



## wwPDB EM Validation Summary Report ⓘ

Oct 6, 2024 – 07:22 PM EDT

PDB ID : 7SCC  
EMDB ID : EMD-25033  
Title : T-cylinder of Synechocystis PCC 6803 Phycobilisome, complex with OCP - local refinement  
Authors : Sauer, P.V.; Sutter, M.; Dominguez-Martin, M.A.; Kirst, H.; Kerfeld, C.A.  
Deposited on : 2021-09-27  
Resolution : 2.60 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev113  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

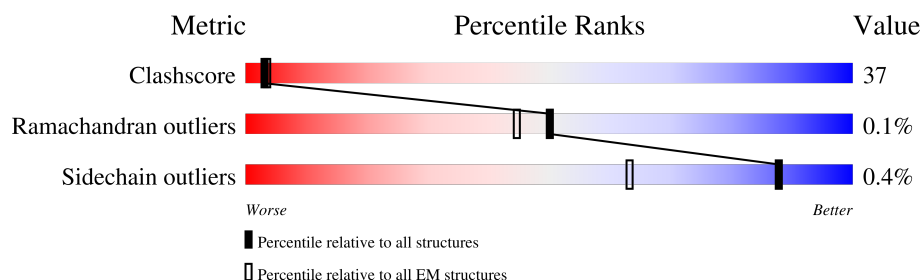
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

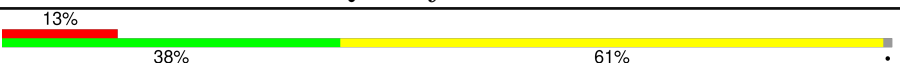
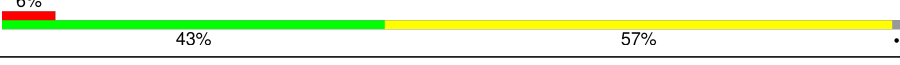

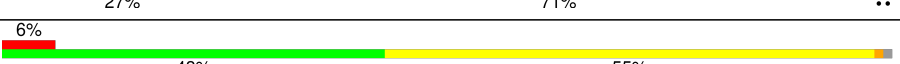

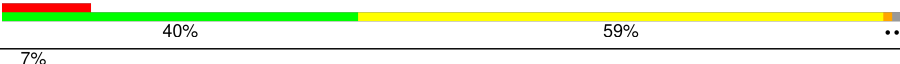


The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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	AA	161	
1	AC	161	
1	AE	161	
1	AH	161	
1	AJ	161	
1	AL	161	
1	AW	161	
1	AY	161	

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Mol	Chain	Length	Quality of chain
1	BA	161	
1	BD	161	
1	BF	161	
1	BH	161	
2	AB	161	
2	AD	161	
2	AF	161	
2	AI	161	
2	AK	161	
2	AM	161	
2	AX	161	
2	AZ	161	
2	BB	161	
2	BE	161	
2	BG	161	
2	BI	161	
3	AO	67	
3	BK	67	
4	AQ	896	
4	BM	896	
5	AS	317	
5	AT	317	
5	BO	317	
5	BP	317	
6	AU	249	

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Mol	Chain	Length	Quality of chain
6	AV	249	<div><div><div></div><div></div><div></div></div><div>6%14%8%</div><div>78%</div></div>
6	BQ	249	<div><div><div></div><div></div><div></div></div><div>12%12%10%</div><div>78%</div></div>
6	BR	249	<div><div><div></div><div></div><div></div></div><div>7%10%12%</div><div>78%</div></div>

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 43008 atoms, of which 104 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 Allophycocyanin alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	160	Total	C	N	O	S	0	0
			1210	754	207	242	7		
1	AC	160	Total	C	N	O	S	0	0
			1210	754	207	242	7		
1	AE	160	Total	C	N	O	S	0	0
			1210	754	207	242	7		
1	AH	160	Total	C	N	O	S	0	0
			1210	754	207	242	7		
1	AJ	160	Total	C	N	O	S	0	0
			1210	754	207	242	7		
1	AL	160	Total	C	N	O	S	0	0
			1210	754	207	242	7		
1	AW	160	Total	C	N	O	S	0	0
			1210	754	207	242	7		
1	AY	160	Total	C	N	O	S	0	0
			1210	754	207	242	7		
1	BA	160	Total	C	N	O	S	0	0
			1210	754	207	242	7		
1	BD	160	Total	C	N	O	S	0	0
			1210	754	207	242	7		
1	BF	160	Total	C	N	O	S	0	0
			1210	754	207	242	7		
1	BH	160	Total	C	N	O	S	0	0
			1210	754	207	242	7		

- Molecule 2 is a protein called Allophycocyanin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AB	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		
2	AD	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		
2	AF	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	AI	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		
2	AK	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		
2	AM	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		
2	AX	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		
2	AZ	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		
2	BB	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		
2	BE	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		
2	BG	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		
2	BI	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AO	67	Total	C	N	O	S	0	0
			546	343	104	94	5		
3	BK	67	Total	C	N	O	S	0	0
			546	343	104	94	5		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AO	36	TRP	SER	conflict	UNP Q01950
BK	36	TRP	SER	conflict	UNP Q01950

- Molecule 4 is a protein called Phycobiliprotein ApcE.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AQ	209	Total	C	N	O	S	0	0
			1687	1081	288	314	4		
4	BM	209	Total	C	N	O	S	0	0
			1687	1081	288	314	4		

- | Mol | Chain | Residues | Atoms         |           |          |          |         | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|-------|
| 5   | AS    | 296      | Total<br>2280 | C<br>1459 | N<br>387 | O<br>423 | S<br>11 | 0       | 0     |
| 5   | AT    | 131      | Total<br>1033 | C<br>665  | N<br>173 | O<br>192 | S<br>3  | 0       | 0     |
| 5   | BO    | 131      | Total<br>1033 | C<br>665  | N<br>173 | O<br>192 | S<br>3  | 0       | 0     |
| 5   | BP    | 296      | Total<br>2280 | C<br>1459 | N<br>387 | O<br>423 | S<br>11 | 0       | 0     |

- | Mol | Chain | Residues | Atoms        |          |         |         |        | AltConf | Trace |
|-----|-------|----------|--------------|----------|---------|---------|--------|---------|-------|
| 6   | AU    | 54       | Total<br>426 | C<br>266 | N<br>83 | O<br>75 | S<br>2 | 0       | 0     |
| 6   | AV    | 54       | Total<br>426 | C<br>266 | N<br>83 | O<br>75 | S<br>2 | 0       | 0     |
| 6   | BQ    | 54       | Total<br>426 | C<br>266 | N<br>83 | O<br>75 | S<br>2 | 0       | 0     |
| 6   | BR    | 54       | Total<br>426 | C<br>266 | N<br>83 | O<br>75 | S<br>2 | 0       | 0     |

- # CYC

Mol	Chain	Residues	Atoms				AltConf
7	AA	1	Total	C	N	O	0
			43	33	4	6	
7	AB	1	Total	C	N	O	0
			43	33	4	6	
7	AC	1	Total	C	N	O	0
			43	33	4	6	
7	AD	1	Total	C	N	O	0
			43	33	4	6	
7	AE	1	Total	C	N	O	0
			43	33	4	6	
7	AF	1	Total	C	N	O	0
			43	33	4	6	
7	AH	1	Total	C	N	O	0
			43	33	4	6	
7	AI	1	Total	C	N	O	0
			43	33	4	6	
7	AJ	1	Total	C	N	O	0
			43	33	4	6	
7	AK	1	Total	C	N	O	0
			43	33	4	6	
7	AL	1	Total	C	N	O	0
			43	33	4	6	
7	AM	1	Total	C	N	O	0
			43	33	4	6	
7	AW	1	Total	C	N	O	0
			43	33	4	6	
7	AX	1	Total	C	N	O	0
			43	33	4	6	
7	AY	1	Total	C	N	O	0
			43	33	4	6	
7	AZ	1	Total	C	N	O	0
			43	33	4	6	
7	BA	1	Total	C	N	O	0
			43	33	4	6	
7	BB	1	Total	C	N	O	0
			43	33	4	6	
7	BD	1	Total	C	N	O	0
			43	33	4	6	
7	BE	1	Total	C	N	O	0
			43	33	4	6	
7	BF	1	Total	C	N	O	0
			43	33	4	6	
7	BG	1	Total	C	N	O	0
			43	33	4	6	

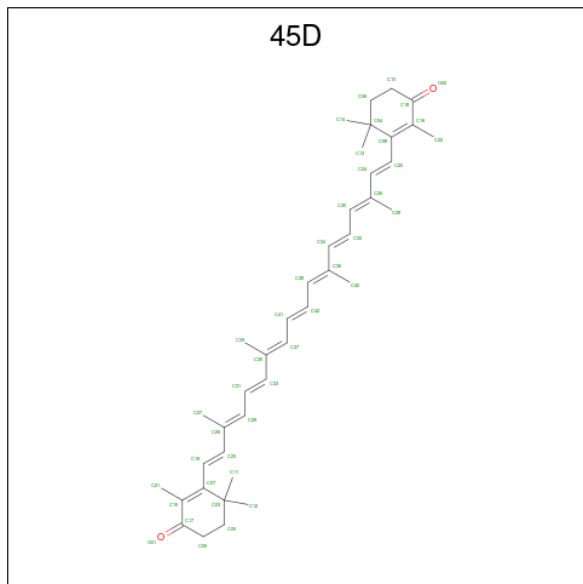
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Mol	Chain	Residues	Atoms				AltConf
7	BH	1	Total	C	N	O	0
			43	33	4	6	
7	BI	1	Total	C	N	O	0
			43	33	4	6	

- Molecule 8 is beta,beta-carotene-4,4'-dione (three-letter code: 45D) (formula:  $C_{40}H_{52}O_2$ ) (labeled as "Ligand of Interest" by depositor).

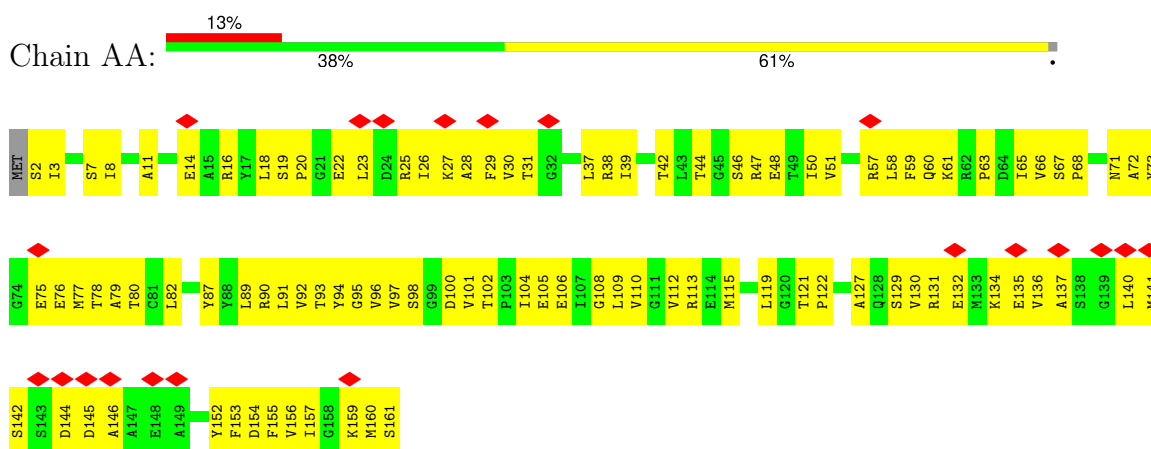


Mol	Chain	Residues	Atoms				AltConf
8	AS	1	Total	C	H	O	0
			94	40	52	2	
8	BP	1	Total	C	H	O	0
			94	40	52	2	

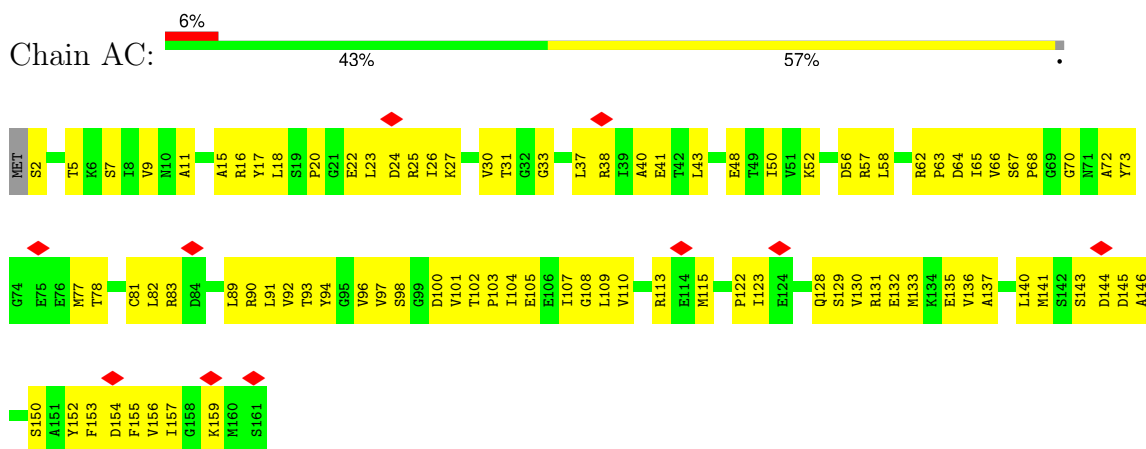
### 3 Residue-property plots

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

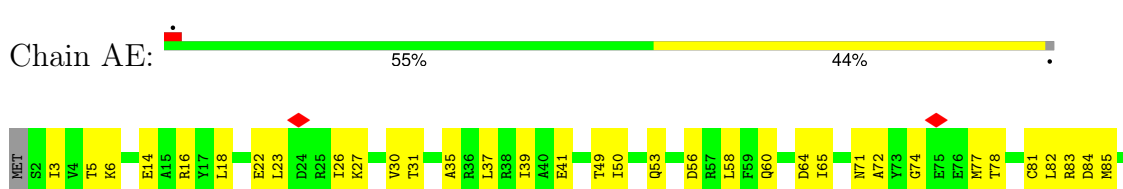
#### • Molecule 1: Allophycocyanin alpha chain



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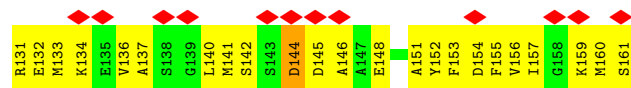
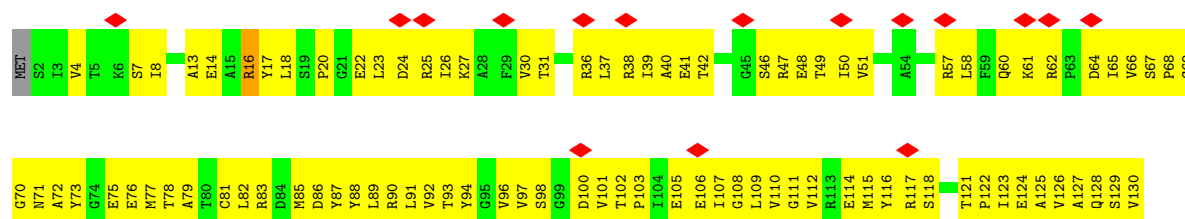


#### • Molecule 1: Allophycocyanin alpha chain

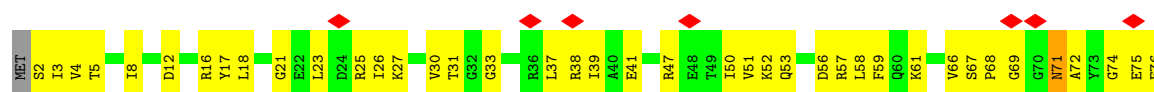
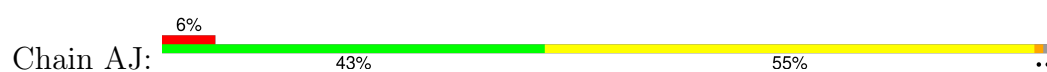




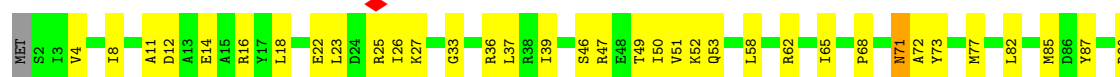
• Molecule 1: Allophycocyanin alpha chain



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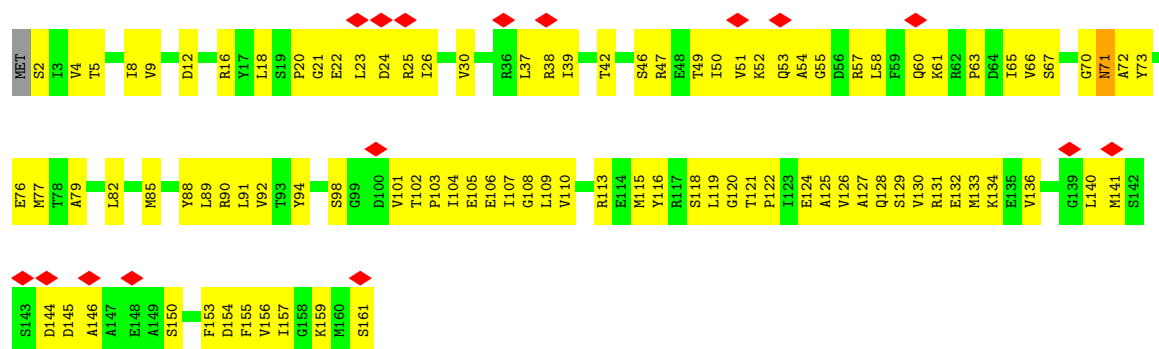


• Molecule 1: Allophycocyanin alpha chain

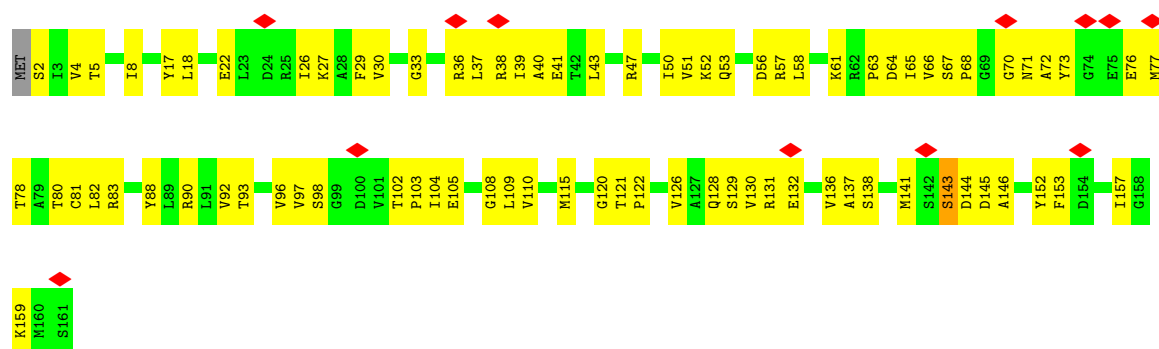


• Molecule 1: Allophycocyanin alpha chain

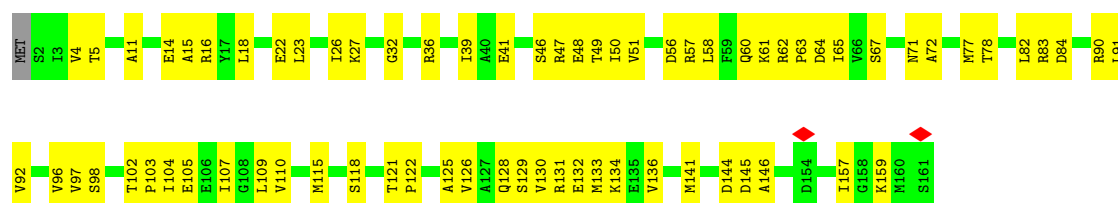




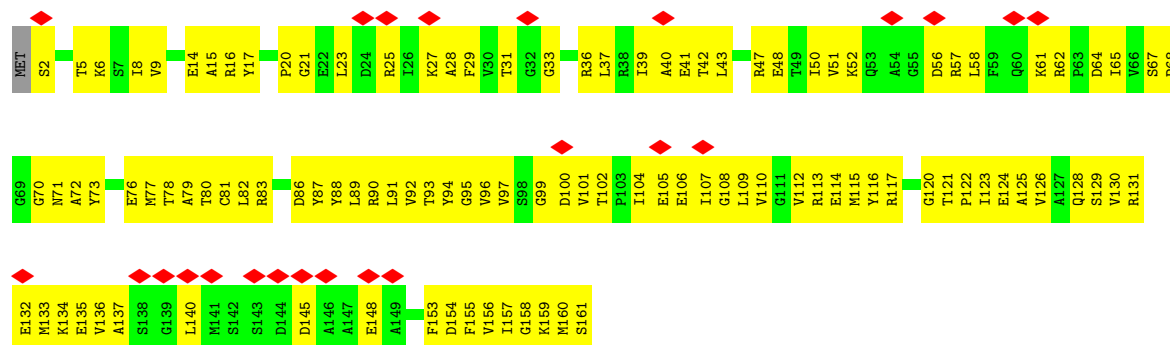
• Molecule 1: Allophycocyanin alpha chain



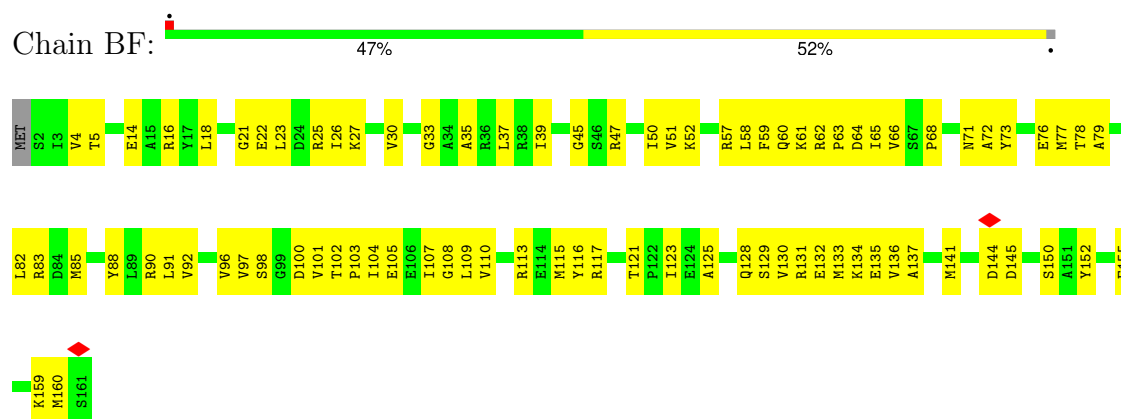
• Molecule 1: Allophycocyanin alpha chain



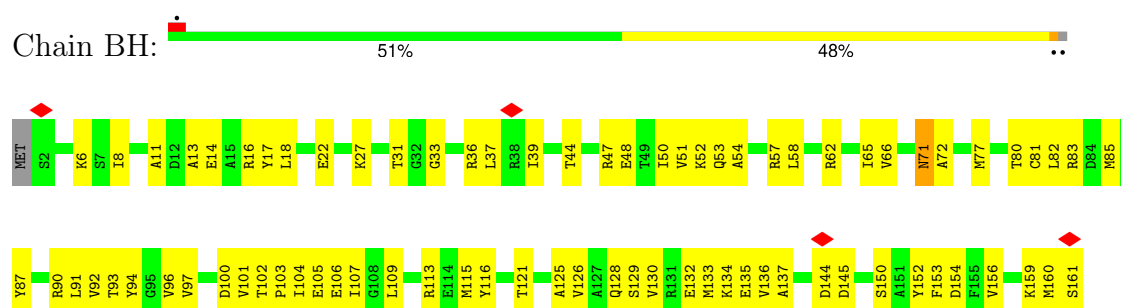
• Molecule 1: Allophycocyanin alpha chain



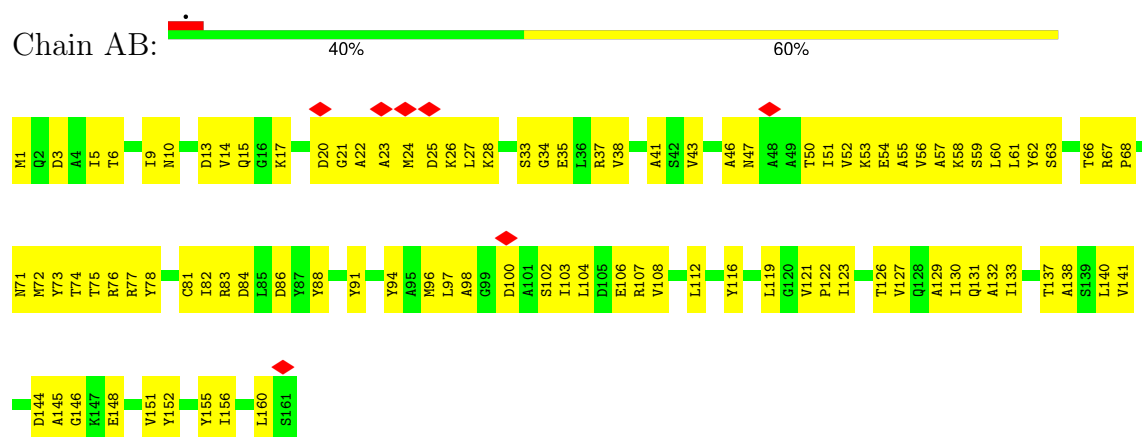
- Molecule 1: Allophycocyanin alpha chain



