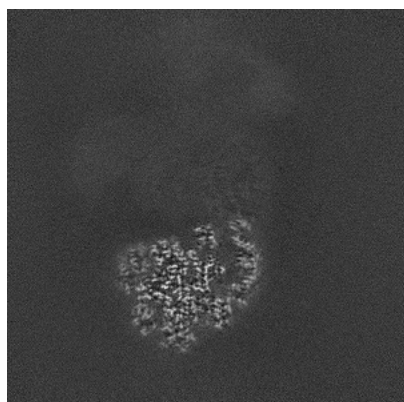


Y Index: 230

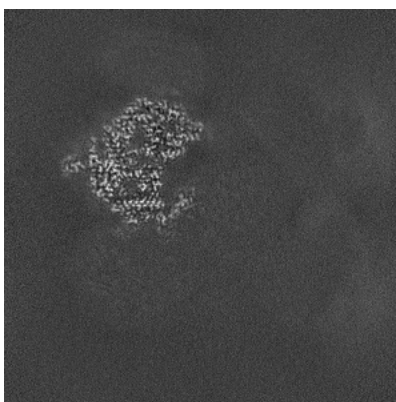


Z Index: 165

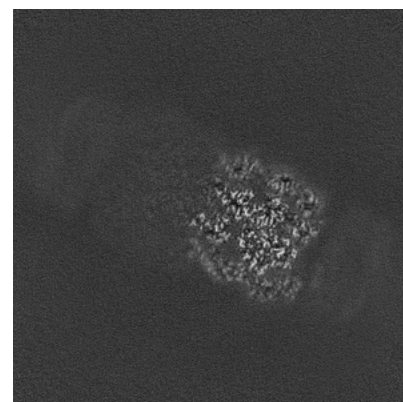
6.3.2 Raw map



X Index: 310



Y Index: 230

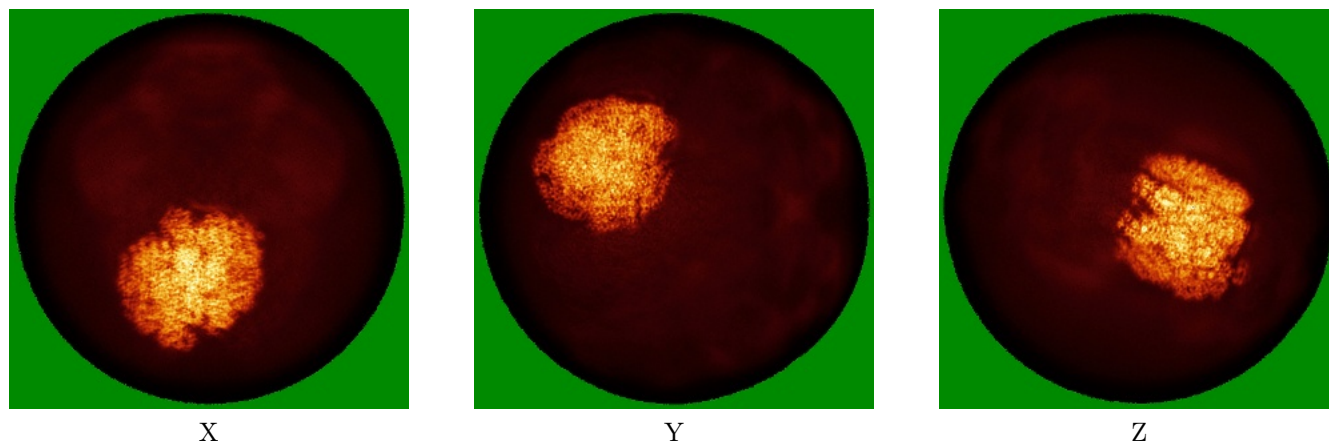


Z Index: 165

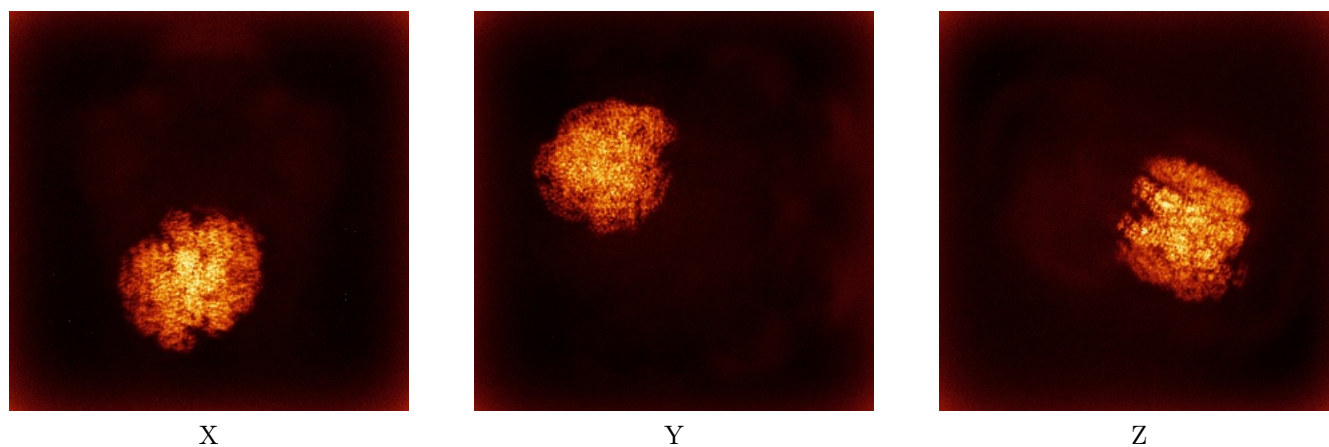
