



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 10:52 AM UTC

PDB ID : 7SUT / pdb_00007sut
Title : Light harvesting phycobiliprotein HaPE645 from the cryptophyte *Hemiselmis andersenii* CCMP644
Authors : Rathbone, H.W.; Michie, K.A.; Laos, A.L.; Curmi, P.M.G.
Deposited on : 2021-11-18
Resolution : 1.49 Å (reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

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

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:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

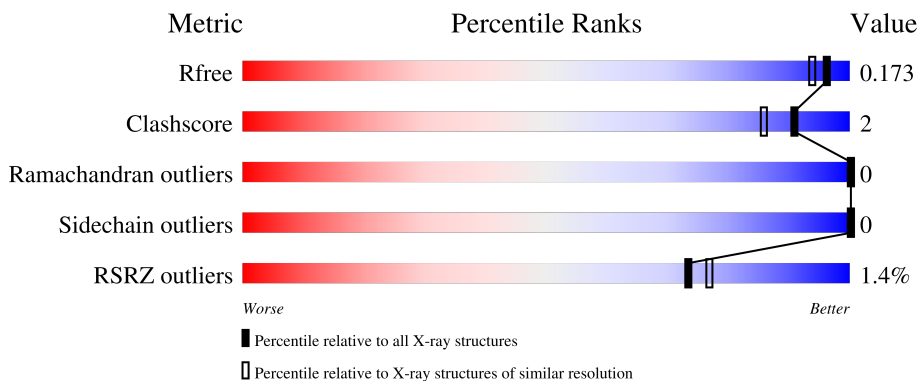
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.49 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.



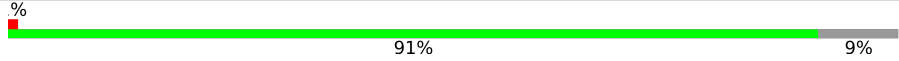
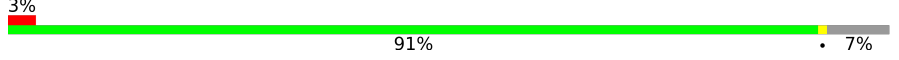
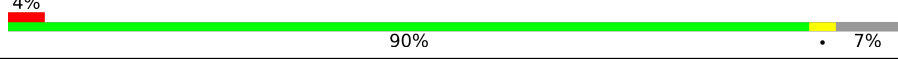
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	80	 94%
1	E	80	 94%
2	B	177	 93% 5%
2	D	177	 91% 9%
2	F	177	 95% 5%

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Mol	Chain	Length	Quality of chain
2	H	177	 <p>% 91% 9%</p>
3	C	68	 <p>3% 91% 7%</p>
3	G	68	 <p>4% 90% 7%</p>

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 16766 atoms, of which 8115 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 HaPE645 alpha-1 subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	78	Total	C	H	N	O	S	0	9	0
			1356	427	671	116	136	6			
1	E	78	Total	C	H	N	O	S	0	3	0
			1256	399	620	106	126	5			

- Molecule 2 is a protein called Phycoerythrin550 beta subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	174	Total	C	H	N	O	S	0	18	0
			2713	831	1362	231	279	10			
2	D	161	Total	C	H	N	O	S	0	4	0
			2395	737	1204	205	239	10			
2	F	176	Total	C	H	N	O	S	0	9	0
			2630	808	1324	222	265	11			
2	H	161	Total	C	H	N	O	S	0	6	0
			2396	737	1201	206	243	9			

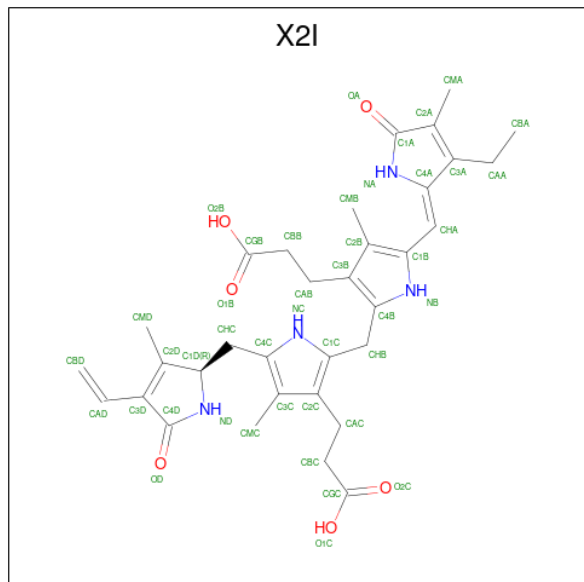
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	172	VAL	GLU	conflict	UNP U5T8W0
D	172	VAL	GLU	conflict	UNP U5T8W0
F	172	VAL	GLU	conflict	UNP U5T8W0
H	172	VAL	GLU	conflict	UNP U5T8W0

- Molecule 3 is a protein called HaPE645 alpha-2 subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	C	63	Total	C	H	N	O	S	0	2	0
			1046	325	525	90	100	6			
3	G	63	Total	C	H	N	O	S	0	4	0
			1075	335	537	92	105	6			

- Molecule 4 is (15,16)-DIHYDROBILIVERDIN (SINGLY LINKED) (CCD ID: X2I) (formula: $C_{33}H_{40}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	H	N			O
4	A	1	Total	C	H	N	O	0	0
			78	33	35	4	6		
4	C	1	Total	C	H	N	O	0	0
			78	33	35	4	6		
4	E	1	Total	C	H	N	O	0	0
			78	33	35	4	6		
4	G	1	Total	C	H	N	O	0	0
			78	33	35	4	6		

- Molecule 5 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).

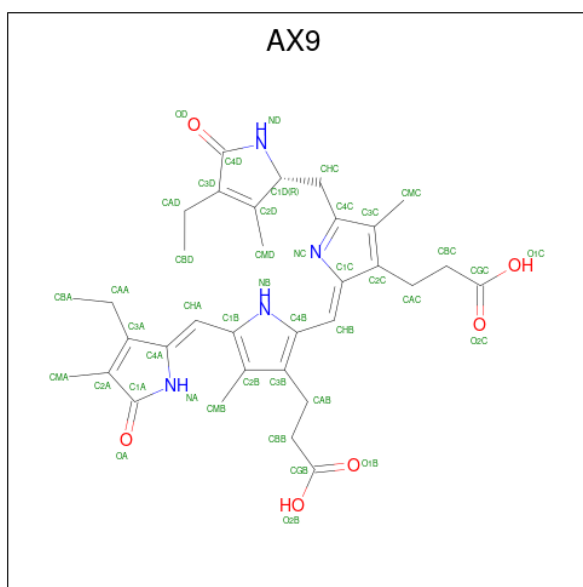


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
5	A	1	Total	C	H	O	0	0
			31	8	18	5		
5	H	1	Total	C	H	O	0	0
			31	8	18	5		

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

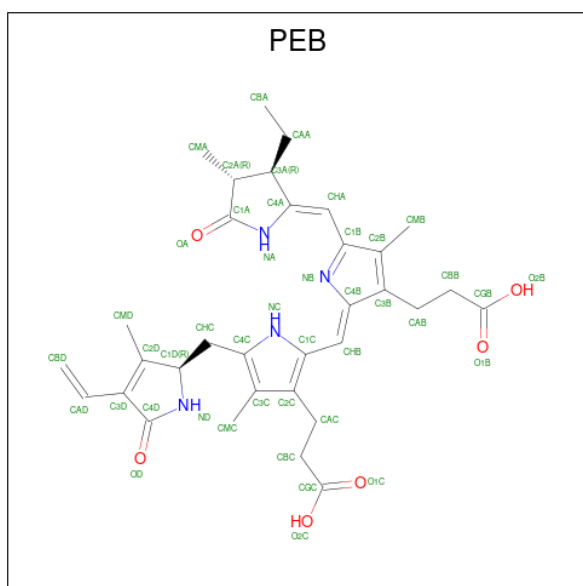
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Cl	0	0
			1	1		

- Molecule 7 is DiCys-(15,16)-Dihydrobiliverdin (CCD ID: AX9) (formula: C₃₃H₄₀N₄O₆) (labeled as "Ligand of Interest" by depositor).



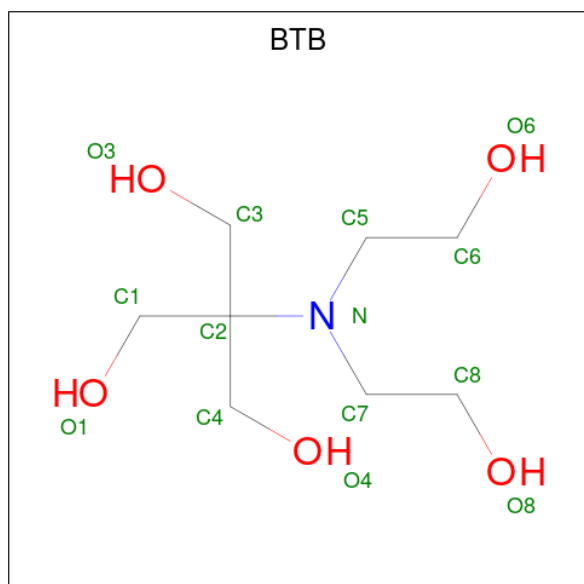
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
7	B	1	Total	C	H	N	O	0	1
			158	66	72	8	12		
7	D	1	Total	C	H	N	O	0	0
			79	33	36	4	6		
7	F	1	Total	C	H	N	O	0	0
			79	33	36	4	6		
7	H	1	Total	C	H	N	O	0	0
			79	33	36	4	6		

- Molecule 8 is PHYCOERYTHROBILIN (CCD ID: PEB) (formula: $C_{33}H_{40}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



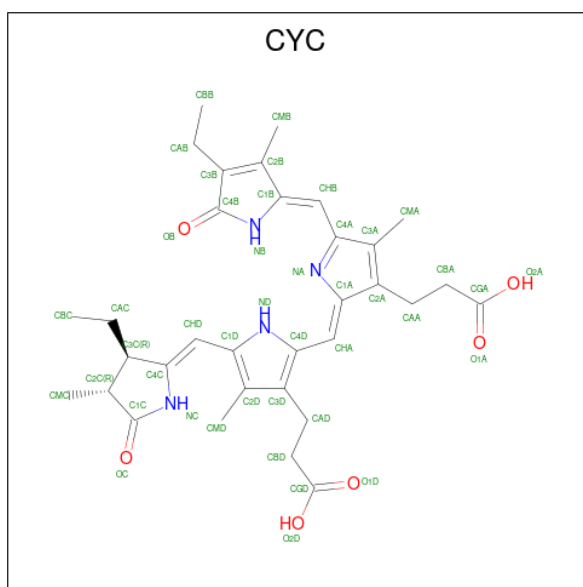
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
8	B	1	Total 80	C 33	H 37	N 4	O 6	0	0
8	B	1	Total 80	C 33	H 37	N 4	O 6	0	0
8	D	1	Total 80	C 33	H 37	N 4	O 6	0	0
8	F	1	Total 80	C 33	H 37	N 4	O 6	0	0
8	F	1	Total 80	C 33	H 37	N 4	O 6	0	0
8	H	1	Total 80	C 33	H 37	N 4	O 6	0	0

- Molecule 9 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (CCD ID: BTB) (formula: C₈H₁₉NO₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
9	B	1	Total 33	C 8	H 19	N 1	O 5	0	0

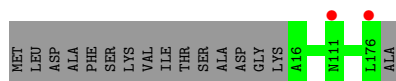
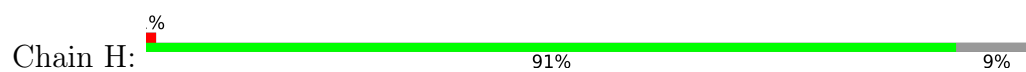
- Molecule 10 is PHYCOCYANOBILIN (CCD ID: CYC) (formula: C₃₃H₄₀N₄O₆) (labeled as "Ligand of Interest" by depositor).



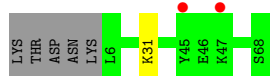
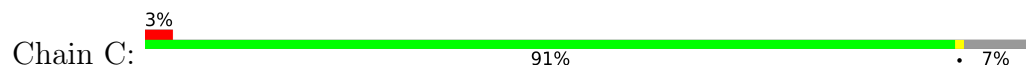
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	H	N			O
10	D	1	80	33	37	4	6	0	0
10	H	1	80	33	37	4	6	0	0

- Molecule 11 is water.

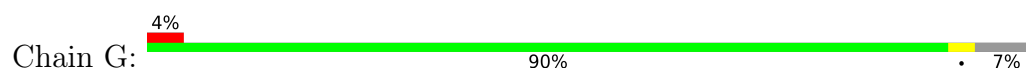
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	65	Total	O	0	1
			65	65		
11	B	80	Total	O	0	0
			80	80		
11	C	41	Total	O	0	0
			41	41		
11	D	82	Total	O	0	0
			82	82		
11	E	45	Total	O	0	0
			45	45		
11	F	58	Total	O	0	0
			58	58		
11	G	28	Total	O	0	1
			28	28		
11	H	57	Total	O	0	0
			57	57		



- Molecule 3: HaPE645 alpha-2 subunit



- Molecule 3: HaPE645 alpha-2 subunit



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.03Å 80.98Å 115.84Å 90.00° 92.21° 90.00°	Depositor
Resolution (Å)	41.43 – 1.49 41.43 – 1.49	Depositor EDS
% Data completeness (in resolution range)	93.3 (41.43-1.49) 87.8 (41.43-1.49)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.78 (at 1.49Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.145 , 0.175 0.144 , 0.173	Depositor DCC
R_{free} test set	1871 reflections (1.15%)	wwPDB-VP
Wilson B-factor (Å ²)	17.6	Xtrriage
Anisotropy	0.101	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 40.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.022 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	16766	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.27% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: CL, BTB, PEB, CYC, AX9, PG4, X2I

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	0.42	0/696	0.57	0/927
1	E	0.40	0/647	0.58	0/864
2	B	0.40	0/1395	0.56	0/1880
2	D	0.46	0/1211	0.62	0/1634
2	F	0.36	0/1345	0.55	0/1814
2	H	0.33	0/1222	0.51	0/1651
3	C	0.45	0/528	0.65	0/704
3	G	0.36	0/545	0.52	0/728
All	All	0.40	0/7589	0.57	0/10202

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	685	671	662	6	0
1	E	636	620	616	3	0
2	B	1351	1362	1315	11	0
2	D	1191	1204	1193	0	0
2	F	1306	1324	1297	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	1195	1201	1180	0	0
3	C	521	525	521	1	0
3	G	538	537	533	3	0
4	A	43	35	0	0	0
4	C	43	35	0	0	0
4	E	43	35	0	0	0
4	G	43	35	0	0	0
5	A	13	18	18	1	0
5	H	13	18	18	0	0
6	A	1	0	0	0	0
7	B	86	72	0	0	0
7	D	43	36	0	0	0
7	F	43	36	0	0	0
7	H	43	36	0	0	0
8	B	86	74	74	3	0
8	D	43	37	37	0	0
8	F	86	74	74	3	0
8	H	43	37	37	1	0
9	B	14	19	19	0	0
10	D	43	37	37	1	0
10	H	43	37	37	0	0
11	A	65	0	0	0	0
11	B	80	0	0	0	0
11	C	41	0	0	1	0
11	D	82	0	0	0	0
11	E	45	0	0	0	0
11	F	58	0	0	0	0
11	G	28	0	0	0	0
11	H	57	0	0	0	0
All	All	8651	8115	7668	27	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 2.