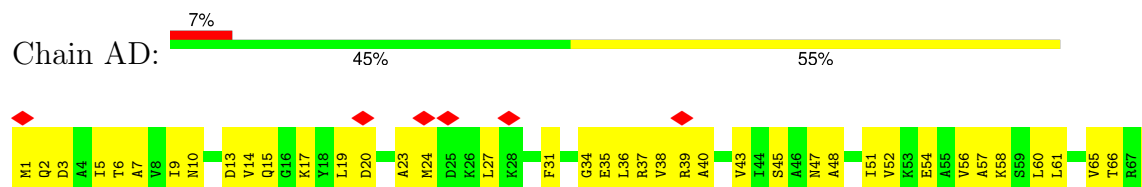
- Molecule 1: Allophycocyanin alpha chain



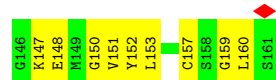
- Molecule 2: Allophycocyanin beta chain



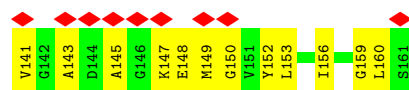
- Molecule 2: Allophycocyanin beta chain



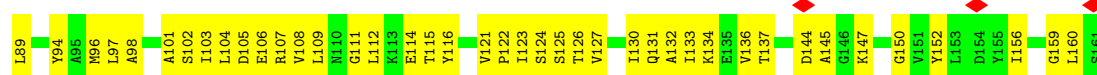
- Molecule 2: Allophycocyanin beta chain



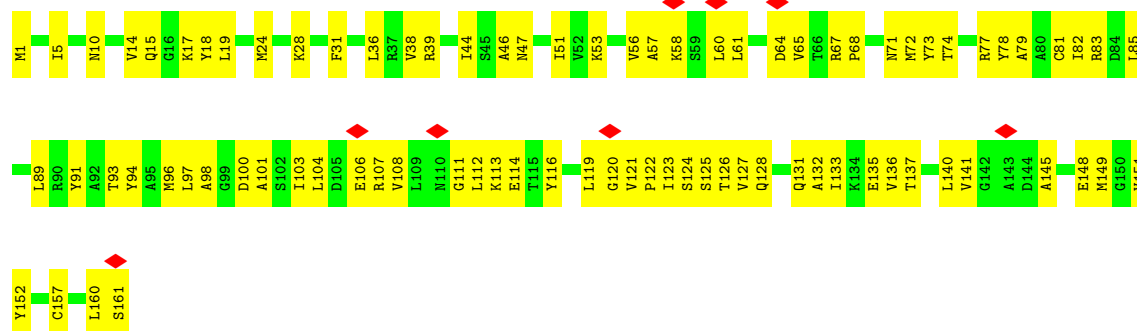
- Molecule 2: Allophycocyanin beta chain



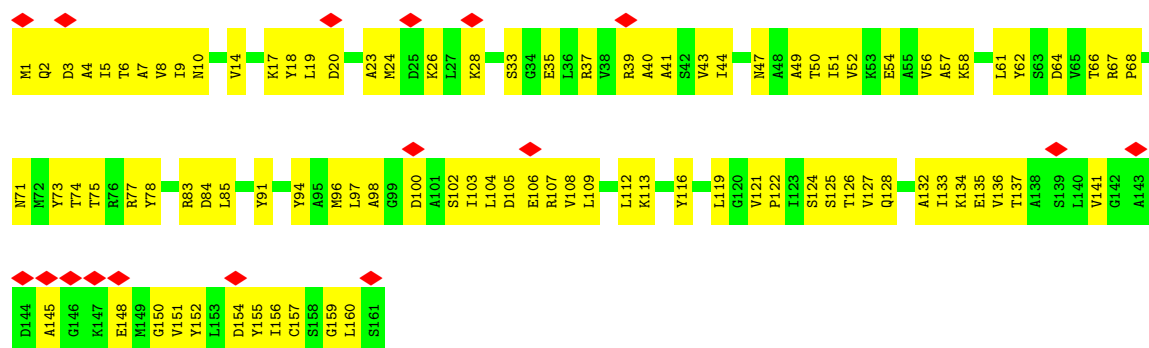
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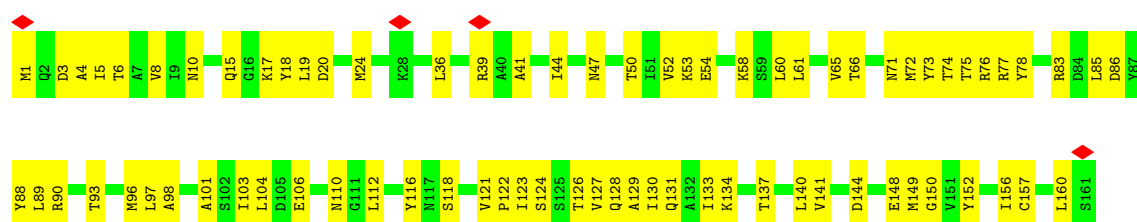
- Molecule 2: Allophycocyanin beta chain



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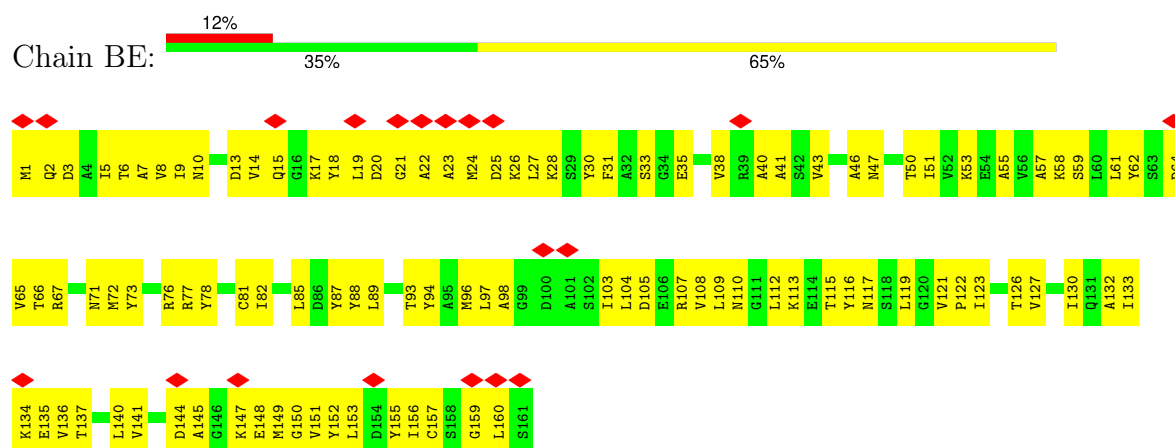
• Molecule 2: Allophycocyanin beta chain



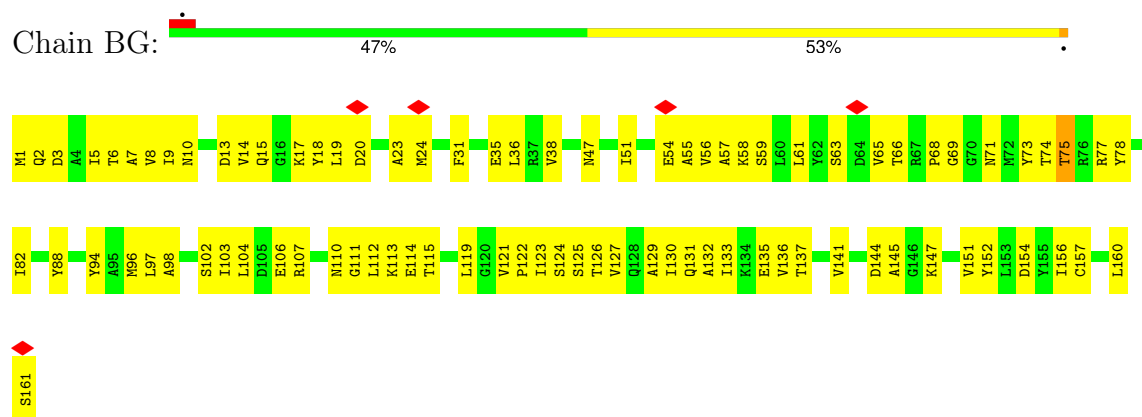
• Molecule 2: Allophycocyanin beta chain



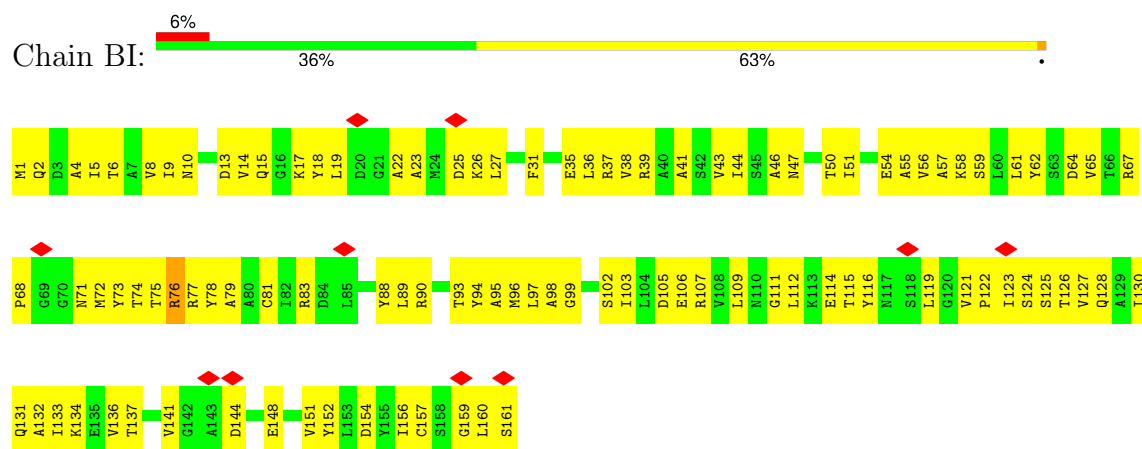
- Molecule 2: Allophycocyanin beta chain



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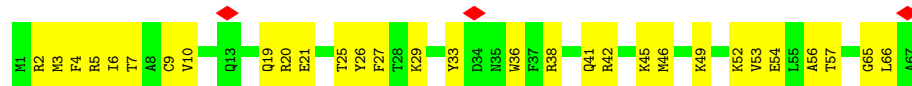
- Molecule 3: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core



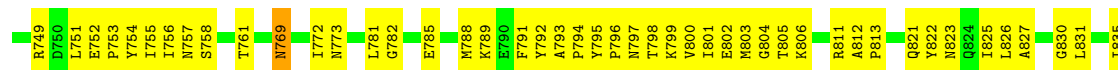
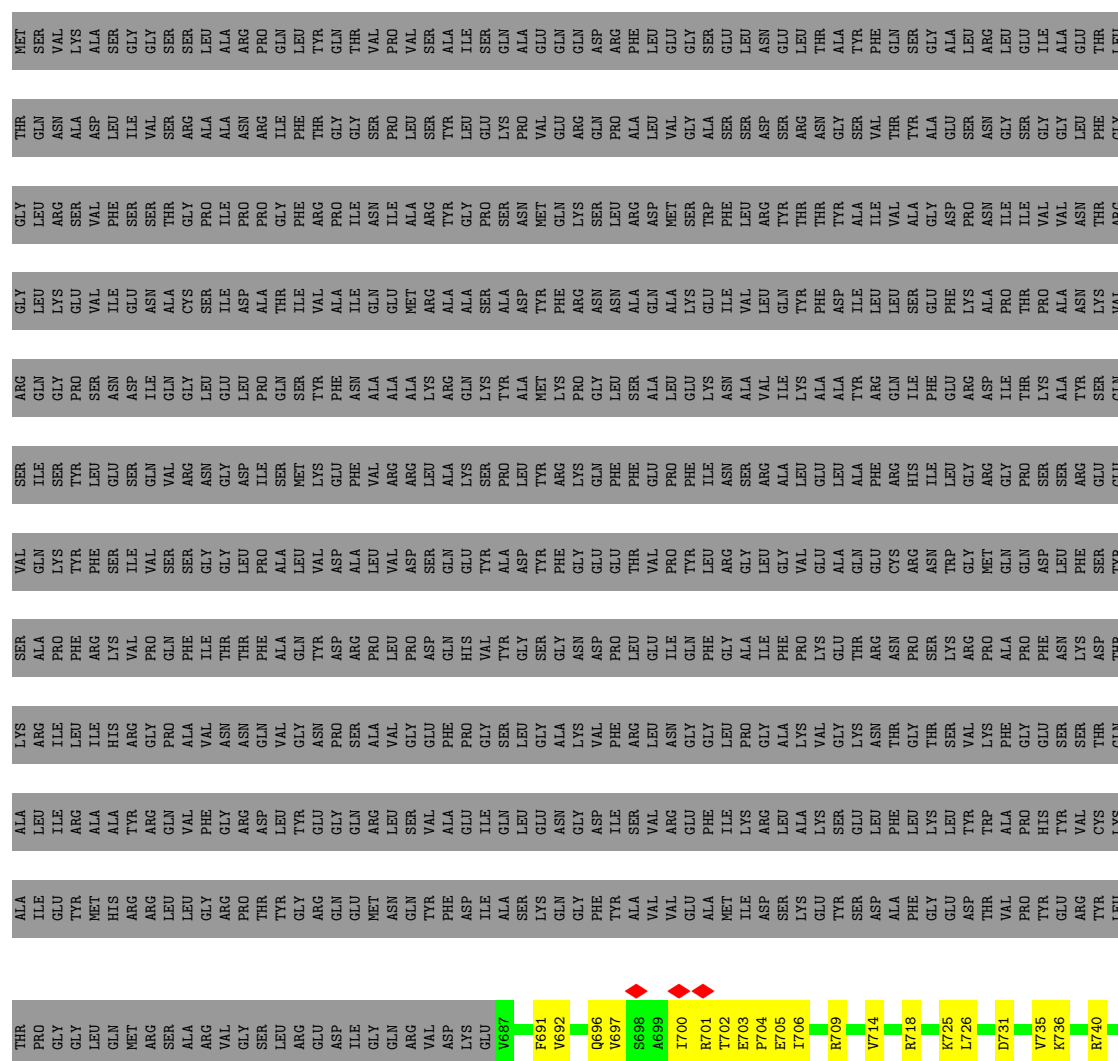


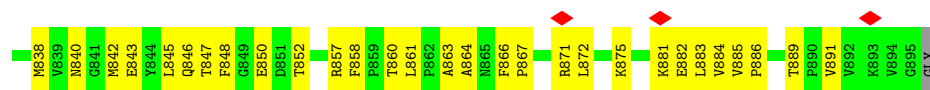


- Molecule 3: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core

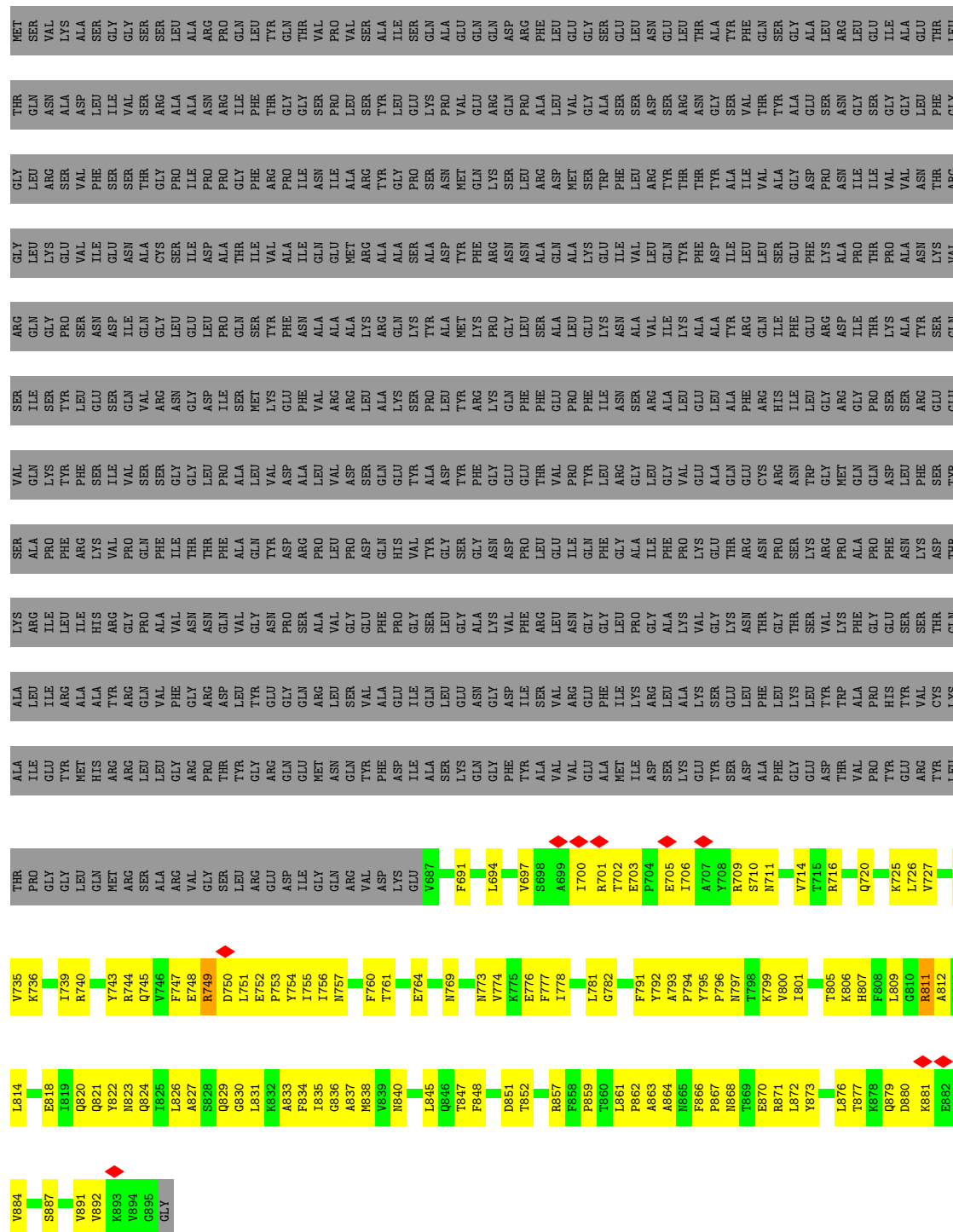


- Molecule 4: Phycobiliprotein ApcE



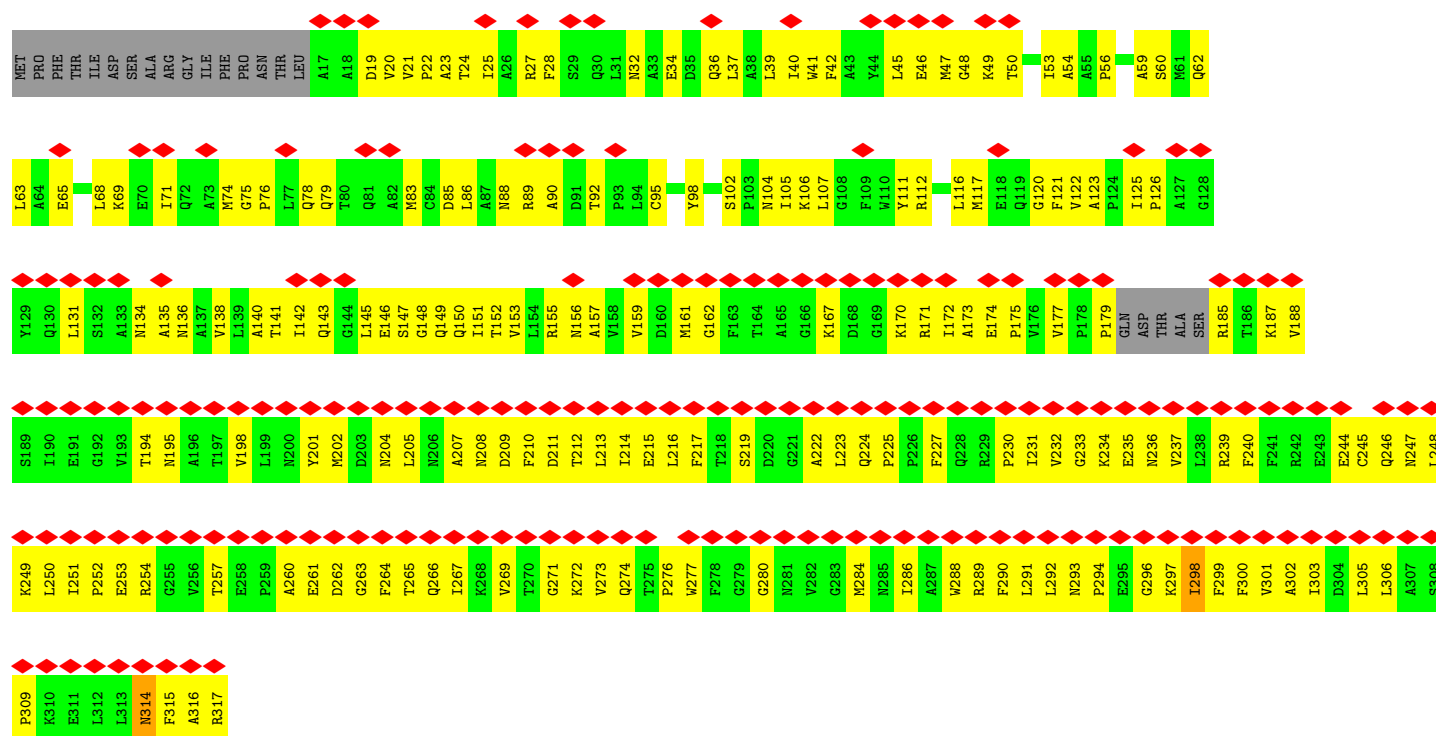


### • Molecule 4: Phycobiliprotein ApcE



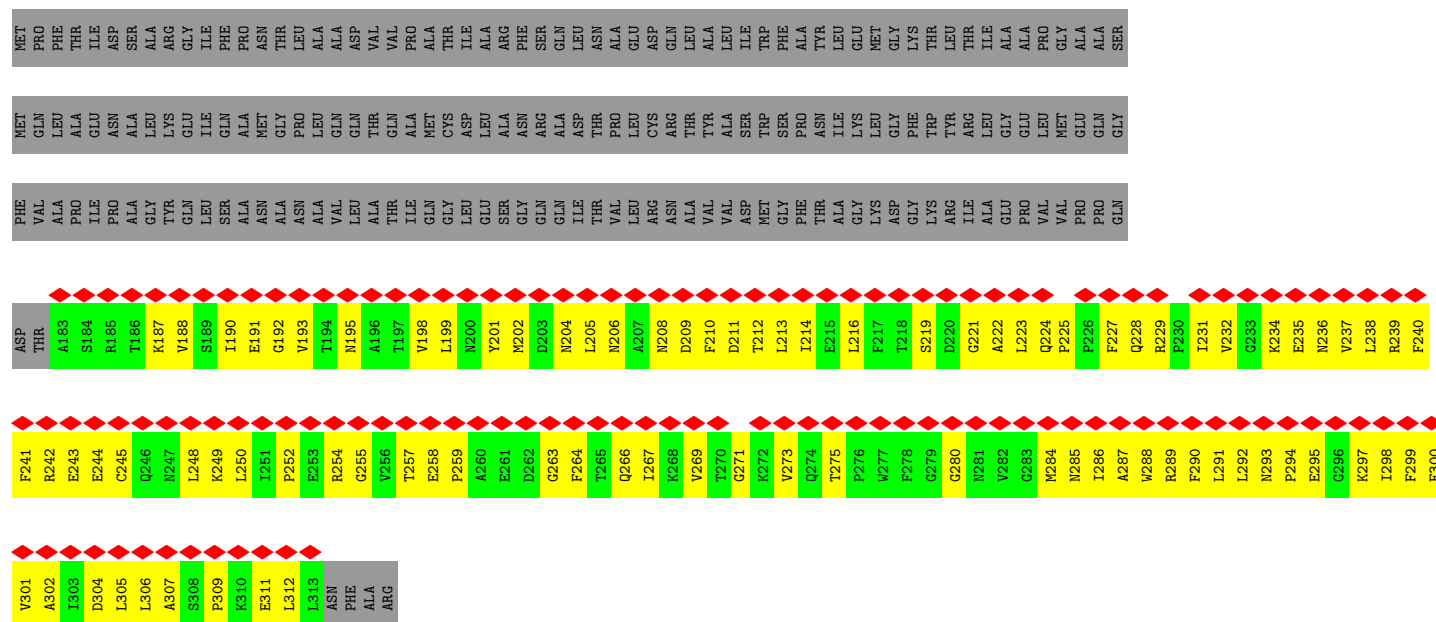
### • Molecule 5: Orange carotenoid-binding protein

