



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 12:32 am BST

PDB ID : 6RSK
Title : Cytochrome c co-crystallized with 20 eq. sulfonato-calix[8]arene and 15 eq. spermine - structure II
Authors : Engilberge, S.; Crowley, P.B.
Deposited on : 2019-05-21
Resolution : 2.31 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

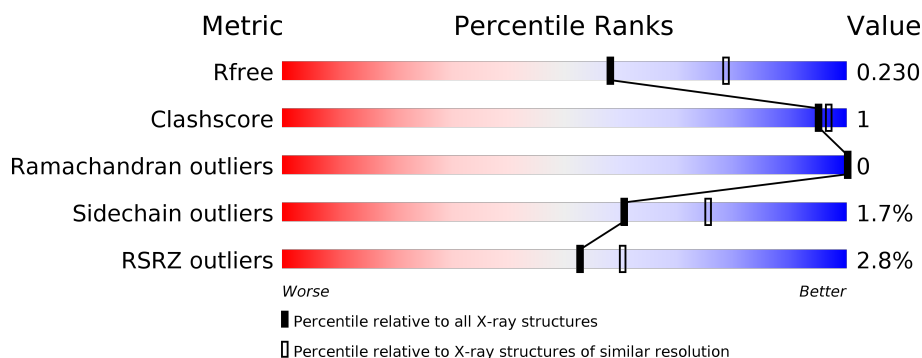
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 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}	130704	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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 on 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	108	<div> <div>%</div> <div>99%</div> </div>
1	B	108	<div> <div>5%</div> <div>97%</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	SPM	A	212	-	-	-	X
5	SPM	B	211	-	-	-	X

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.

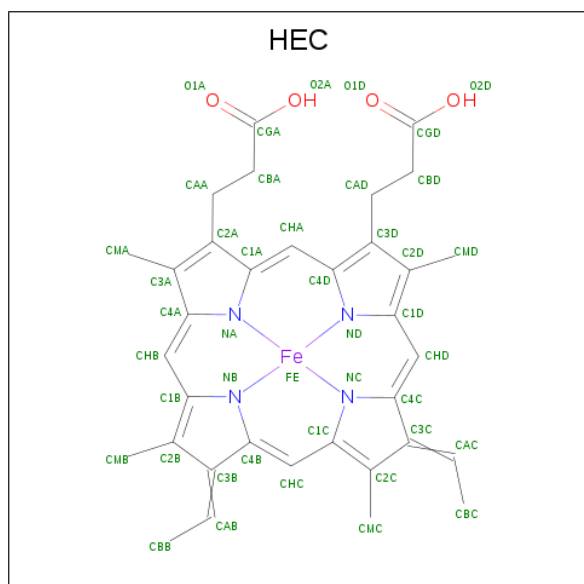
- Molecule 1 is a protein called Cytochrome c iso-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	108	Total 846	C 534	N 151	O 157	S 4	0	0	0
1	B	108	Total 846	C 534	N 151	O 157	S 4	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

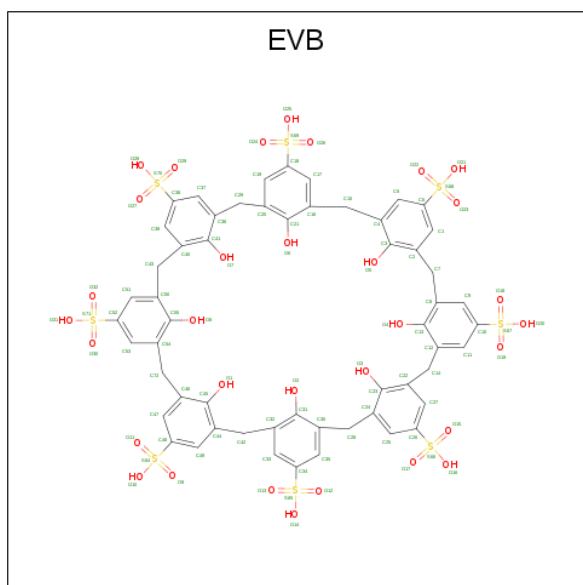
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	ALA	-	expression tag	UNP P00044
A	102	THR	CYS	engineered mutation	UNP P00044
B	-5	ALA	-	expression tag	UNP P00044
B	102	THR	CYS	engineered mutation	UNP P00044

- Molecule 2 is HEME C (three-letter code: HEC) (formula: $\text{C}_{34}\text{H}_{34}\text{FeN}_4\text{O}_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is sulfonato-calix[8]arene (three-letter code: EVB) (formula: $C_{56}H_{48}O_{32}S_8$) (labeled as "Ligand of Interest" by author).



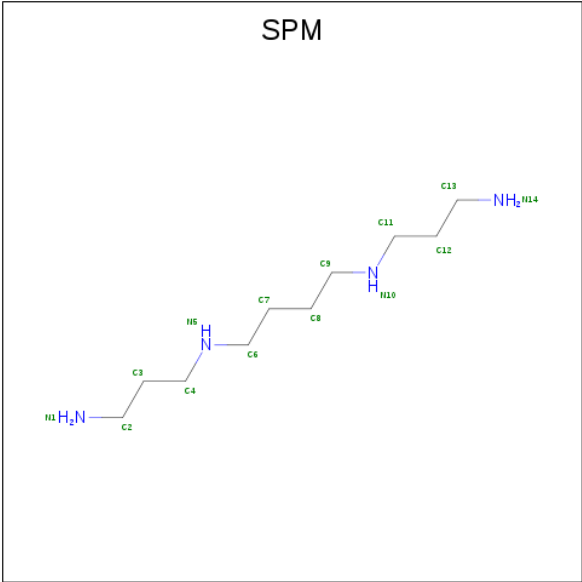
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			96	56	32	8		
3	A	1	Total	C	O	S	0	0
			96	56	32	8		
3	A	1	Total	C	O	S	0	0
			96	56	32	8		
3	B	1	Total	C	O	S	0	0
			96	56	32	8		
3	B	1	Total	C	O	S	0	0
			96	56	32	8		
3	B	1	Total	C	O	S	0	0
			96	56	32	8		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is SPERMINE (three-letter code: SPM) (formula: C₁₀H₂₆N₄) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	N	0	0
			14	10	4		
5	A	1	Total	C	N	0	0
			14	10	4		
5	B	1	Total	C	N	0	0
			14	10	4		
5	B	1	Total	C	N	0	0
			14	10	4		

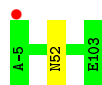
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	132	Total	O	0	0
			132	132		
6	B	47	Total	O	0	0
			47	47		

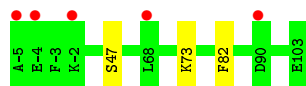
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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 electron 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Cytochrome c iso-1



- Molecule 1: Cytochrome c iso-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	100.46 Å 100.46 Å 89.54 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	66.84 – 2.31 71.04 – 2.31	Depositor EDS
% Data completeness (in resolution range)	100.0 (66.84-2.31) 100.0 (71.04-2.31)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 2.32 Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.183 , 0.222 0.191 , 0.230	Depositor DCC
R_{free} test set	1095 reflections (5.27%)	wwPDB-VP
Wilson B-factor (Å ²)	44.9	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 58.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2644	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.78% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EVB, HEC, SPM, SO4

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	0.50	0/864	0.63	0/1155
1	B	0.40	0/864	0.60	0/1155
All	All	0.45	0/1728	0.61	0/2310

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

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	846	0	849	0	0
1	B	846	0	849	1	0
2	A	43	0	30	2	0
2	B	43	0	30	3	0
3	A	288	0	0	0	0
3	B	288	0	0	0	0
4	A	30	0	0	0	0
4	B	25	0	0	0	0
5	A	28	0	52	0	0
5	B	28	0	52	0	0
6	A	132	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	47	0	0	0	0
All	All	2644	0	1862	5	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 1.