The worst 5 of 27 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:F:142:ILE:O	8:F:203:PEB:HAA2	2.04	0.58
8:H:203:PEB:HBA3	8:H:203:PEB:HHA1	1.86	0.57
1:A:6:LEU:CD1	2:B:12:ALA:HB1	2.35	0.56
1:A:43[B]:MET:HG3	2:B:9:ILE:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:11[B]:ILE:HD13	3:G:43:VAL:HG13	1.93	0.51

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 X-ray entries followed by that with respect to entries of similar resolution.

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	85/80 (106%)	81 (95%)	4 (5%)	0	100	100
1	E	79/80 (99%)	75 (95%)	4 (5%)	0	100	100
2	B	190/177 (107%)	186 (98%)	4 (2%)	0	100	100
2	D	163/177 (92%)	161 (99%)	2 (1%)	0	100	100
2	F	183/177 (103%)	181 (99%)	2 (1%)	0	100	100
2	H	165/177 (93%)	163 (99%)	2 (1%)	0	100	100
3	C	63/68 (93%)	63 (100%)	0	0	100	100
3	G	65/68 (96%)	64 (98%)	1 (2%)	0	100	100
All	All	993/1004 (99%)	974 (98%)	19 (2%)	0	100	100

There are no Ramachandran outliers to report.

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 X-ray entries followed by that with respect to entries of similar resolution.

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	77/70 (110%)	77 (100%)	0	100	100
1	E	71/70 (101%)	71 (100%)	0	100	100
2	B	155/140 (111%)	155 (100%)	0	100	100
2	D	132/140 (94%)	132 (100%)	0	100	100
2	F	147/140 (105%)	147 (100%)	0	100	100
2	H	134/140 (96%)	134 (100%)	0	100	100
3	C	57/60 (95%)	57 (100%)	0	100	100
3	G	59/60 (98%)	59 (100%)	0	100	100
All	All	832/820 (102%)	832 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	145	ASN
2	F	25	GLN
2	F	145	ASN
2	H	111	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](#)

Of 21 ligands modelled in this entry, 1 is monoatomic - leaving 20 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	CYC	H	202	2	46,46,46	2.81	12 (26%)	63,67,67	2.16	14 (22%)
7	AX9	B	201[B]	2	45,46,46	1.81	7 (15%)	54,67,67	1.20	5 (9%)
8	PEB	F	203	2	46,46,46	4.11	33 (71%)	56,67,67	2.01	17 (30%)
4	X2I	E	101	1	46,46,46	1.59	7 (15%)	59,67,67	1.64	16 (27%)
8	PEB	H	203	2	46,46,46	3.93	32 (69%)	56,67,67	2.29	22 (39%)
5	PG4	A	102	-	12,12,12	0.17	0	11,11,11	0.59	0
8	PEB	B	202	2	46,46,46	3.78	33 (71%)	56,67,67	2.11	18 (32%)
7	AX9	B	201[A]	2	45,46,46	1.79	7 (15%)	54,67,67	1.22	6 (11%)
7	AX9	D	201	2	45,46,46	1.67	8 (17%)	54,67,67	1.15	7 (12%)
4	X2I	C	101	3	46,46,46	1.59	7 (15%)	59,67,67	1.50	11 (18%)
8	PEB	D	203	2	46,46,46	3.48	30 (65%)	56,67,67	1.87	18 (32%)
4	X2I	A	101	1	46,46,46	1.45	5 (10%)	59,67,67	1.63	15 (25%)
10	CYC	D	202	2	46,46,46	2.48	11 (23%)	63,67,67	2.41	16 (25%)
8	PEB	B	203	2	46,46,46	3.60	31 (67%)	56,67,67	1.97	21 (37%)
5	PG4	H	204	-	12,12,12	0.16	0	11,11,11	0.61	0
4	X2I	G	101	3	46,46,46	1.64	7 (15%)	59,67,67	1.73	15 (25%)
8	PEB	F	202	2	46,46,46	4.33	34 (73%)	56,67,67	2.20	24 (42%)
9	BTB	B	204	-	13,13,13	0.63	0	7,16,16	0.41	0
7	AX9	H	201	2	45,46,46	1.82	9 (20%)	54,67,67	1.09	3 (5%)
7	AX9	F	201	2	45,46,46	1.79	8 (17%)	54,67,67	1.29	5 (9%)

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	H	202	2	-	6/26/74/74	0/4/4/4
7	AX9	B	201[B]	2	-	4/26/74/74	0/4/4/4
8	PEB	F	203	2	-	5/26/74/74	0/4/4/4
4	X2I	E	101	1	-	7/26/58/58	0/4/4/4
8	PEB	H	203	2	-	7/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PG4	A	102	-	-	4/10/10/10	-
8	PEB	B	202	2	-	4/26/74/74	0/4/4/4
7	AX9	B	201[A]	2	-	7/26/74/74	0/4/4/4
7	AX9	D	201	2	-	5/26/74/74	0/4/4/4
4	X2I	C	101	3	-	7/26/58/58	0/4/4/4
8	PEB	D	203	2	-	6/26/74/74	0/4/4/4
4	X2I	A	101	1	-	7/26/58/58	0/4/4/4
10	CYC	D	202	2	-	8/26/74/74	0/4/4/4
8	PEB	B	203	2	-	4/26/74/74	0/4/4/4
5	PG4	H	204	-	-	1/10/10/10	-
4	X2I	G	101	3	-	6/26/58/58	0/4/4/4
8	PEB	F	202	2	-	6/26/74/74	0/4/4/4
9	BTB	B	204	-	-	0/21/21/21	-
7	AX9	H	201	2	-	4/26/74/74	0/4/4/4
7	AX9	F	201	2	-	4/26/74/74	0/4/4/4

The worst 5 of 281 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	H	202	CYC	C1C-NC	-9.77	1.24	1.37
10	D	202	CYC	C1C-NC	-9.12	1.25	1.37
8	F	202	PEB	C4D-ND	8.94	1.46	1.35
8	F	202	PEB	CHB-C1C	8.88	1.60	1.40
8	F	202	PEB	C1A-NA	8.87	1.49	1.37

The worst 5 of 233 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	202	CYC	OC-C1C-C2C	-9.88	118.32	126.17
10	D	202	CYC	C2C-C1C-NC	8.10	115.03	108.29
10	H	202	CYC	C2C-C1C-NC	8.01	114.95	108.29
10	H	202	CYC	OC-C1C-C2C	-7.87	119.91	126.17
10	D	202	CYC	C3C-C4C-NC	5.97	115.63	107.94

There are no chirality outliers.

5 of 102 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	202	PEB	NB-C1B-CHA-C4A

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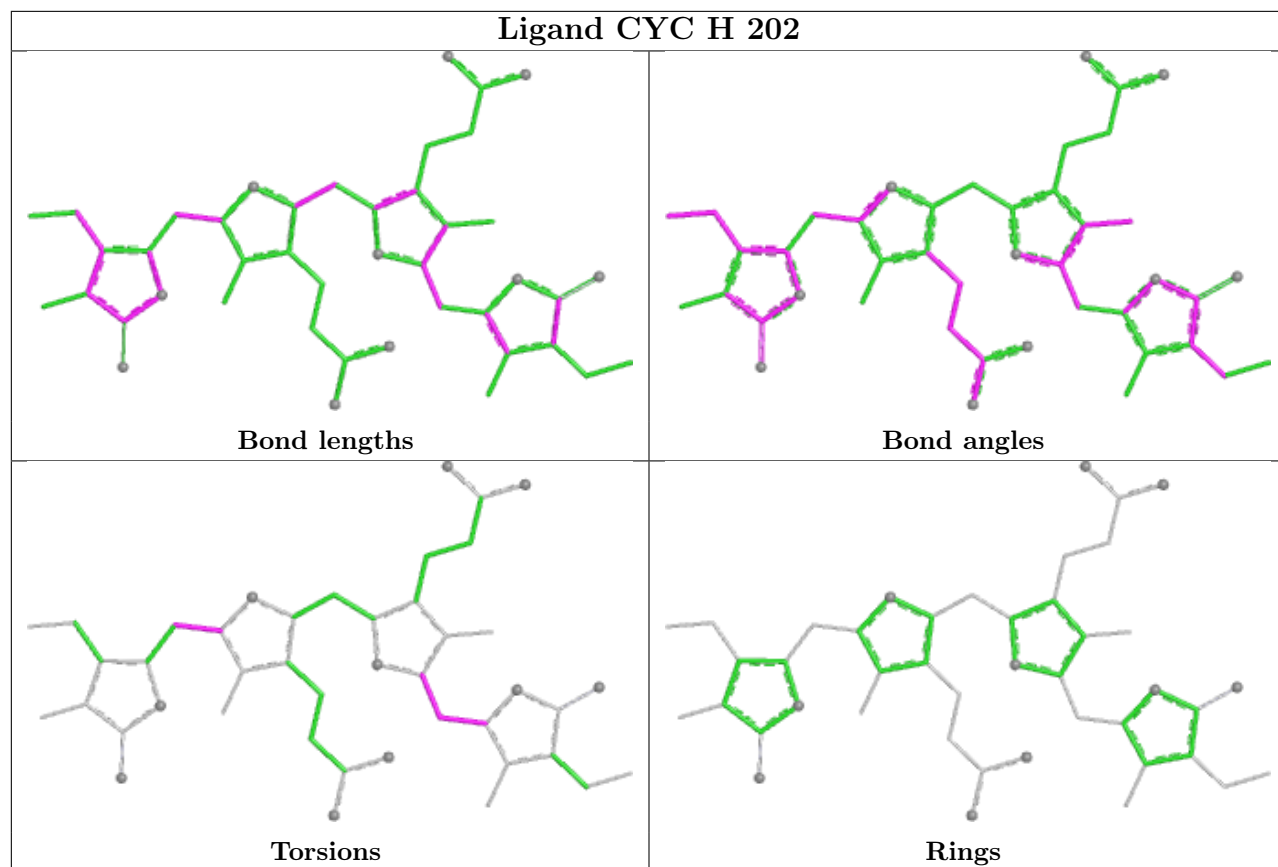
Mol	Chain	Res	Type	Atoms
8	B	202	PEB	C2B-C1B-CHA-C4A
8	B	203	PEB	NB-C1B-CHA-C4A
8	B	203	PEB	C2B-C1B-CHA-C4A
8	D	203	PEB	NA-C4A-CHA-C1B

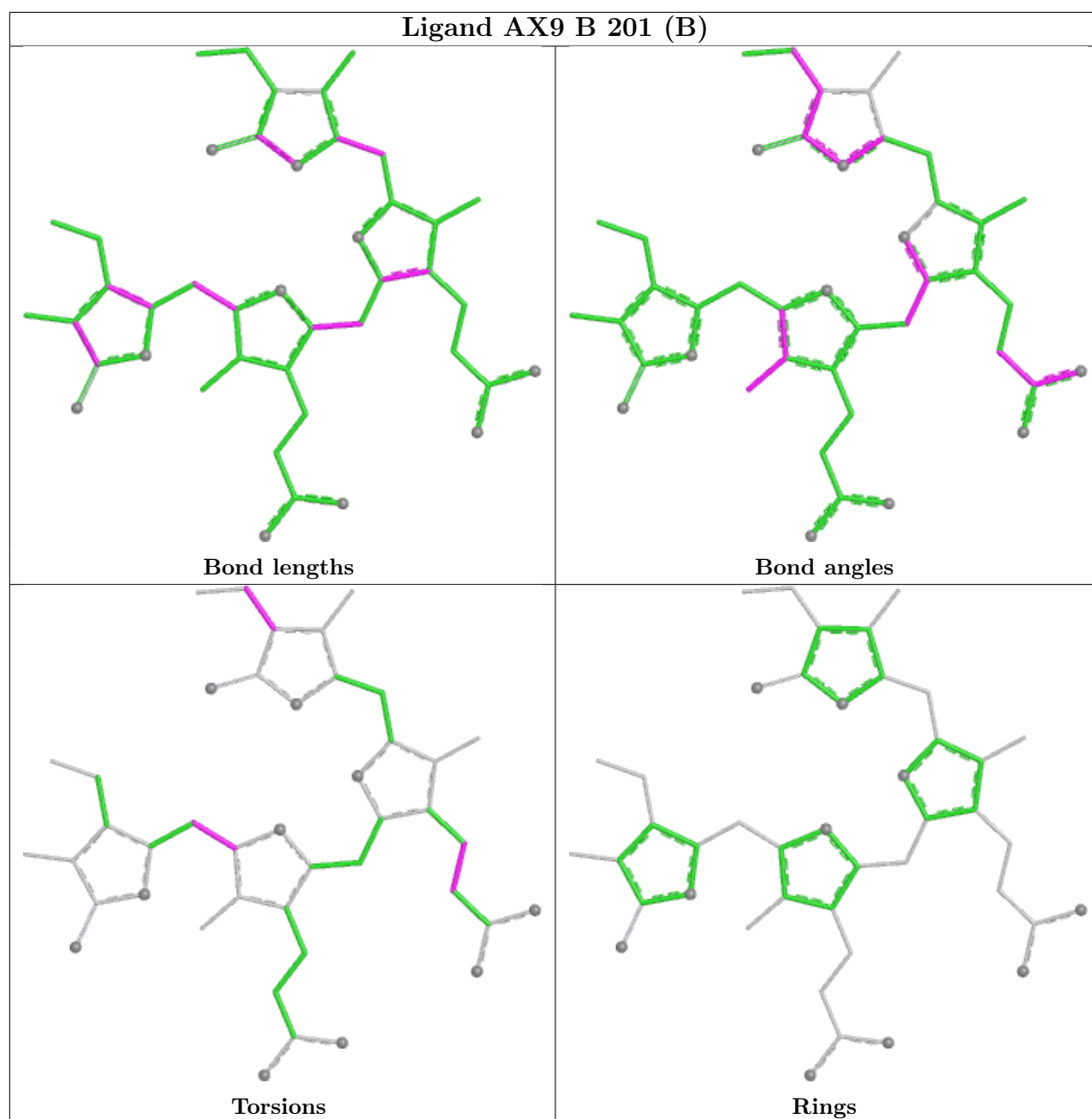
There are no ring outliers.