Chain AS: 



• Molecule 5: Orange carotenoid-binding protein

Chain AT: 

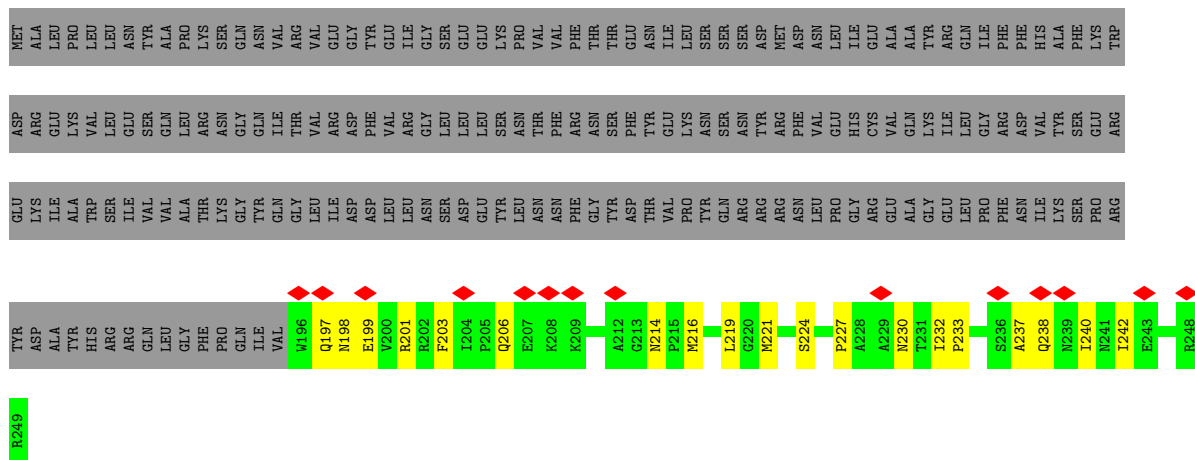


• Molecule 5: Orange carotenoid-binding protein

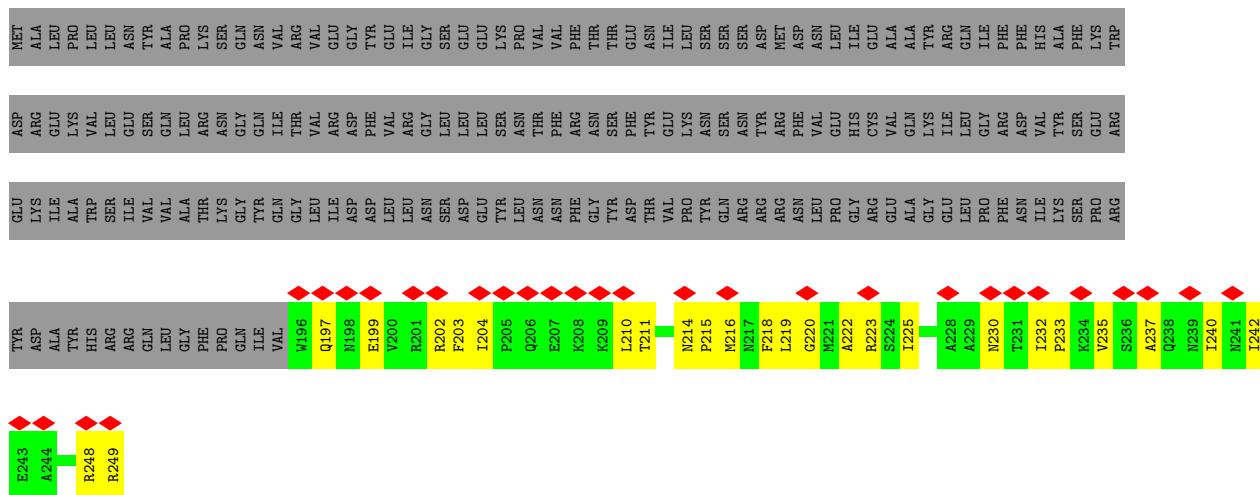
Chain BO: 



- Molecule 6: Phycobilisome rod-core linker polypeptide CpcG



- Molecule 6: Phycobilisome rod-core linker polypeptide CpcG



- Molecule 6: Phycobilisome rod-core linker polypeptide CpcG





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	176804	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 ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.674	Depositor
Minimum map value	-0.669	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.066	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	377.99997, 377.99997, 377.99997	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CYC, 45D

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	AA	0.27	0/1225	0.50	0/1652
1	AC	0.26	0/1225	0.53	0/1652
1	AE	0.26	0/1225	0.52	1/1652 (0.1%)
1	AH	0.27	0/1225	0.58	1/1652 (0.1%)
1	AJ	0.27	0/1225	0.55	1/1652 (0.1%)
1	AL	0.26	0/1225	0.49	0/1652
1	AW	0.27	0/1225	0.52	0/1652
1	AY	0.26	0/1225	0.52	0/1652
1	BA	0.25	0/1225	0.47	0/1652
1	BD	0.27	0/1225	0.54	0/1652
1	BF	0.26	0/1225	0.47	0/1652
1	BH	0.26	0/1225	0.50	0/1652
2	AB	0.28	0/1220	0.49	0/1650
2	AD	0.27	0/1220	0.45	0/1650
2	AF	0.27	0/1220	0.47	0/1650
2	AI	0.26	0/1220	0.53	0/1650
2	AK	0.27	0/1220	0.46	0/1650
2	AM	0.27	0/1220	0.46	0/1650
2	AX	0.26	0/1220	0.48	0/1650
2	AZ	0.29	0/1220	0.47	0/1650
2	BB	0.26	0/1220	0.46	0/1650
2	BE	0.27	0/1220	0.50	0/1650
2	BG	0.26	0/1220	0.47	0/1650
2	BI	0.27	0/1220	0.49	0/1650
3	AO	0.27	0/555	0.58	0/743
3	BK	0.25	0/555	0.57	0/743
4	AQ	0.26	0/1722	0.50	1/2330 (0.0%)
4	BM	0.26	0/1722	0.49	0/2330
5	AS	0.25	0/2327	0.47	0/3164
5	AT	0.26	0/1055	0.52	0/1432
5	BO	0.26	0/1055	0.51	0/1432
5	BP	0.25	0/2327	0.47	0/3164



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
6	AU	0.26	0/434	0.57	0/587
6	AV	0.27	0/434	0.51	0/587
6	BQ	0.26	0/434	0.57	0/587
6	BR	0.28	0/434	0.57	0/587
All	All	0.26	0/42394	0.50	4/57310 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AE	154	ASP	CB-CG-OD1	6.41	124.06	118.30
1	AH	144	ASP	CB-CG-OD1	5.78	123.51	118.30
1	AJ	56	ASP	CB-CG-OD1	5.61	123.35	118.30
4	AQ	731	ASP	CB-CG-OD1	5.50	123.25	118.30

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	AA	1210	0	1210	131	0
1	AC	1210	0	1210	105	0
1	AE	1210	0	1210	73	0
1	AH	1210	0	1210	148	0
1	AJ	1210	0	1210	126	0
1	AL	1210	0	1210	63	0
1	AW	1210	0	1210	129	0
1	AY	1210	0	1210	104	0
1	BA	1210	0	1210	68	0
1	BD	1210	0	1210	169	0
1	BF	1210	0	1210	103	0
1	BH	1210	0	1210	83	0
2	AB	1206	0	1218	123	0
2	AD	1206	0	1218	91	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	AF	1206	0	1218	102	0
2	AI	1206	0	1218	148	0
2	AK	1206	0	1218	108	0
2	AM	1206	0	1218	100	0
2	AX	1206	0	1218	122	0
2	AZ	1206	0	1218	85	0
2	BB	1206	0	1218	78	0
2	BE	1206	0	1218	143	0
2	BG	1206	0	1218	91	0
2	BI	1206	0	1218	126	0
3	AO	546	0	568	50	0
3	BK	546	0	568	41	0
4	AQ	1687	0	1702	100	0
4	BM	1687	0	1702	114	0
5	AS	2280	0	2286	218	0
5	AT	1033	0	1035	96	0
5	BO	1033	0	1035	107	0
5	BP	2280	0	2286	183	0
6	AU	426	0	437	47	0
6	AV	426	0	437	33	0
6	BQ	426	0	437	39	0
6	BR	426	0	437	52	0
7	AA	43	0	37	13	0
7	AB	43	0	37	9	0
7	AC	43	0	37	12	0
7	AD	43	0	37	9	0
7	AE	43	0	37	13	0
7	AF	43	0	37	9	0
7	AH	43	0	37	15	0
7	AI	43	0	37	10	0
7	AJ	43	0	37	13	0
7	AK	43	0	37	12	0
7	AL	43	0	37	13	0
7	AM	43	0	37	19	0
7	AW	43	0	37	16	0
7	AX	43	0	37	11	0
7	AY	43	0	37	18	0
7	AZ	43	0	37	8	0
7	BA	43	0	37	13	0
7	BB	43	0	37	11	0
7	BD	43	0	37	10	0
7	BE	43	0	37	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	BF	43	0	37	11	0
7	BG	43	0	37	9	0
7	BH	43	0	37	13	0
7	BI	43	0	37	7	0
8	AS	42	52	52	17	0
8	BP	42	52	52	8	0
All	All	42904	104	43058	3206	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 37.

The worst 5 of 3206 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:AK:147:LYS:HE2	4:BM:700:ILE:HG21	1.28	1.08
5:BO:214:ILE:HD13	5:BO:238:LEU:HD22	1.34	1.04
5:AS:224:GLN:HB3	5:AS:302:ALA:HA	1.40	1.04
5:BP:224:GLN:HB3	5:BP:302:ALA:HA	1.37	1.03
2:AI:8:VAL:HG21	2:AI:27:LEU:HD21	1.39	1.01

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	AA	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
1	AC	158/161 (98%)	152 (96%)	6 (4%)	0	100	100
1	AE	158/161 (98%)	158 (100%)	0	0	100	100
1	AH	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
1	AJ	158/161 (98%)	153 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AL	158/161 (98%)	158 (100%)	0	0	100	100
1	AW	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
1	AY	158/161 (98%)	153 (97%)	4 (2%)	1 (1%)	22	43
1	BA	158/161 (98%)	158 (100%)	0	0	100	100
1	BD	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
1	BF	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
1	BH	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
2	AB	159/161 (99%)	157 (99%)	2 (1%)	0	100	100
2	AD	159/161 (99%)	155 (98%)	4 (2%)	0	100	100
2	AF	159/161 (99%)	156 (98%)	3 (2%)	0	100	100
2	AI	159/161 (99%)	151 (95%)	8 (5%)	0	100	100
2	AK	159/161 (99%)	151 (95%)	7 (4%)	1 (1%)	22	43
2	AM	159/161 (99%)	155 (98%)	4 (2%)	0	100	100
2	AX	159/161 (99%)	157 (99%)	2 (1%)	0	100	100
2	AZ	159/161 (99%)	154 (97%)	5 (3%)	0	100	100
2	BB	159/161 (99%)	156 (98%)	3 (2%)	0	100	100
2	BE	159/161 (99%)	149 (94%)	10 (6%)	0	100	100
2	BG	159/161 (99%)	149 (94%)	9 (6%)	1 (1%)	22	43
2	BI	159/161 (99%)	157 (99%)	2 (1%)	0	100	100
3	AO	65/67 (97%)	62 (95%)	3 (5%)	0	100	100
3	BK	65/67 (97%)	64 (98%)	1 (2%)	0	100	100
4	AQ	207/896 (23%)	200 (97%)	7 (3%)	0	100	100
4	BM	207/896 (23%)	200 (97%)	7 (3%)	0	100	100
5	AS	292/317 (92%)	281 (96%)	10 (3%)	1 (0%)	37	59
5	AT	129/317 (41%)	122 (95%)	7 (5%)	0	100	100
5	BO	129/317 (41%)	124 (96%)	5 (4%)	0	100	100
5	BP	292/317 (92%)	280 (96%)	11 (4%)	1 (0%)	37	59
6	AU	52/249 (21%)	44 (85%)	8 (15%)	0	100	100
6	AV	52/249 (21%)	46 (88%)	6 (12%)	0	100	100
6	BQ	52/249 (21%)	45 (86%)	7 (14%)	0	100	100
6	BR	52/249 (21%)	50 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	5398/8054 (67%)	5233 (97%)	160 (3%)	5 (0%)	50	71

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AK	75	THR
5	AS	298	ILE
2	BG	75	THR
5	BP	298	ILE
1	AY	143	SER

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AA	128/129 (99%)	128 (100%)	0	100	100
1	AC	128/129 (99%)	128 (100%)	0	100	100
1	AE	128/129 (99%)	128 (100%)	0	100	100
1	AH	128/129 (99%)	127 (99%)	1 (1%)	79	91
1	AJ	128/129 (99%)	127 (99%)	1 (1%)	79	91
1	AL	128/129 (99%)	127 (99%)	1 (1%)	79	91
1	AW	128/129 (99%)	127 (99%)	1 (1%)	79	91
1	AY	128/129 (99%)	128 (100%)	0	100	100
1	BA	128/129 (99%)	127 (99%)	1 (1%)	79	91
1	BD	128/129 (99%)	128 (100%)	0	100	100
1	BF	128/129 (99%)	128 (100%)	0	100	100
1	BH	128/129 (99%)	127 (99%)	1 (1%)	79	91
2	AB	125/125 (100%)	125 (100%)	0	100	100
2	AD	125/125 (100%)	125 (100%)	0	100	100
2	AF	125/125 (100%)	125 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AI	125/125 (100%)	125 (100%)	0	100	100
2	AK	125/125 (100%)	125 (100%)	0	100	100
2	AM	125/125 (100%)	125 (100%)	0	100	100
2	AX	125/125 (100%)	125 (100%)	0	100	100
2	AZ	125/125 (100%)	125 (100%)	0	100	100
2	BB	125/125 (100%)	125 (100%)	0	100	100
2	BE	125/125 (100%)	125 (100%)	0	100	100
2	BG	125/125 (100%)	125 (100%)	0	100	100
2	BI	125/125 (100%)	124 (99%)	1 (1%)	79	91
3	AO	58/58 (100%)	58 (100%)	0	100	100
3	BK	58/58 (100%)	58 (100%)	0	100	100
4	AQ	184/753 (24%)	181 (98%)	3 (2%)	58	79
4	BM	184/753 (24%)	182 (99%)	2 (1%)	70	86
5	AS	239/257 (93%)	237 (99%)	2 (1%)	79	91
5	AT	113/257 (44%)	113 (100%)	0	100	100
5	BO	113/257 (44%)	112 (99%)	1 (1%)	75	90
5	BP	239/257 (93%)	237 (99%)	2 (1%)	79	91
6	AU	46/221 (21%)	45 (98%)	1 (2%)	47	72
6	AV	46/221 (21%)	46 (100%)	0	100	100
6	BQ	46/221 (21%)	46 (100%)	0	100	100
6	BR	46/221 (21%)	45 (98%)	1 (2%)	47	72
All	All	4408/6582 (67%)	4389 (100%)	19 (0%)	88	96

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	BM	811	ARG
5	BP	314	ASN
6	BR	234	LYS
5	BP	171	ARG
6	AU	209	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
2	AX	71	ASN
6	BR	230	ASN
2	BB	10	ASN
2	BI	128	GLN
2	AZ	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 oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

26 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	$\# Z  > 2$
7	CYC	AY	200	1	42,46,46	0.55	1 (2%)	52,67,67	0.90	3 (5%)
7	CYC	BG	200	2	42,46,46	0.58	1 (2%)	52,67,67	0.95	4 (7%)
7	CYC	AE	200	1	42,46,46	0.51	1 (2%)	52,67,67	0.70	3 (5%)
7	CYC	AJ	200	1	42,46,46	0.55	1 (2%)	52,67,67	0.76	4 (7%)
7	CYC	AH	200	1	42,46,46	0.48	1 (2%)	52,67,67	0.93	3 (5%)
7	CYC	AA	200	1	42,46,46	0.52	1 (2%)	52,67,67	0.88	4 (7%)
7	CYC	BI	200	2	42,46,46	0.53	1 (2%)	52,67,67	0.74	2 (3%)
7	CYC	AM	200	2	42,46,46	0.53	1 (2%)	52,67,67	0.78	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	CYC	AW	200	1	42,46,46	0.56	1 (2%)	52,67,67	0.58	2 (3%)
7	CYC	AC	200	1	42,46,46	0.45	1 (2%)	52,67,67	0.83	3 (5%)
7	CYC	BD	200	1	42,46,46	0.58	1 (2%)	52,67,67	0.96	2 (3%)
7	CYC	BB	200	2	42,46,46	0.57	1 (2%)	52,67,67	1.12	4 (7%)
7	CYC	AL	200	1	42,46,46	0.54	1 (2%)	52,67,67	0.79	3 (5%)
7	CYC	AK	200	2	42,46,46	0.56	1 (2%)	52,67,67	1.15	5 (9%)
7	CYC	BE	200	2	42,46,46	0.54	1 (2%)	52,67,67	1.37	4 (7%)
7	CYC	AX	200	2	42,46,46	0.55	1 (2%)	52,67,67	0.83	3 (5%)
7	CYC	BA	200	1	42,46,46	0.55	1 (2%)	52,67,67	0.93	3 (5%)
7	CYC	AF	200	2	42,46,46	0.58	1 (2%)	52,67,67	1.12	4 (7%)
7	CYC	BF	200	1	42,46,46	0.54	1 (2%)	52,67,67	1.00	4 (7%)
7	CYC	BH	200	1	42,46,46	0.54	1 (2%)	52,67,67	0.96	3 (5%)
7	CYC	AI	200	2	42,46,46	0.54	1 (2%)	52,67,67	1.33	4 (7%)
7	CYC	AB	200	2	42,46,46	0.54	1 (2%)	52,67,67	0.80	3 (5%)
8	45D	BP	400	-	43,43,43	1.00	1 (2%)	54,60,60	1.54	11 (20%)
7	CYC	AZ	200	2	42,46,46	0.54	1 (2%)	52,67,67	0.88	4 (7%)
8	45D	AS	400	-	43,43,43	1.00	2 (4%)	54,60,60	1.46	11 (20%)
7	CYC	AD	200	2	42,46,46	0.53	1 (2%)	52,67,67	0.91	3 (5%)

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
7	CYC	AY	200	1	-	13/25/74/74	0/4/4/4
7	CYC	BG	200	2	-	7/25/74/74	0/4/4/4
7	CYC	AE	200	1	-	6/25/74/74	0/4/4/4
7	CYC	AJ	200	1	-	11/25/74/74	0/4/4/4
7	CYC	AH	200	1	-	9/25/74/74	0/4/4/4
7	CYC	AA	200	1	-	8/25/74/74	0/4/4/4
7	CYC	BI	200	2	-	6/25/74/74	0/4/4/4
7	CYC	AM	200	2	-	7/25/74/74	0/4/4/4
7	CYC	AW	200	1	-	6/25/74/74	0/4/4/4
7	CYC	AC	200	1	-	13/25/74/74	0/4/4/4
7	CYC	BD	200	1	-	9/25/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	CYC	BB	200	2	-	5/25/74/74	0/4/4/4
7	CYC	AL	200	1	-	10/25/74/74	0/4/4/4
7	CYC	AK	200	2	-	10/25/74/74	0/4/4/4
7	CYC	BE	200	2	-	10/25/74/74	0/4/4/4
7	CYC	AX	200	2	-	5/25/74/74	0/4/4/4
7	CYC	BA	200	1	-	7/25/74/74	0/4/4/4
7	CYC	AF	200	2	-	6/25/74/74	0/4/4/4
7	CYC	BF	200	1	-	6/25/74/74	0/4/4/4
7	CYC	BH	200	1	-	7/25/74/74	0/4/4/4
7	CYC	AI	200	2	-	9/25/74/74	0/4/4/4
7	CYC	AB	200	2	-	7/25/74/74	0/4/4/4
8	45D	BP	400	-	-	15/29/69/69	0/2/2/2
7	CYC	AZ	200	2	-	7/25/74/74	0/4/4/4
8	45D	AS	400	-	-	12/29/69/69	0/2/2/2
7	CYC	AD	200	2	-	8/25/74/74	0/4/4/4

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	AS	400	45D	C34-C36	3.67	1.53	1.46
8	BP	400	45D	C34-C36	3.57	1.53	1.46
7	BG	200	CYC	CHA-C1A	3.26	1.38	1.35
7	AW	200	CYC	CHA-C1A	3.22	1.38	1.35
7	AY	200	CYC	CHA-C1A	3.20	1.38	1.35

The worst 5 of 101 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	BE	200	CYC	C1D-CHD-C4C	8.19	139.71	128.47
7	AI	200	CYC	C1D-CHD-C4C	7.66	138.99	128.47
7	AK	200	CYC	C1D-CHD-C4C	5.84	136.49	128.47
7	AF	200	CYC	C1B-CHB-C4A	5.42	141.36	128.06
7	BD	200	CYC	C1B-CHB-C4A	5.21	140.84	128.06

There are no chirality outliers.

5 of 219 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	AA	200	CYC	NA-C4A-CHB-C1B
7	AA	200	CYC	C3A-C4A-CHB-C1B
7	AB	200	CYC	NA-C4A-CHB-C1B
7	AB	200	CYC	C3A-C4A-CHB-C1B
7	AC	200	CYC	C1A-C2A-CAA-CBA

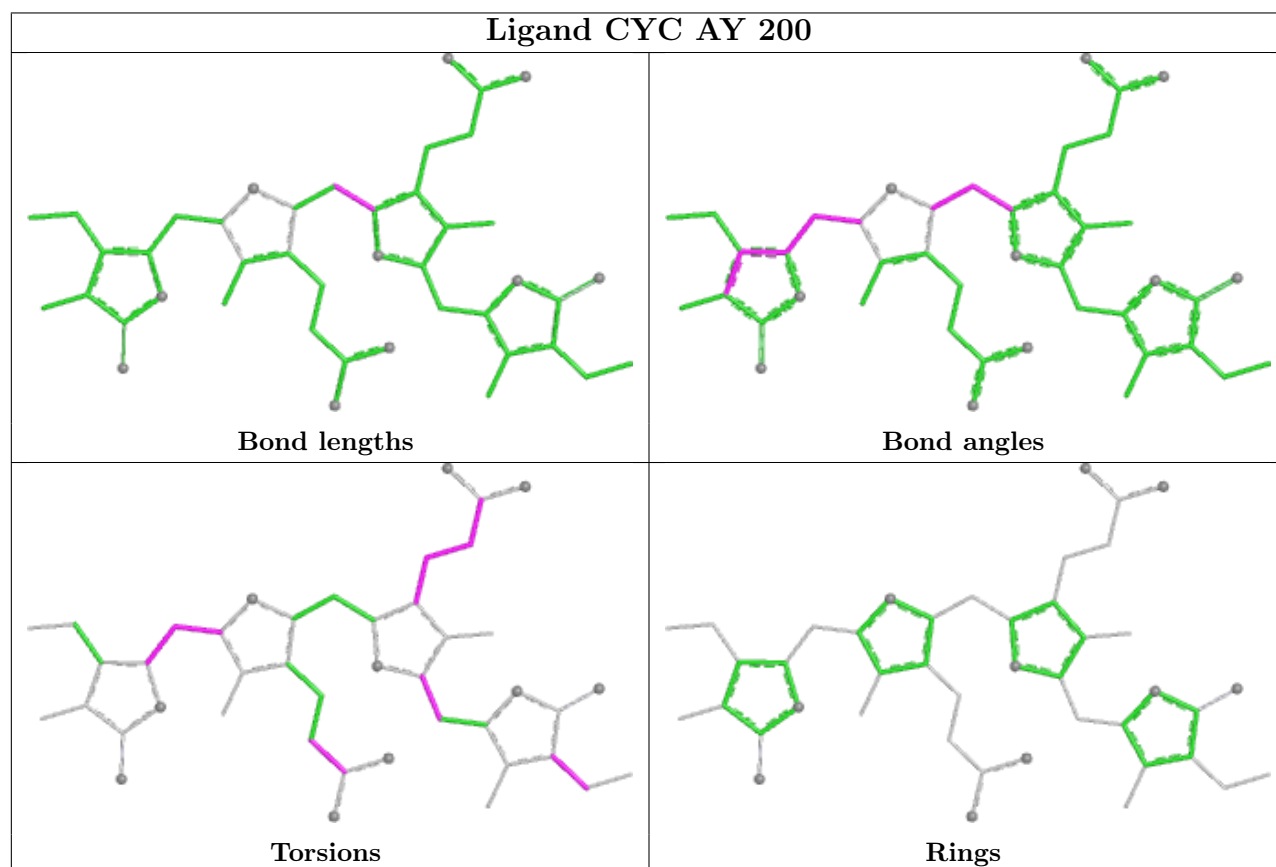
There are no ring outliers.