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



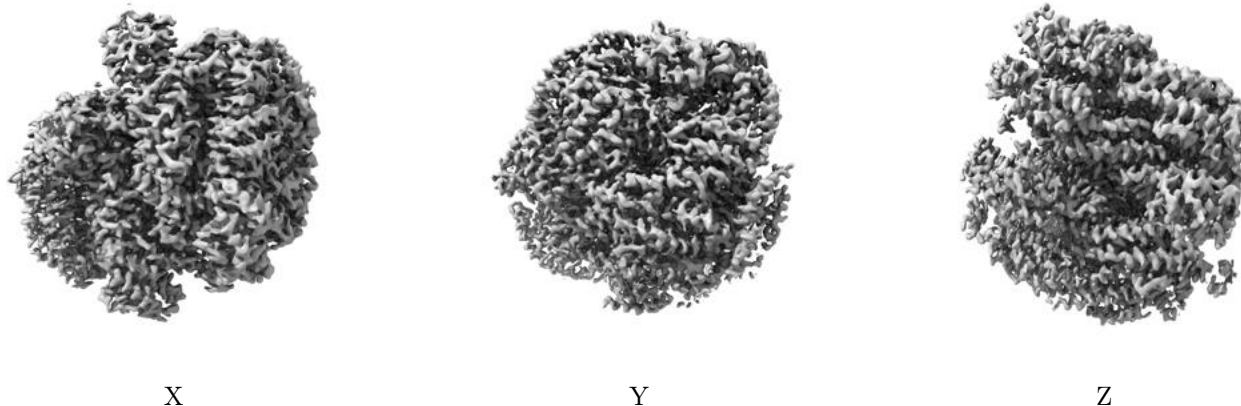
6.4.2 Raw map



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.

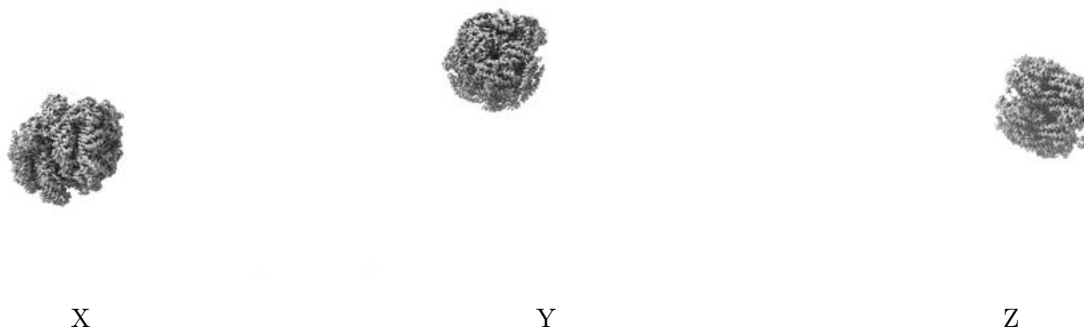
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.3. 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.