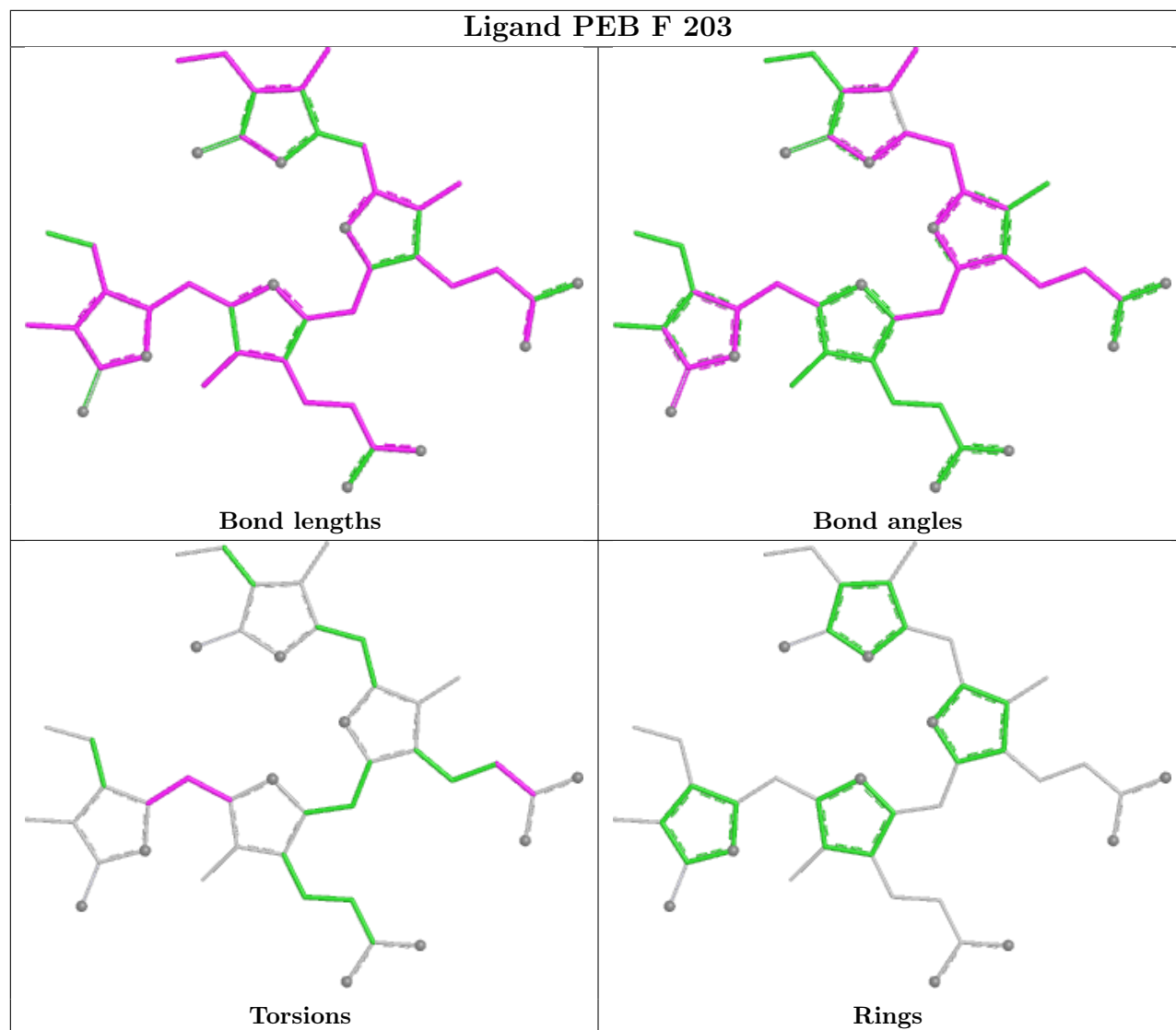
7 monomers are involved in 9 short contacts:

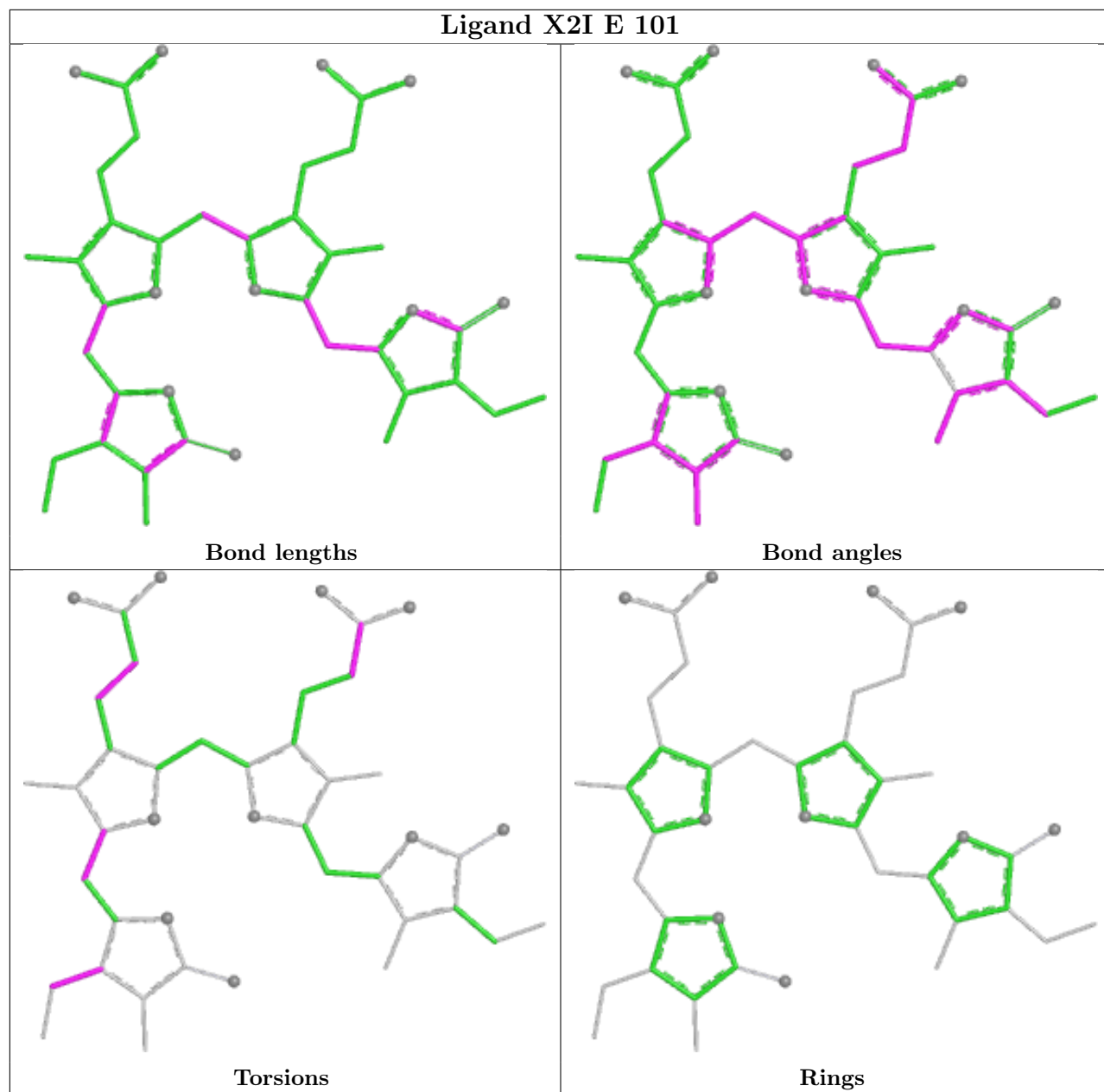
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	F	203	PEB	2	0
8	H	203	PEB	1	0
5	A	102	PG4	1	0
8	B	202	PEB	1	0
10	D	202	CYC	1	0
8	B	203	PEB	2	0
8	F	202	PEB	1	0

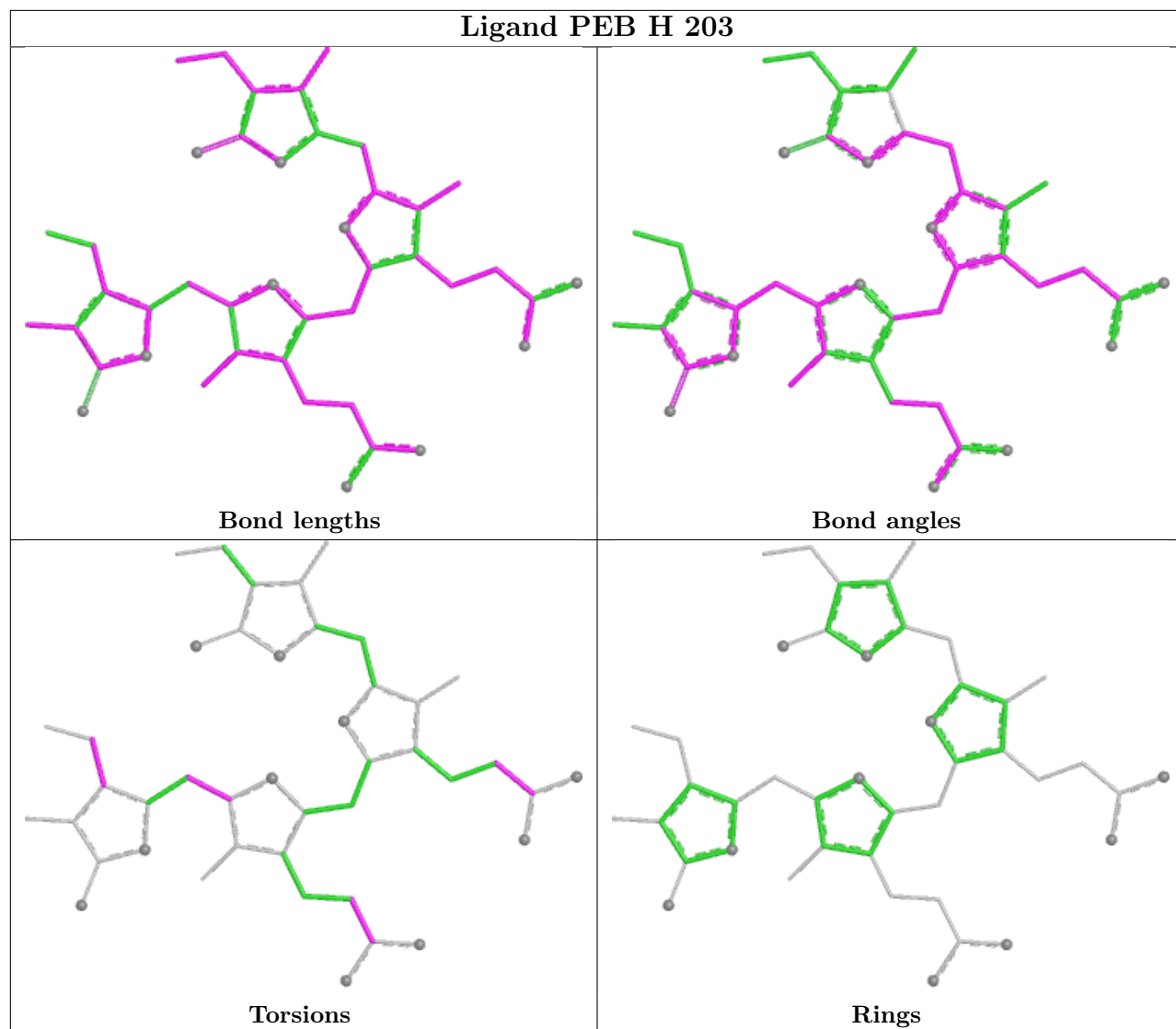
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