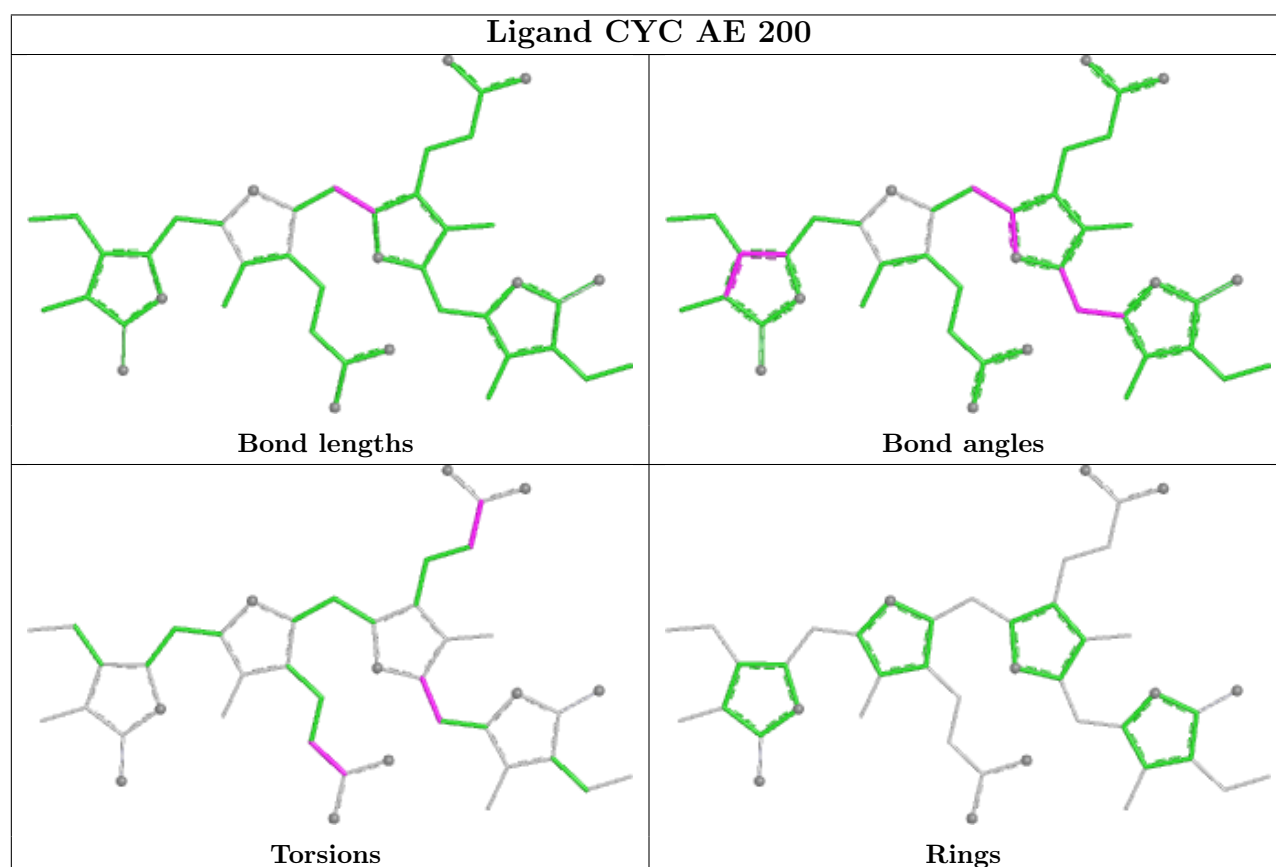
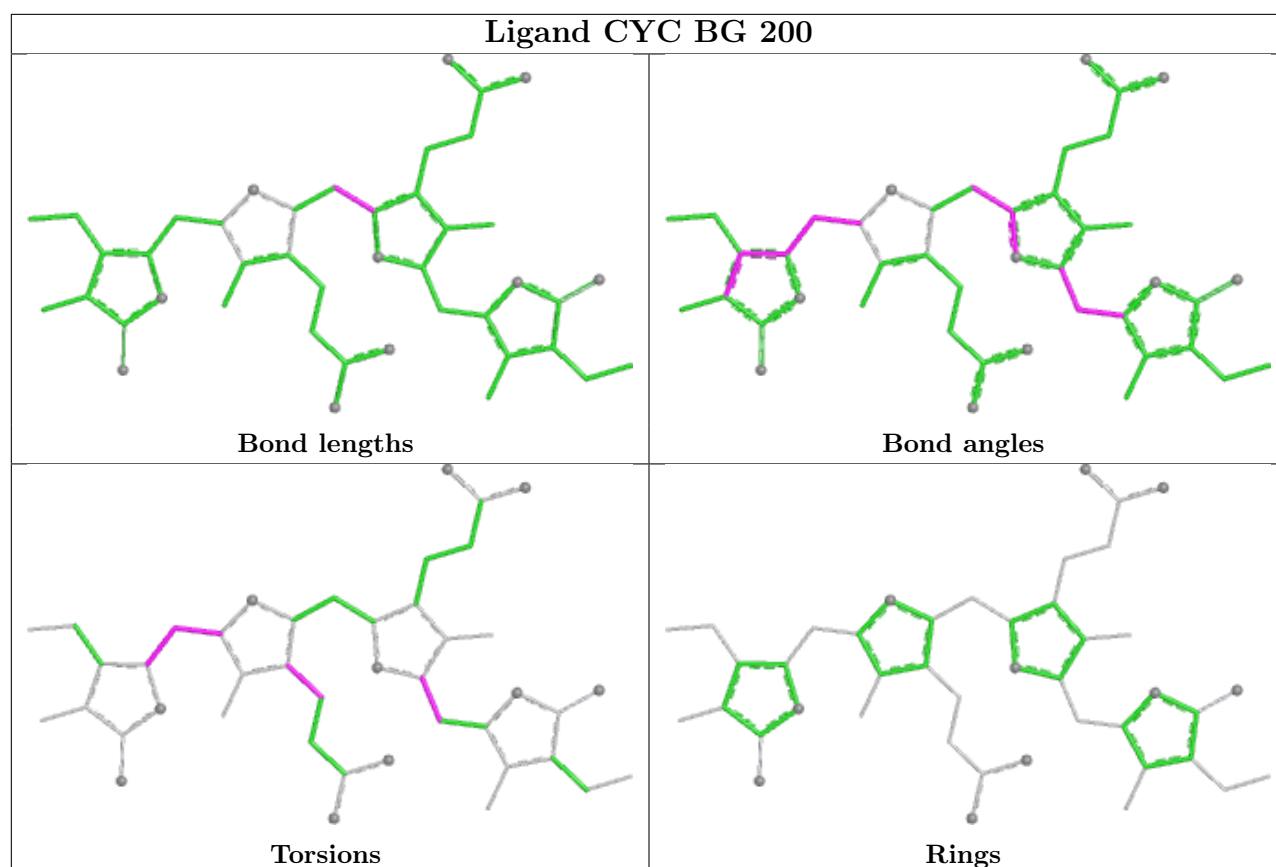
26 monomers are involved in 314 short contacts:

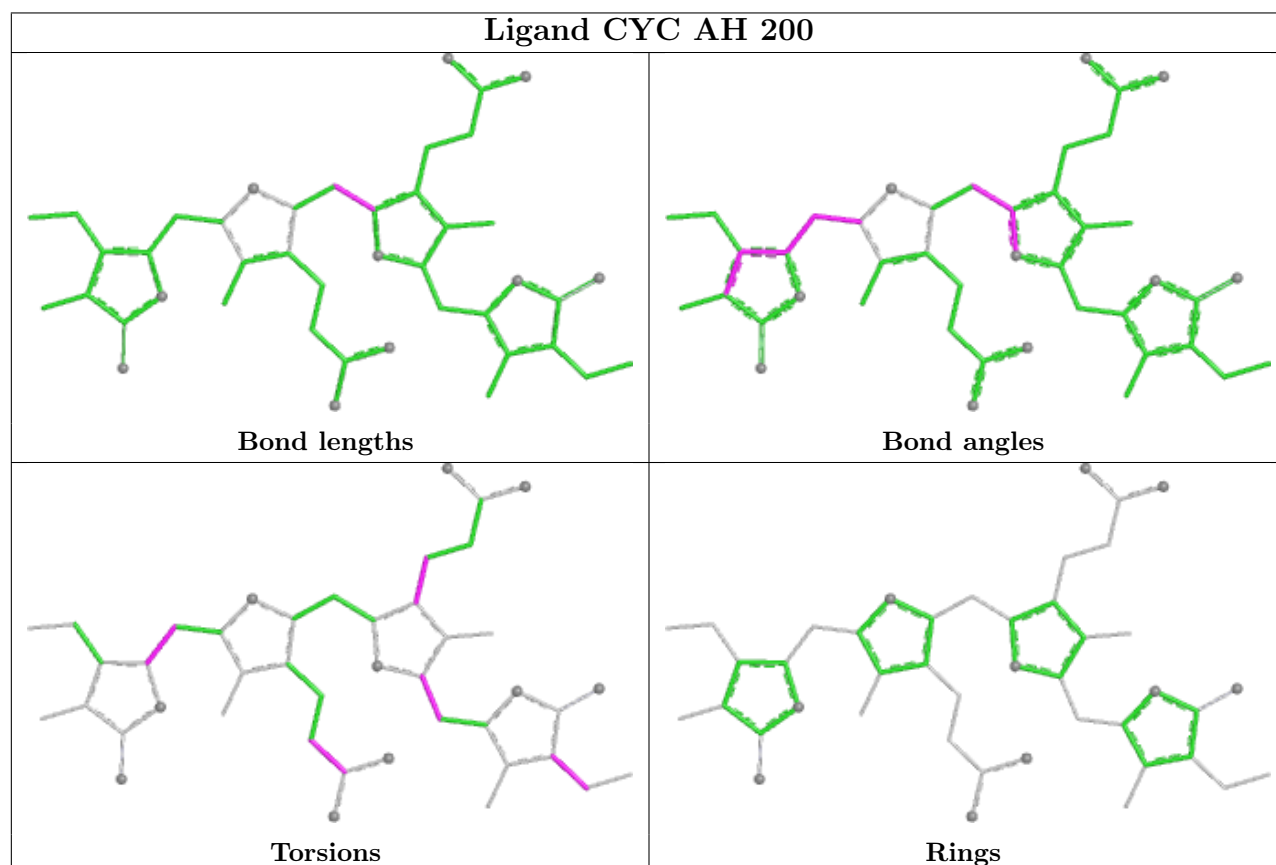
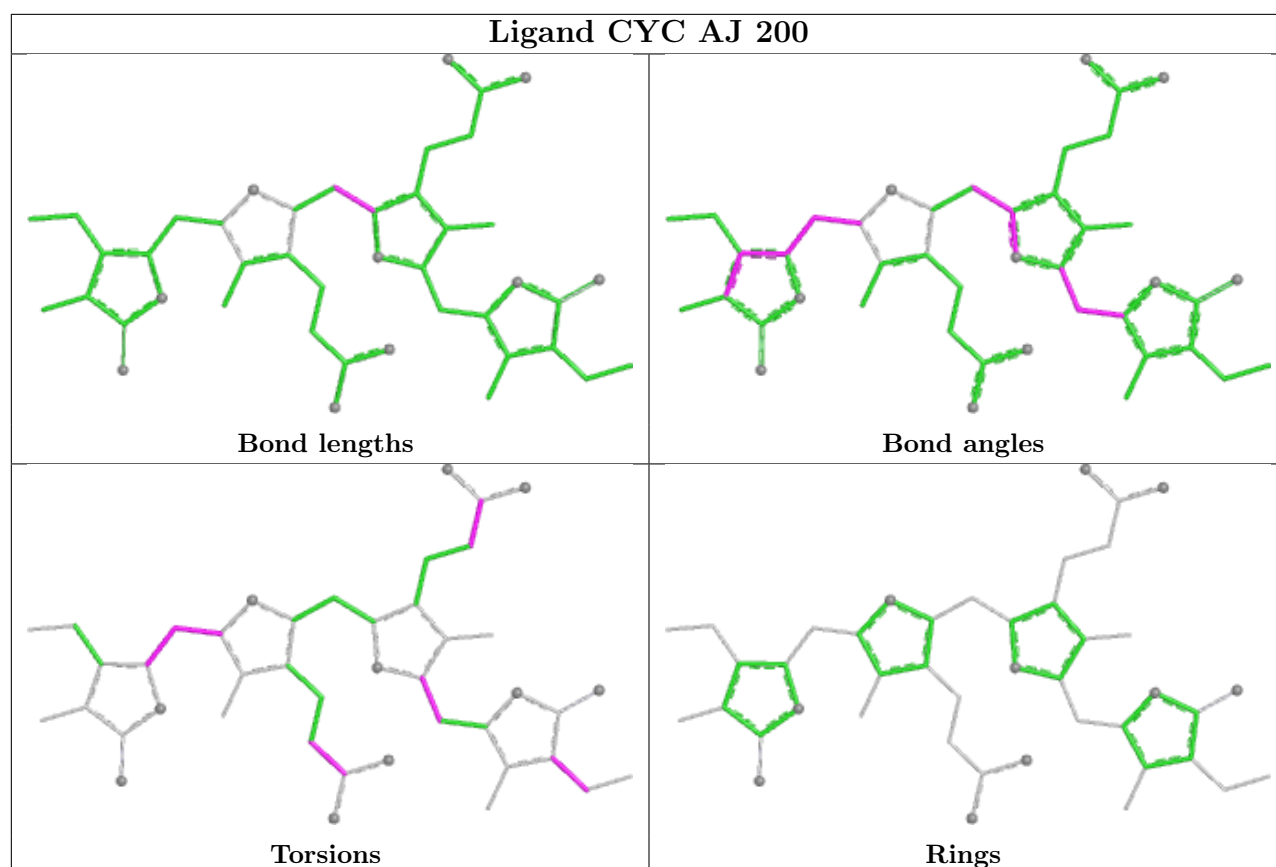
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	AY	200	CYC	18	0
7	BG	200	CYC	9	0
7	AE	200	CYC	13	0
7	AJ	200	CYC	13	0
7	AH	200	CYC	15	0
7	AA	200	CYC	13	0
7	BI	200	CYC	7	0
7	AM	200	CYC	19	0
7	AW	200	CYC	16	0
7	AC	200	CYC	12	0
7	BD	200	CYC	10	0
7	BB	200	CYC	11	0
7	AL	200	CYC	13	0
7	AK	200	CYC	12	0
7	BE	200	CYC	15	0
7	AX	200	CYC	11	0
7	BA	200	CYC	13	0
7	AF	200	CYC	9	0
7	BF	200	CYC	11	0
7	BH	200	CYC	13	0
7	AI	200	CYC	10	0
7	AB	200	CYC	9	0
8	BP	400	45D	8	0
7	AZ	200	CYC	8	0
8	AS	400	45D	17	0
7	AD	200	CYC	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

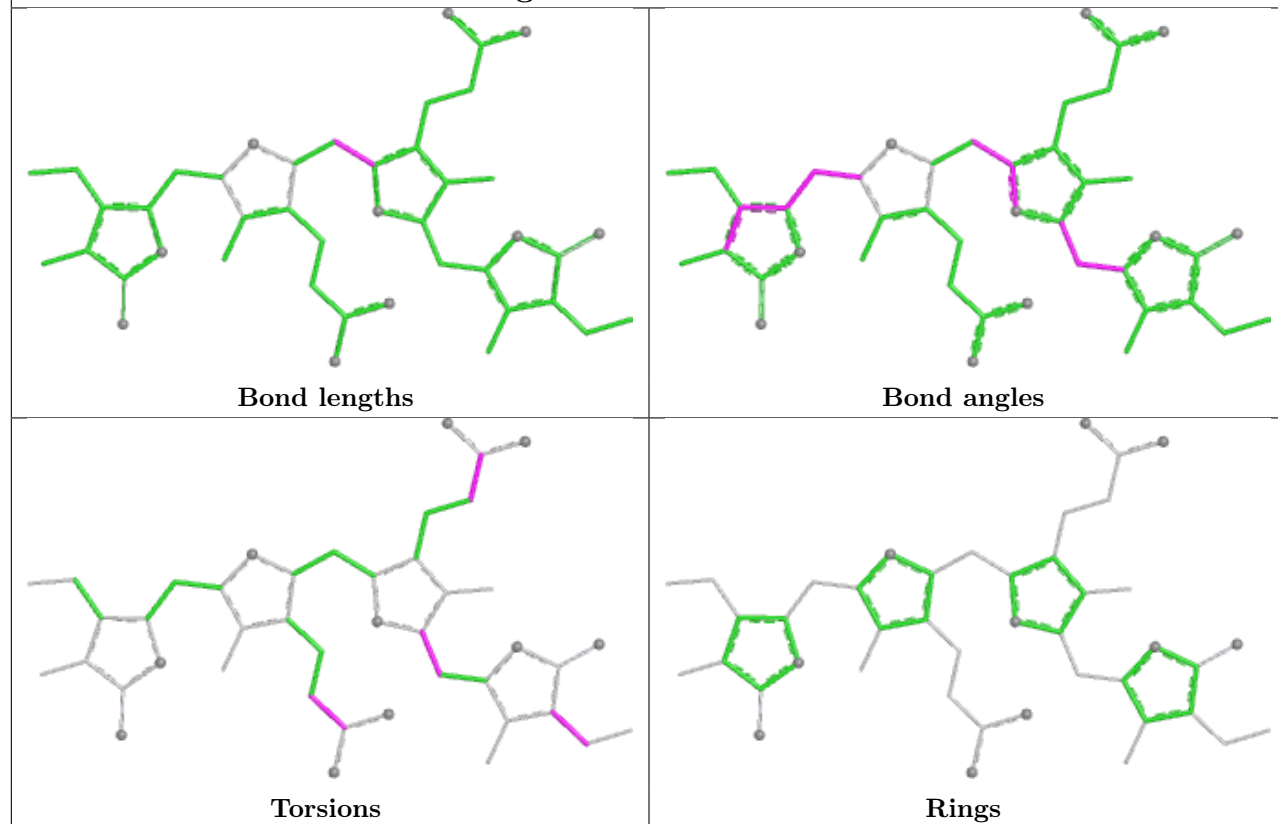
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified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