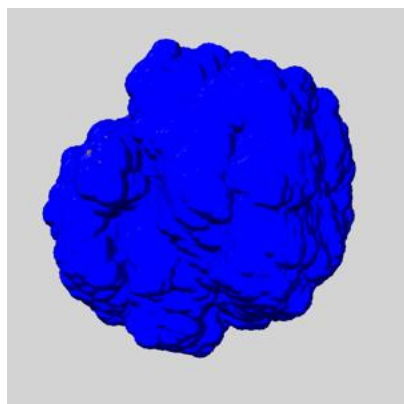
6.6 Mask visualisation [i](#)

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

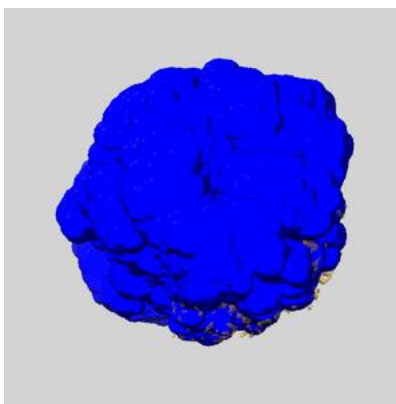
A mask typically either:

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

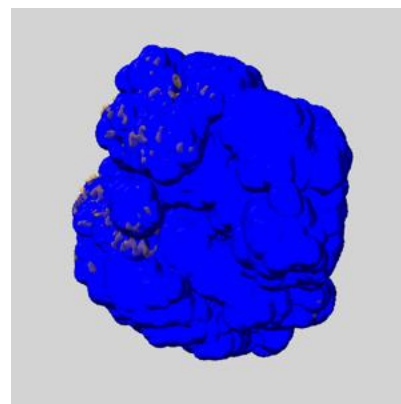
6.6.1 emd_41434_msk_1.map [i](#)