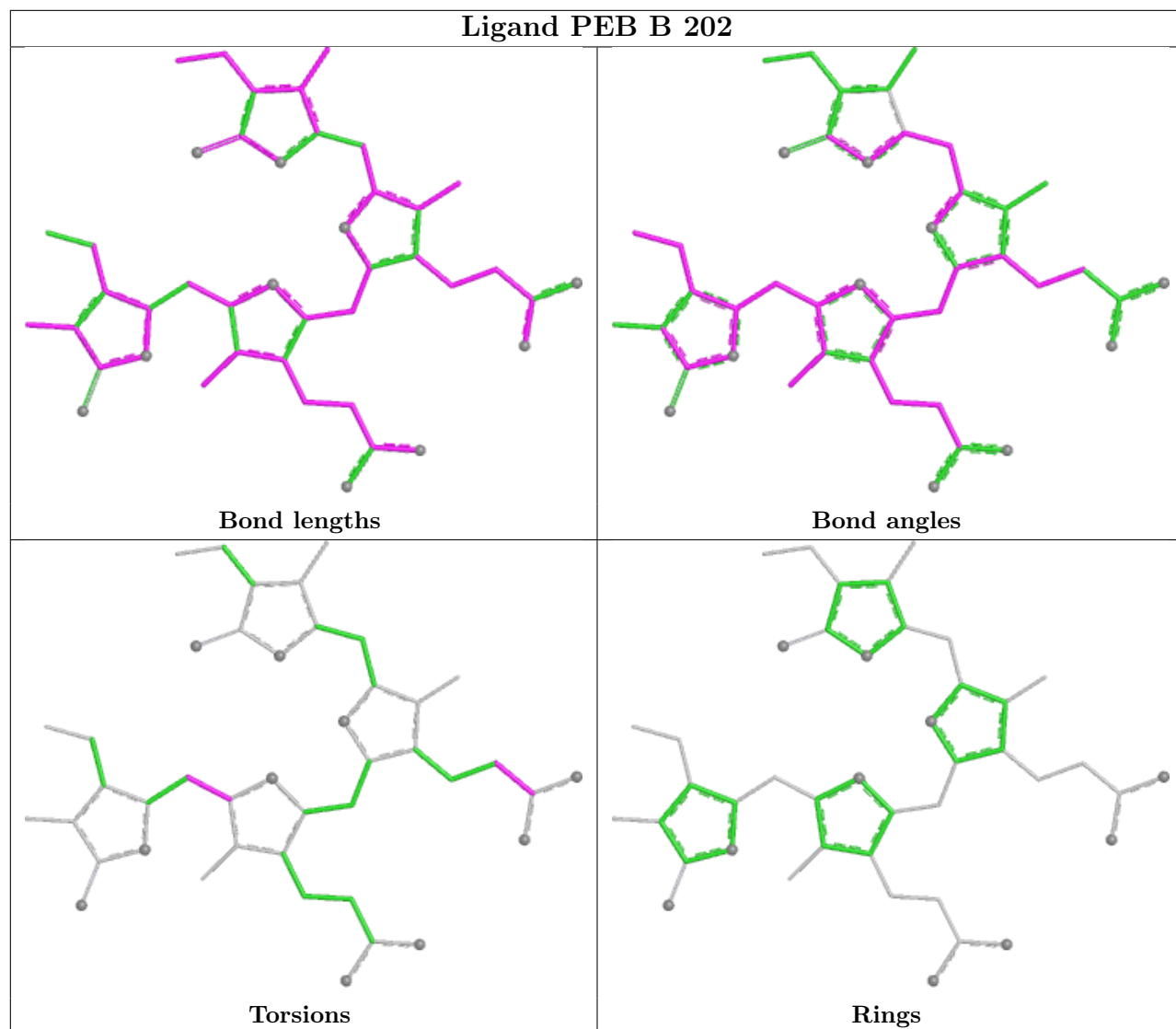


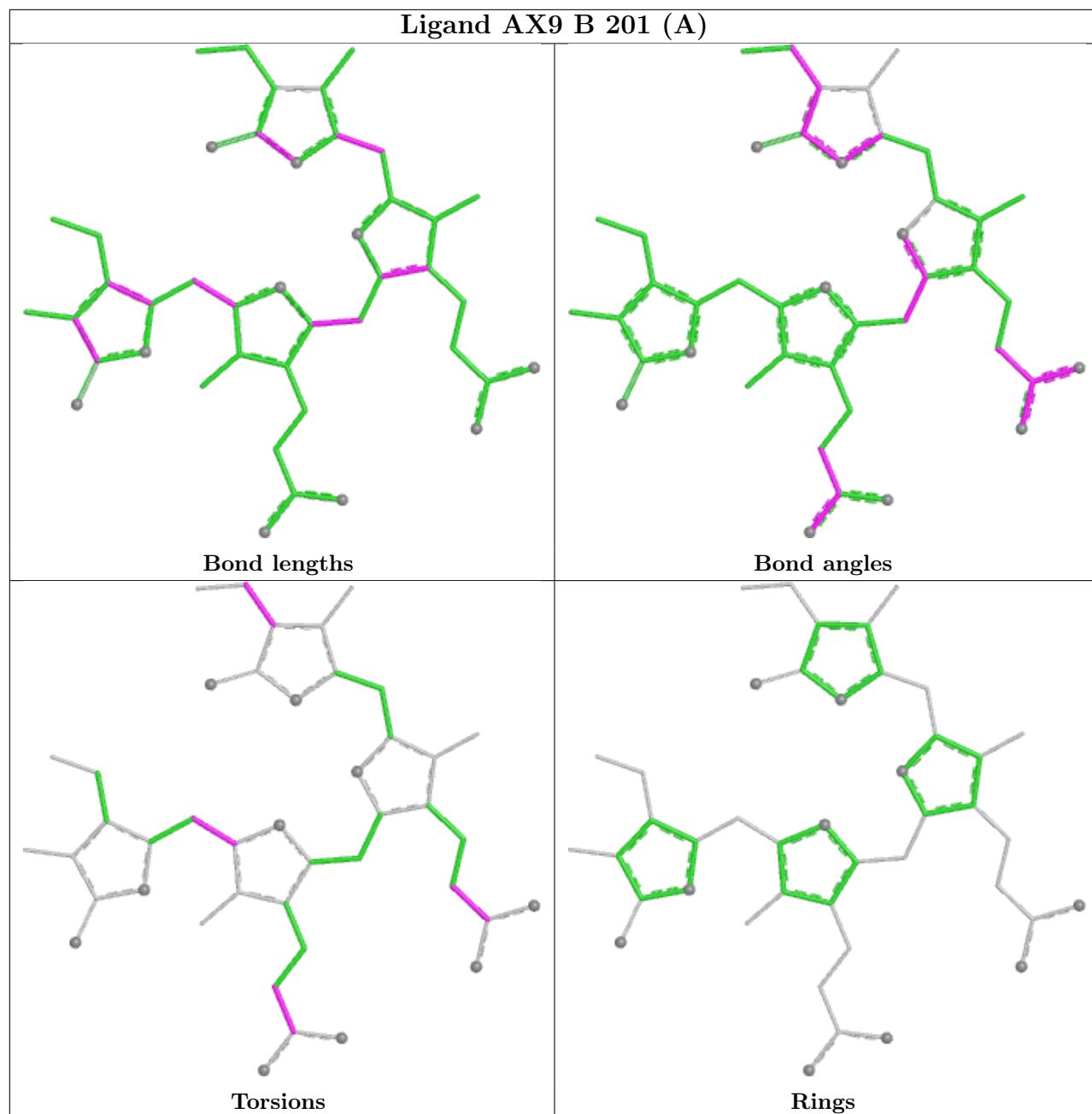


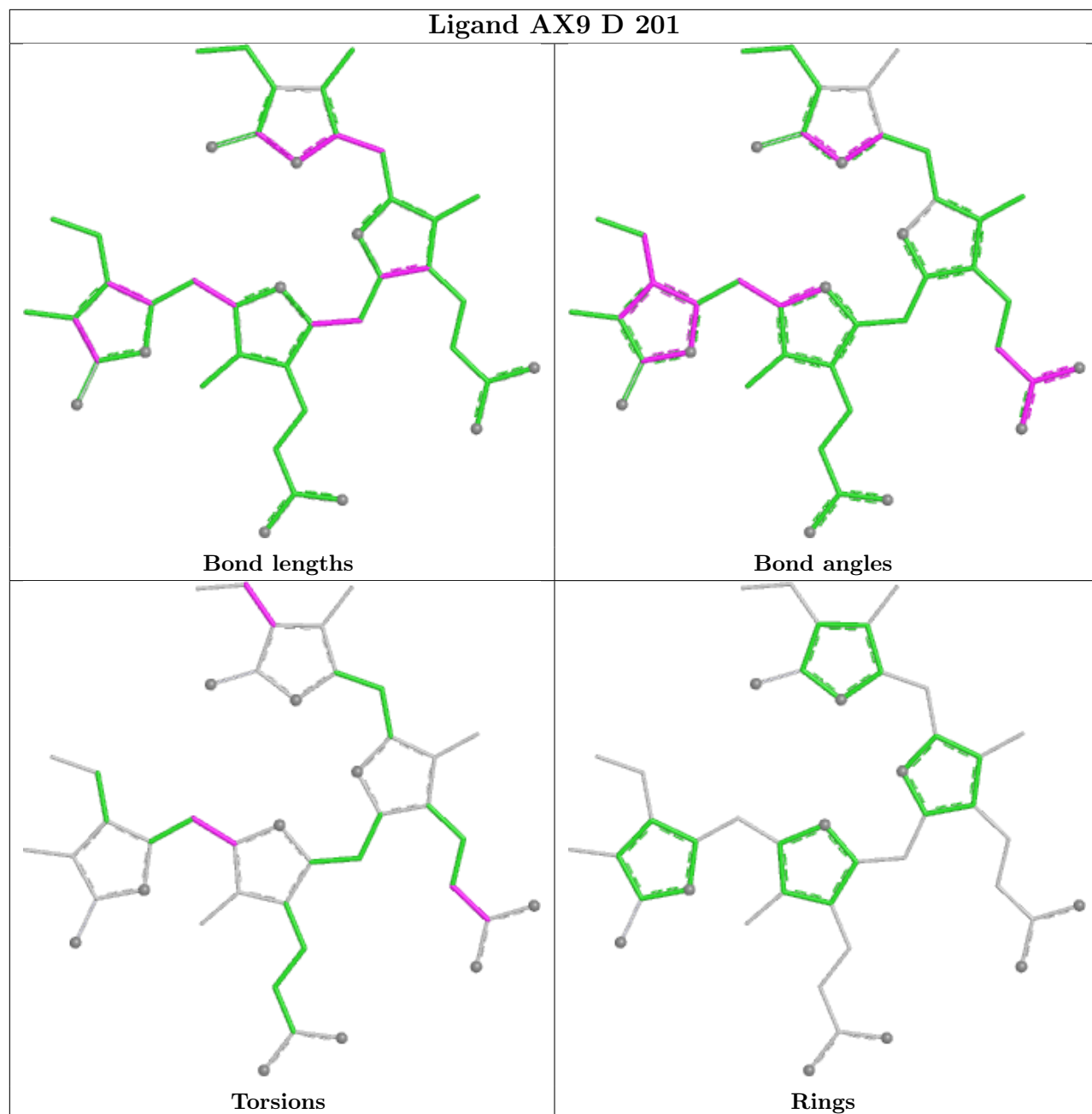


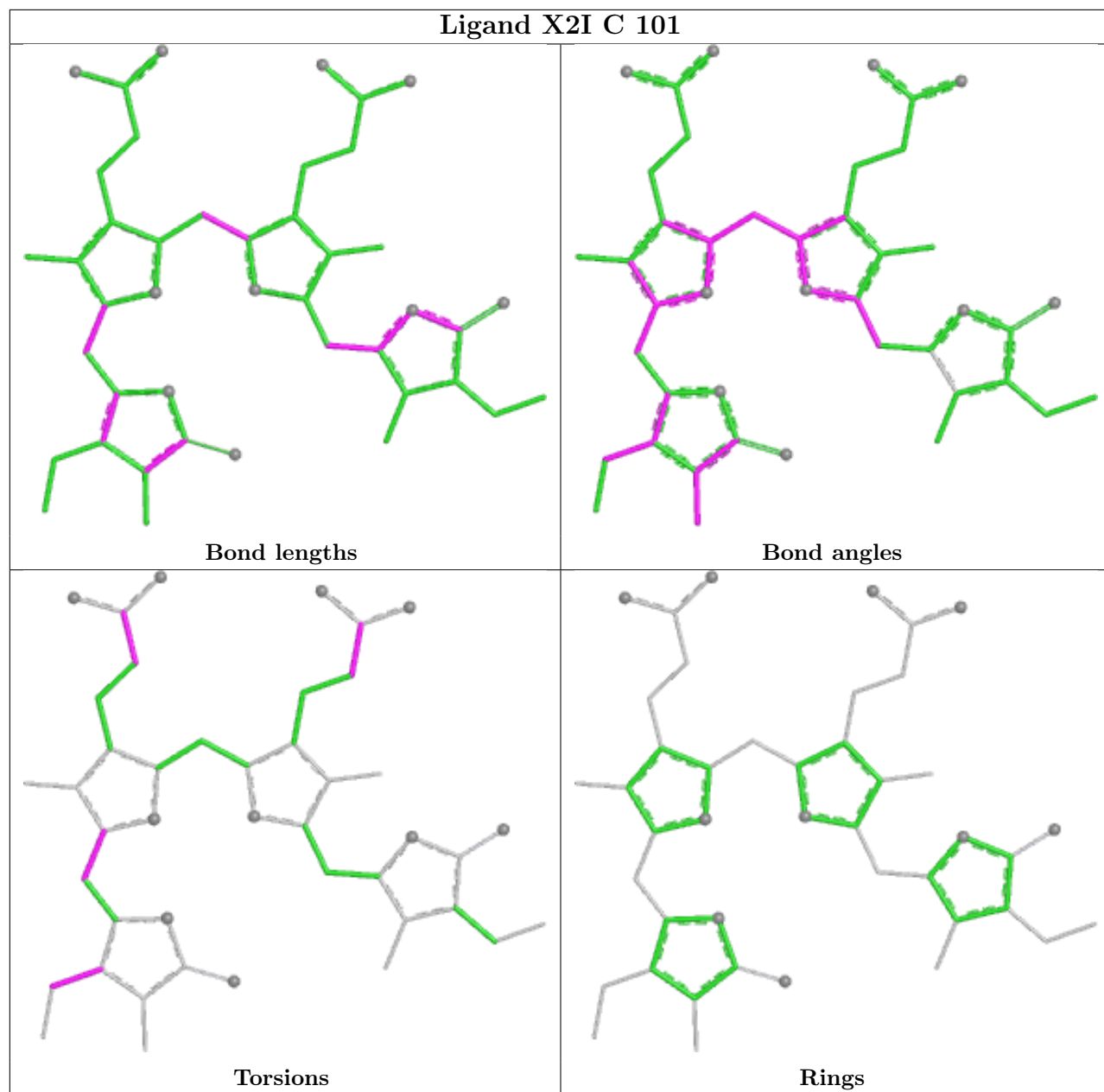


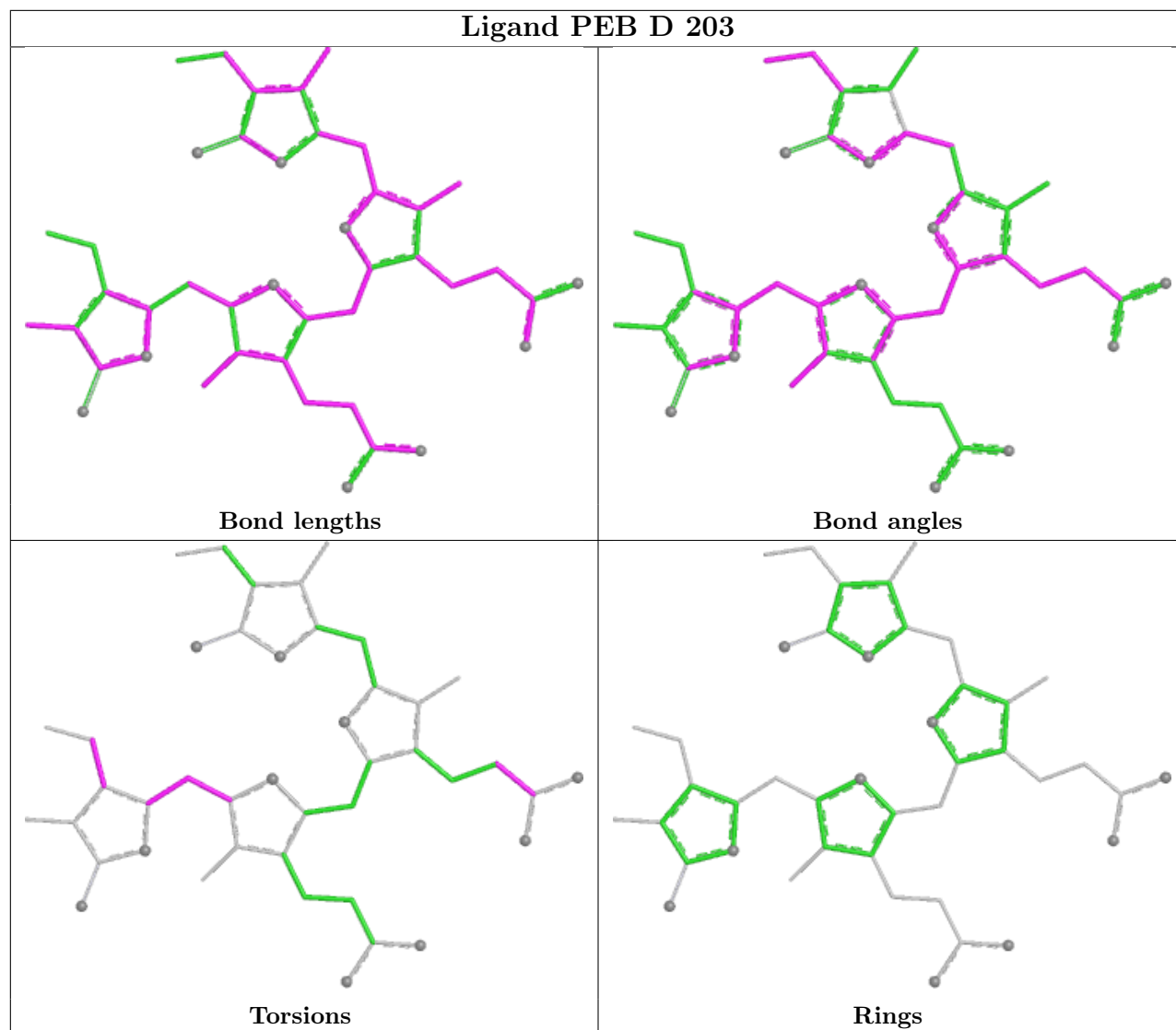


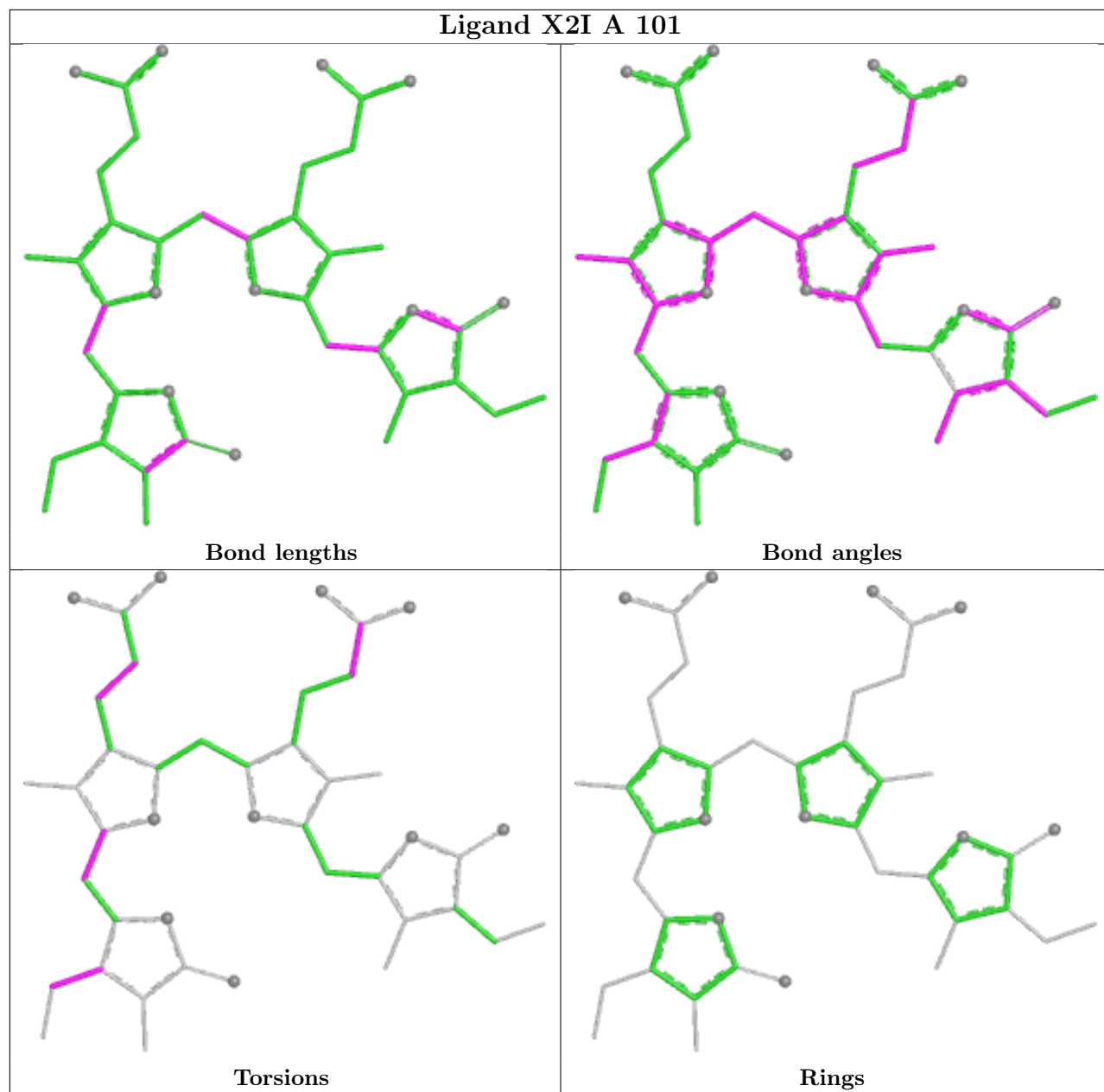


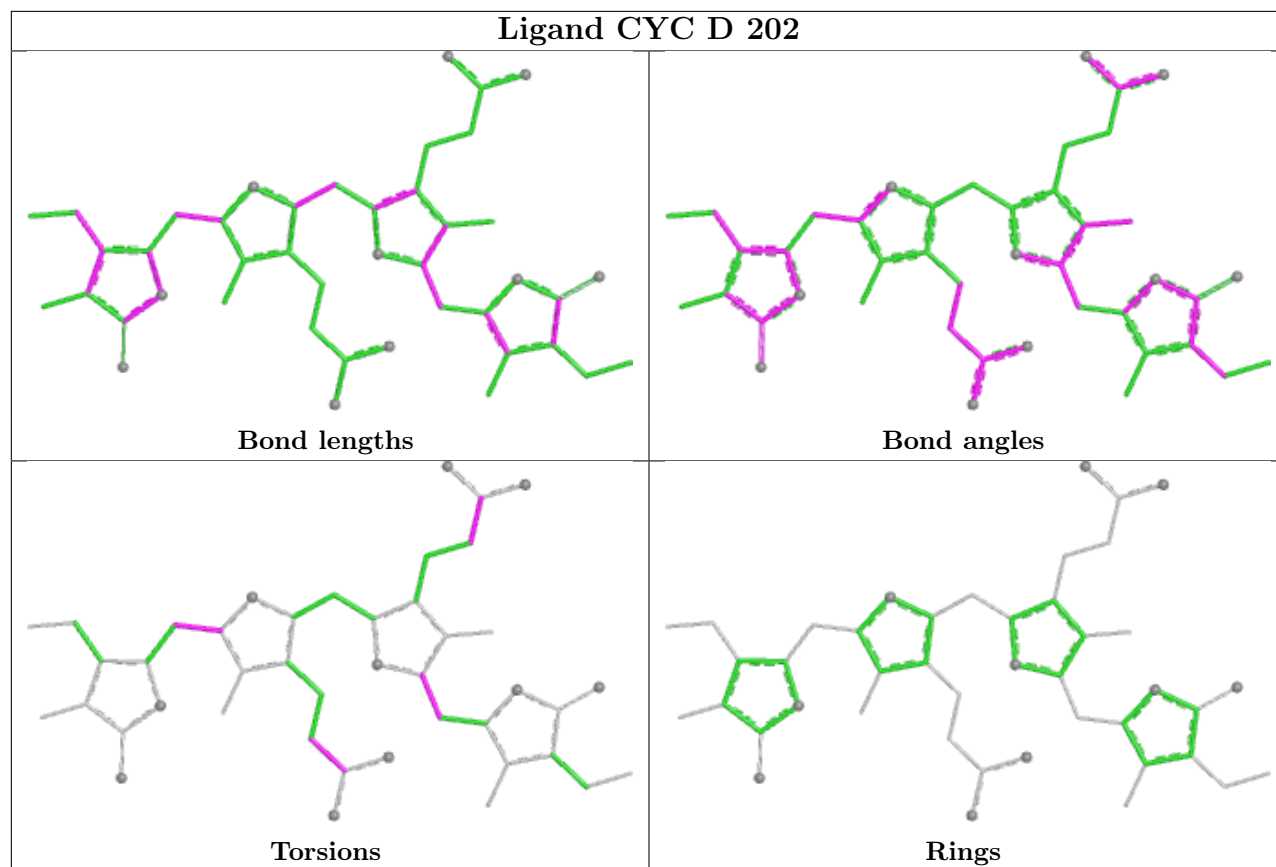


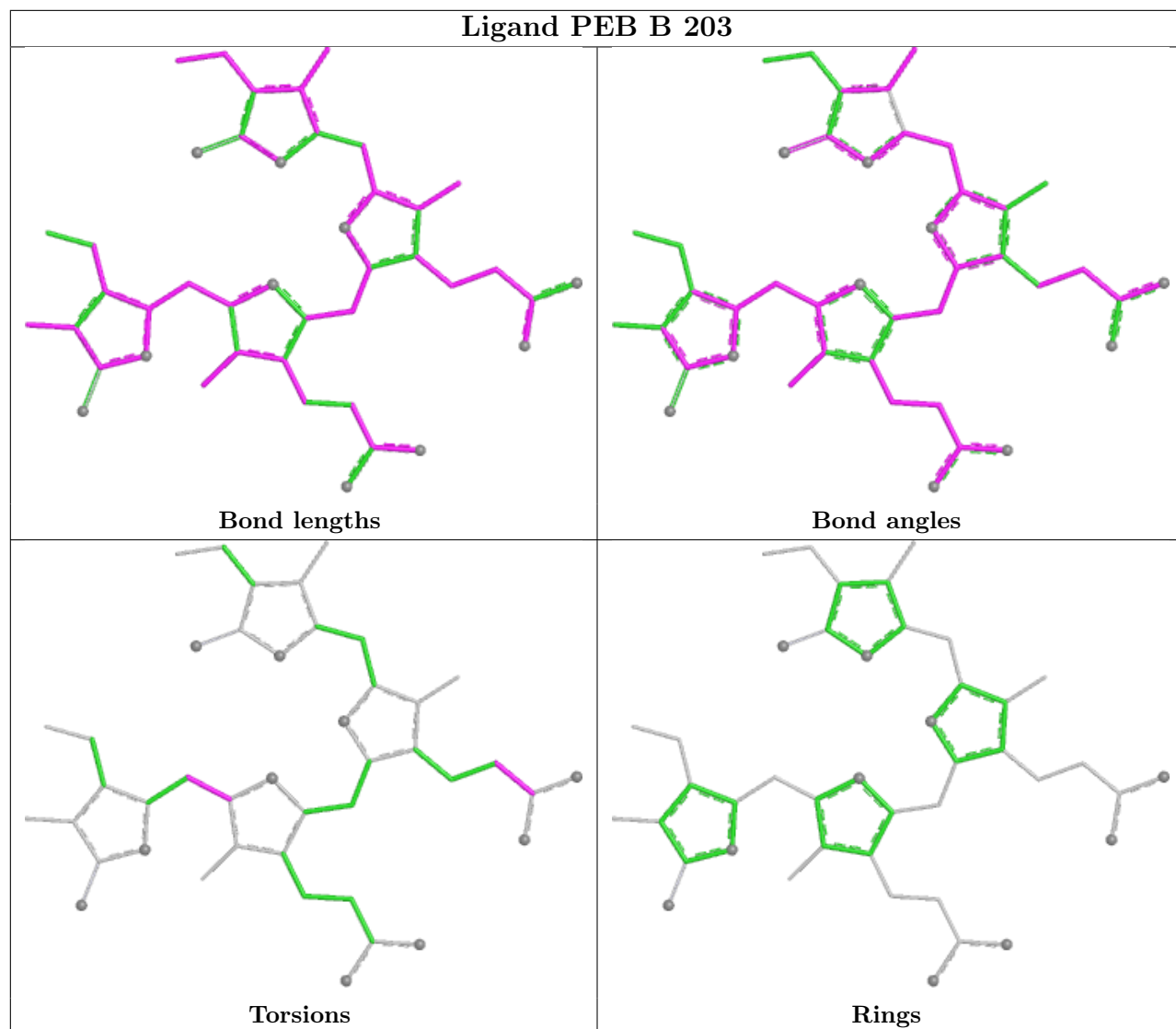


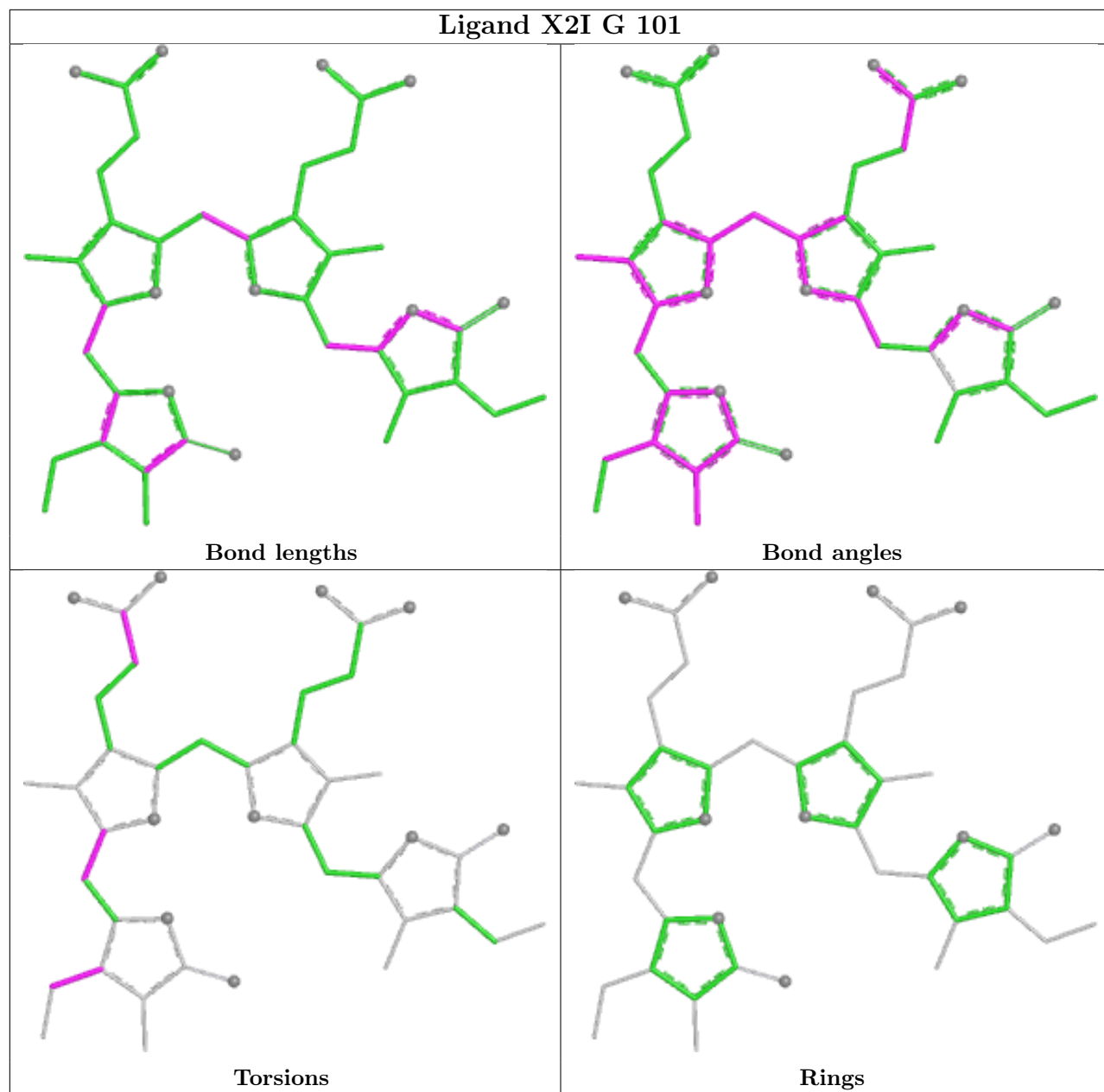


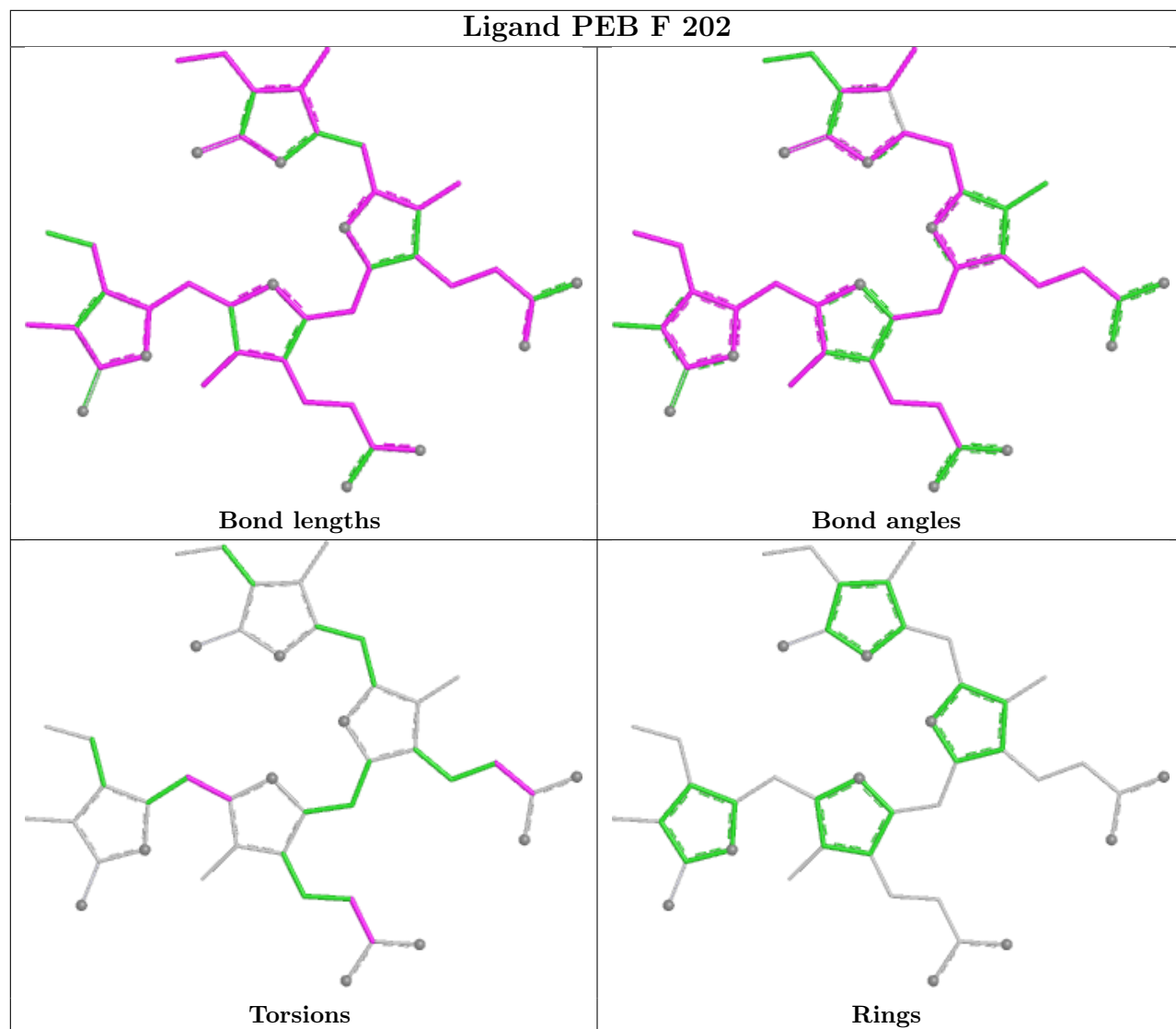


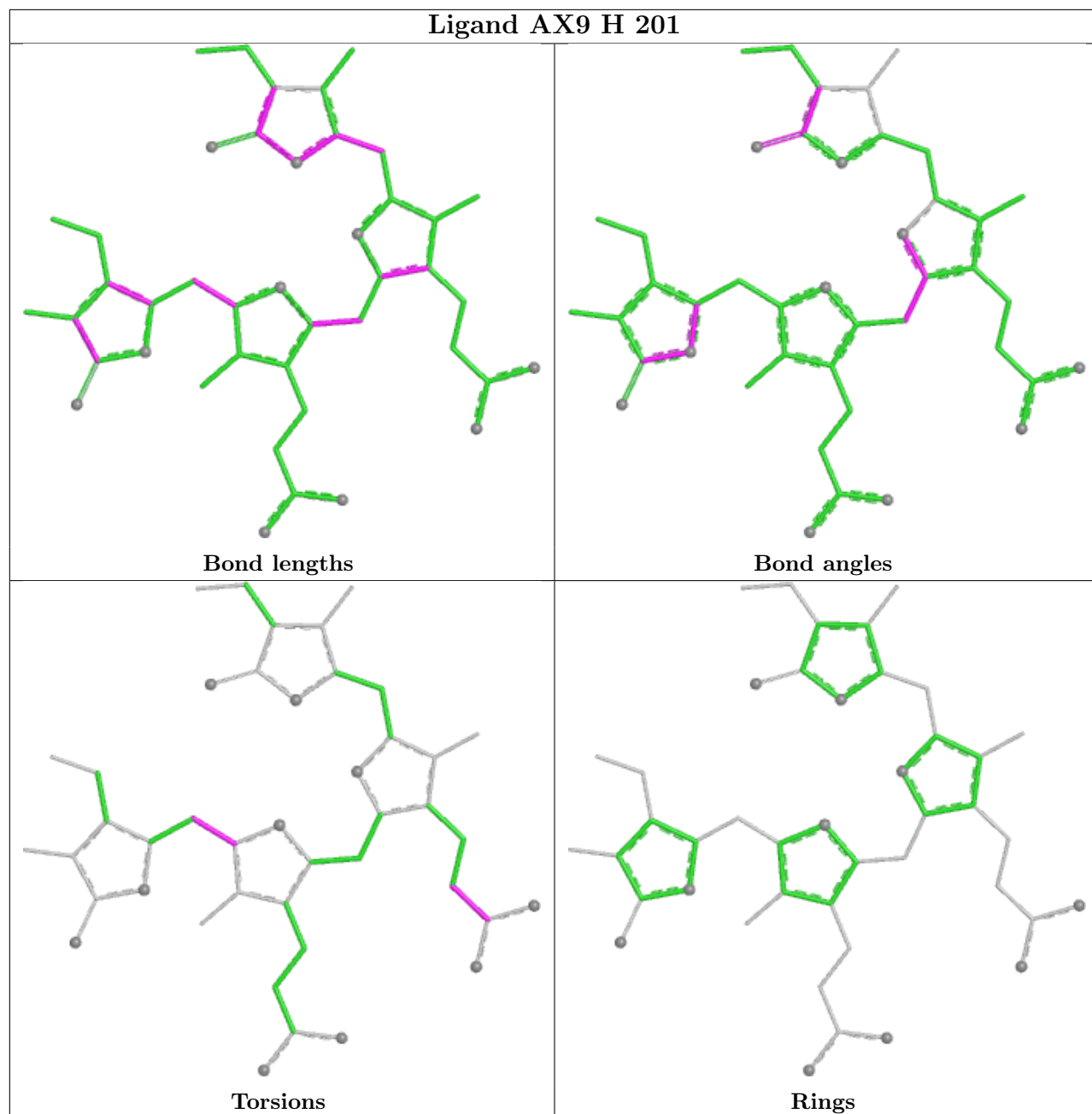


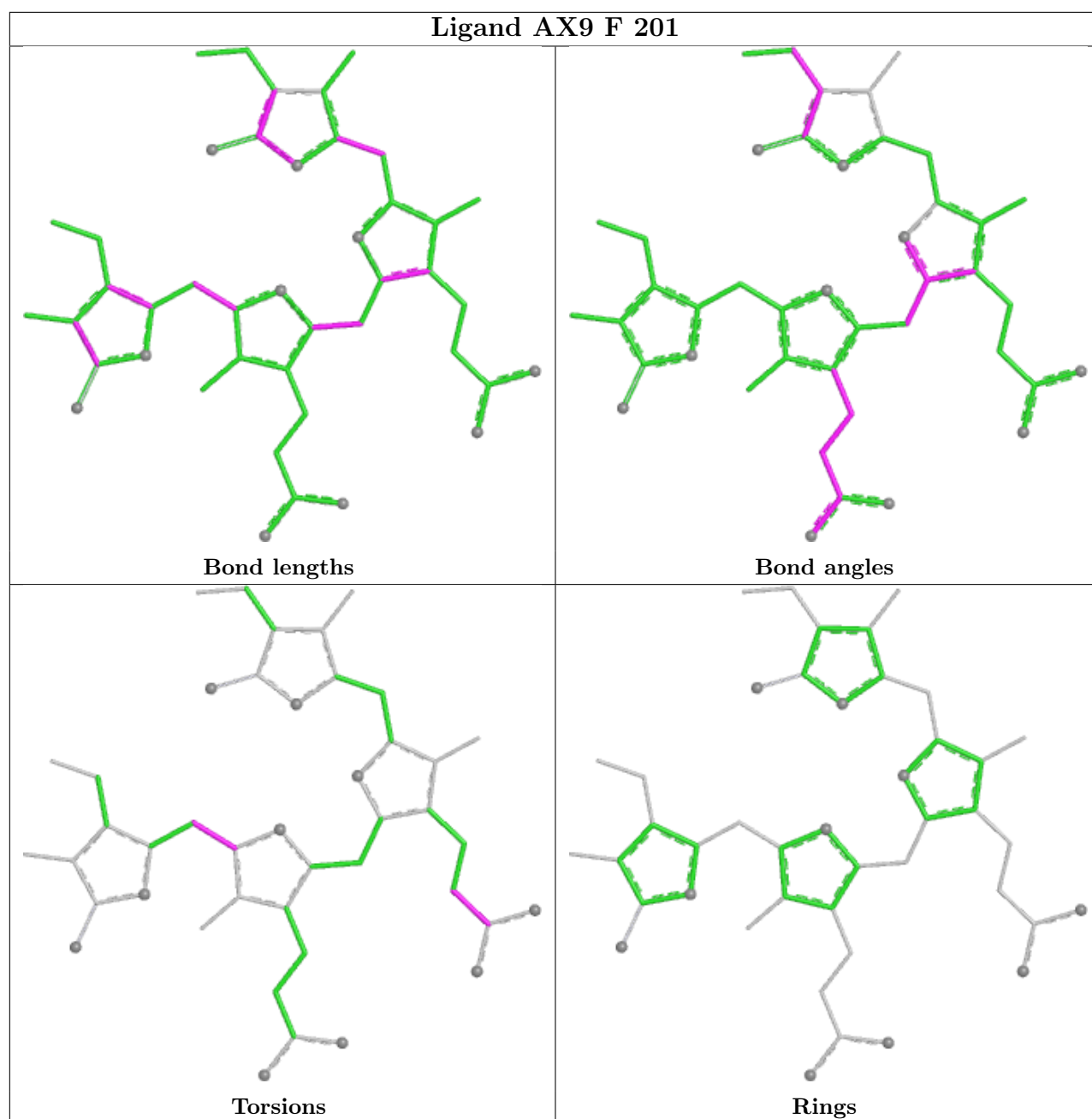












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	78/80 (97%)	-0.52	0 100 100	9, 21, 37, 78	9 (11%)
1	E	78/80 (97%)	-0.21	1 (1%) 75 78	12, 29, 55, 65	3 (3%)
2	B	174/177 (98%)	-0.37	2 (1%) 78 81	9, 23, 47, 79	14 (8%)
2	D	161/177 (90%)	-0.62	0 100 100	10, 21, 38, 55	3 (1%)
2	F	176/177 (99%)	-0.15	3 (1%) 69 72	11, 31, 48, 78	5 (2%)
2	H	161/177 (90%)	-0.17	2 (1%) 76 80	12, 31, 53, 65	4 (2%)