All (5) 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:B:201:HEC:HMC1	2:B:201:HEC:HBC2	1.78	0.64
2:B:201:HEC:HMC1	2:B:201:HEC:CBC	2.43	0.49
1:B:82:PHE:CD1	2:B:201:HEC:HMC2	2.55	0.42
2:A:201:HEC:HMC1	2:A:201:HEC:CBC	2.51	0.40
2:A:201:HEC:HAC	2:A:201:HEC:HHD	1.84	0.40

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	106/108 (98%)	102 (96%)	4 (4%)	0	100	100
1	B	106/108 (98%)	103 (97%)	3 (3%)	0	100	100
All	All	212/216 (98%)	205 (97%)	7 (3%)	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	88/88 (100%)	87 (99%)	1 (1%)	73	85
1	B	88/88 (100%)	86 (98%)	2 (2%)	50	66
All	All	176/176 (100%)	173 (98%)	3 (2%)	60	75

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	B	47	SER
1	B	73	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

23 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$
5	SPM	A	212	-	13,13,13	0.36	0	12,12,12	0.50	0
3	EVB	B	202	-	104,104,104	2.12	28 (26%)	168,168,168	0.91	6 (3%)
4	SO4	A	209	-	4,4,4	0.15	0	6,6,6	0.12	0
3	EVB	B	204	-	104,104,104	2.23	30 (28%)	168,168,168	0.78	1 (0%)
4	SO4	A	205	-	4,4,4	0.16	0	6,6,6	0.26	0
4	SO4	A	208	-	4,4,4	0.20	0	6,6,6	0.08	0
3	EVB	B	203	-	104,104,104	2.27	32 (30%)	168,168,168	0.78	0
4	SO4	A	207	-	4,4,4	0.15	0	6,6,6	0.14	0
4	SO4	B	206	-	4,4,4	0.15	0	6,6,6	0.23	0
3	EVB	A	202	-	104,104,104	2.07	28 (26%)	168,168,168	0.93	5 (2%)
4	SO4	B	205	-	4,4,4	0.15	0	6,6,6	0.08	0
4	SO4	A	206	-	4,4,4	0.14	0	6,6,6	0.25	0
2	HEC	B	201	1,6	26,50,50	2.00	6 (23%)	18,82,82	1.75	4 (22%)
4	SO4	B	207	-	4,4,4	0.15	0	6,6,6	0.10	0
4	SO4	B	209	-	4,4,4	0.24	0	6,6,6	0.09	0
5	SPM	B	211	-	13,13,13	0.35	0	12,12,12	0.43	0
2	HEC	A	201	1,6	26,50,50	2.09	5 (19%)	18,82,82	1.89	3 (16%)
4	SO4	B	208	-	4,4,4	0.13	0	6,6,6	0.06	0
3	EVB	A	204	-	104,104,104	2.28	31 (29%)	168,168,168	0.87	4 (2%)
5	SPM	A	211	-	13,13,13	0.43	0	12,12,12	0.66	0
3	EVB	A	203	-	104,104,104	2.04	28 (26%)	168,168,168	0.93	5 (2%)
5	SPM	B	210	-	13,13,13	0.36	0	12,12,12	0.45	0
4	SO4	A	210	-	4,4,4	0.16	0	6,6,6	0.14	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEC	A	201	1,6	-	0/6/54/54	-
5	SPM	A	212	-	-	6/11/11/11	-
3	EVB	B	202	-	-	0/80/80/80	-
5	SPM	B	211	-	-	10/11/11/11	-
3	EVB	A	204	-	-	4/80/80/80	-
5	SPM	A	211	-	-	4/11/11/11	-
2	HEC	B	201	1,6	-	0/6/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EVB	A	203	-	-	4/80/80/80	-
3	EVB	B	203	-	-	5/80/80/80	-
5	SPM	B	210	-	-	8/11/11/11	-
3	EVB	B	204	-	-	4/80/80/80	-
3	EVB	A	202	-	-	0/80/80/80	-