X



Y

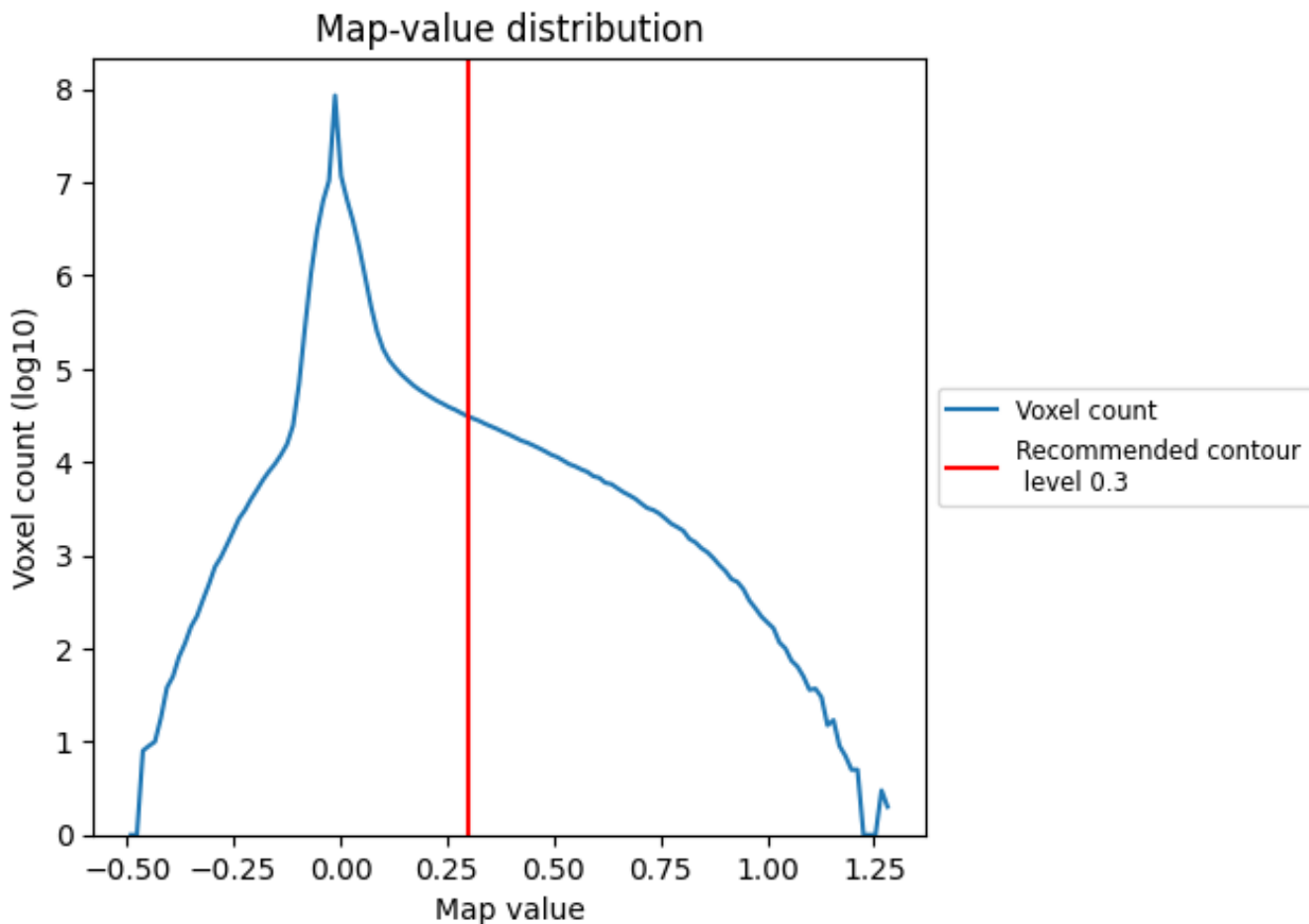


Z

7 Map analysis [i](#)

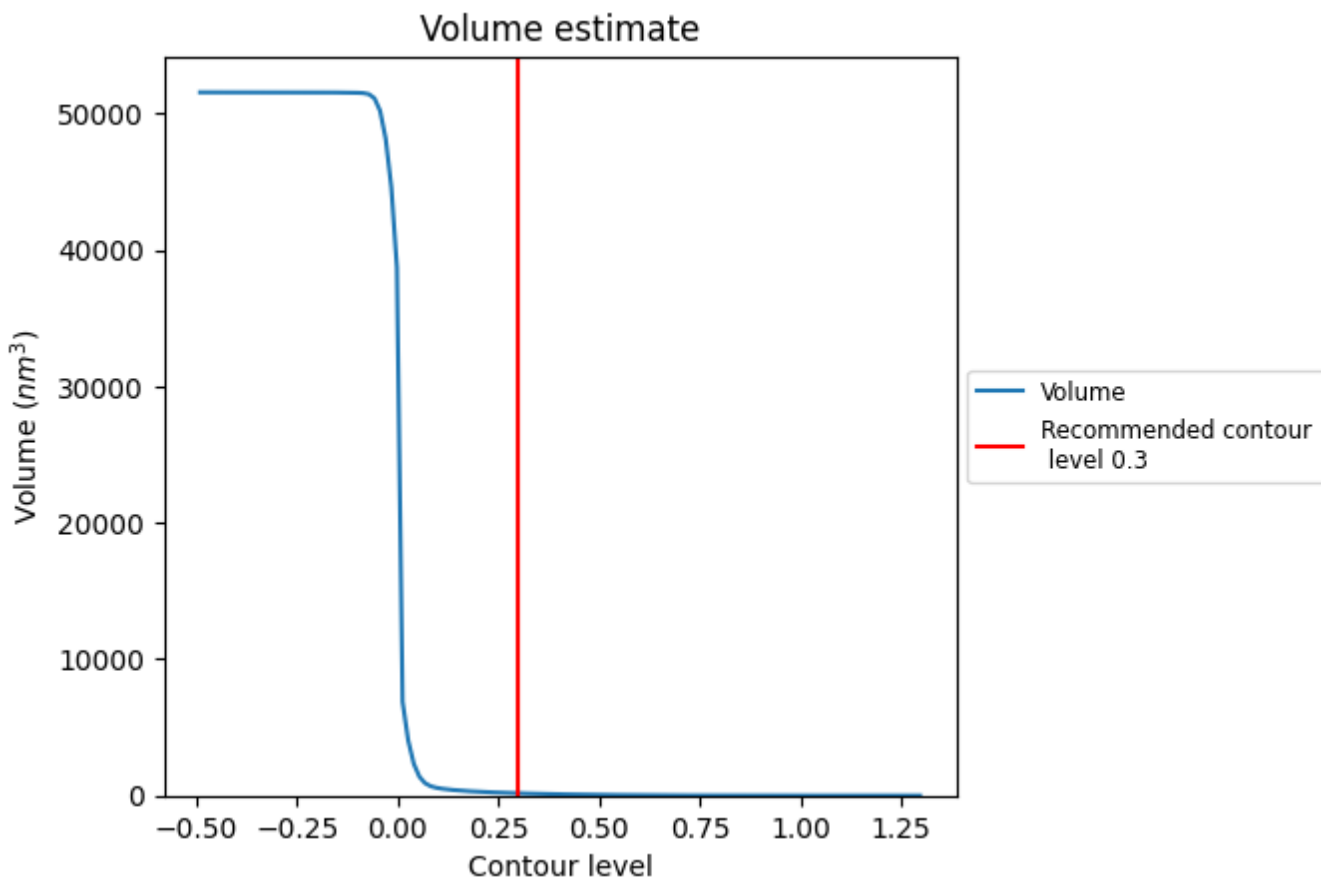
This section contains the results of statistical analysis of the map.

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.