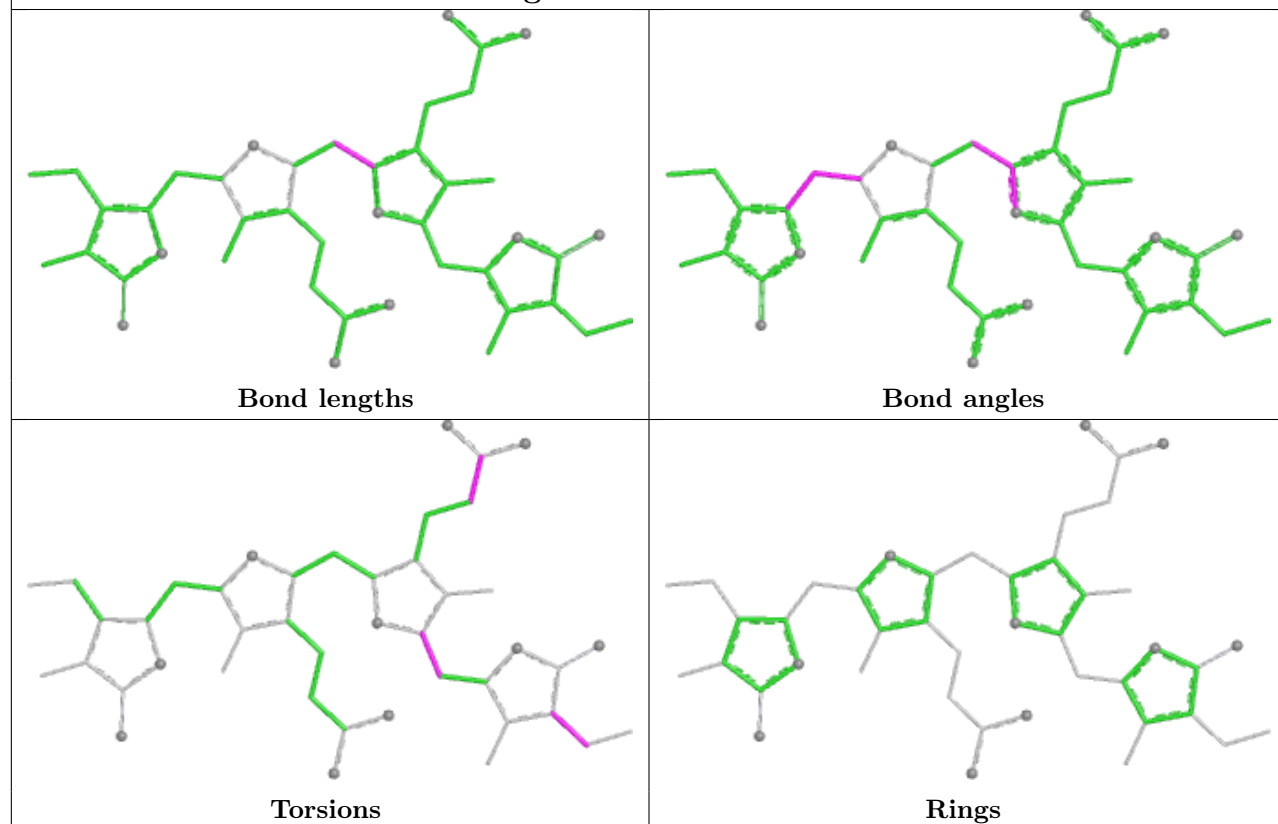




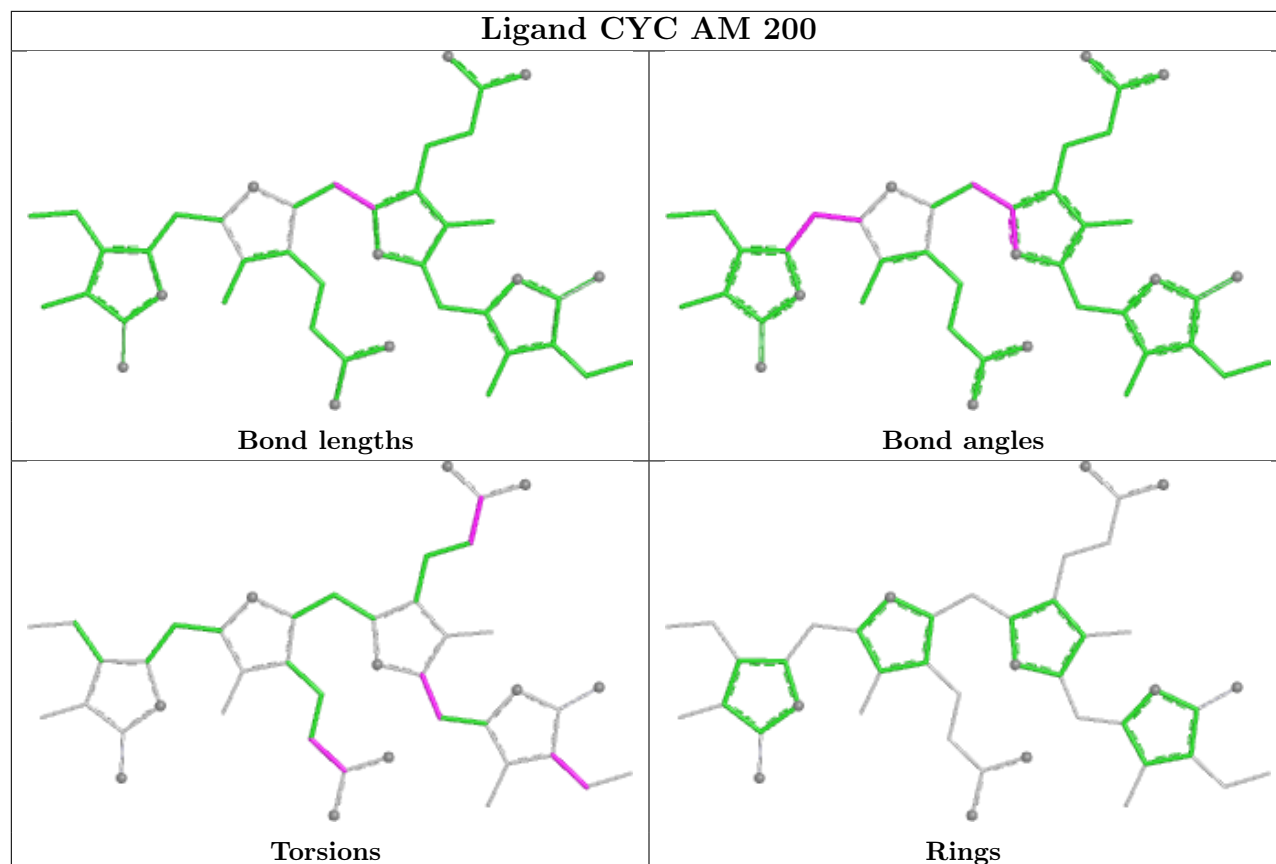
## Ligand CYC AA 200



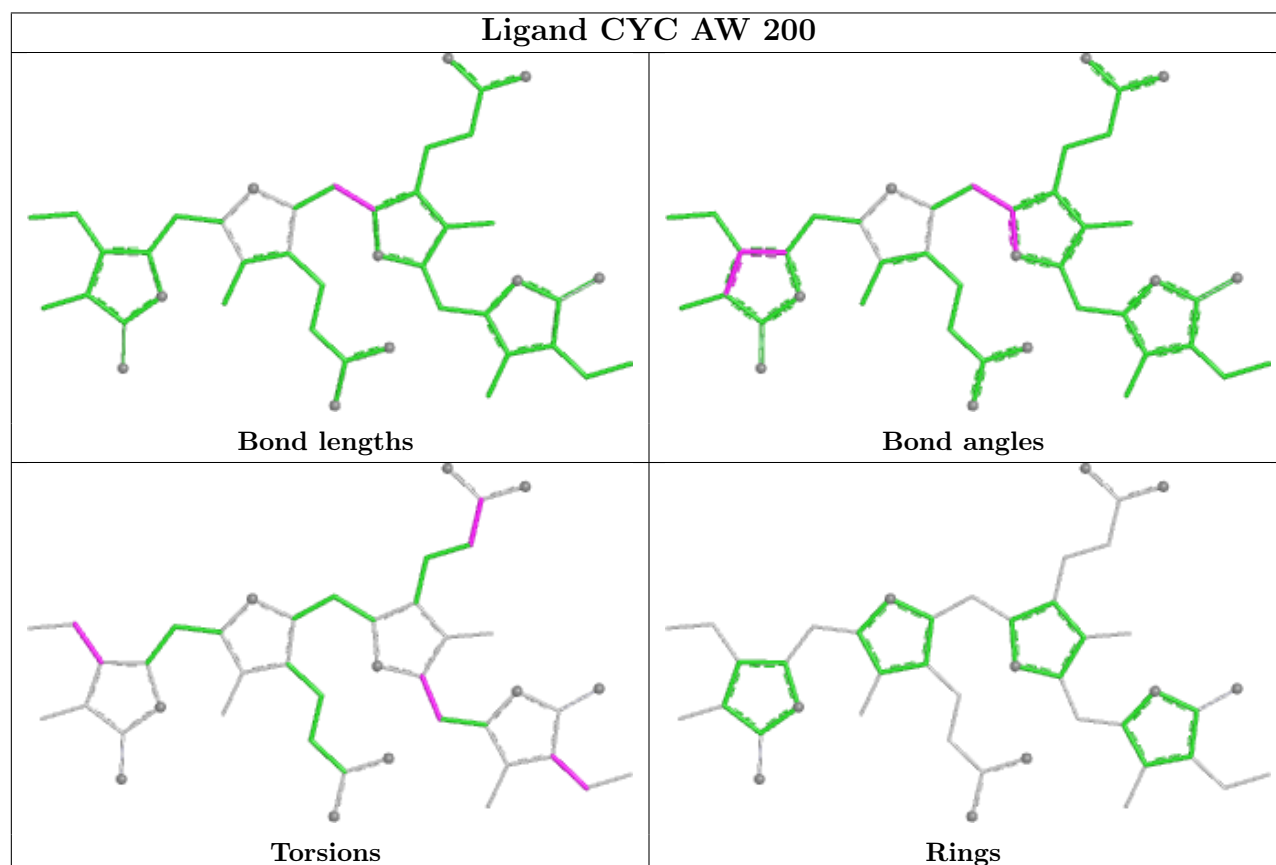
## Ligand CYC BI 200

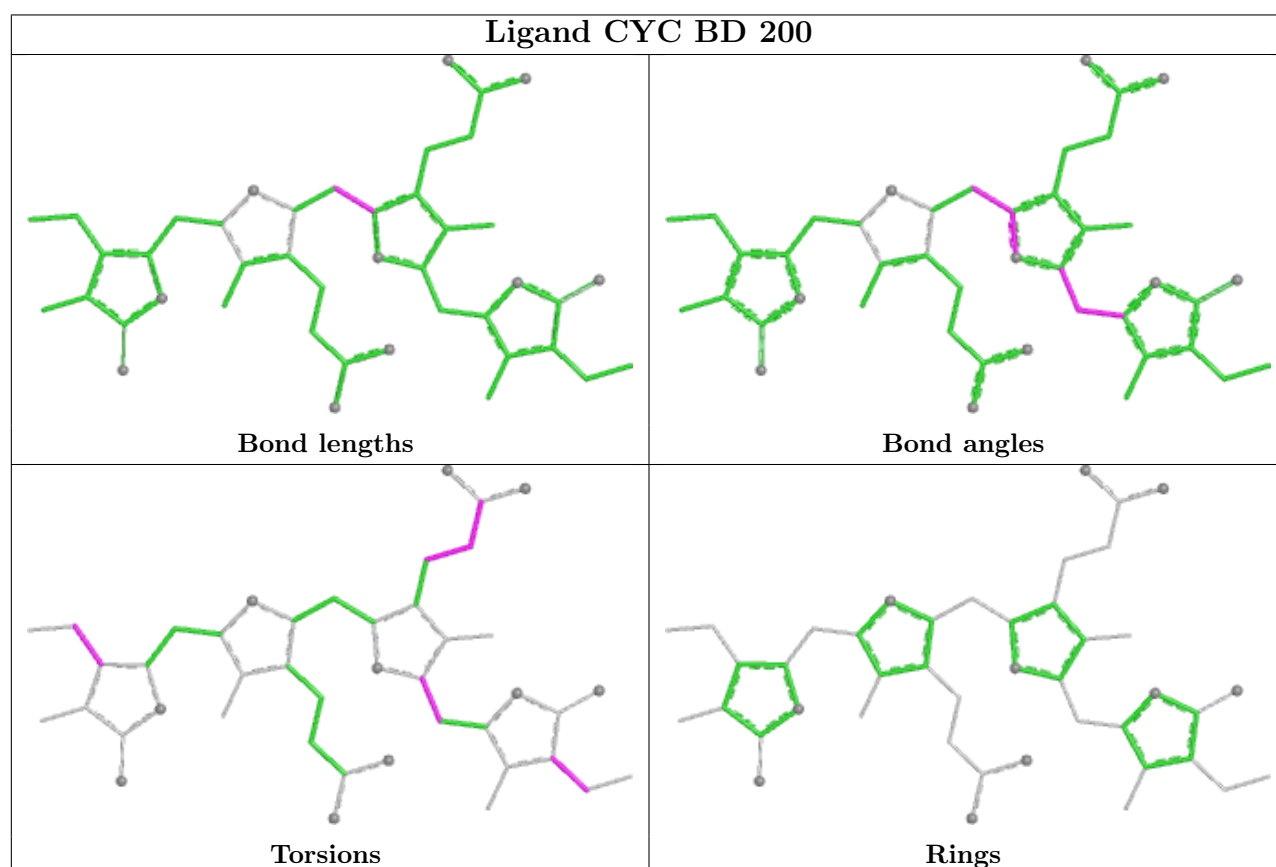
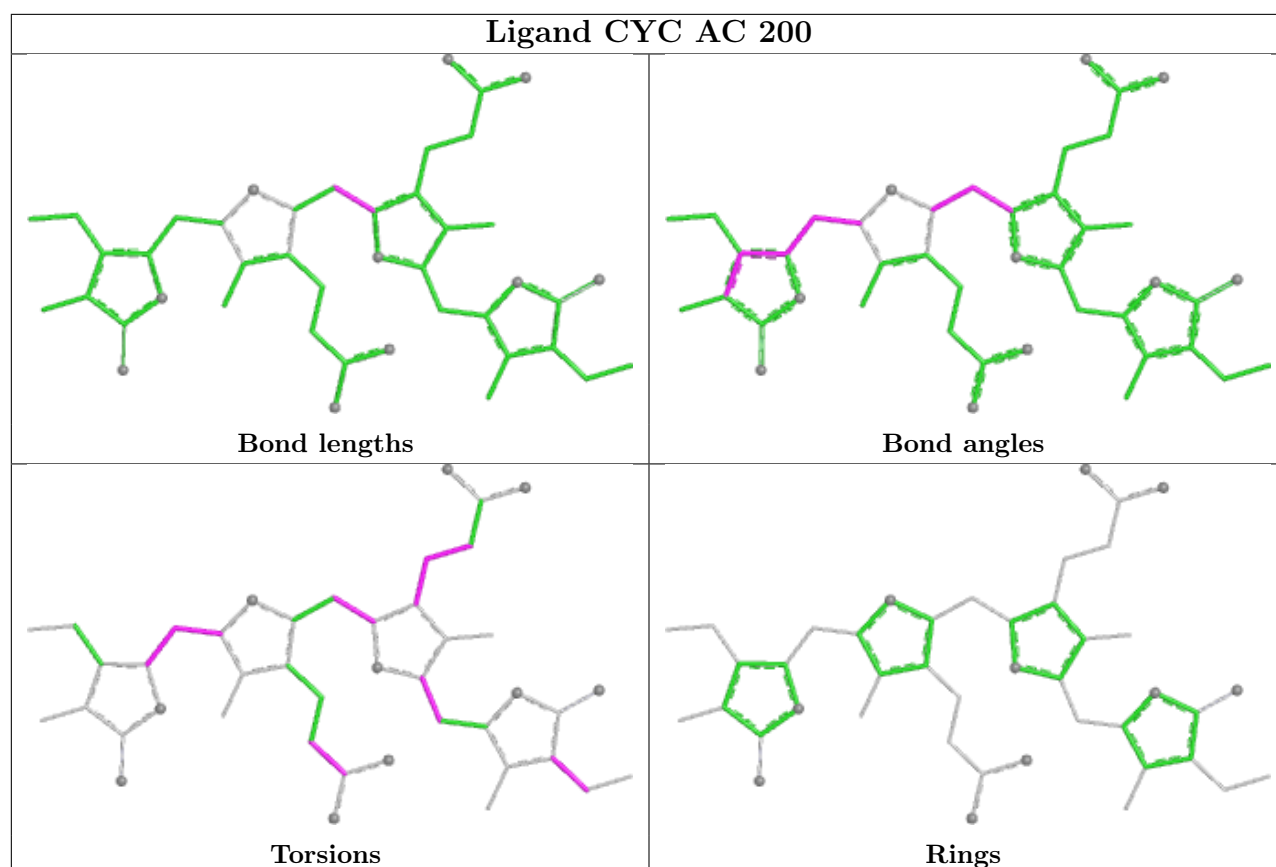


## Ligand CYC AM 200

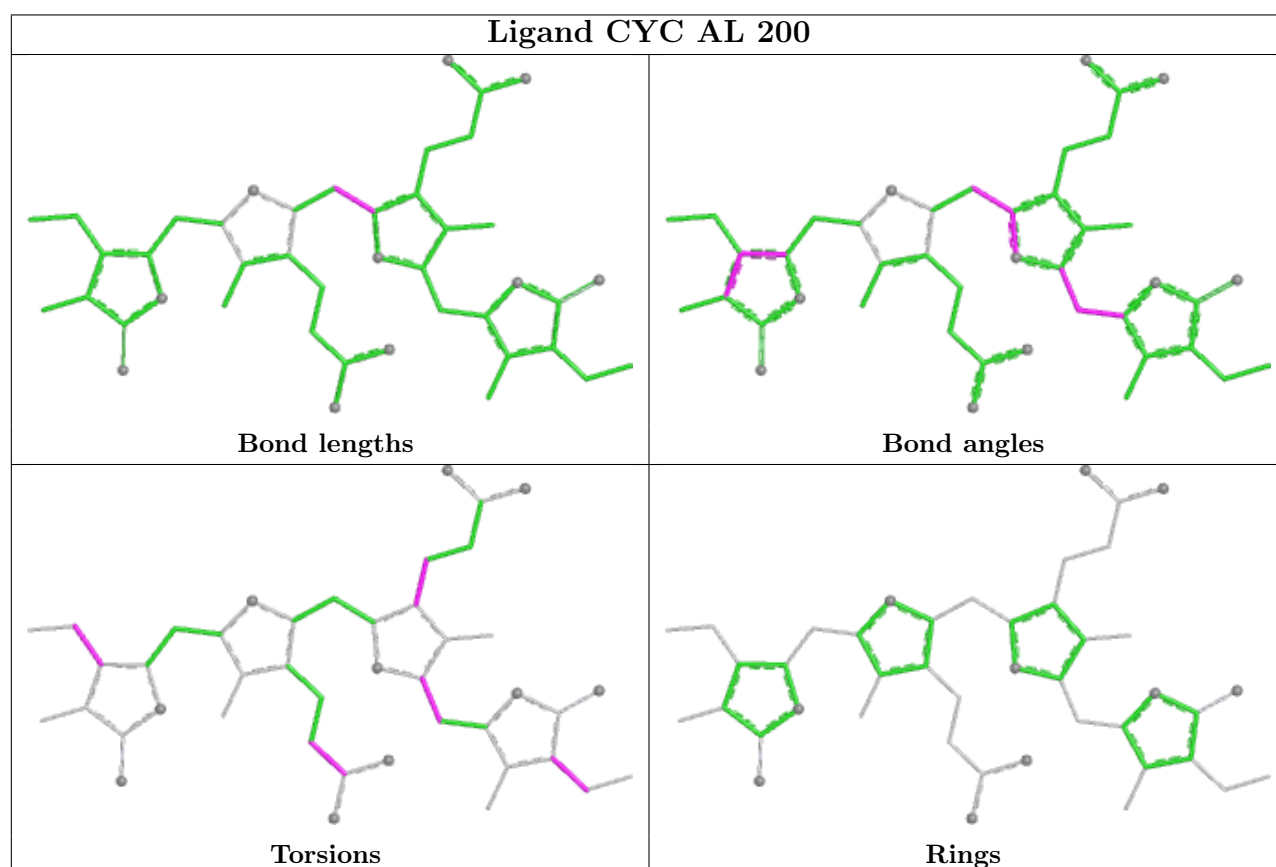
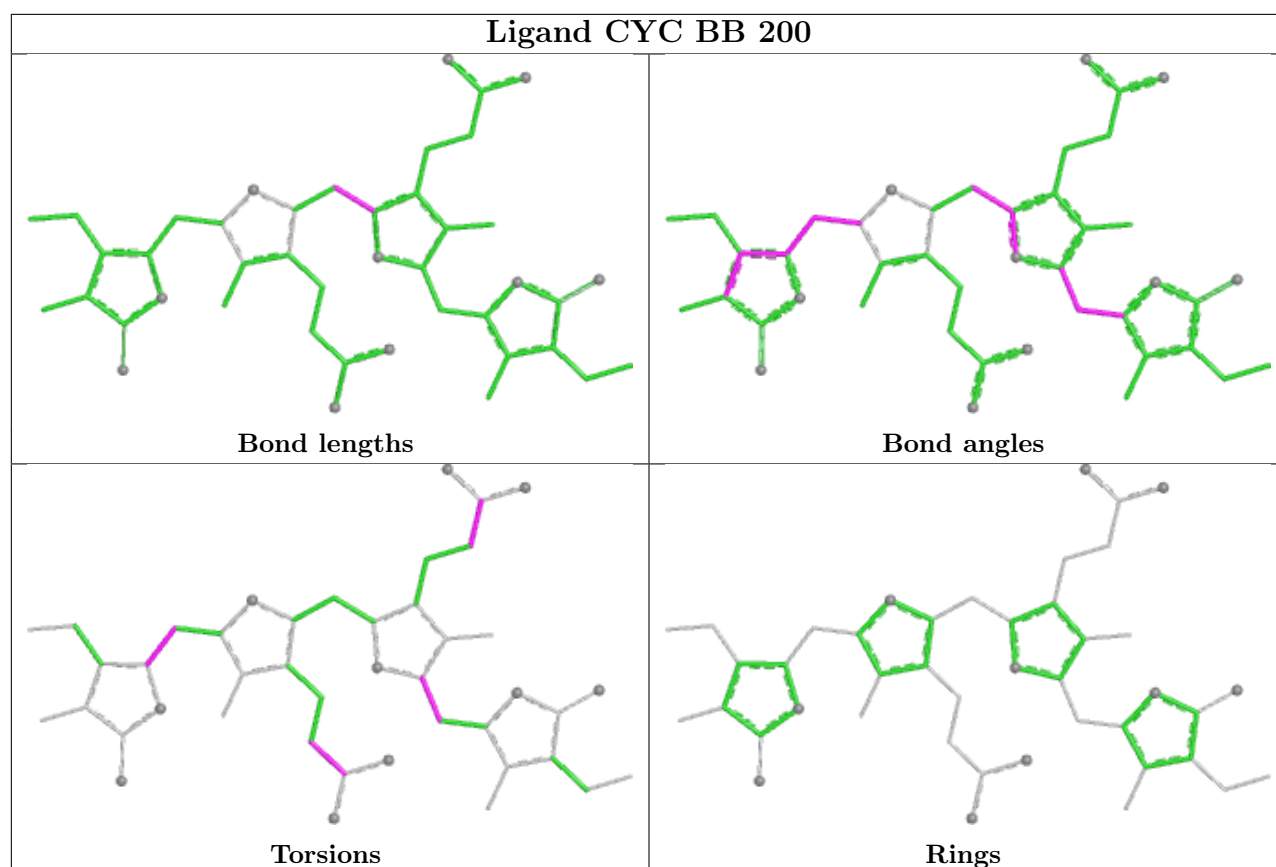