All (188) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	201	HEC	C3B-C2B	5.87	1.46	1.40
2	B	201	HEC	C3B-C2B	5.42	1.46	1.40
2	B	201	HEC	C3C-C2C	5.24	1.46	1.40
3	A	204	EVB	O9-S64	4.57	1.66	1.43
3	A	204	EVB	O24-S69	4.57	1.66	1.43
3	A	204	EVB	O11-S64	4.56	1.66	1.43
3	B	204	EVB	O11-S64	4.54	1.66	1.43
2	A	201	HEC	C3B-C4B	4.53	1.51	1.43
3	B	203	EVB	O9-S64	4.52	1.66	1.43
3	A	204	EVB	O26-S69	4.52	1.66	1.43
3	B	204	EVB	O9-S64	4.50	1.66	1.43
3	A	204	EVB	O22-S68	4.50	1.66	1.43
3	B	203	EVB	O17-S66	4.49	1.66	1.43
3	A	204	EVB	O18-S67	4.49	1.66	1.43
3	B	203	EVB	O23-S68	4.48	1.66	1.43
3	A	204	EVB	O17-S66	4.48	1.66	1.43
3	B	203	EVB	O11-S64	4.47	1.66	1.43
3	B	204	EVB	O19-S67	4.47	1.66	1.43
3	B	203	EVB	O13-S65	4.47	1.66	1.43
3	B	204	EVB	O17-S66	4.46	1.66	1.43
3	B	204	EVB	O18-S67	4.46	1.66	1.43
3	B	203	EVB	O32-S71	4.46	1.66	1.43
3	B	203	EVB	O12-S65	4.46	1.66	1.43
3	A	204	EVB	O13-S65	4.45	1.66	1.43
3	B	203	EVB	O26-S69	4.45	1.66	1.43
3	B	203	EVB	O24-S69	4.45	1.66	1.43
3	B	204	EVB	O15-S66	4.44	1.66	1.43
3	A	204	EVB	O15-S66	4.44	1.66	1.43
3	A	204	EVB	O30-S71	4.44	1.66	1.43
3	B	204	EVB	O13-S65	4.44	1.66	1.43
3	A	204	EVB	O23-S68	4.44	1.66	1.43
2	A	201	HEC	C4D-ND	4.44	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	204	EVB	O24-S69	4.43	1.66	1.43
3	B	203	EVB	O29-S70	4.43	1.66	1.43
3	A	204	EVB	O32-S71	4.43	1.66	1.43
3	B	203	EVB	O22-S68	4.43	1.65	1.43
3	B	202	EVB	O11-S64	4.42	1.65	1.43
3	B	203	EVB	O18-S67	4.42	1.65	1.43
3	A	204	EVB	O19-S67	4.42	1.65	1.43
3	B	202	EVB	O9-S64	4.41	1.65	1.43
3	B	204	EVB	O23-S68	4.41	1.65	1.43
3	B	204	EVB	O26-S69	4.41	1.65	1.43
3	B	203	EVB	O19-S67	4.41	1.65	1.43
3	B	202	EVB	O15-S66	4.41	1.65	1.43
3	A	204	EVB	O29-S70	4.40	1.65	1.43
3	A	204	EVB	O12-S65	4.40	1.65	1.43
3	B	204	EVB	O22-S68	4.40	1.65	1.43
3	B	204	EVB	O12-S65	4.39	1.65	1.43
3	B	203	EVB	O30-S71	4.39	1.65	1.43
3	B	202	EVB	O17-S66	4.38	1.65	1.43
3	A	204	EVB	O27-S70	4.38	1.65	1.43
3	B	203	EVB	O27-S70	4.38	1.65	1.43
3	B	204	EVB	O29-S70	4.35	1.65	1.43
3	A	202	EVB	O11-S64	4.35	1.65	1.43
3	B	203	EVB	O15-S66	4.33	1.65	1.43
3	B	202	EVB	O19-S67	4.33	1.65	1.43
3	B	204	EVB	O32-S71	4.33	1.65	1.43
3	B	204	EVB	O27-S70	4.32	1.65	1.43
3	A	202	EVB	O17-S66	4.31	1.65	1.43
3	A	202	EVB	O23-S68	4.29	1.65	1.43
3	B	204	EVB	O30-S71	4.29	1.65	1.43
3	A	203	EVB	O15-S66	4.29	1.65	1.43
3	A	202	EVB	O18-S67	4.27	1.65	1.43
3	B	202	EVB	O24-S69	4.27	1.65	1.43
3	B	202	EVB	O27-S70	4.26	1.65	1.43
3	B	202	EVB	O29-S70	4.25	1.65	1.43
3	B	202	EVB	O13-S65	4.25	1.65	1.43
3	A	202	EVB	O9-S64	4.24	1.65	1.43
3	B	202	EVB	O26-S69	4.23	1.65	1.43
3	A	202	EVB	O15-S66	4.22	1.64	1.43
3	B	202	EVB	O23-S68	4.21	1.64	1.43
3	B	202	EVB	O22-S68	4.20	1.64	1.43
3	A	203	EVB	O9-S64	4.20	1.64	1.43
3	A	202	EVB	O19-S67	4.20	1.64	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	202	EVB	O29-S70	4.19	1.64	1.43
3	B	203	EVB	O14-S65	4.17	1.66	1.45
3	A	204	EVB	O14-S65	4.16	1.66	1.45
3	B	202	EVB	O32-S71	4.15	1.64	1.43
3	A	203	EVB	O26-S69	4.15	1.64	1.43
3	B	202	EVB	O30-S71	4.15	1.64	1.43
3	B	204	EVB	O14-S65	4.15	1.66	1.45
3	B	203	EVB	O10-S64	4.14	1.66	1.45
3	A	204	EVB	O25-S69	4.14	1.66	1.45
3	A	203	EVB	O13-S65	4.13	1.64	1.43
2	B	201	HEC	C3B-C4B	4.13	1.50	1.43
3	A	202	EVB	O22-S68	4.13	1.64	1.43
3	A	202	EVB	O13-S65	4.12	1.64	1.43
3	A	203	EVB	O12-S65	4.12	1.64	1.43
3	A	204	EVB	O21-S68	4.11	1.66	1.45
3	B	202	EVB	O18-S67	4.11	1.64	1.43
3	A	204	EVB	O10-S64	4.11	1.66	1.45
3	B	203	EVB	O31-S71	4.10	1.66	1.45
3	B	203	EVB	O21-S68	4.10	1.66	1.45
3	A	204	EVB	O31-S71	4.09	1.66	1.45
3	A	203	EVB	O30-S71	4.09	1.64	1.43
3	B	204	EVB	O25-S69	4.08	1.66	1.45
3	B	204	EVB	O10-S64	4.08	1.66	1.45
3	B	203	EVB	O25-S69	4.07	1.66	1.45
3	A	202	EVB	O24-S69	4.07	1.64	1.43
3	B	204	EVB	O21-S68	4.07	1.66	1.45
3	A	203	EVB	O17-S66	4.07	1.64	1.43
3	B	204	EVB	O20-S67	4.06	1.65	1.45
3	B	204	EVB	O31-S71	4.06	1.65	1.45
3	A	203	EVB	O24-S69	4.05	1.64	1.43
3	A	203	EVB	O23-S68	4.04	1.64	1.43
3	B	204	EVB	O16-S66	4.04	1.65	1.45
3	B	203	EVB	O28-S70	4.03	1.65	1.45
3	A	204	EVB	O16-S66	4.03	1.65	1.45
3	A	202	EVB	O27-S70	4.03	1.64	1.43
3	A	202	EVB	O32-S71	4.03	1.64	1.43
3	A	203	EVB	O19-S67	4.03	1.64	1.43
3	A	203	EVB	O11-S64	4.03	1.63	1.43
3	A	204	EVB	O28-S70	4.03	1.65	1.45
3	B	203	EVB	O20-S67	4.02	1.65	1.45
3	A	203	EVB	O22-S68	4.02	1.63	1.43
3	A	202	EVB	O10-S64	4.01	1.65	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	203	EVB	O16-S66	4.01	1.65	1.45
3	A	203	EVB	O14-S65	4.01	1.65	1.45
3	B	204	EVB	O28-S70	3.99	1.65	1.45
3	B	202	EVB	O25-S69	3.98	1.65	1.45
3	A	203	EVB	O32-S71	3.98	1.63	1.43
3	A	204	EVB	O20-S67	3.97	1.65	1.45
3	B	202	EVB	O16-S66	3.95	1.65	1.45
3	B	202	EVB	O31-S71	3.93	1.65	1.45
3	A	202	EVB	O30-S71	3.92	1.63	1.43
3	A	203	EVB	O18-S67	3.92	1.63	1.43
3	A	202	EVB	O26-S69	3.91	1.63	1.43
3	B	202	EVB	O12-S65	3.91	1.63	1.43
3	A	203	EVB	O27-S70	3.91	1.63	1.43
3	B	202	EVB	O14-S65	3.90	1.65	1.45
3	B	202	EVB	O10-S64	3.90	1.65	1.45
3	B	202	EVB	O20-S67	3.85	1.64	1.45
3	A	203	EVB	O20-S67	3.82	1.64	1.45
3	B	202	EVB	O21-S68	3.82	1.64	1.45
3	B	202	EVB	O28-S70	3.81	1.64	1.45
3	A	203	EVB	O21-S68	3.78	1.64	1.45
3	A	202	EVB	O31-S71	3.77	1.64	1.45
3	A	202	EVB	O14-S65	3.76	1.64	1.45
3	A	203	EVB	O25-S69	3.74	1.64	1.45
3	A	203	EVB	O29-S70	3.73	1.62	1.43
3	A	203	EVB	O10-S64	3.72	1.64	1.45
3	A	202	EVB	O25-S69	3.69	1.64	1.45
3	A	202	EVB	O20-S67	3.68	1.64	1.45
3	A	202	EVB	O21-S68	3.67	1.63	1.45
3	A	203	EVB	O31-S71	3.66	1.63	1.45
3	A	202	EVB	O16-S66	3.66	1.63	1.45
3	A	202	EVB	O12-S65	3.61	1.61	1.43
3	A	203	EVB	O28-S70	3.56	1.63	1.45
3	A	203	EVB	O16-S66	3.51	1.63	1.45
3	A	202	EVB	O28-S70	3.39	1.62	1.45
2	A	201	HEC	C3C-C4C	3.02	1.48	1.43
2	A	201	HEC	C1B-NB	3.00	1.42	1.36
3	A	202	EVB	C34-S65	2.94	1.83	1.77
2	B	201	HEC	C3C-C4C	2.93	1.48	1.43
3	A	204	EVB	C34-S65	2.93	1.83	1.77
3	B	203	EVB	C48-S64	2.87	1.83	1.77
3	B	204	EVB	C26-S66	2.86	1.83	1.77
3	A	204	EVB	C52-S71	2.78	1.83	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	203	EVB	C34-S65	2.66	1.82	1.77
3	A	204	EVB	C26-S66	2.66	1.82	1.77
3	B	203	EVB	C26-S66	2.54	1.82	1.77
3	A	202	EVB	C6-S68	2.51	1.82	1.77
3	B	204	EVB	C34-S65	2.49	1.82	1.77
3	B	203	EVB	C52-S71	2.48	1.82	1.77
3	A	204	EVB	C6-S68	2.45	1.82	1.77
3	B	203	EVB	C18-S69	2.43	1.82	1.77
3	A	203	EVB	C26-S66	2.43	1.82	1.77
3	B	204	EVB	C6-S68	2.41	1.82	1.77
3	B	202	EVB	C48-S64	2.39	1.82	1.77
3	B	204	EVB	C48-S64	2.30	1.82	1.77
2	B	201	HEC	C1C-NC	2.29	1.40	1.36
3	B	202	EVB	C26-S66	2.27	1.81	1.77
3	B	203	EVB	C6-S68	2.24	1.81	1.77
3	A	202	EVB	C48-S64	2.22	1.81	1.77
3	A	204	EVB	C48-S64	2.21	1.81	1.77
3	B	203	EVB	C10-S67	2.19	1.81	1.77
3	A	203	EVB	C52-S71	2.18	1.81	1.77
3	B	203	EVB	C38-S70	2.16	1.81	1.77
3	A	202	EVB	C18-S69	2.12	1.81	1.77
3	B	204	EVB	C52-S71	2.12	1.81	1.77
3	B	202	EVB	C34-S65	2.12	1.81	1.77
3	A	203	EVB	C34-S65	2.11	1.81	1.77
3	B	202	EVB	C10-S67	2.10	1.81	1.77
3	A	204	EVB	C18-S69	2.09	1.81	1.77
3	A	203	EVB	C10-S67	2.06	1.81	1.77
2	B	201	HEC	C1D-ND	2.06	1.40	1.36
3	B	204	EVB	C10-S67	2.04	1.81	1.77
3	A	204	EVB	C10-S67	2.03	1.81	1.77

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	201	HEC	C4B-C3B-C2B	-4.79	101.18	106.35
2	A	201	HEC	CBD-CAD-C3D	-4.35	104.46	112.49
2	B	201	HEC	CBD-CAD-C3D	-3.84	105.40	112.49
2	B	201	HEC	C4B-C3B-C2B	-3.69	102.37	106.35
3	A	202	EVB	C30-C28-C24	-2.98	104.46	112.67
2	A	201	HEC	CMB-C2B-C1B	-2.75	124.23	128.46
3	B	202	EVB	C29-C20-C19	-2.75	115.99	120.23
2	B	201	HEC	C1D-C2D-C3D	-2.55	105.22	107.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	203	EVB	O25-S69-C18	2.47	113.07	106.69
3	A	203	EVB	C32-C33-C34	-2.47	117.37	120.69
3	B	202	EVB	C53-C52-C51	2.45	123.66	120.31
3	B	202	EVB	C30-C28-C24	-2.39	106.08	112.67
3	A	204	EVB	C43-C40-C39	-2.37	116.58	120.23
3	B	202	EVB	C29-C20-C21	2.32	124.97	121.38
3	A	202	EVB	C40-C39-C38	-2.29	117.61	120.69
3	A	202	EVB	C42-C32-C33	-2.25	116.76	120.23
3	A	203	EVB	O19-S67-C10	2.22	111.76	106.65
3	A	204	EVB	C14-C12-C11	-2.21	116.83	120.23
3	A	204	EVB	C72-C46-C47	-2.20	116.85	120.23
3	B	202	EVB	C9-C8-C13	2.19	121.10	118.41
2	B	201	HEC	CMC-C2C-C3C	2.19	128.39	125.82
3	A	203	EVB	O29-S70-C38	2.13	111.55	106.65
3	A	202	EVB	C29-C20-C19	-2.13	116.96	120.23
3	A	203	EVB	C7-C2-C3	-2.10	118.14	121.38
3	B	204	EVB	C29-C20-C19	-2.10	117.00	120.23
3	A	202	EVB	C51-C52-S71	-2.09	116.30	119.89
3	B	202	EVB	C7-C2-C1	-2.05	117.08	120.23
3	A	204	EVB	C17-C18-S69	2.04	123.41	119.89