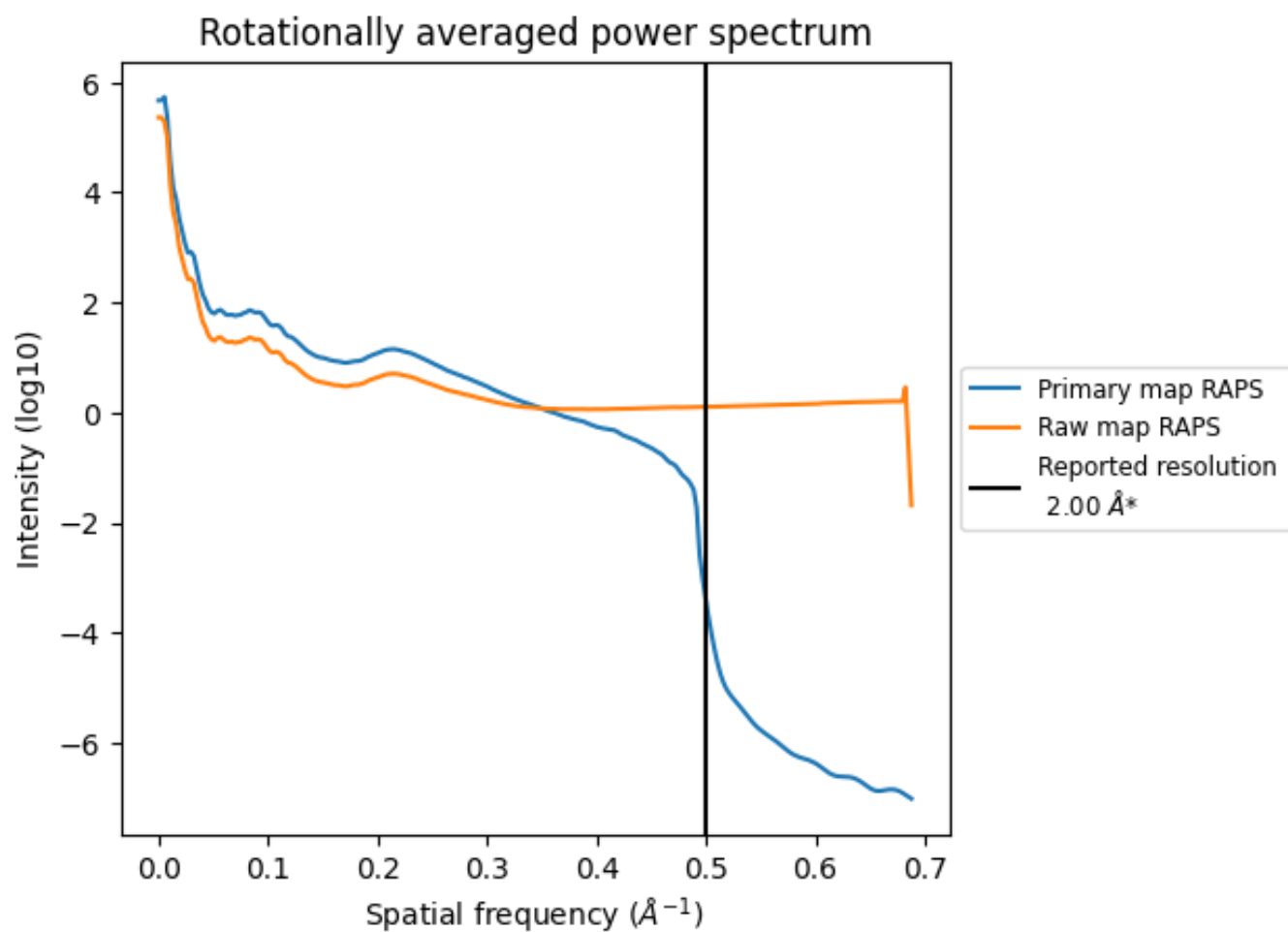
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 167 nm³; this corresponds to an approximate mass of 150 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