## Ligand CYC AW 200

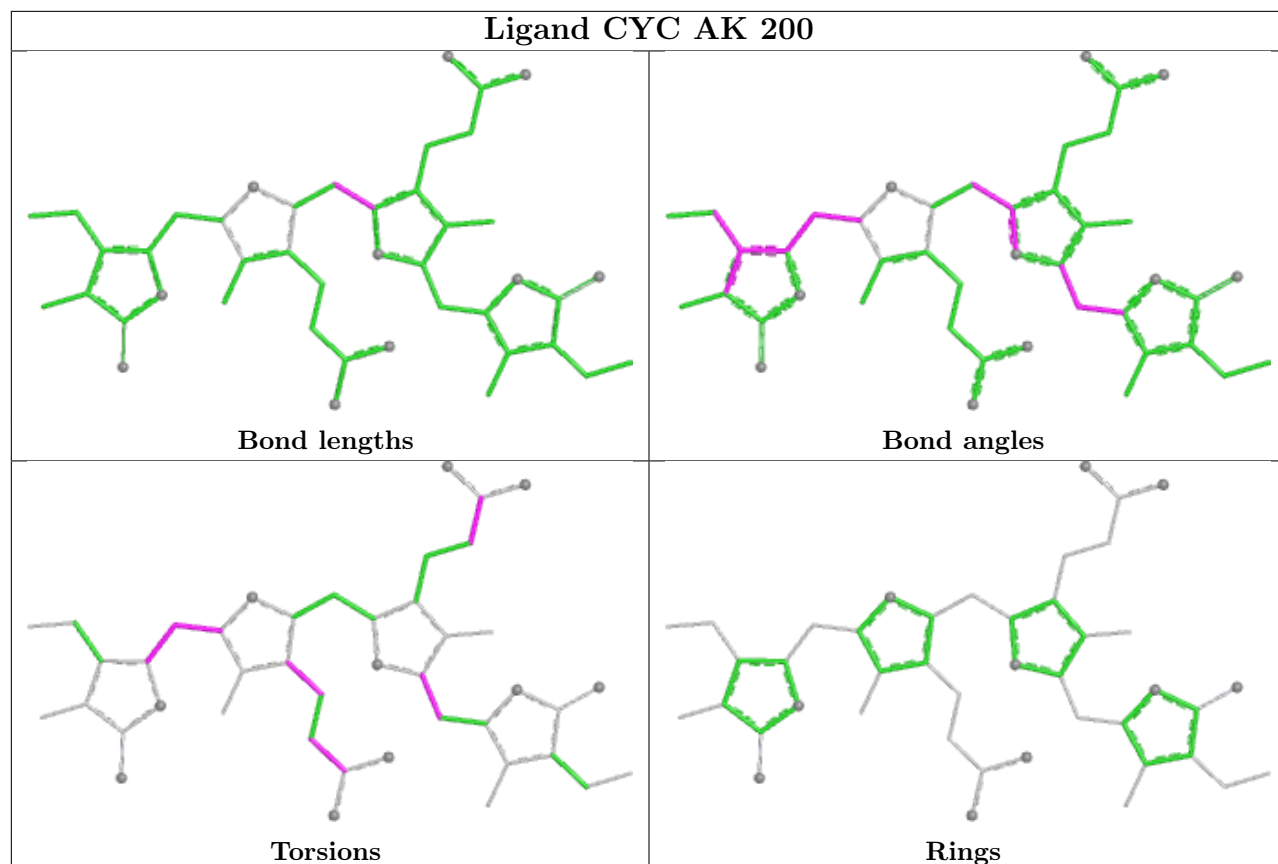




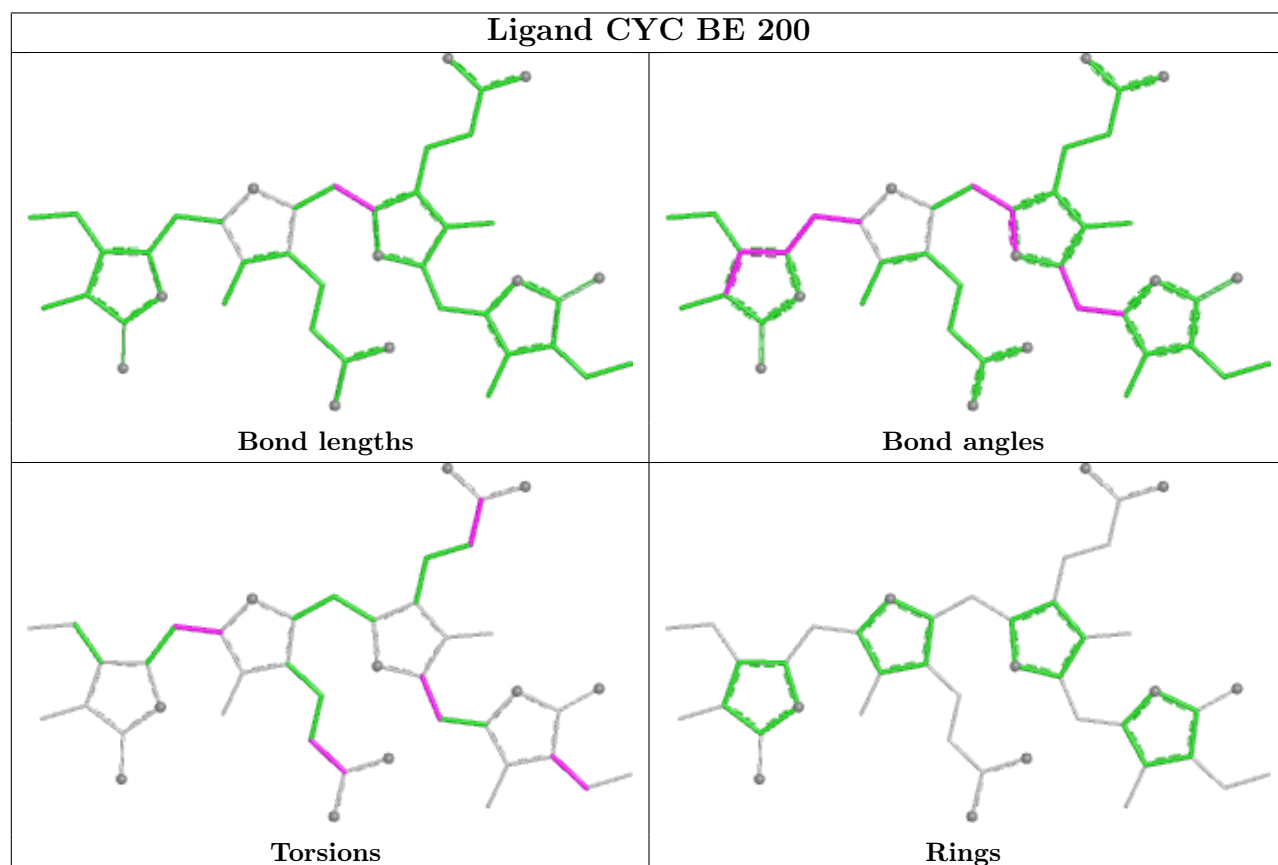


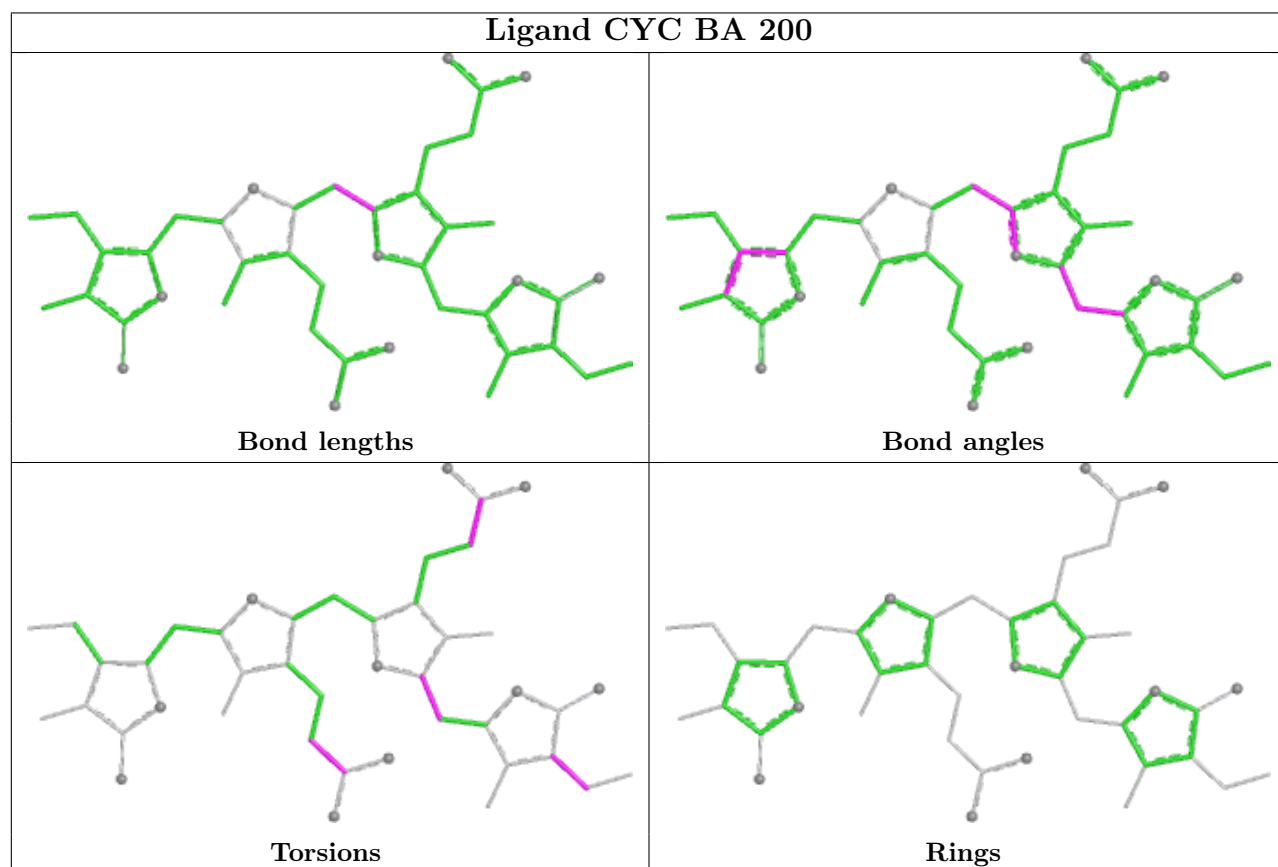
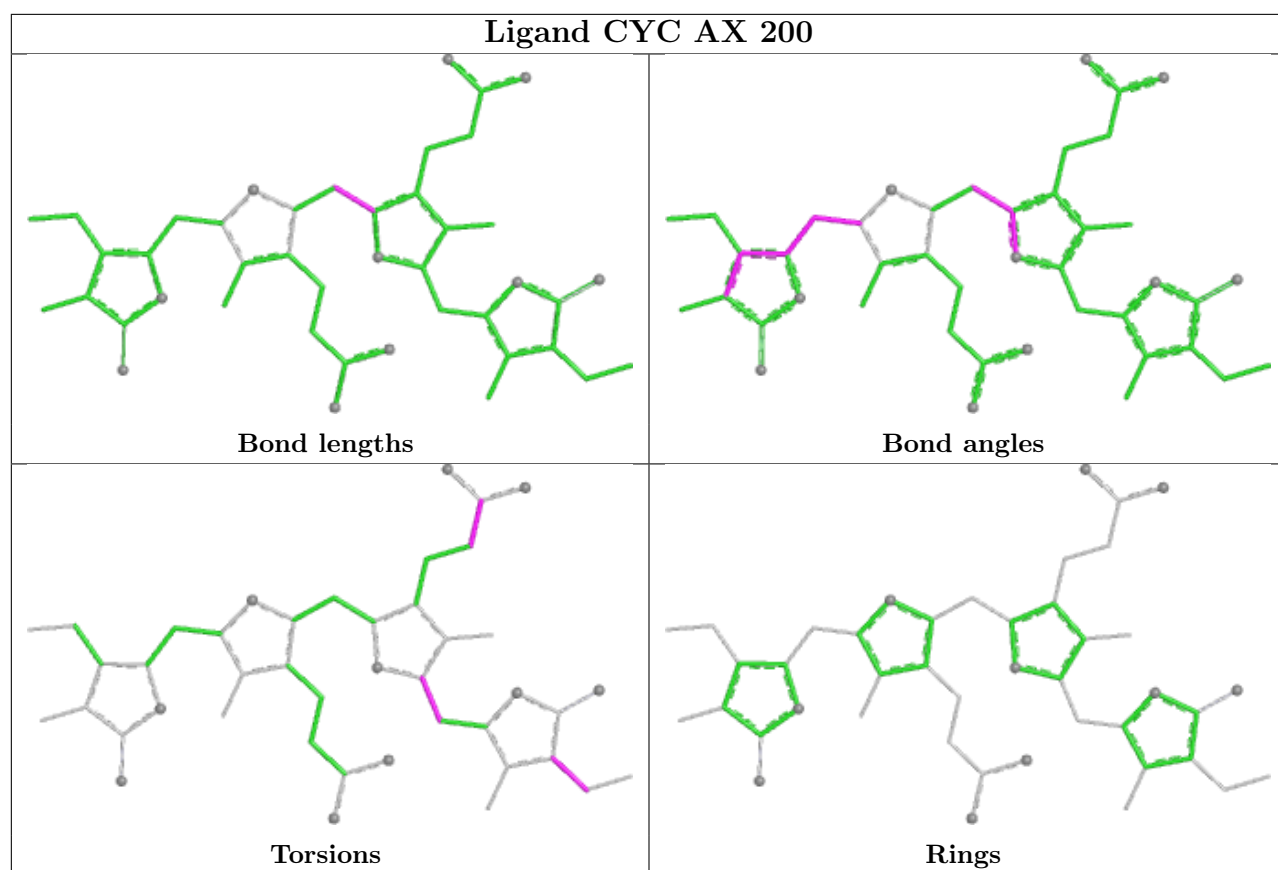


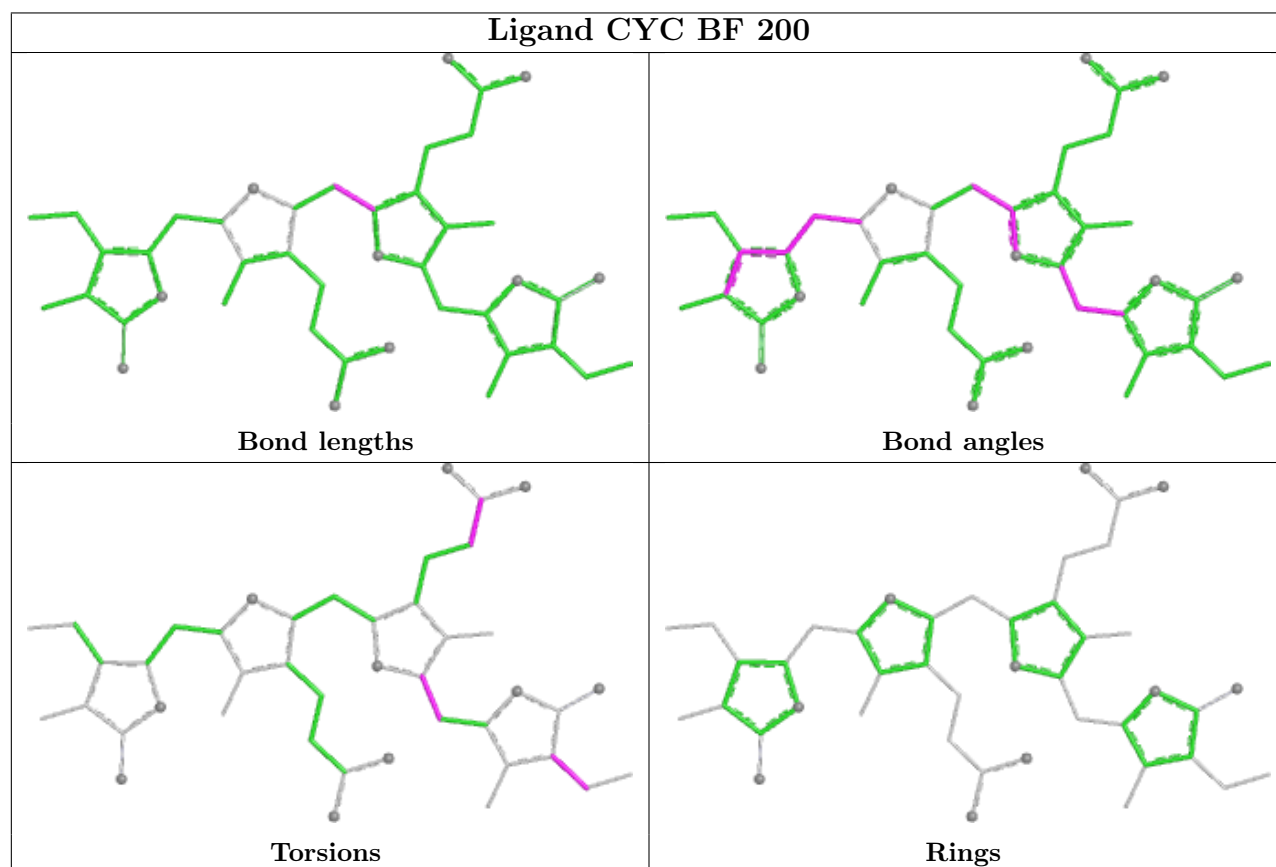
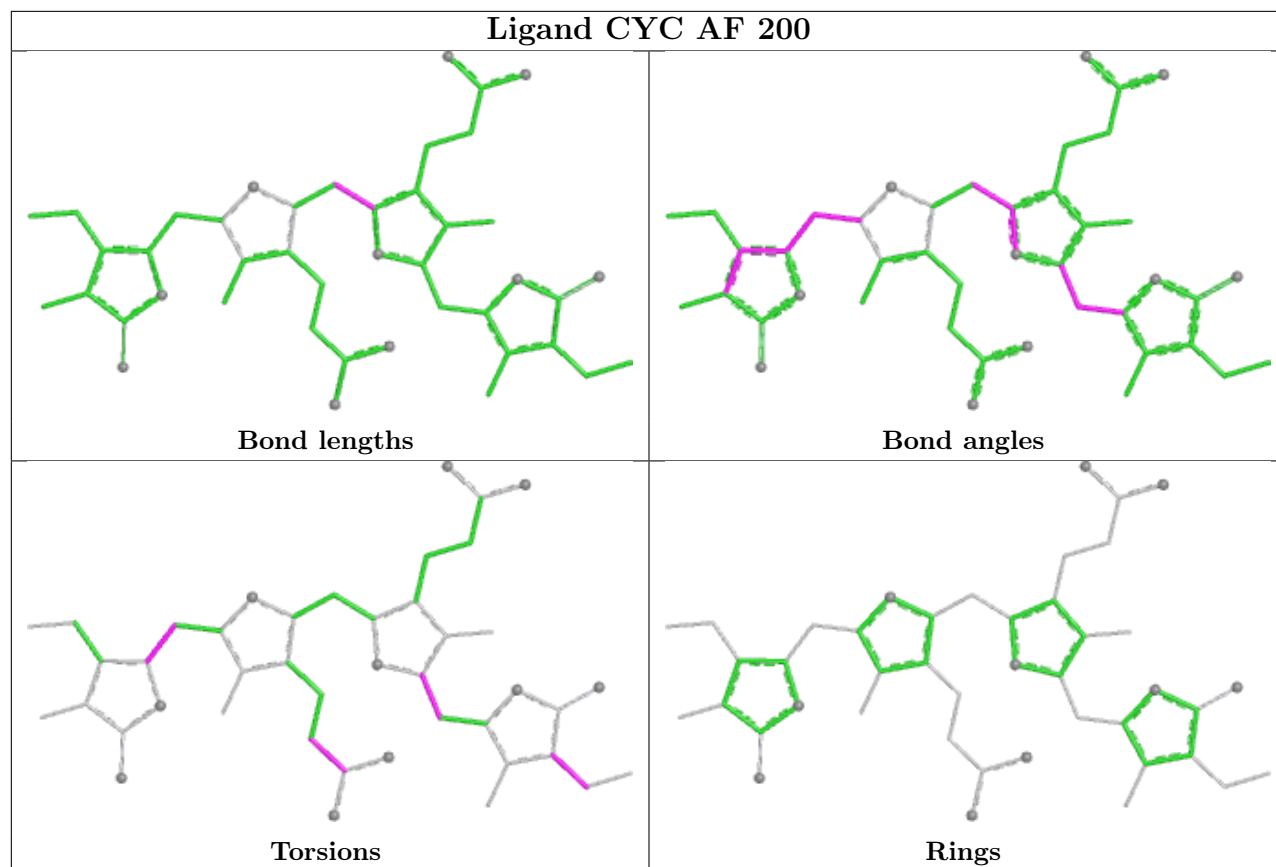
## Ligand CYC AK 200

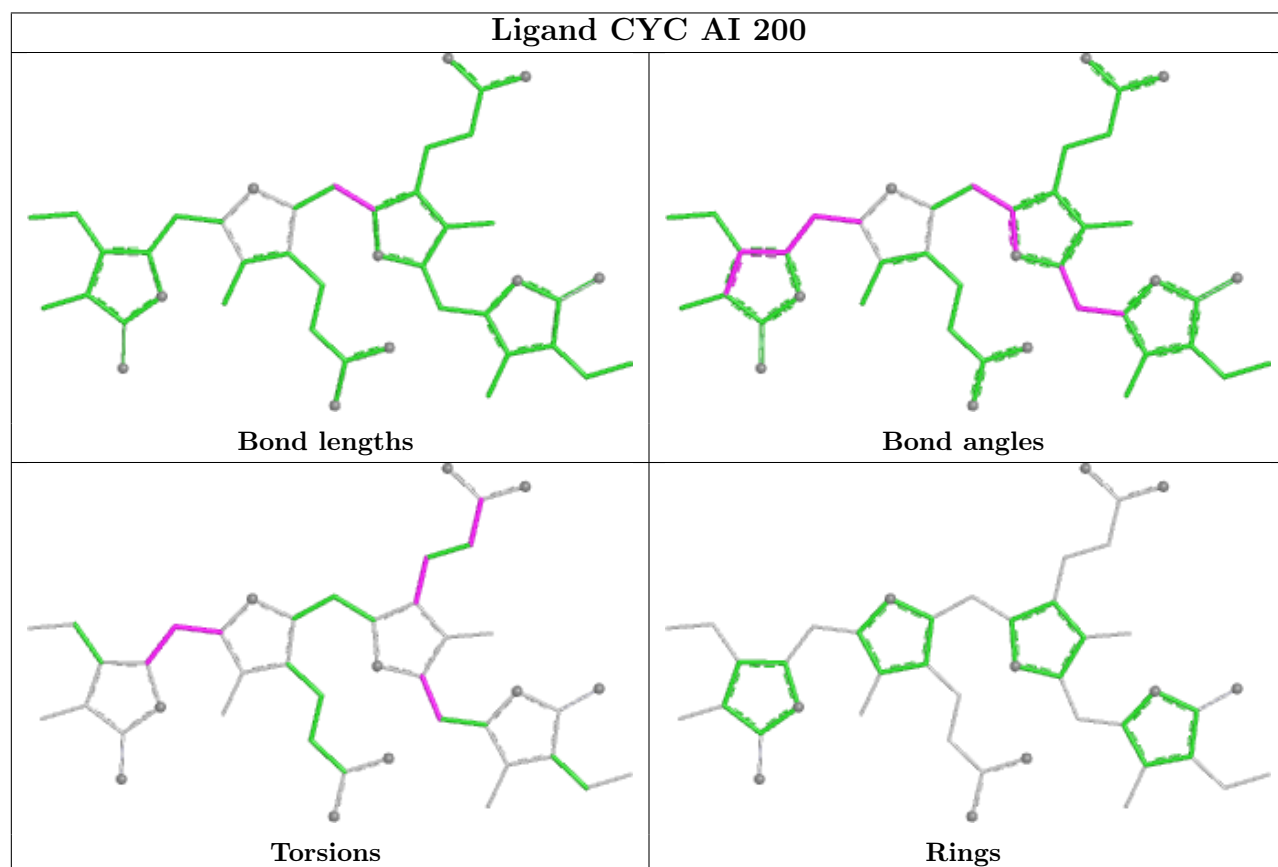
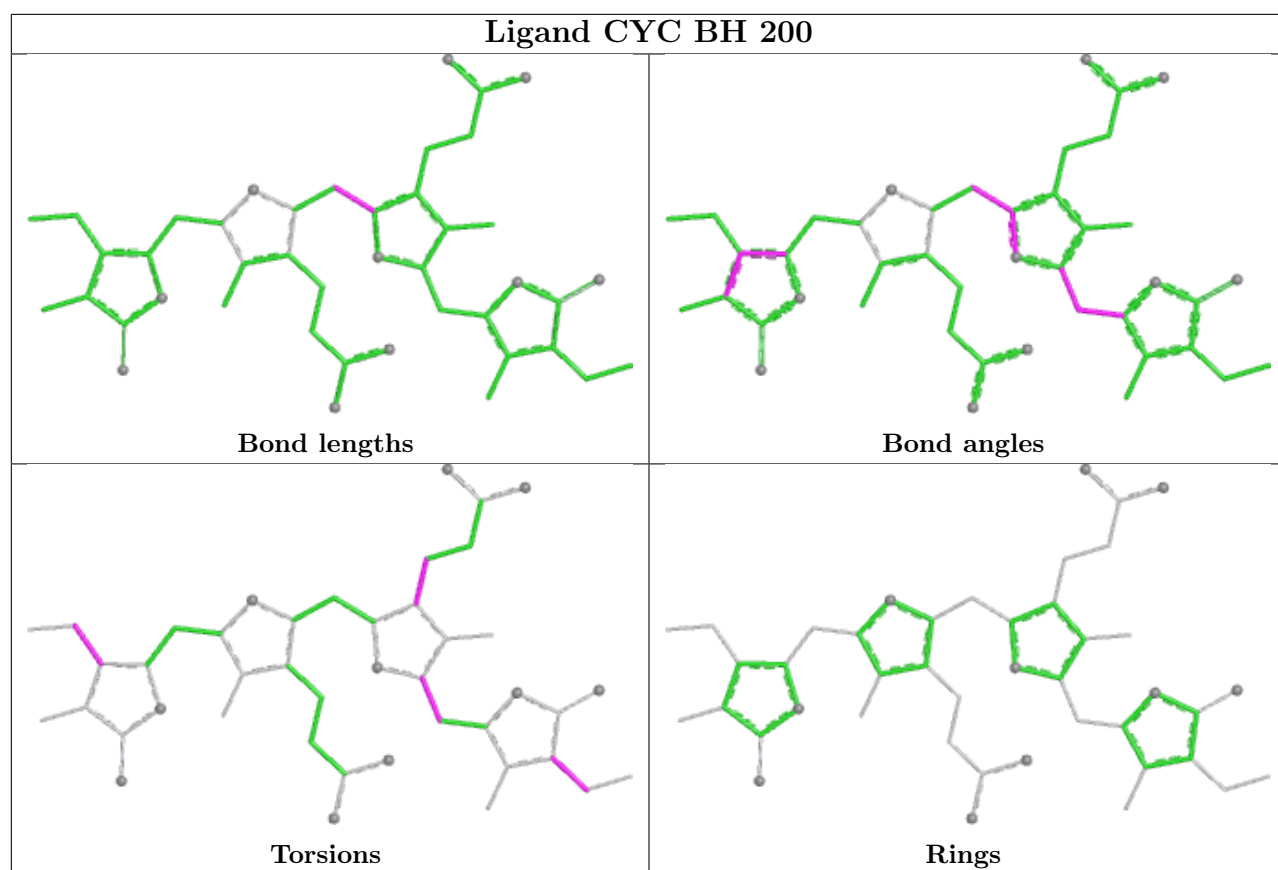


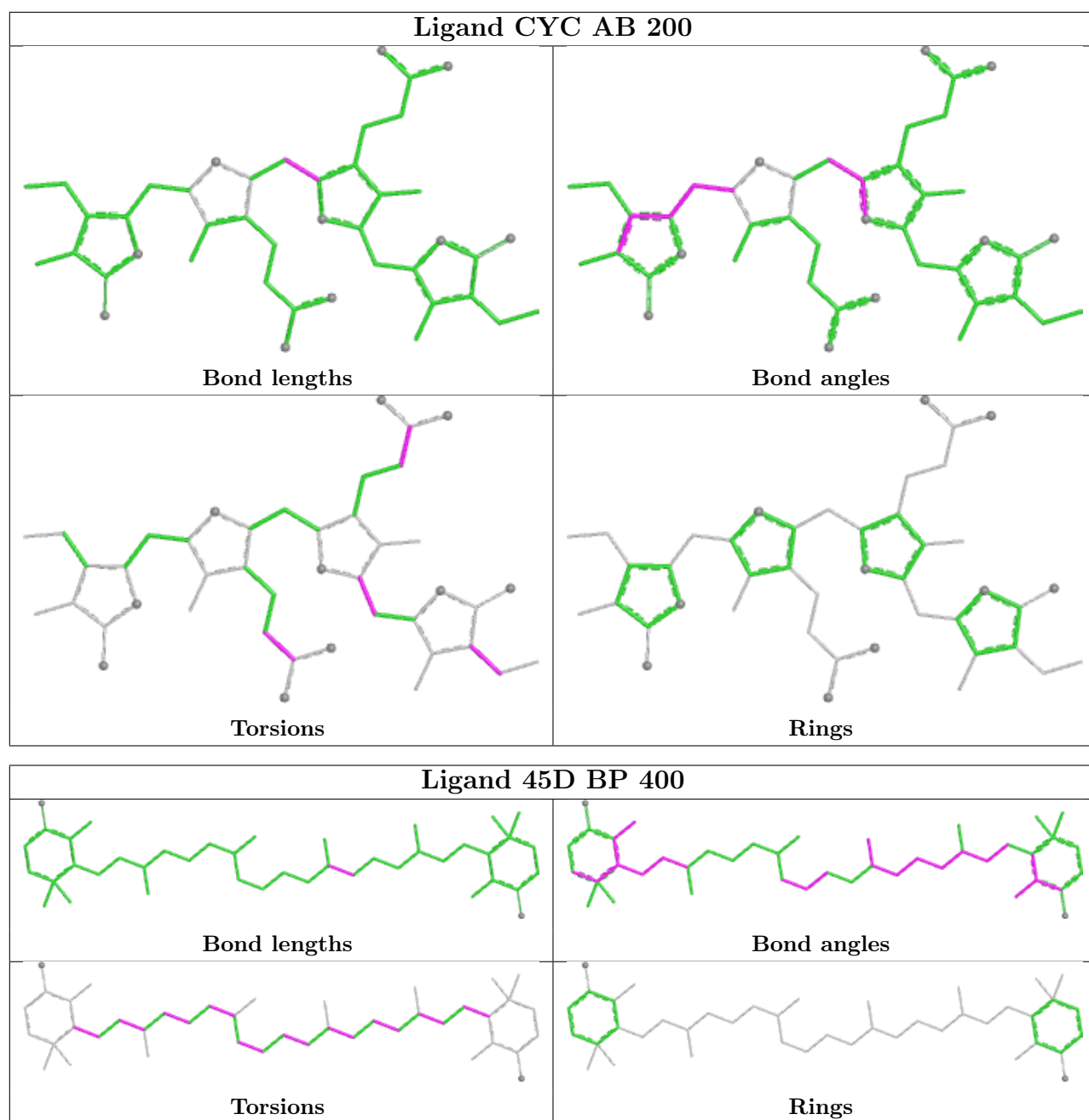
## Ligand CYC BE 200

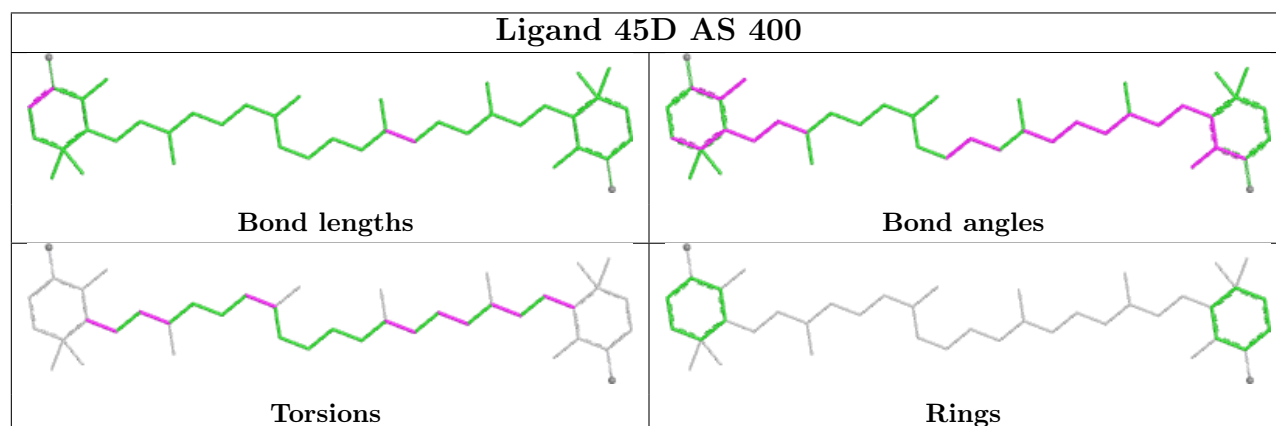
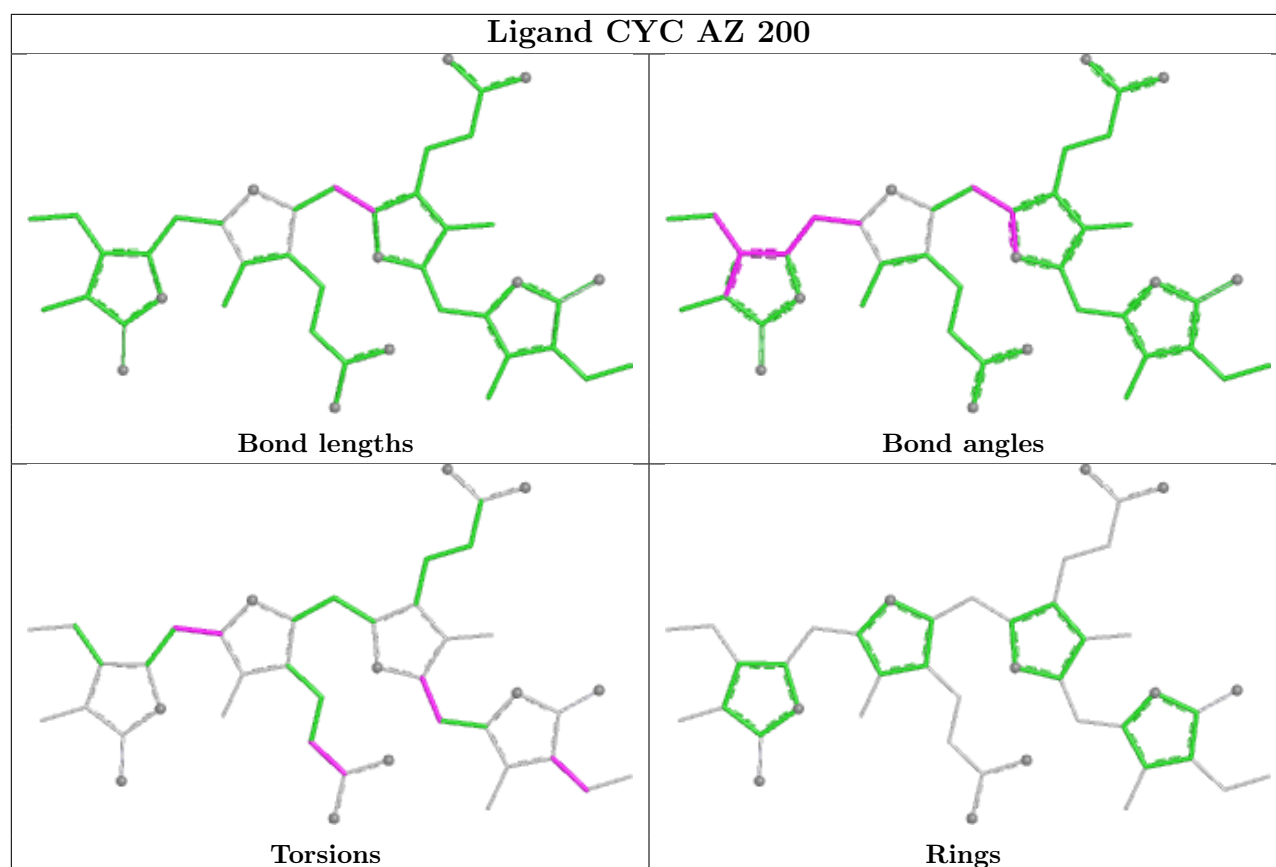