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	210	SPM	C2-C3-C4-N5
5	A	212	SPM	C7-C8-C9-N10
5	B	211	SPM	N5-C6-C7-C8
5	B	210	SPM	N10-C11-C12-C13
5	B	210	SPM	N5-C6-C7-C8
5	B	211	SPM	C12-C11-N10-C9
5	A	211	SPM	C8-C9-N10-C11
5	B	210	SPM	C7-C6-N5-C4
5	A	212	SPM	N5-C6-C7-C8
5	B	211	SPM	C3-C4-N5-C6
5	B	210	SPM	C6-C7-C8-C9
5	B	211	SPM	C6-C7-C8-C9
5	A	212	SPM	C12-C11-N10-C9
5	B	211	SPM	C8-C9-N10-C11
5	A	211	SPM	C11-C12-C13-N14
5	B	211	SPM	C7-C8-C9-N10
5	A	211	SPM	N5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
5	B	210	SPM	C12-C11-N10-C9
5	B	211	SPM	C7-C6-N5-C4
5	A	212	SPM	C8-C9-N10-C11
5	B	210	SPM	C3-C4-N5-C6
3	B	203	EVB	C55-C54-C72-C46
3	A	204	EVB	C2-C7-C8-C13
3	A	203	EVB	C1-C2-C7-C8
3	A	204	EVB	C2-C7-C8-C9
3	B	204	EVB	C4-C15-C16-C21
3	A	203	EVB	C45-C46-C72-C54
3	B	204	EVB	C31-C32-C42-C44
3	B	203	EVB	C53-C54-C72-C46
3	A	203	EVB	C3-C2-C7-C8
5	B	210	SPM	C11-C12-C13-N14
3	B	204	EVB	C4-C15-C16-C17
3	B	203	EVB	C16-C15-C4-C3
3	A	203	EVB	C47-C46-C72-C54
3	A	204	EVB	C32-C42-C44-C45
3	B	204	EVB	C33-C32-C42-C44
3	B	203	EVB	C16-C15-C4-C5
5	B	211	SPM	N1-C2-C3-C4
3	A	204	EVB	C32-C42-C44-C49
5	A	212	SPM	C7-C6-N5-C4
5	B	211	SPM	C2-C3-C4-N5
5	A	212	SPM	C11-C12-C13-N14
5	B	211	SPM	C11-C12-C13-N14
5	A	211	SPM	C7-C8-C9-N10
3	B	203	EVB	C19-C18-S69-O25

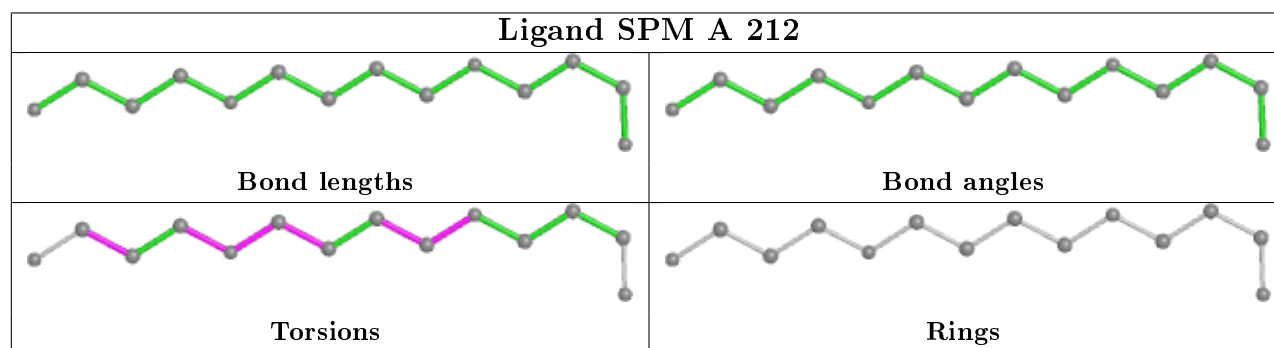
There are no ring outliers.

2 monomers are involved in 5 short contacts:

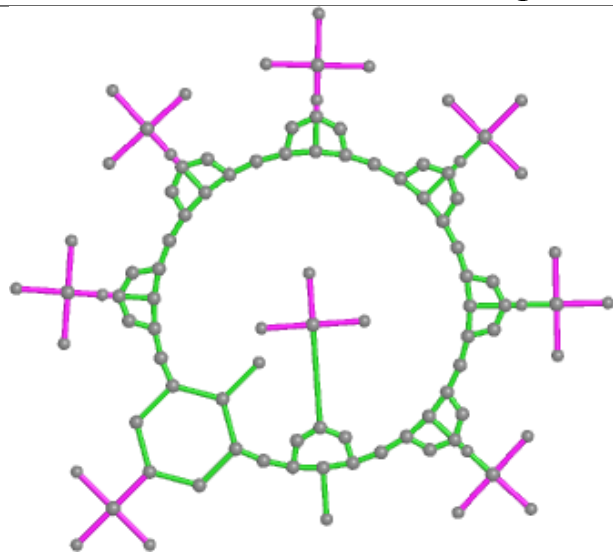
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	201	HEC	3	0
2	A	201	HEC	2	0

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

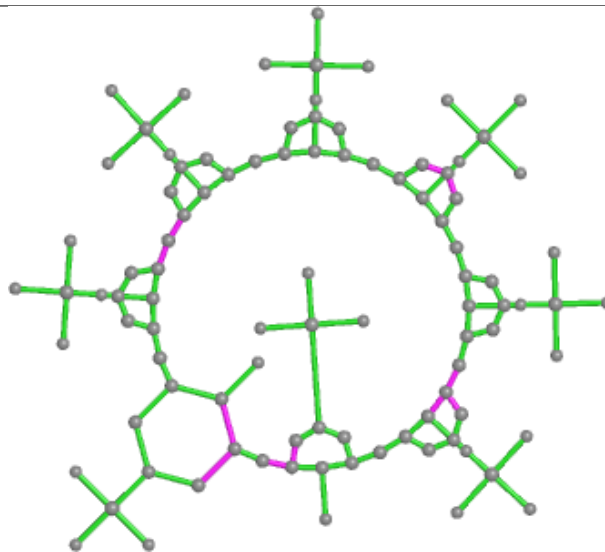
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified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