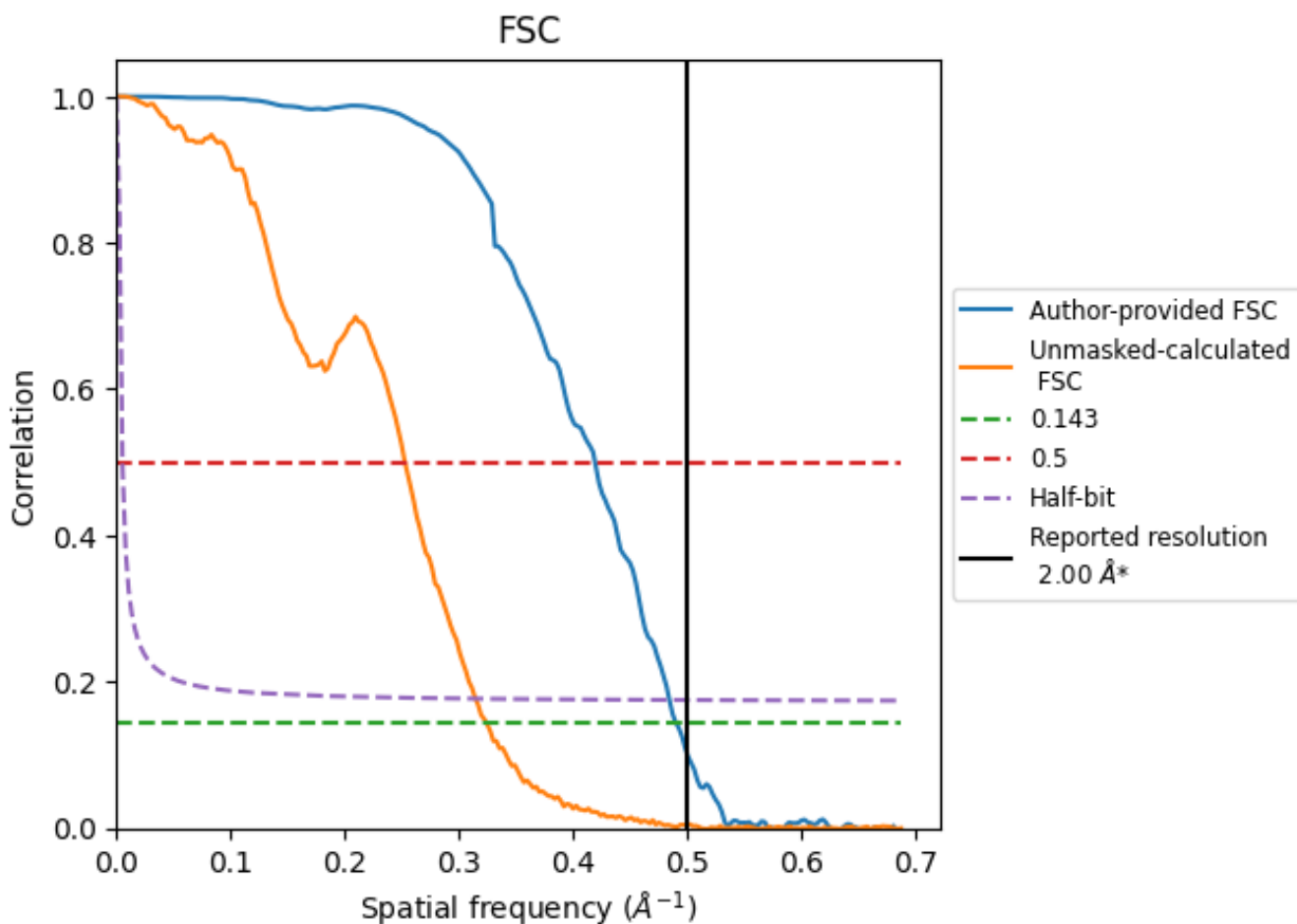


*Reported resolution corresponds to spatial frequency of 0.500 Å⁻¹

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 0.500 Å⁻¹

8.2 Resolution estimates [i](#)

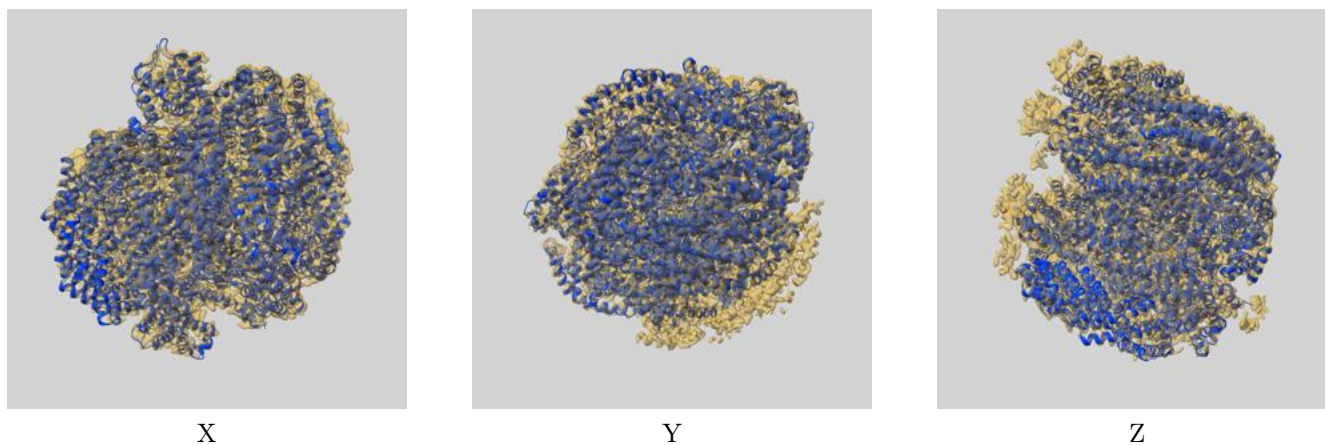
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.00	-	-
Author-provided FSC curve	2.04	2.38	2.06
Unmasked-calculated*	3.08	3.95	3.18