3	C	63/68 (92%)	-0.51	2 (3%) 50 54	16, 22, 43, 75	2 (3%)
3	G	63/68 (92%)	0.00	3 (4%) 35 39	13, 30, 57, 74	4 (6%)
All	All	954/1004 (95%)	-0.32	13 (1%) 73 77	9, 27, 49, 79	44 (4%)

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	45[A]	TYR	5.3
3	C	45[A]	TYR	3.9
2	F	176	LEU	3.1
2	F	1	MET	3.0
2	B	3	ASP	2.6

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

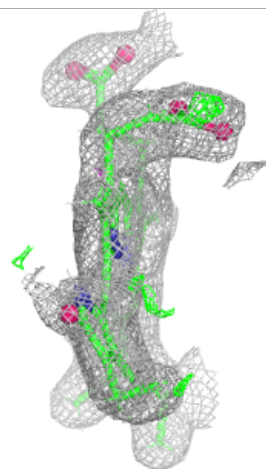
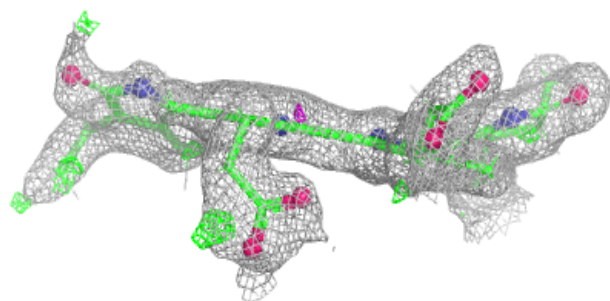
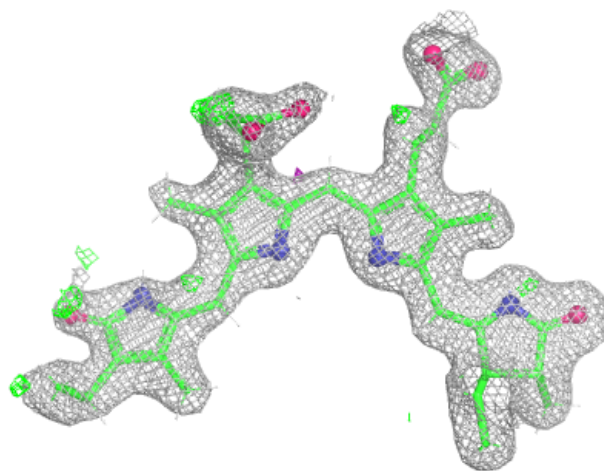
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	PG4	A	102	13/13	0.87	0.14	33,51,70,72	0
5	PG4	H	204	13/13	0.91	0.11	34,47,63,75	0
10	CYC	H	202	43/43	0.93	0.11	22,38,83,100	4
8	PEB	B	202	43/43	0.94	0.09	16,24,34,40	4
8	PEB	F	202	43/43	0.94	0.09	22,32,45,50	4
8	PEB	F	203	43/43	0.94	0.10	19,30,54,67	4
4	X2I	G	101	43/43	0.94	0.09	22,30,41,80	4
7	AX9	B	201[A]	43/43	0.95	0.07	9,19,31,35	79
7	AX9	B	201[B]	43/43	0.95	0.07	8,17,23,27	79
8	PEB	H	203	43/43	0.95	0.08	21,29,40,44	4