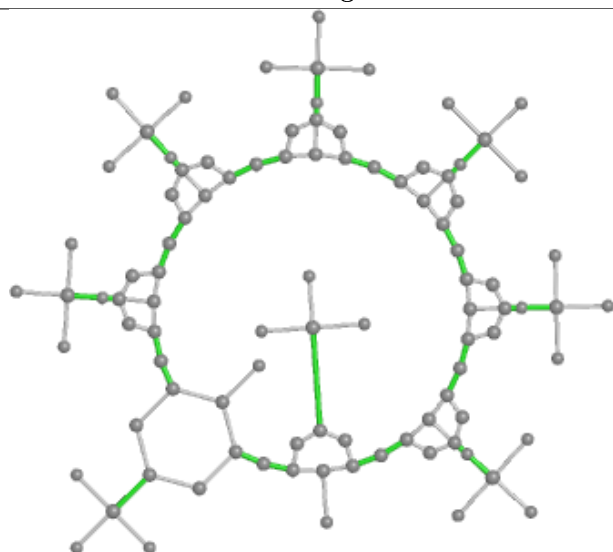
Ligand EVB B 202



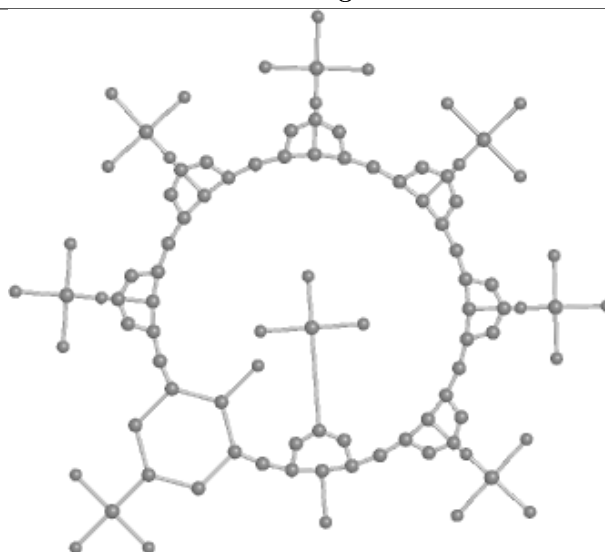
Bond lengths



Bond angles

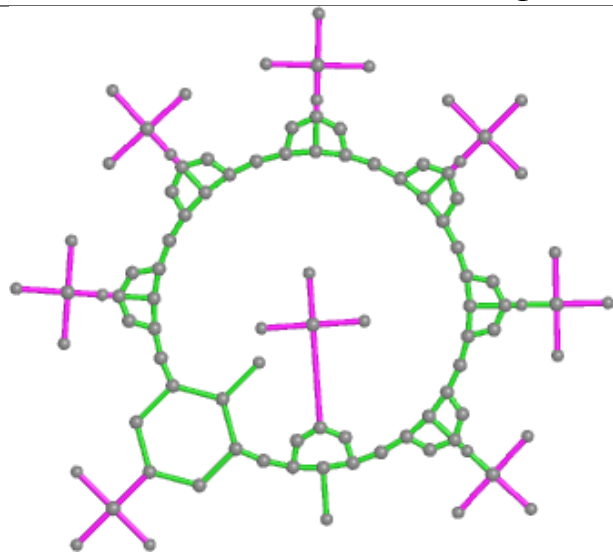


Torsions

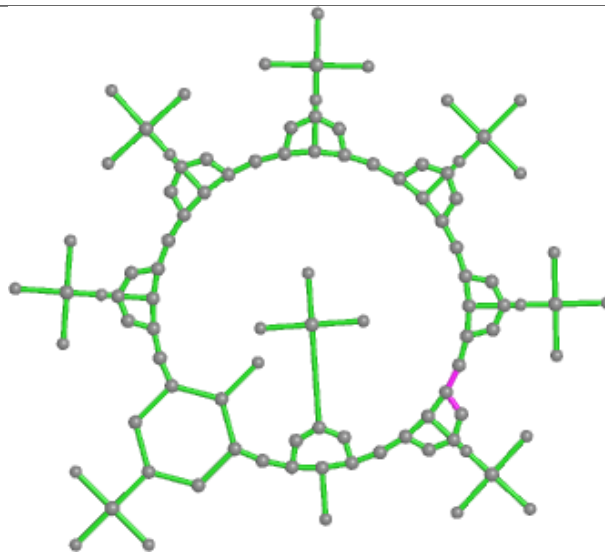


Rings

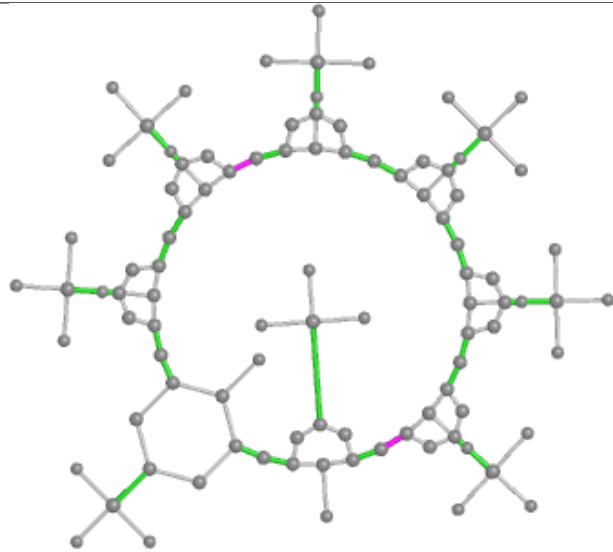
Ligand EVB B 204



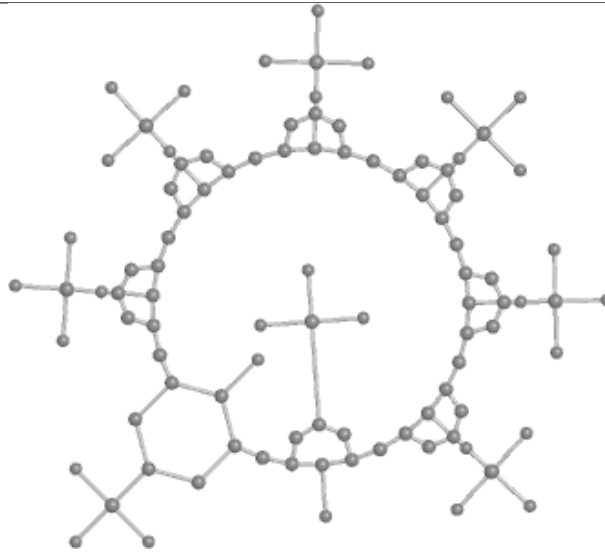
Bond lengths



Bond angles

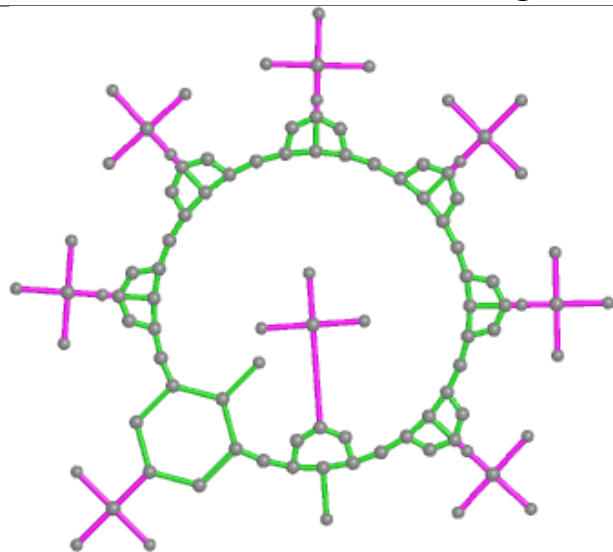


Torsions

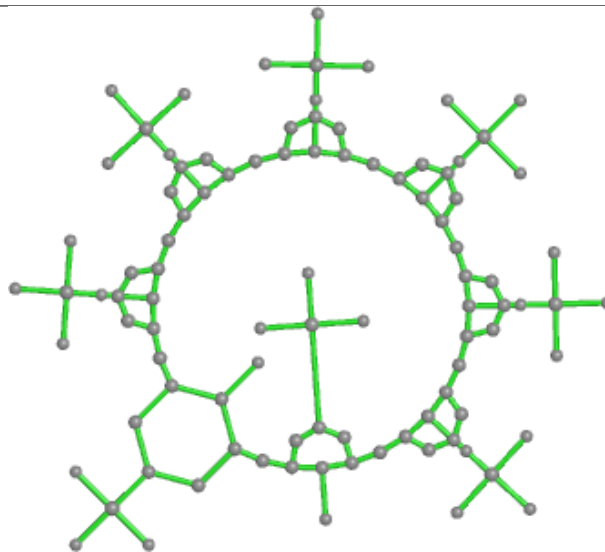


Rings

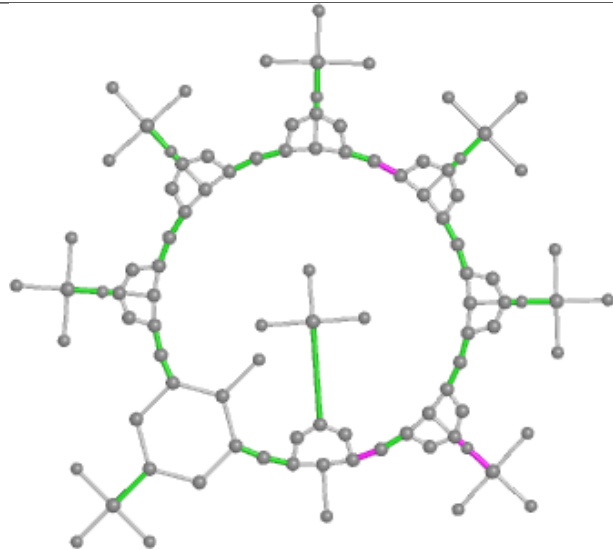
Ligand EVB B 203



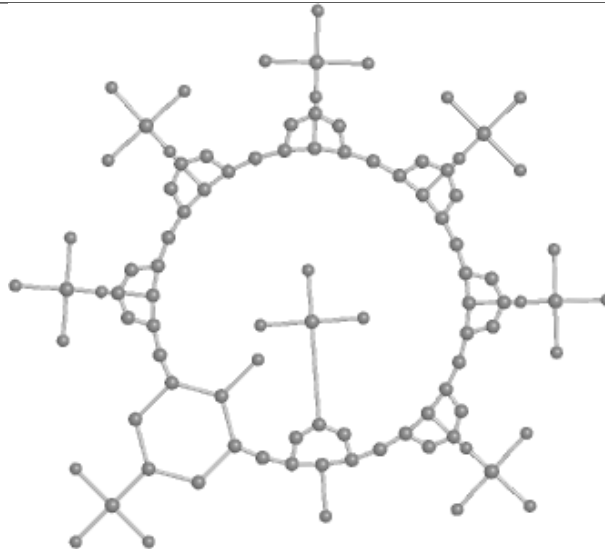
Bond lengths



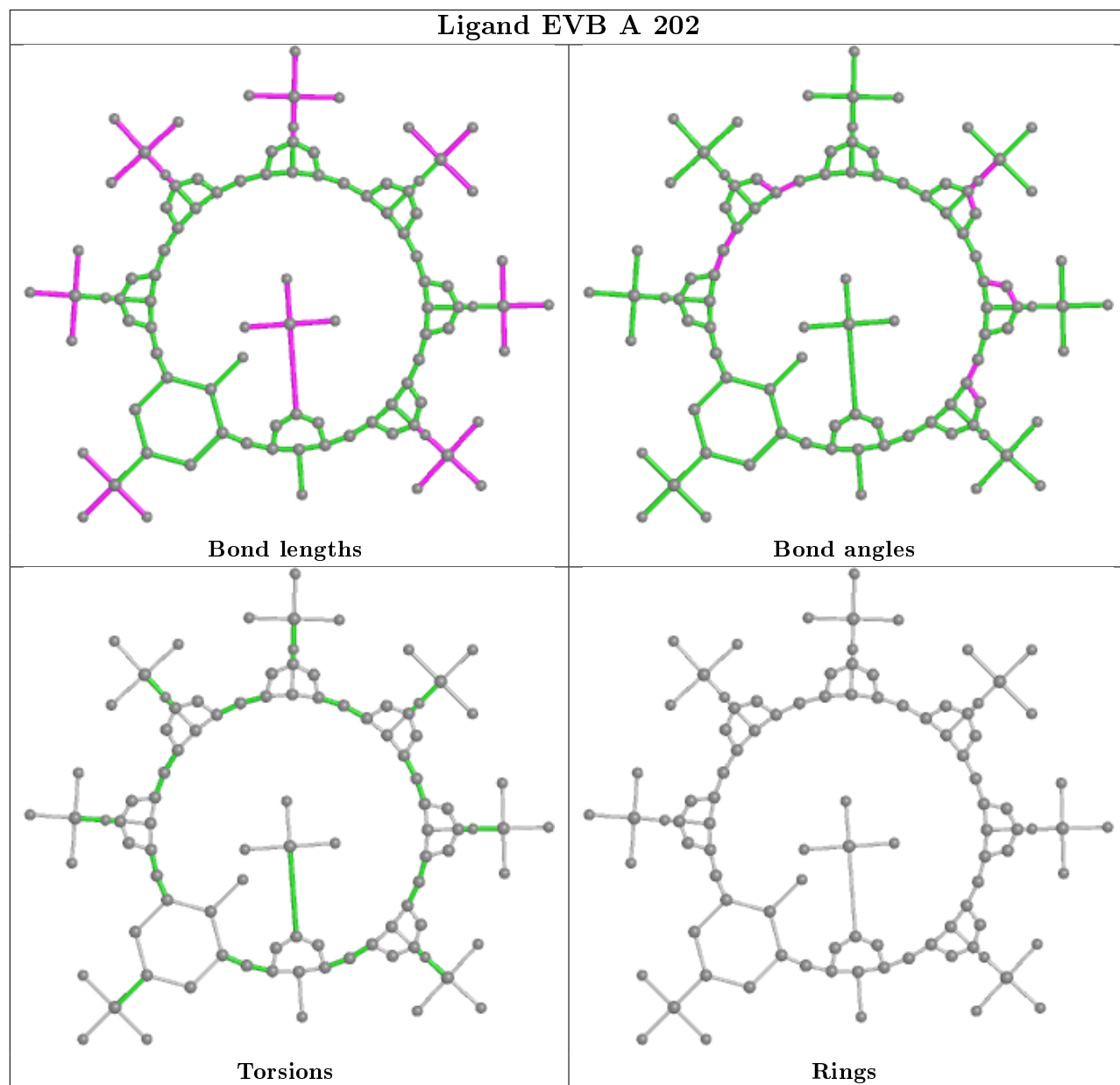
Bond angles

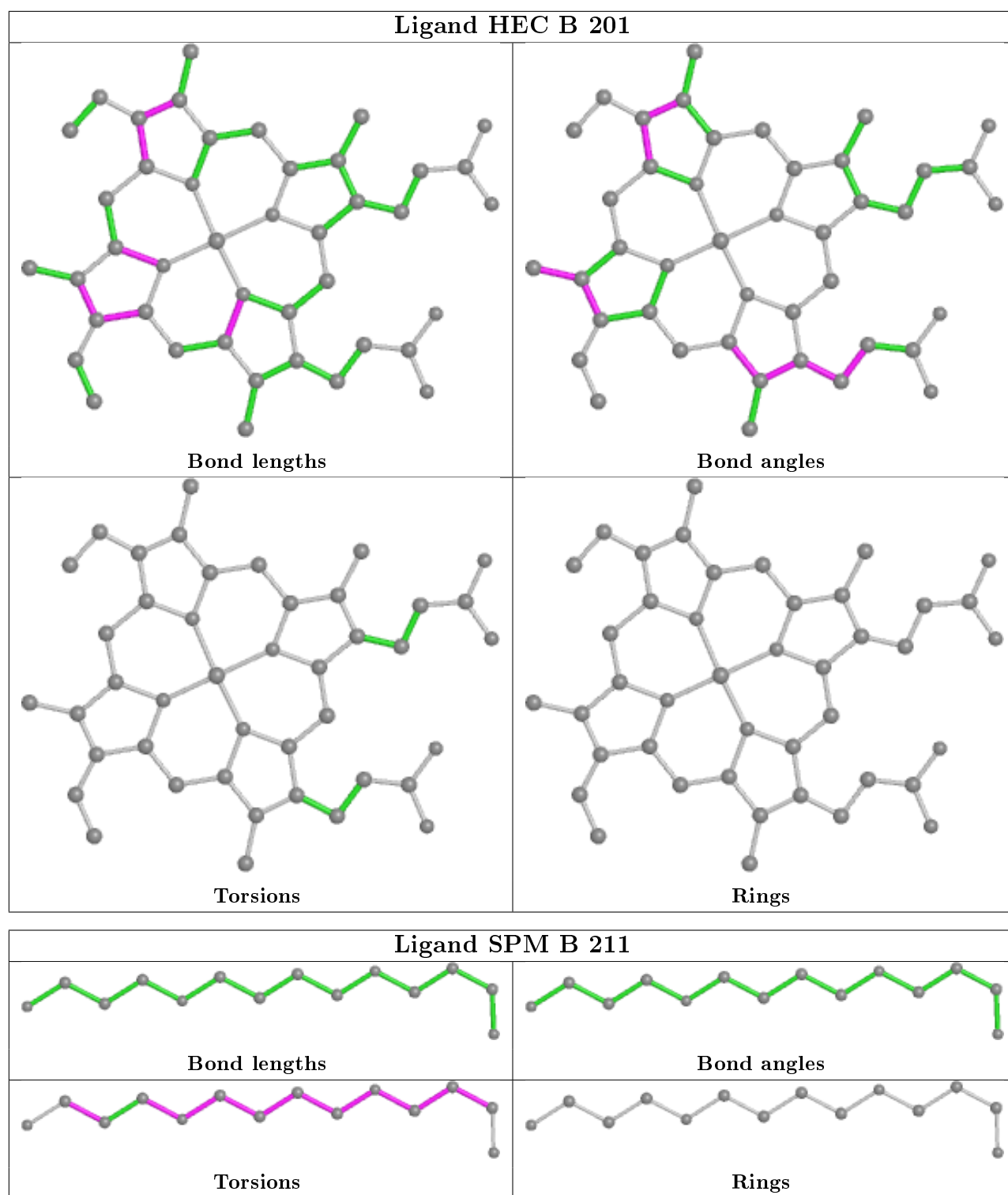