*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 3.08 differs from the reported value 2.0 by more than 10 %

9 Map-model fit [i](#)

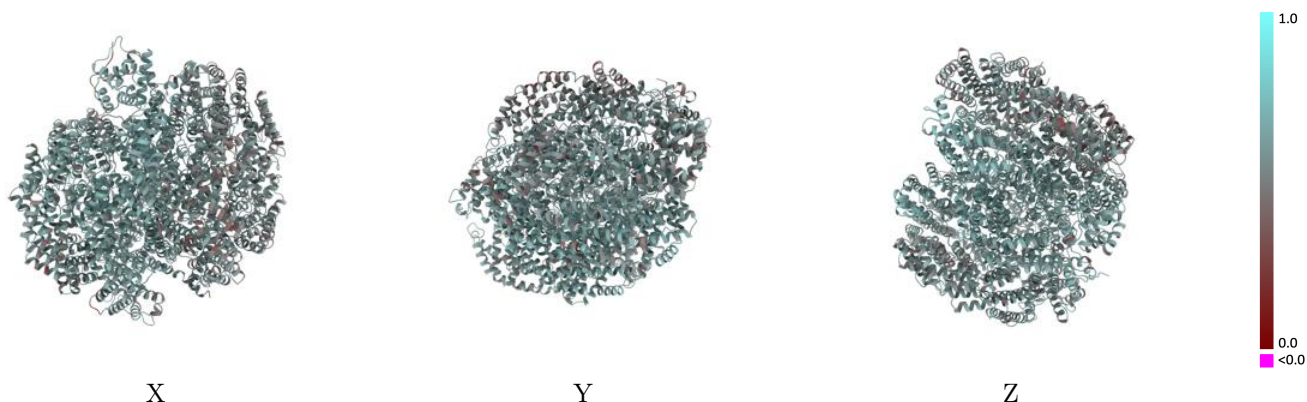
This section contains information regarding the fit between EMDB map EMD-41434 and PDB model 8TO2. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



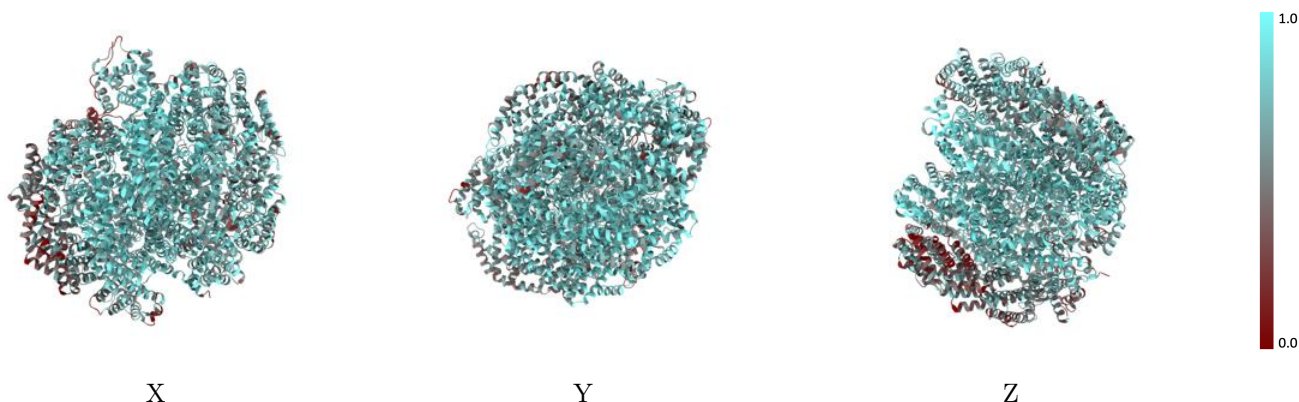
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