10	CYC	D	202	43/43	0.95	0.09	15,27,42,67	4
4	X2I	E	101	43/43	0.95	0.08	21,32,51,73	4
9	BTB	B	204	14/14	0.96	0.07	14,18,21,22	33
8	PEB	B	203	43/43	0.96	0.07	16,22,33,36	4
7	AX9	F	201	43/43	0.96	0.07	13,24,47,59	8
4	X2I	A	101	43/43	0.97	0.06	14,21,28,58	4
8	PEB	D	203	43/43	0.97	0.06	13,19,33,49	4
7	AX9	H	201	43/43	0.97	0.06	13,24,31,38	8
4	X2I	C	101	43/43	0.97	0.06	15,21,31,37	4
7	AX9	D	201	43/43	0.98	0.05	13,17,24,28	8
6	CL	A	103	1/1	0.99	0.07	32,32,32,32	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

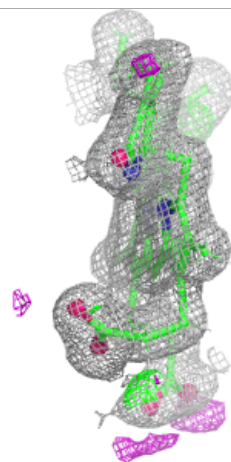
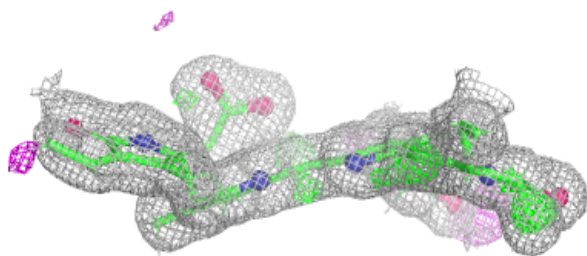
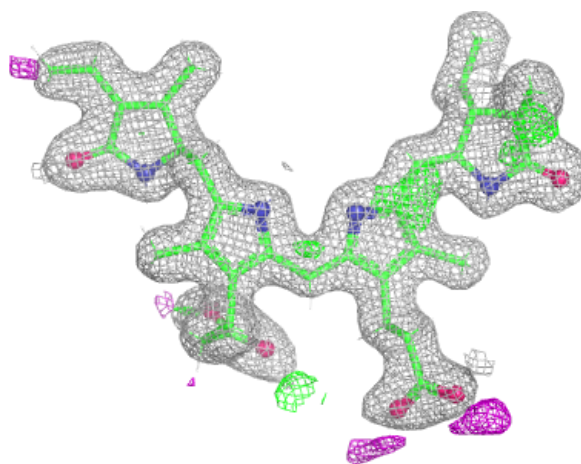
Electron density around CYC H 202:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



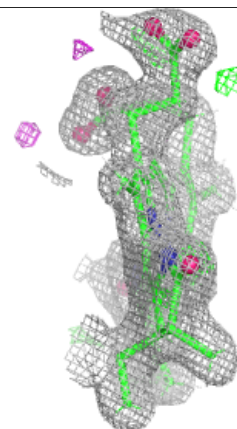
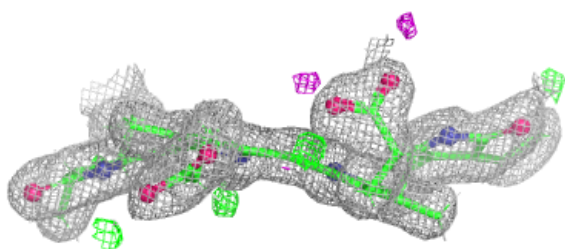
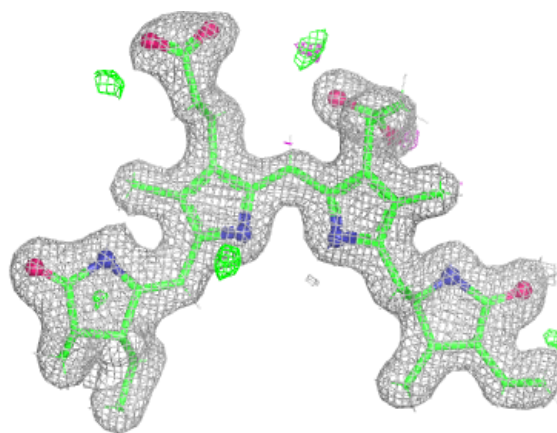
Electron density around PEB B 202:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