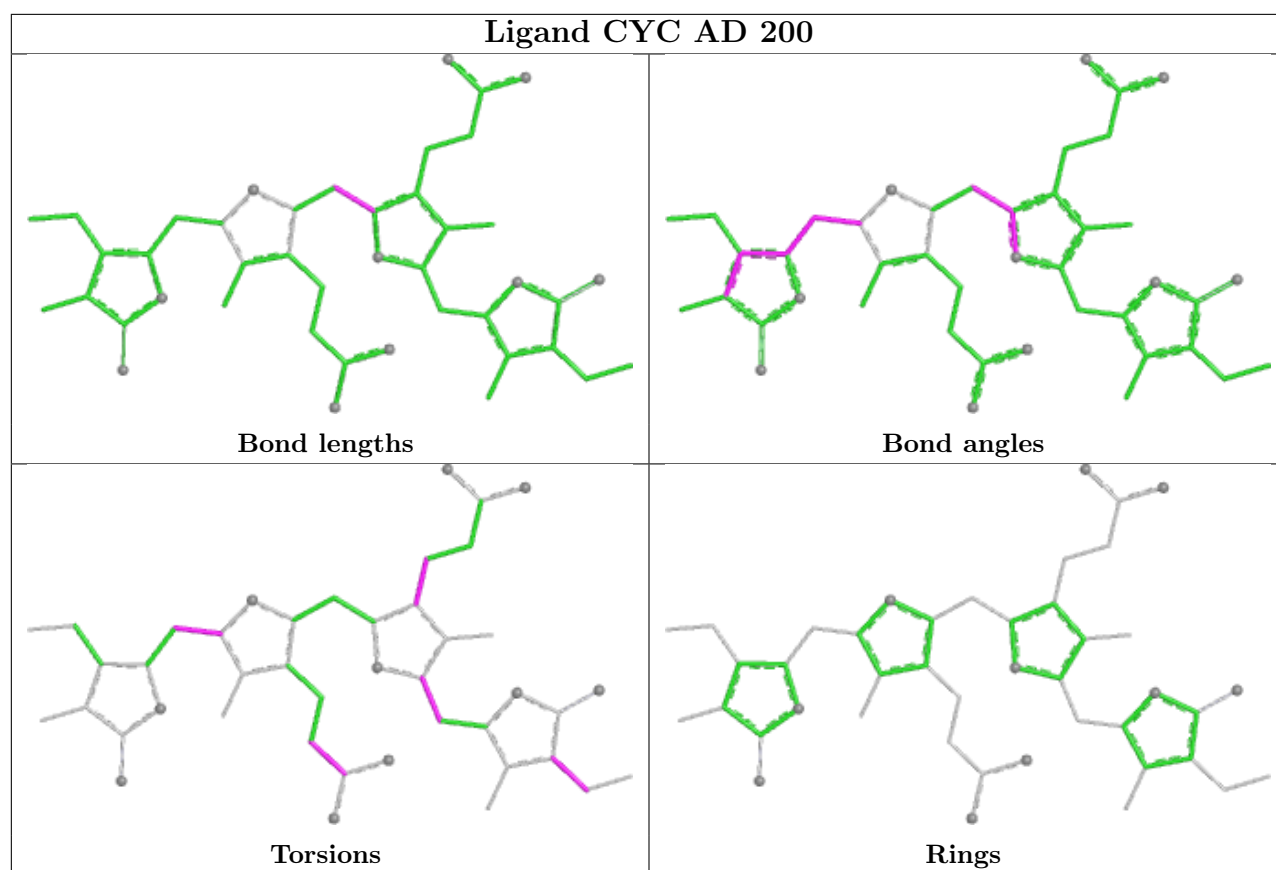












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



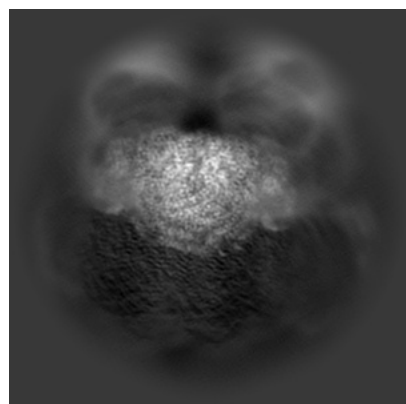
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25033. These allow visual inspection of the internal detail of the map and identification of artifacts.

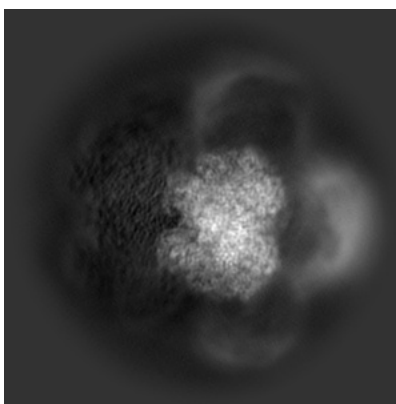
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

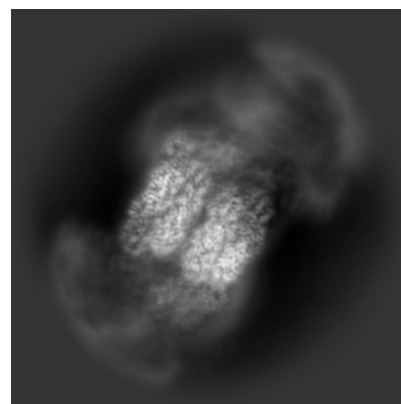
#### 6.1.1 Primary map



X

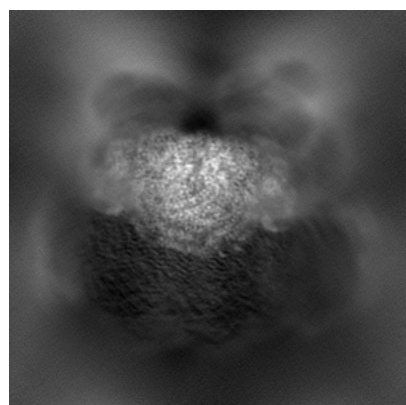


Y

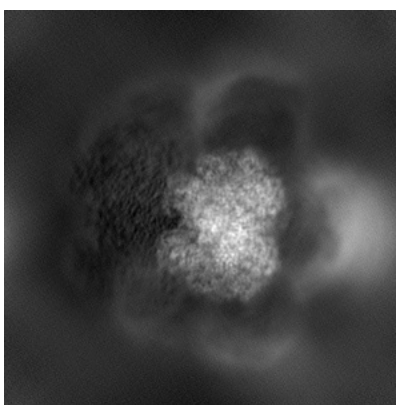


Z

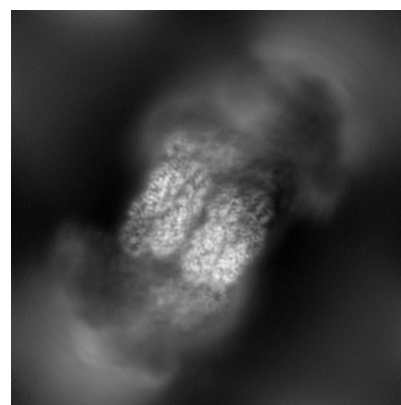
#### 6.1.2 Raw map



X



Y

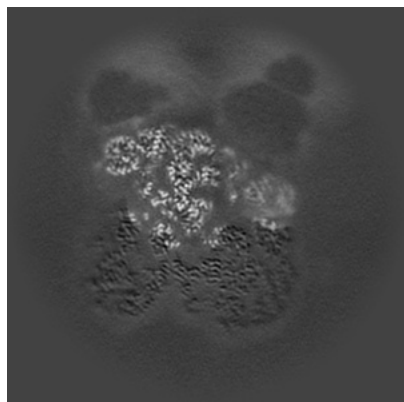


Z

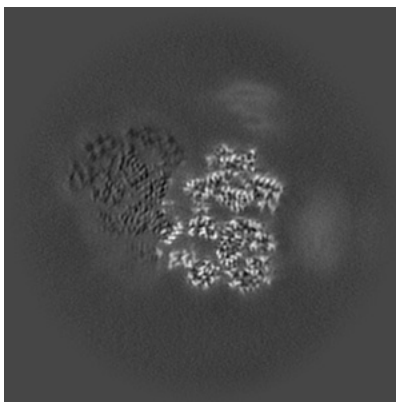
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

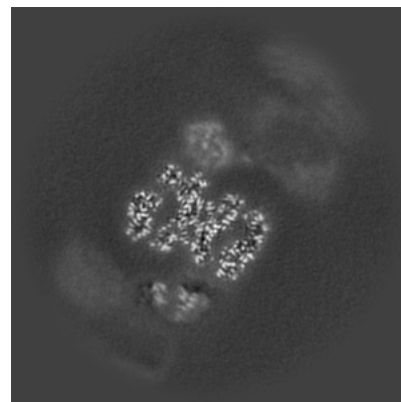
### 6.2.1 Primary map



X Index: 180

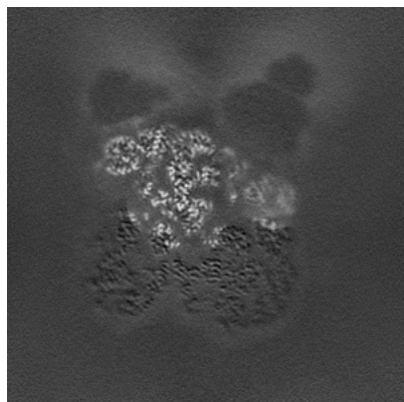


Y Index: 180

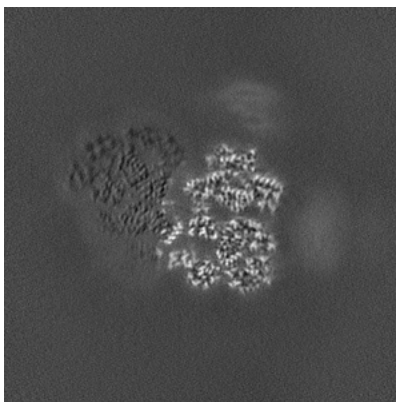


Z Index: 180

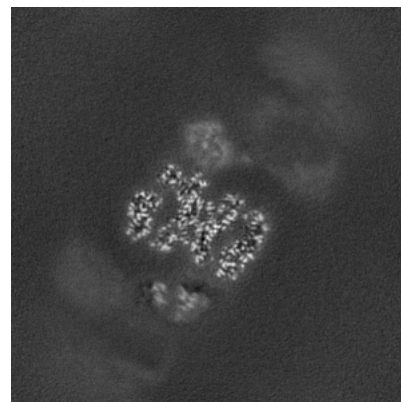
### 6.2.2 Raw map



X Index: 180



Y Index: 180

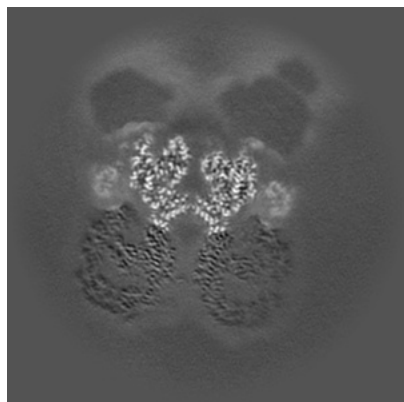


Z Index: 180

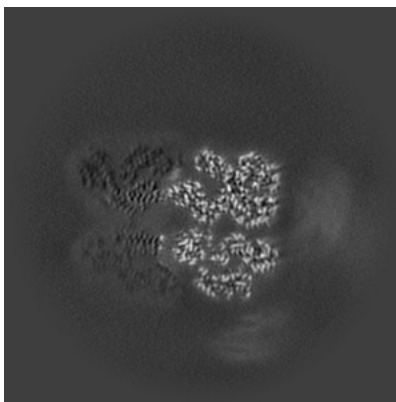
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

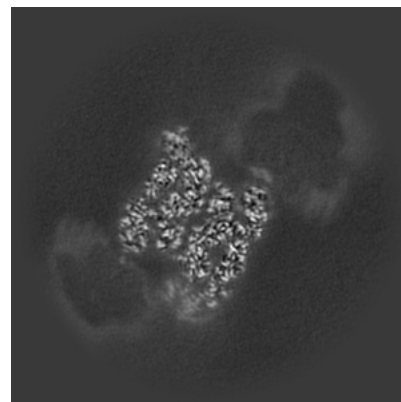
### 6.3.1 Primary map



X Index: 167

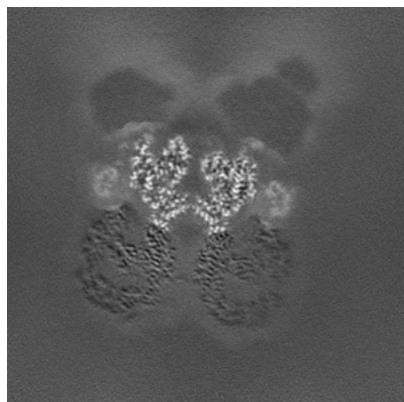


Y Index: 159

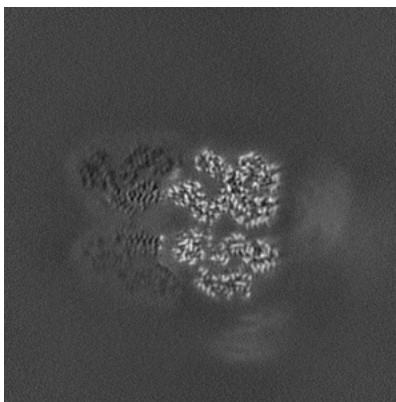


Z Index: 213

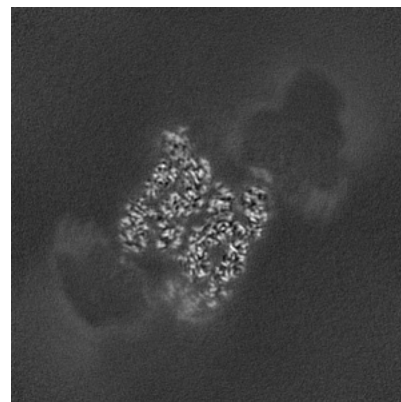
### 6.3.2 Raw map



X Index: 167



Y Index: 159

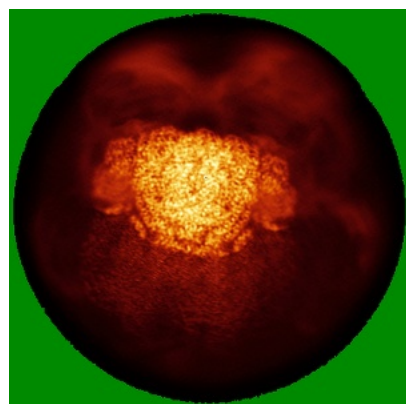


Z Index: 213

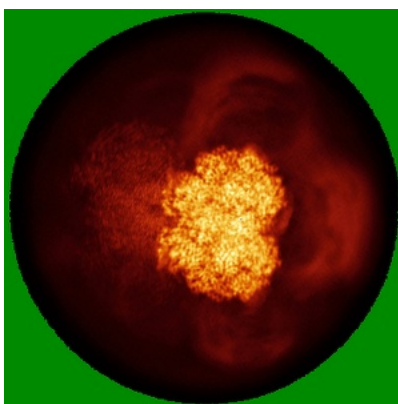
The images above show the largest variance slices of the map in three orthogonal directions.

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

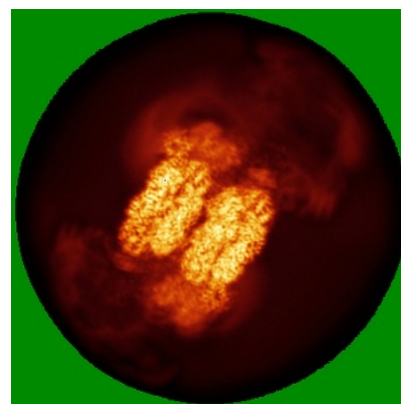
### 6.4.1 Primary map



X

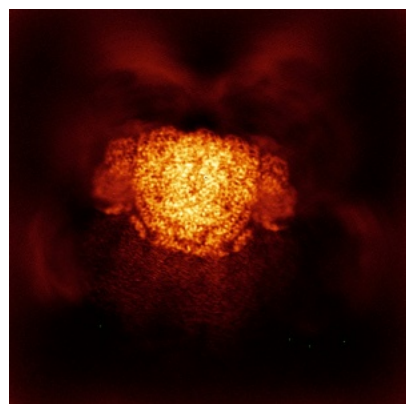


Y

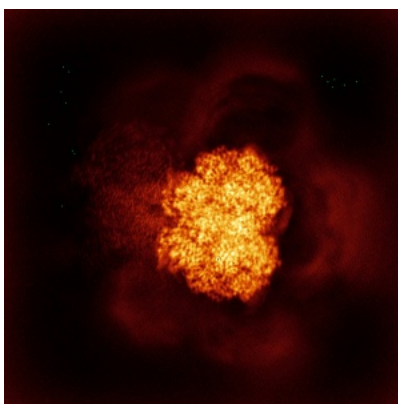


Z

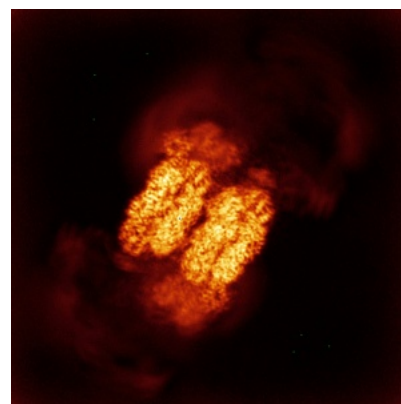
### 6.4.2 Raw map



X



Y



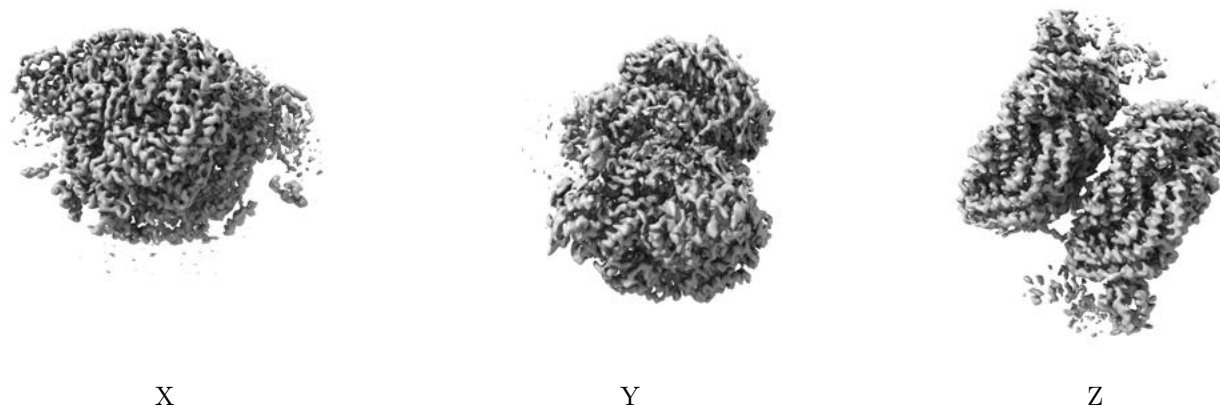
Z

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 0.5. 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.