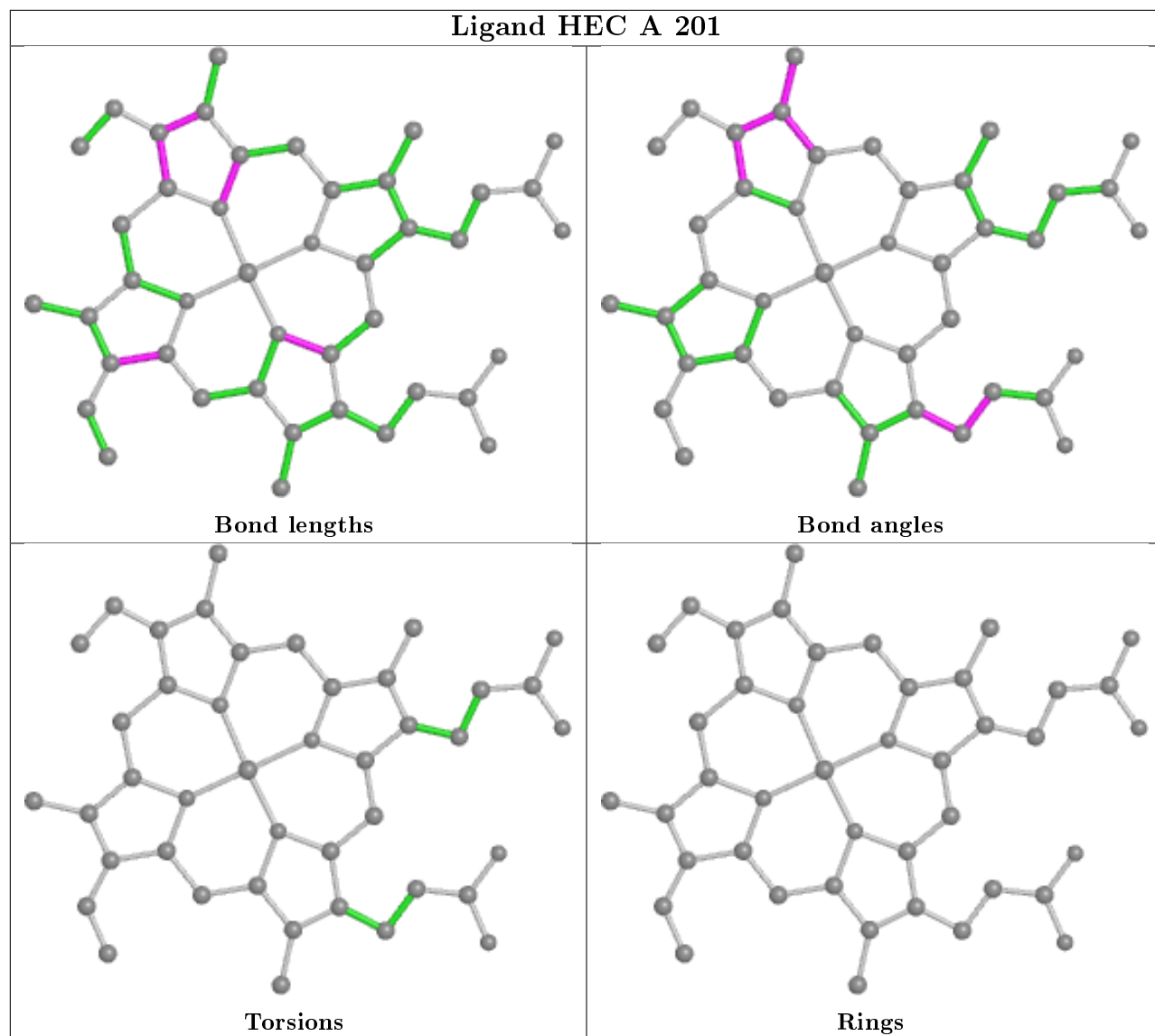
Torsions

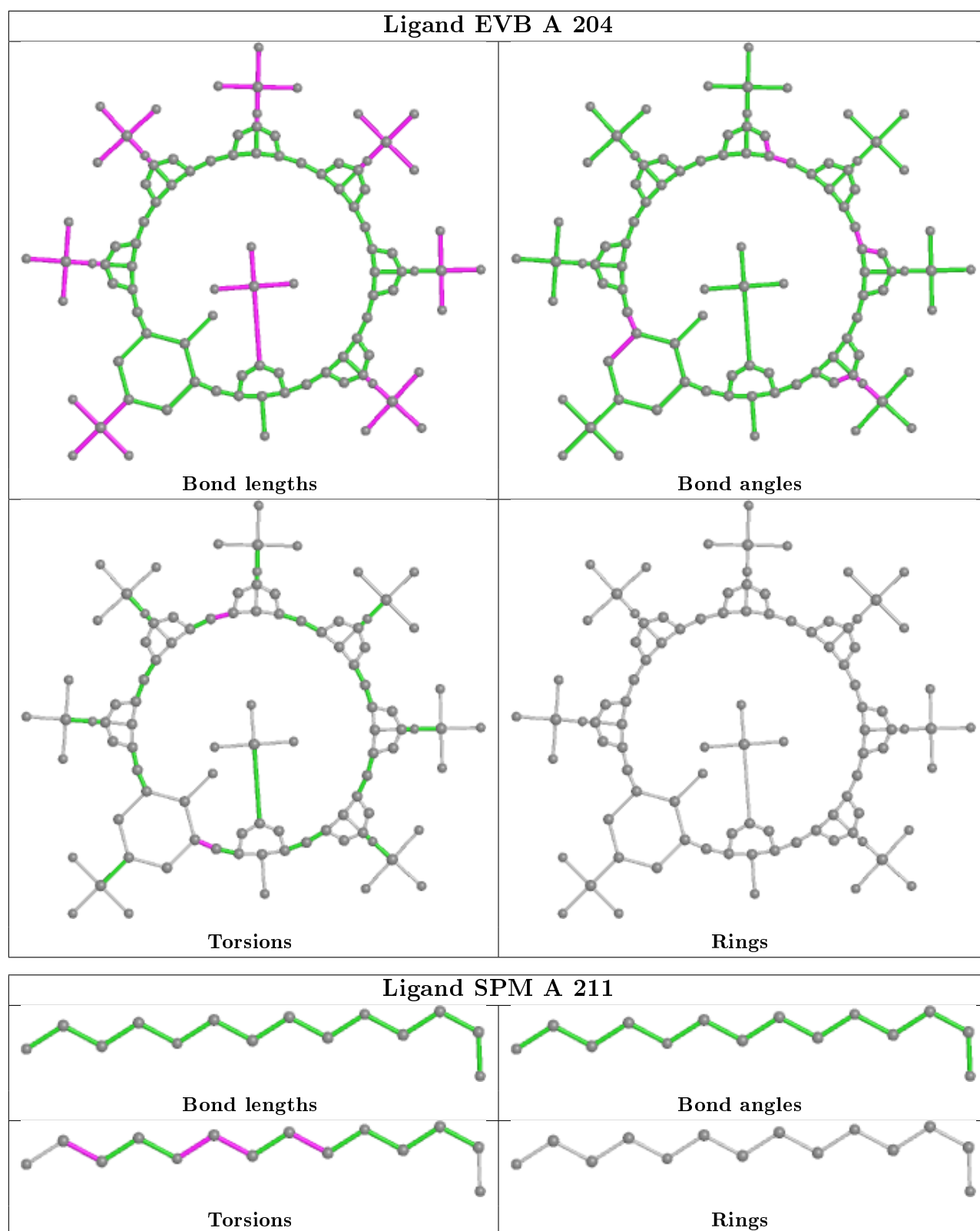


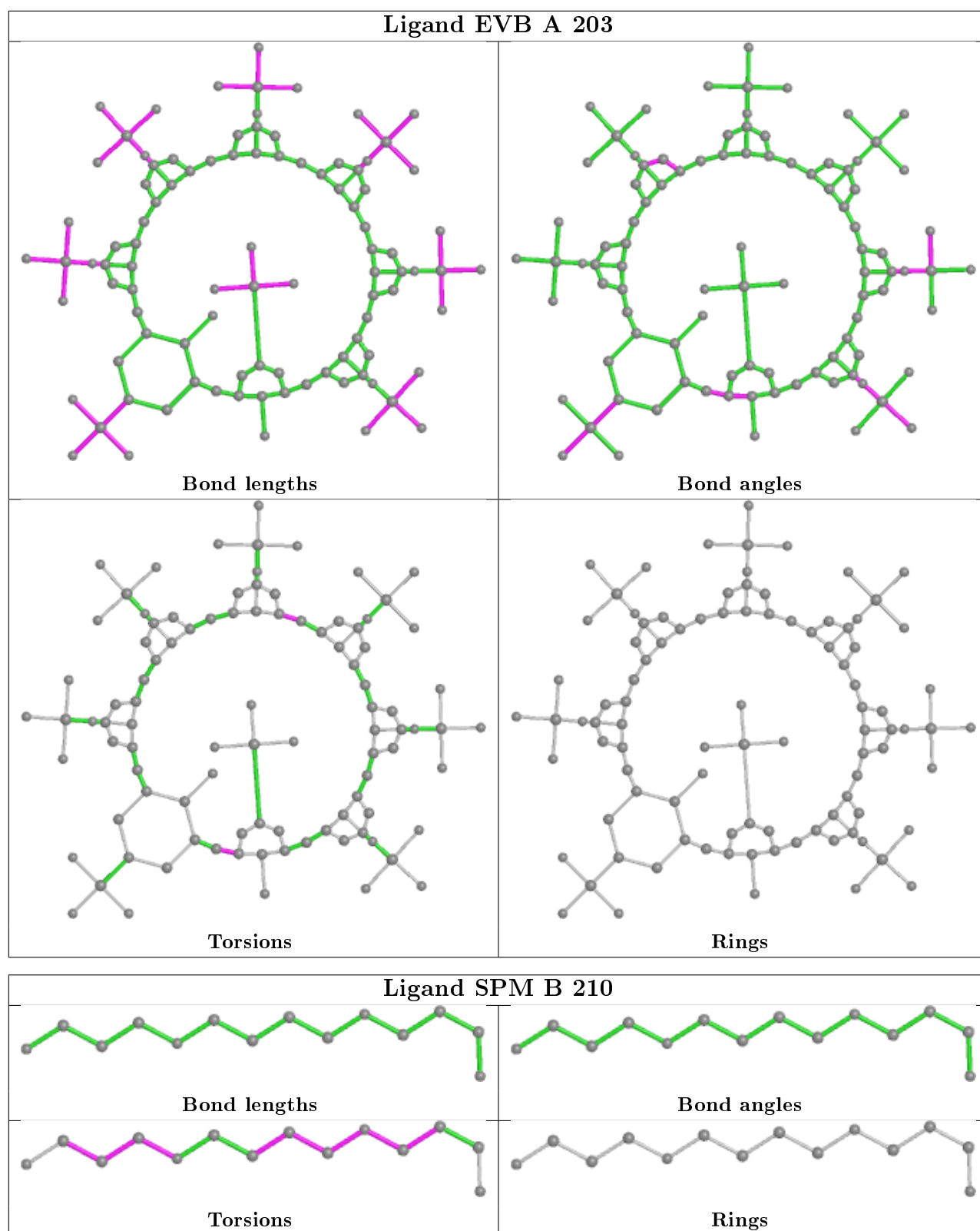
Rings











5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	108/108 (100%)	0.09	1 (0%) 84 88	26, 39, 68, 112	0
1	B	108/108 (100%)	0.42	5 (4%) 32 40	40, 64, 116, 150	0
All	All	216/216 (100%)	0.25	6 (2%) 53 60	26, 48, 101, 150	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	-5	ALA	7.1
1	B	-4	GLU	3.8
1	B	90	ASP	3.5
1	A	-5	ALA	3.2
1	B	-2	LYS	2.9
1	B	68	LEU	2.2

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 carbohydrates in this entry.

6.4 Ligands [i](#)

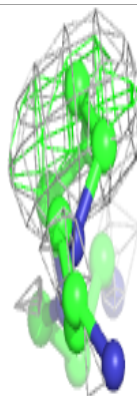
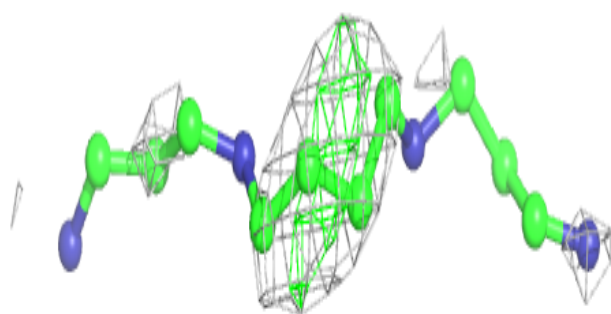