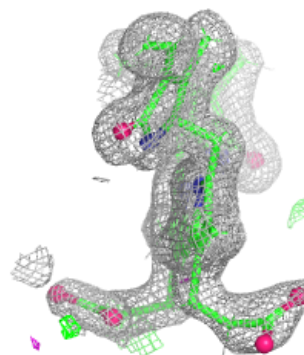
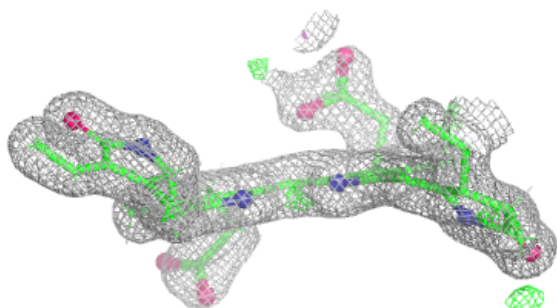
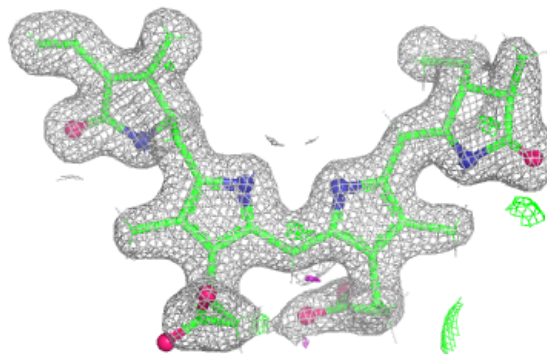


Electron density around PEB F 202:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

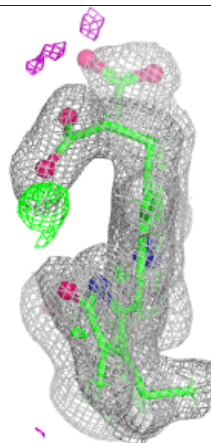
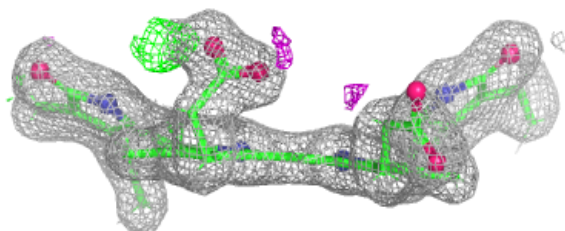
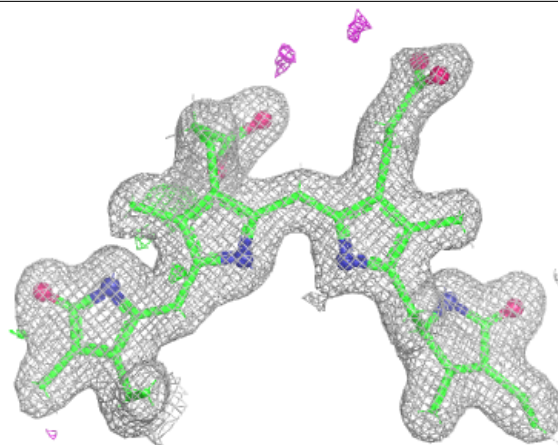
**Electron density around PEB F 203:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



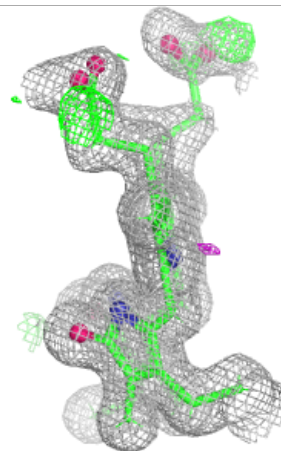
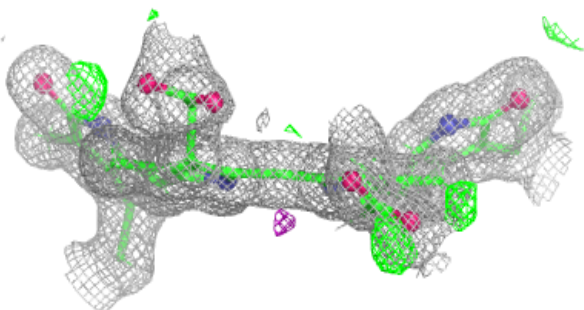
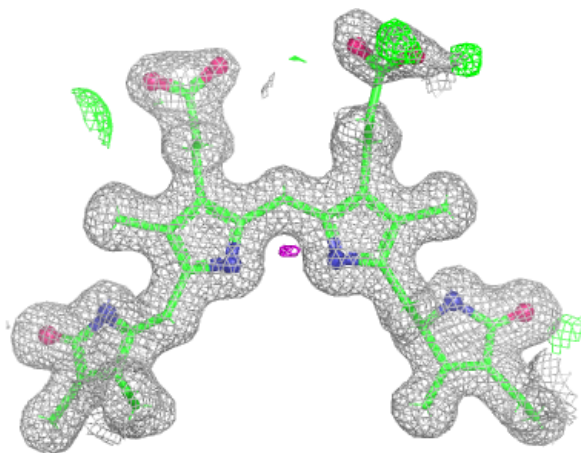
Electron density around X2I G 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



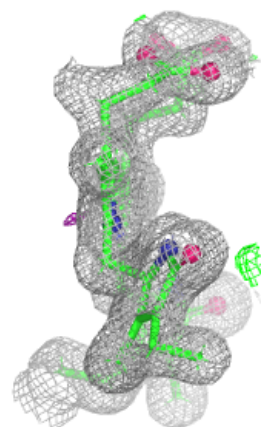
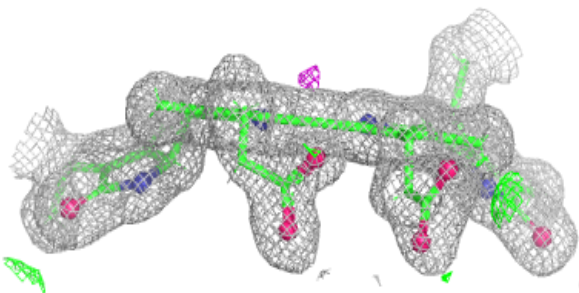
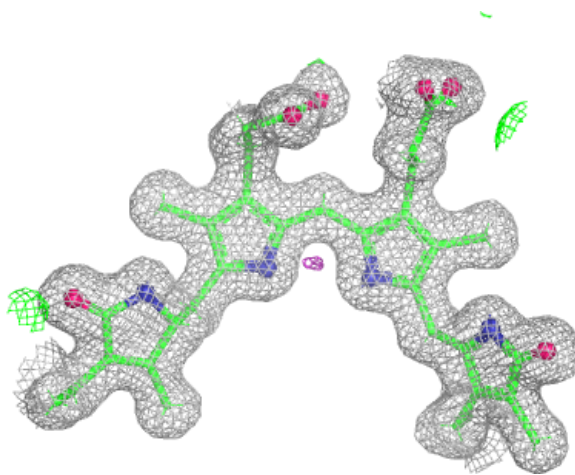
Electron density around AX9 B 201 (A):

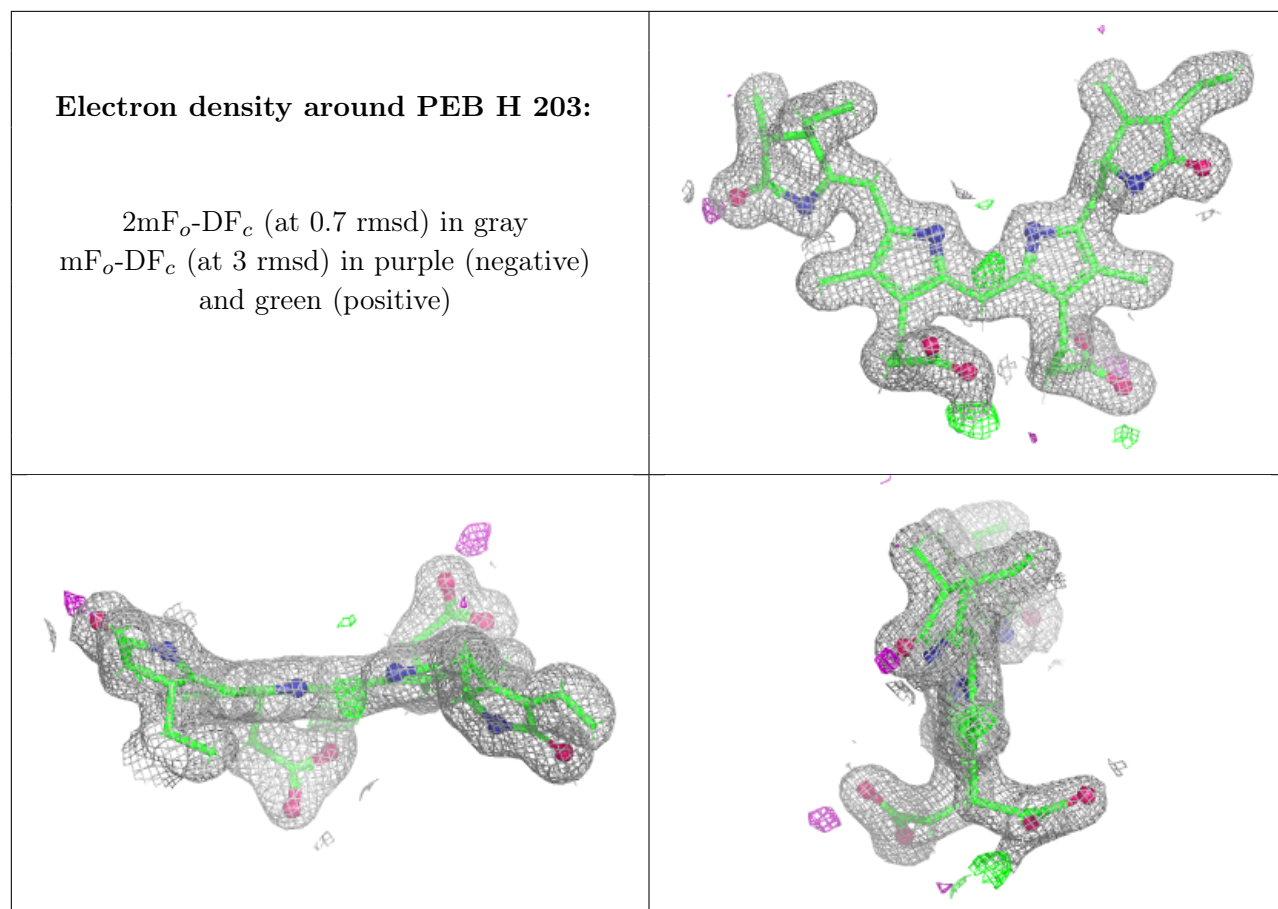
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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around AX9 B 201 (B):

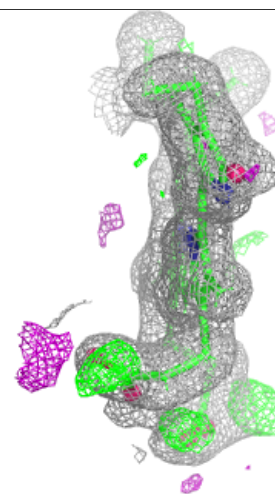
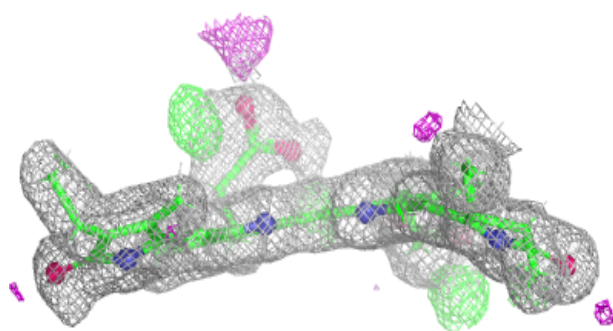
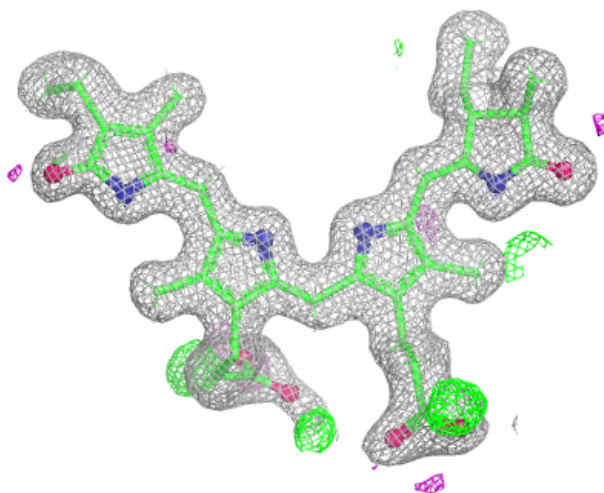
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





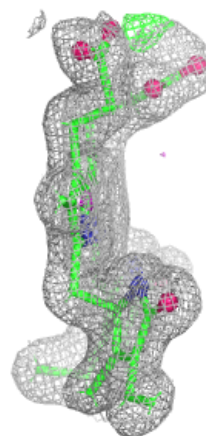
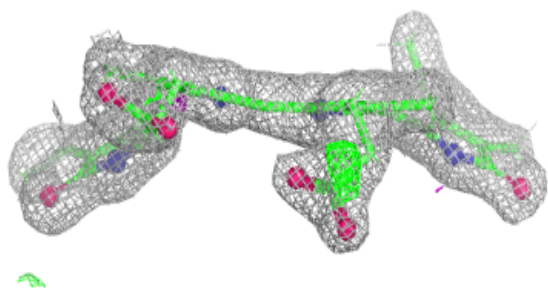
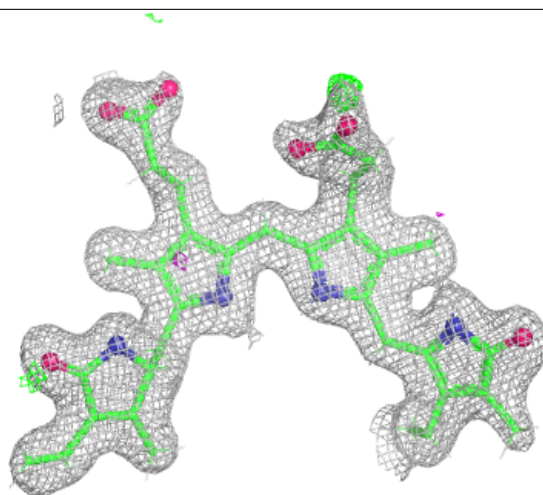
Electron density around CYC D 202:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