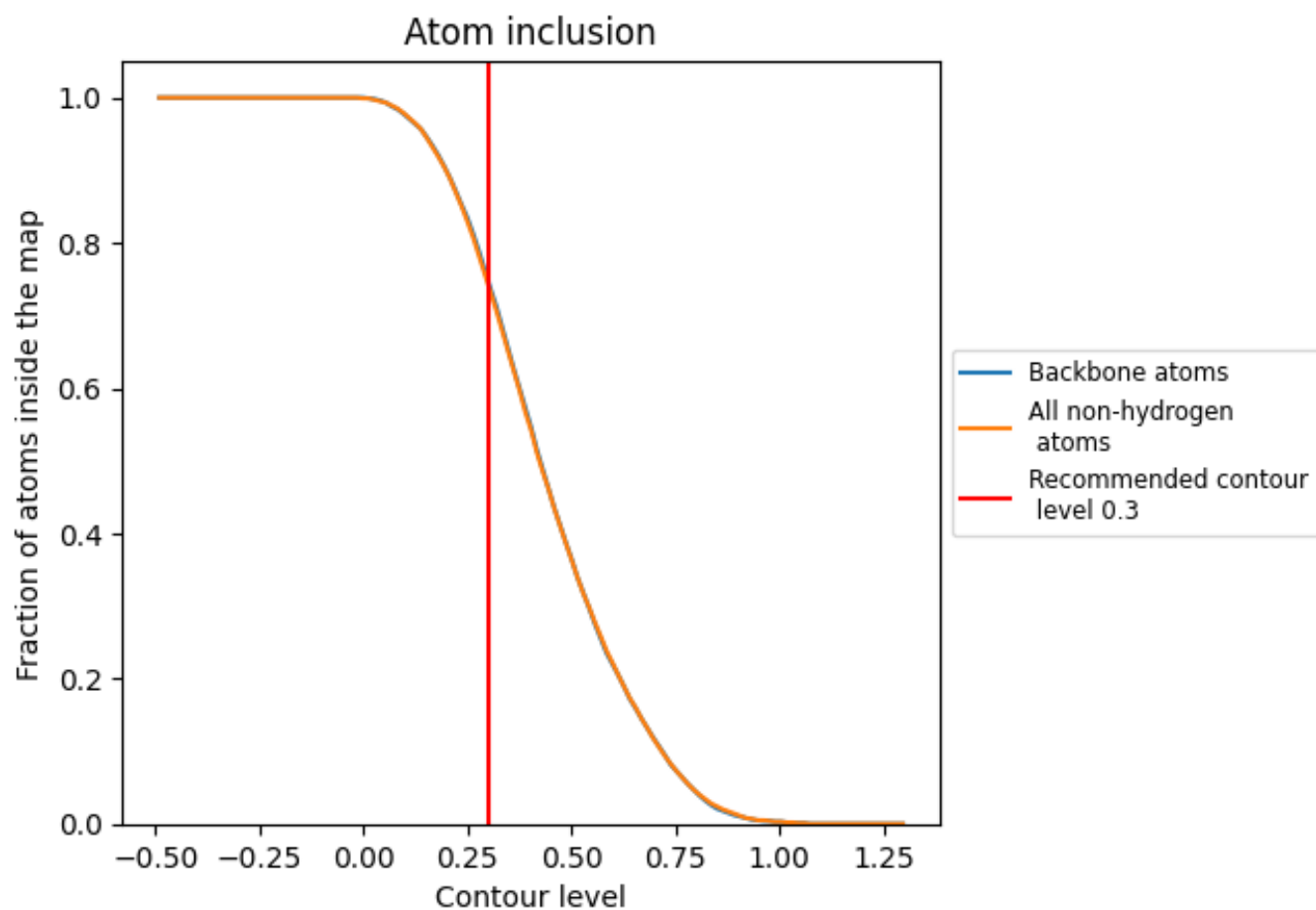
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.3).





























































9.4 Atom inclusion [i](#)



At the recommended contour level, 75% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7420	 0.5920
A	 0.8450	 0.6300
B	 0.6410	 0.5660
C	 0.5960	 0.5590
D	 0.6800	 0.5320
E	 0.6950	 0.5280
F	 0.6940	 0.5140
G	 0.6990	 0.4960
H	 0.7070	 0.5270
I	 0.7430	 0.5320
J	 0.8160	 0.5820
K	 0.8910	 0.6200
L	 0.8290	 0.5970
M	 0.8690	 0.6400
N	 0.8530	 0.6240
O	 0.9120	 0.6550
P	 0.7250	 0.5800
c	 0.7250	 0.6170
d	 0.6490	 0.5900
e	 0.5870	 0.5730
f	 0.3910	 0.5440
g	 0.5750	 0.5820
h	 0.5020	 0.5720
i	 0.6170	 0.5830
j	 0.8840	 0.6390
k	 0.9010	 0.6540
l	 0.8290	 0.6150
m	 0.8920	 0.6320
o	 0.8760	 0.6460
p	 0.7660	 0.5830