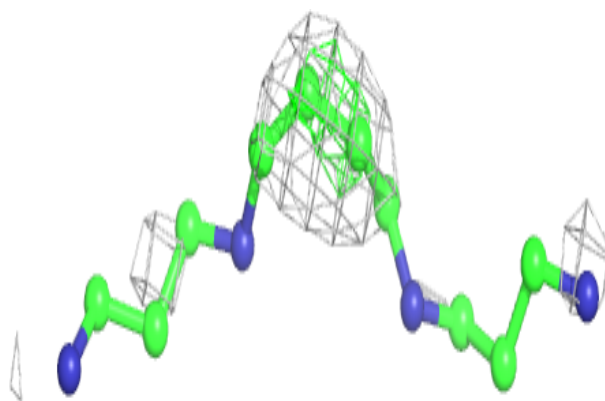
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	SPM	B	211	14/14	0.37	0.41	107,111,115,115	14
5	SPM	B	210	14/14	0.53	0.28	92,94,99,99	0
5	SPM	A	211	14/14	0.65	0.33	66,70,83,85	0
5	SPM	A	212	14/14	0.74	0.47	57,70,81,83	0
4	SO4	B	208	5/5	0.74	0.25	109,109,109,109	5
3	EVB	B	203	96/96	0.80	0.23	89,122,135,137	0
4	SO4	A	209	5/5	0.82	0.28	135,136,136,136	0
4	SO4	B	206	5/5	0.84	0.26	124,125,125,127	0
4	SO4	A	207	5/5	0.85	0.20	125,125,126,126	0
3	EVB	A	204	96/96	0.85	0.24	63,98,111,115	0
4	SO4	B	209	5/5	0.86	0.43	134,135,135,135	0
3	EVB	B	204	96/96	0.86	0.19	74,95,113,114	96
4	SO4	B	205	5/5	0.89	0.21	138,138,138,138	0