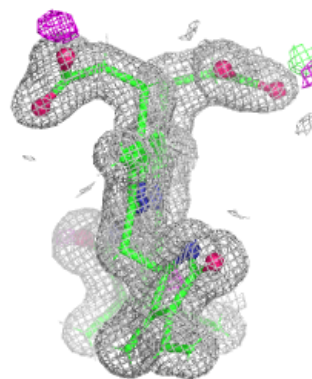
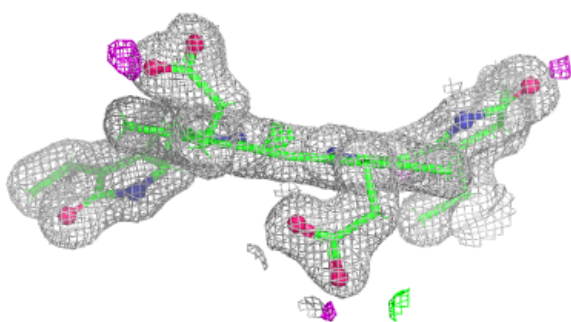
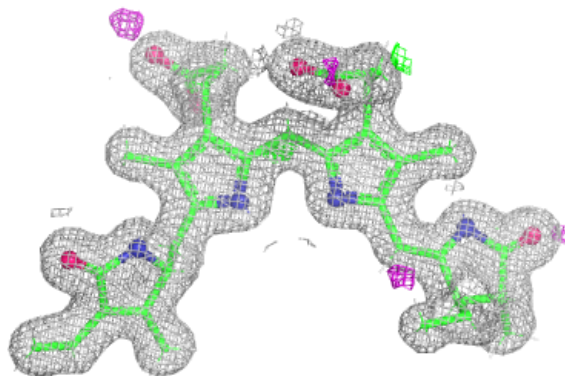
Electron density around X2I E 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



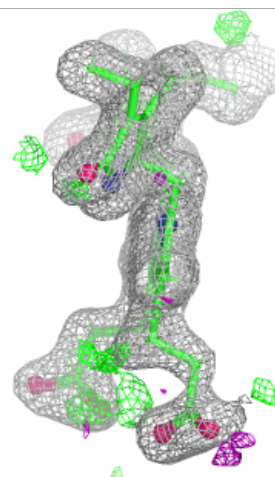
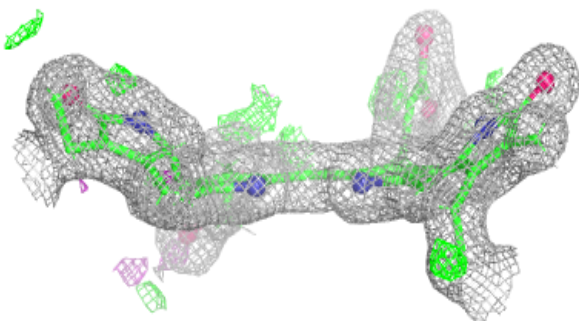
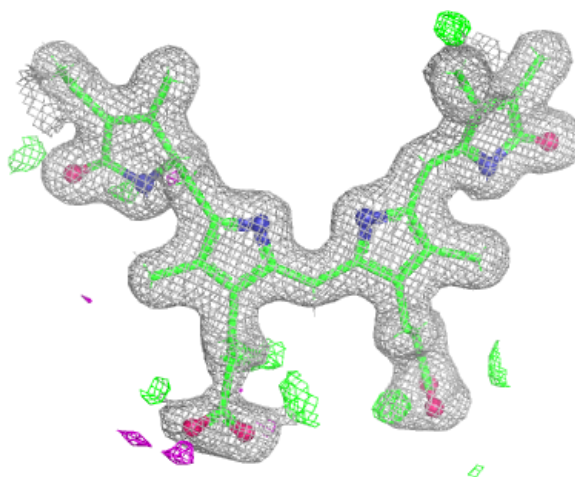
Electron density around PEB B 203:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



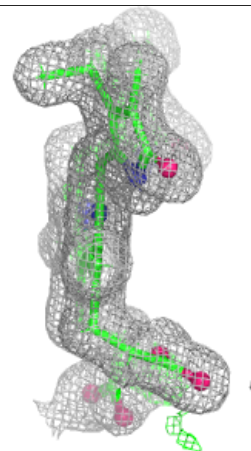
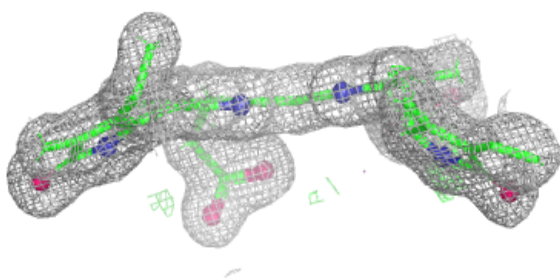
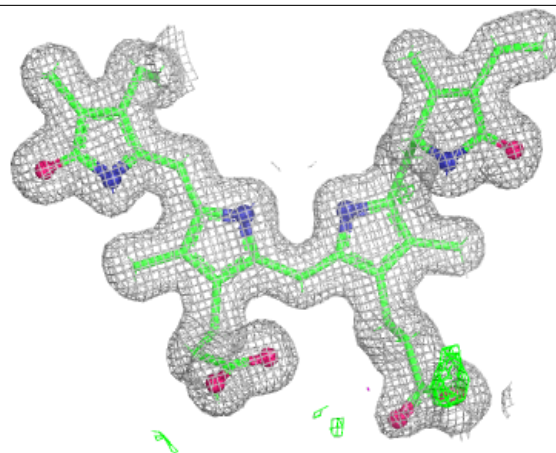
Electron density around AX9 F 201:

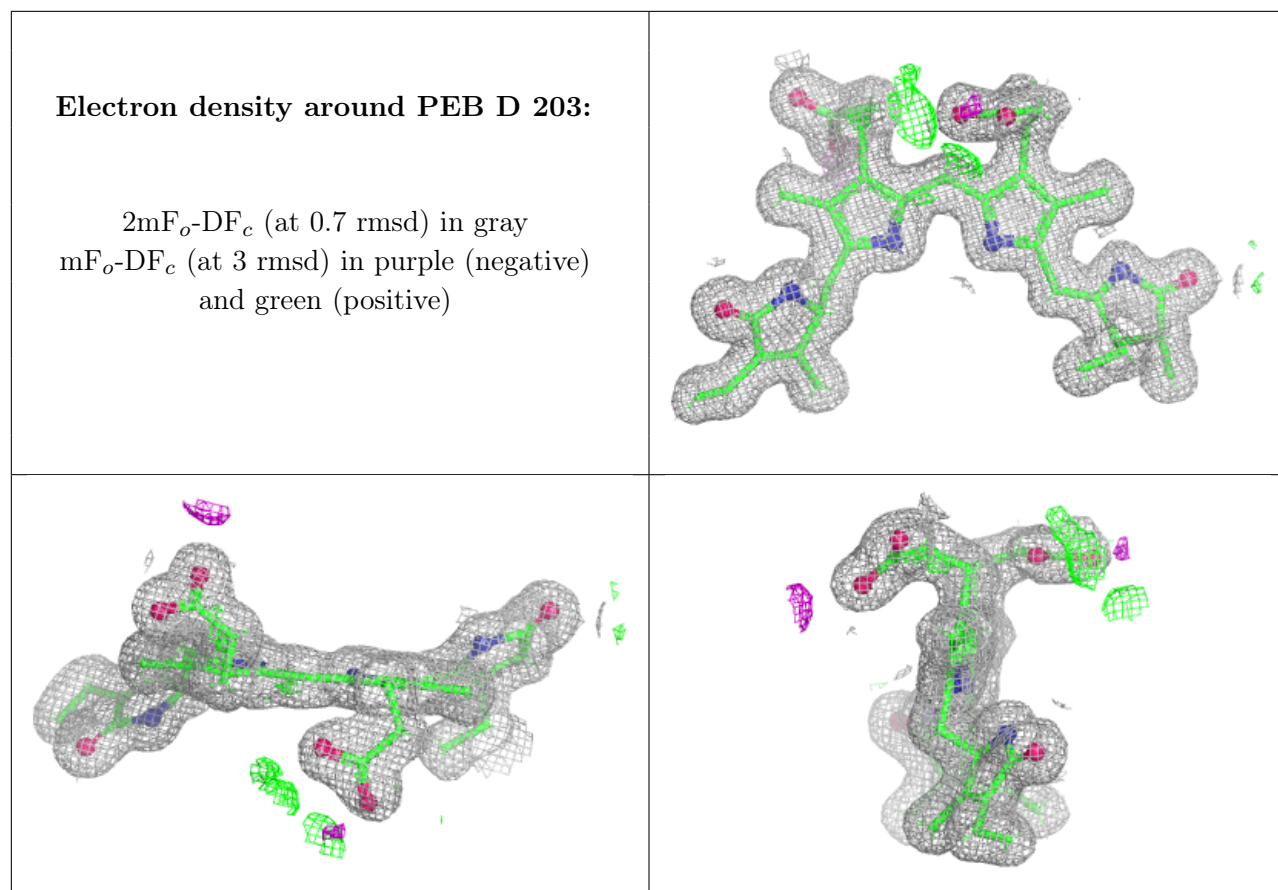
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around X2I A 101:

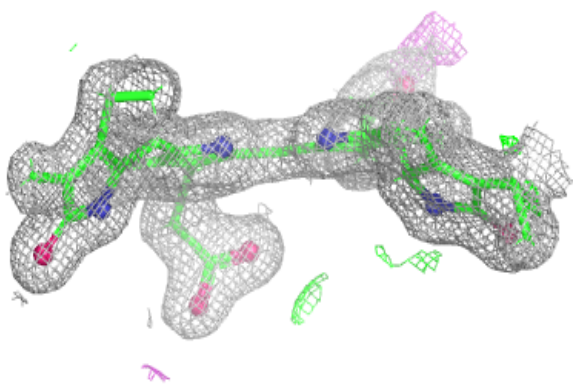
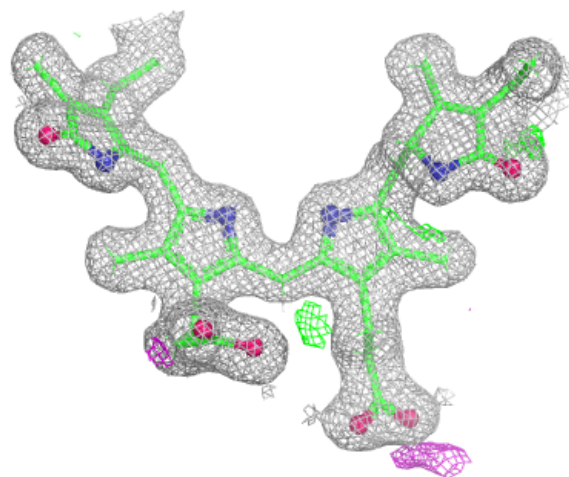
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





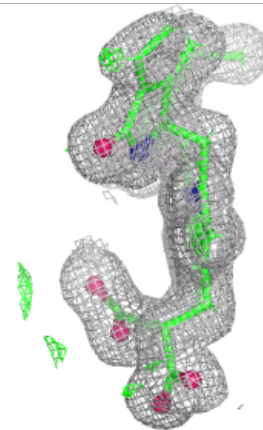
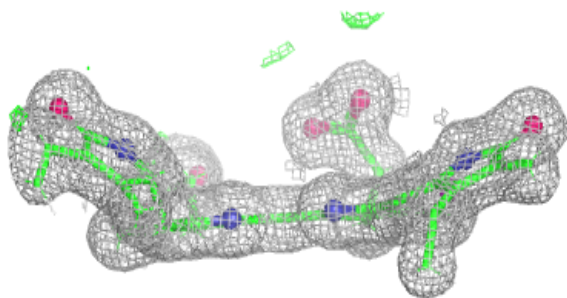
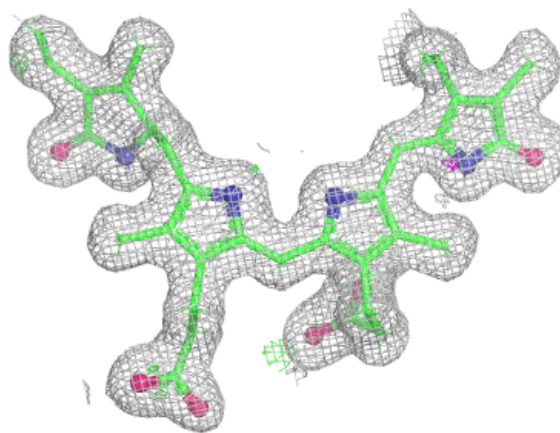
Electron density around AX9 H 201:

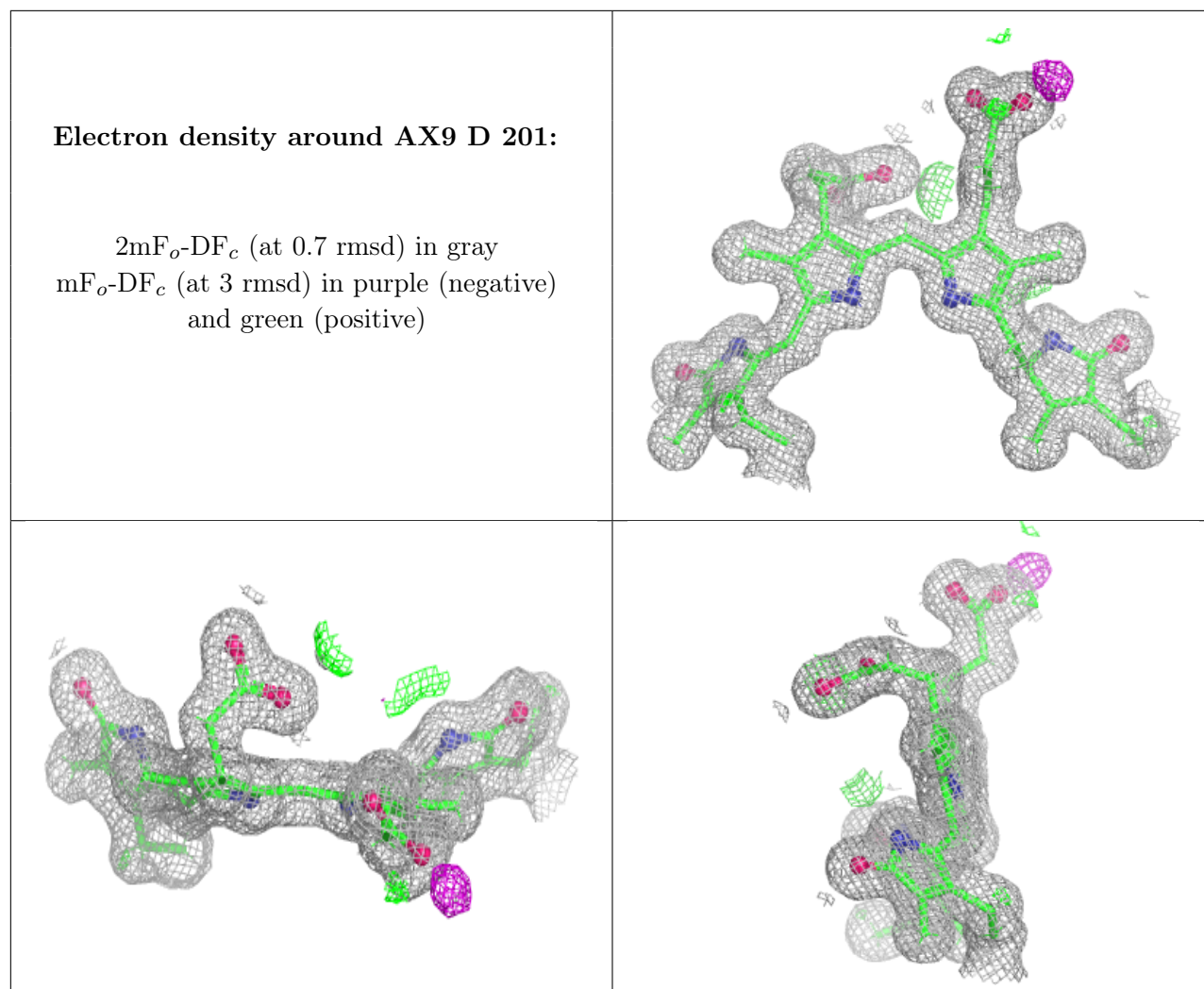
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around X2I C 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.