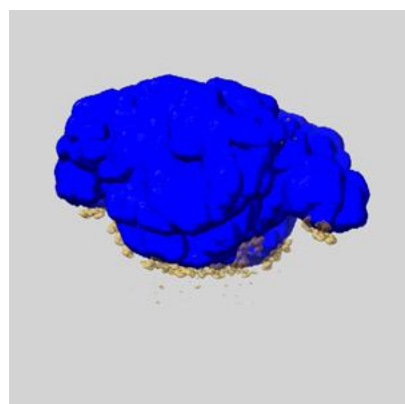
## 6.6 Mask visualisation [i](#)

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

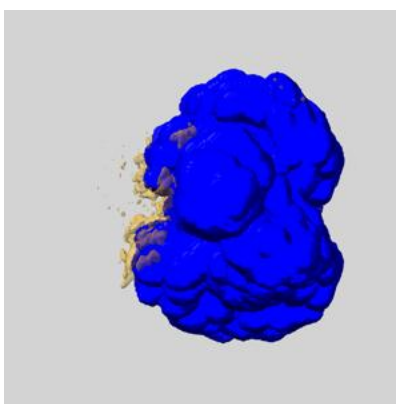
A mask typically either:

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

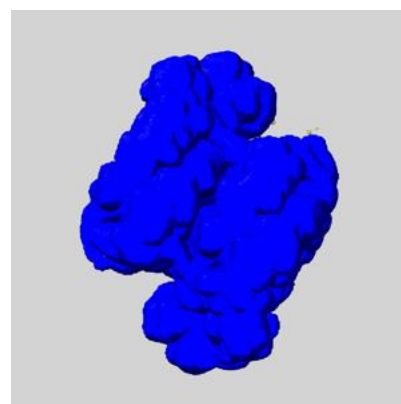
### 6.6.1 emd\_25033\_msk\_1.map [i](#)



X



Y

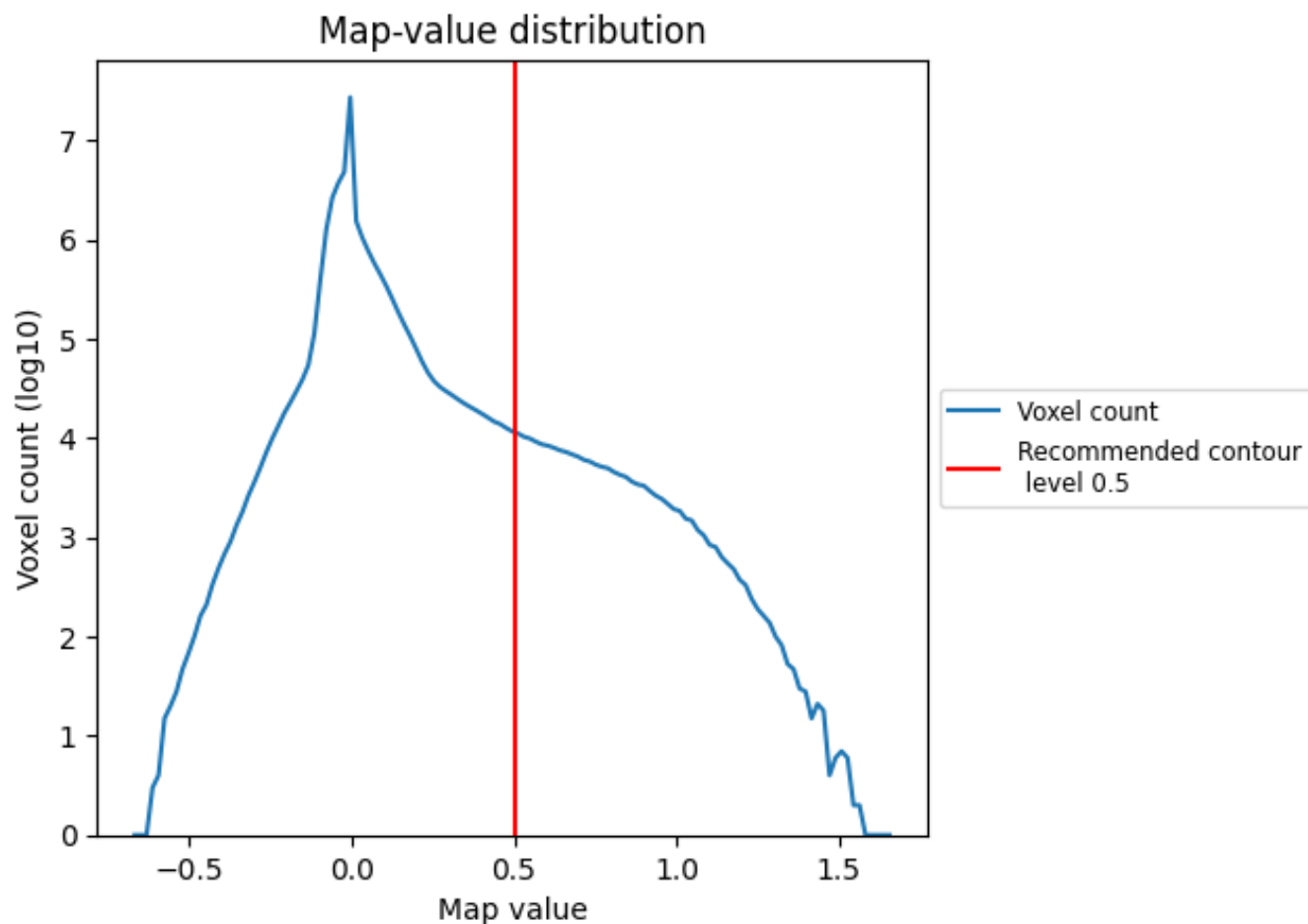


Z

## 7 Map analysis [i](#)

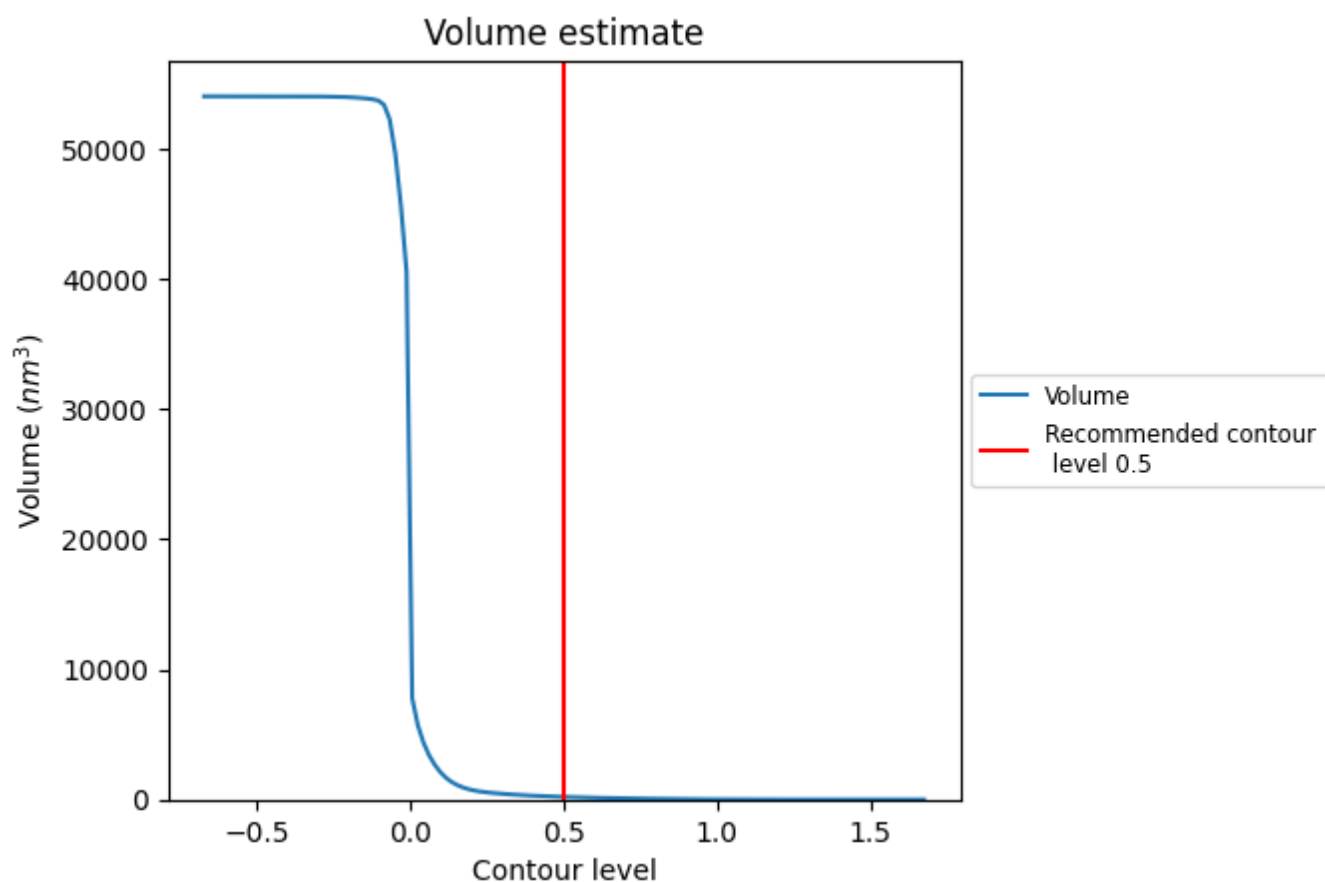
This section contains the results of statistical analysis of the map.

### 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](#)

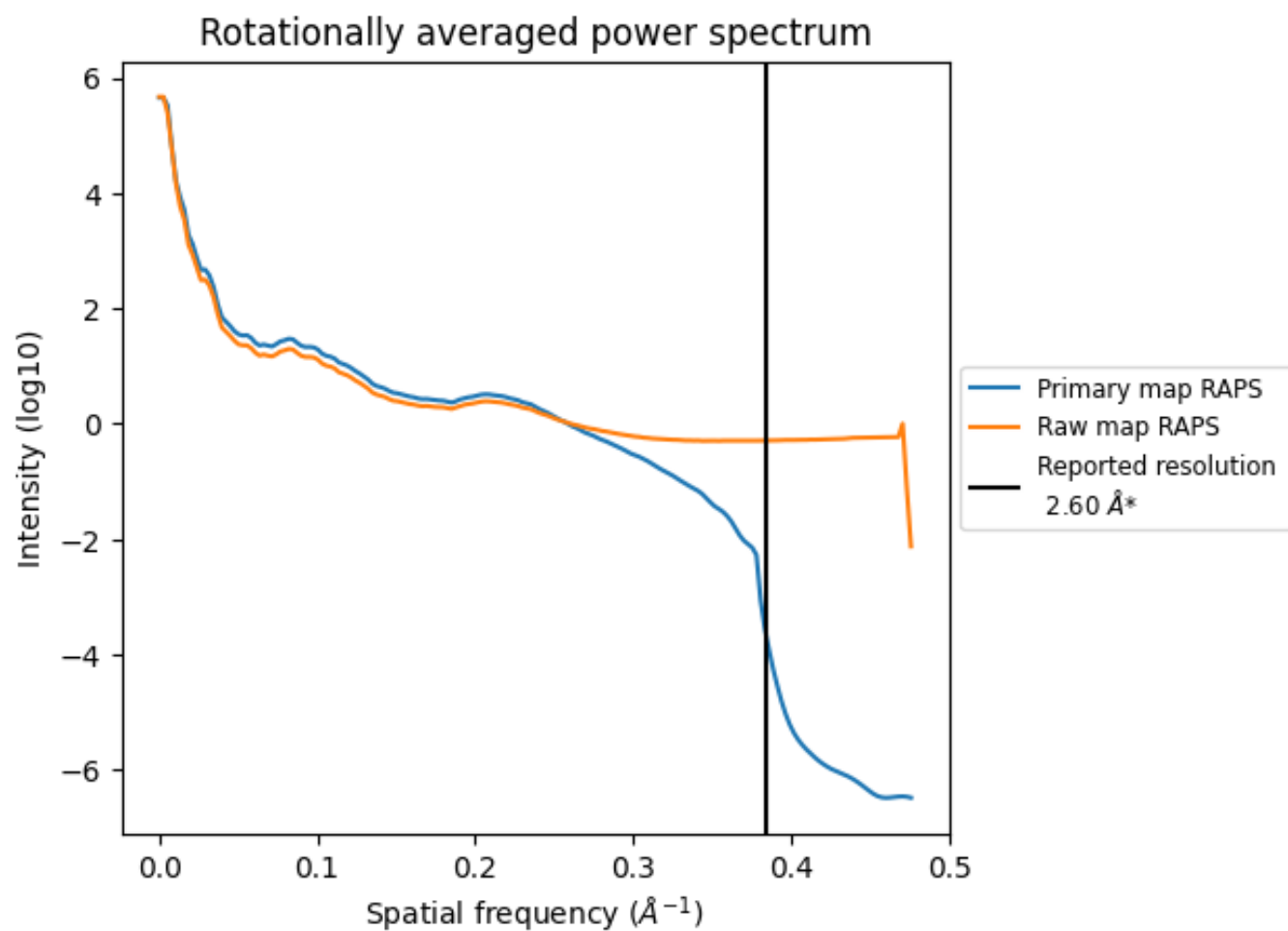


The volume at the recommended contour level is 205 nm<sup>3</sup>; this corresponds to an approximate mass of 185 kDa.

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



### 7.3 Rotationally averaged power spectrum ⓘ

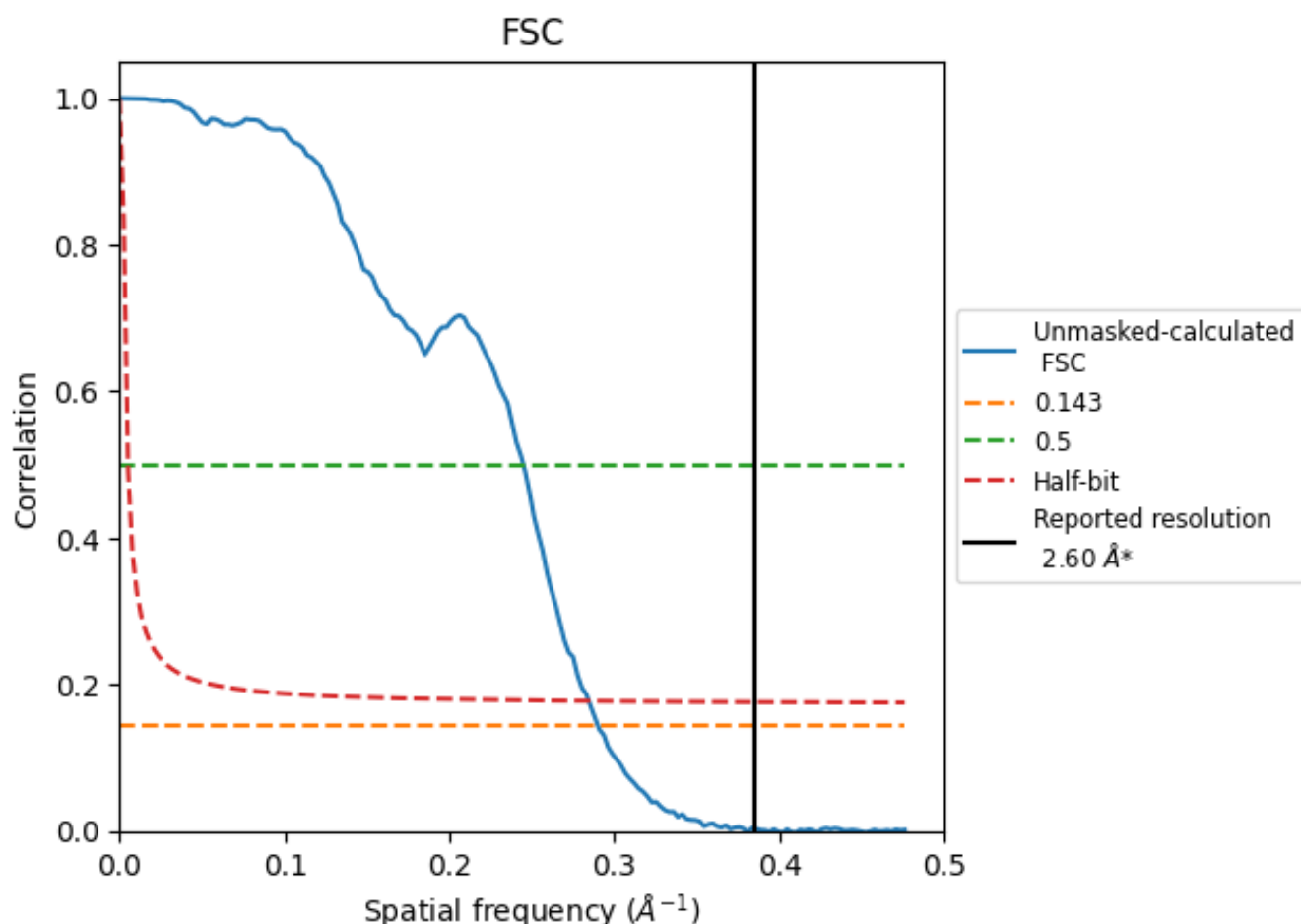


\*Reported resolution corresponds to spatial frequency of 0.385  $\text{\AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.385 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

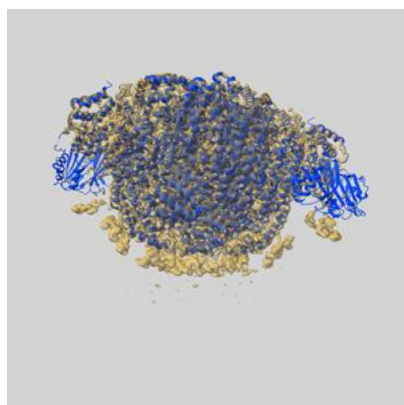
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.45	4.08	3.51

\*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 3.45 differs from the reported value 2.6 by more than 10 %

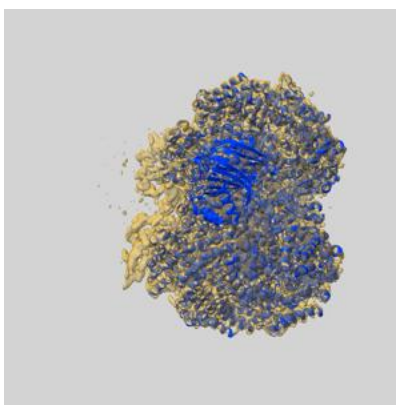
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-25033 and PDB model 7SCC. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

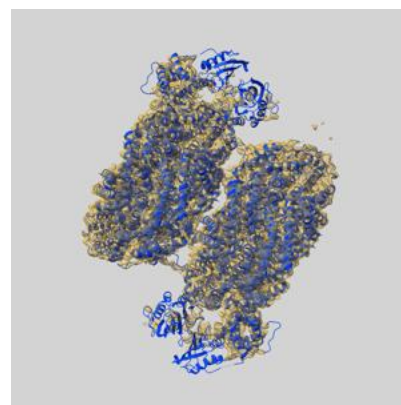
### 9.1 Map-model overlay [i](#)



X



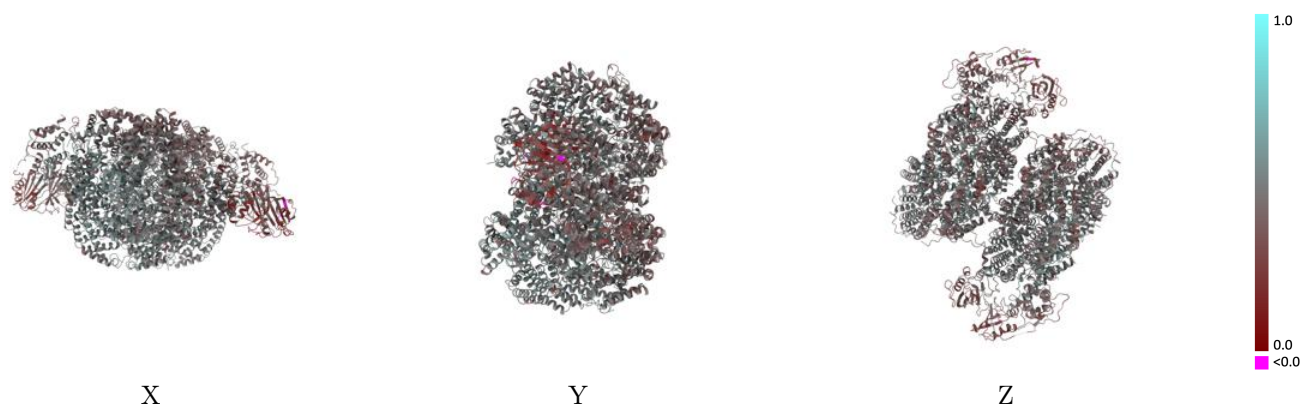
Y



Z

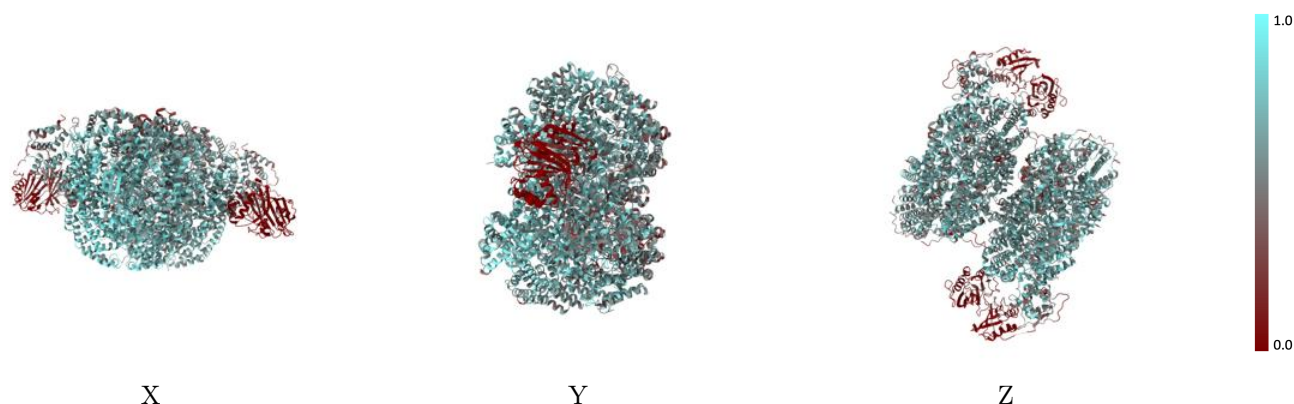
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



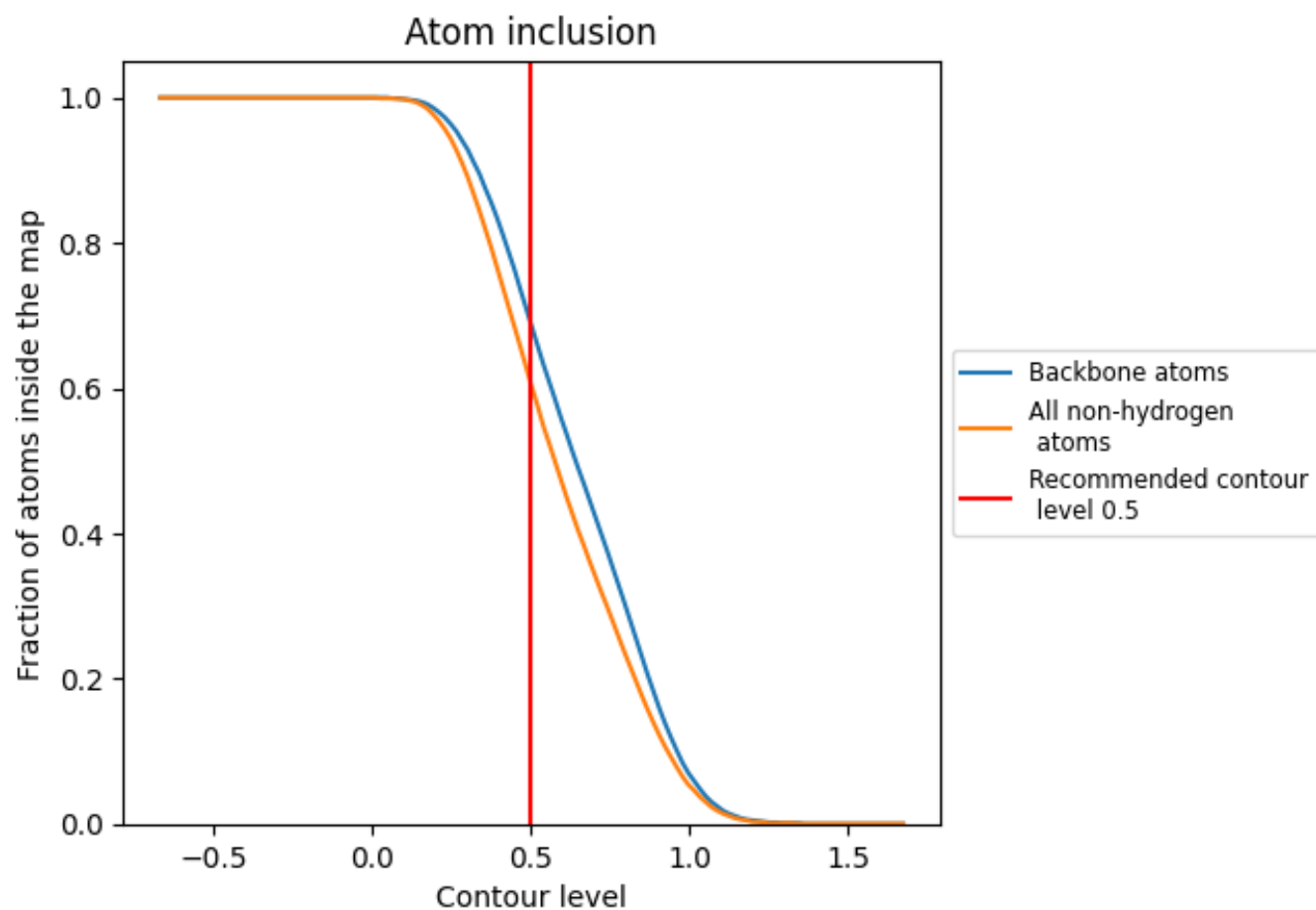
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.5).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 61% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6060	0.4580
AA	0.6340	0.4240
AB	0.6770	0.4710
AC	0.6150	0.4750
AD	0.6690	0.5090
AE	0.7330	0.5050
AF	0.7410	0.4830
AH	0.6070	0.4310
AI	0.5920	0.4300
AJ	0.6810	0.4540
AK	0.7250	0.4970
AL	0.7520	0.5130
AM	0.7050	0.4810
AO	0.7720	0.5160
AQ	0.7340	0.5210
AS	0.2790	0.3510
AT	0.0740	0.2930
AU	0.4140	0.3930
AV	0.5760	0.4550
AW	0.6540	0.4560
AX	0.6510	0.4580
AY	0.6460	0.4480
AZ	0.7380	0.5010
BA	0.7740	0.5090
BB	0.7820	0.5190
BD	0.6010	0.4120
BE	0.6300	0.4540
BF	0.7380	0.5000
BG	0.7450	0.5010
BH	0.7400	0.5060
BI	0.6560	0.4460
BK	0.7680	0.5360
BM	0.7180	0.5120
BO	0.0770	0.3340
BP	0.3060	0.3880



*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
BQ	 0.3980	 0.4230
BR	 0.5200	 0.4240