4	SO4	B	207	5/5	0.89	0.26	126,127,127,127	0
4	SO4	A	208	5/5	0.90	0.29	122,122,122,123	0
4	SO4	A	210	5/5	0.90	0.40	105,108,109,110	0
4	SO4	A	206	5/5	0.95	0.28	88,89,89,93	0
4	SO4	A	205	5/5	0.96	0.15	80,84,85,85	0
3	EVB	B	202	96/96	0.97	0.15	44,54,65,69	0
3	EVB	A	203	96/96	0.98	0.16	33,38,52,56	0
3	EVB	A	202	96/96	0.98	0.15	32,38,52,54	0
2	HEC	B	201	43/43	0.98	0.15	47,49,55,58	0
2	HEC	A	201	43/43	0.99	0.15	27,29,35,36	0

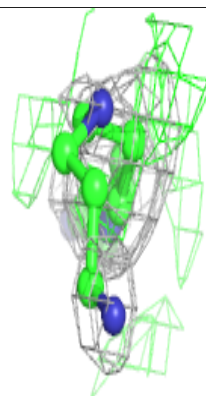
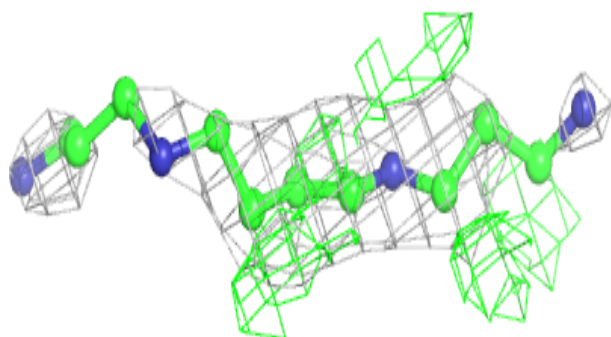
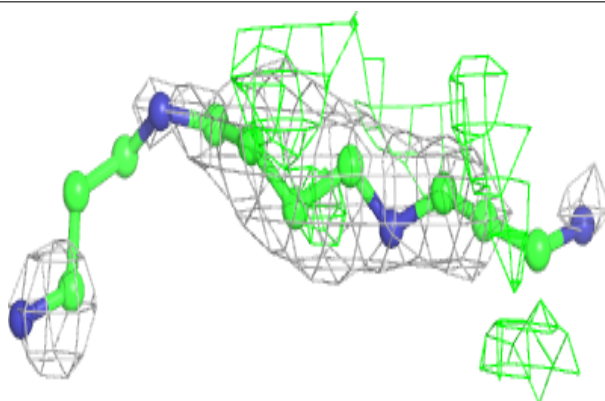
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SPM B 211:

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

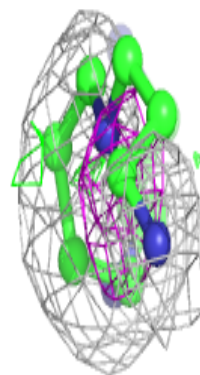
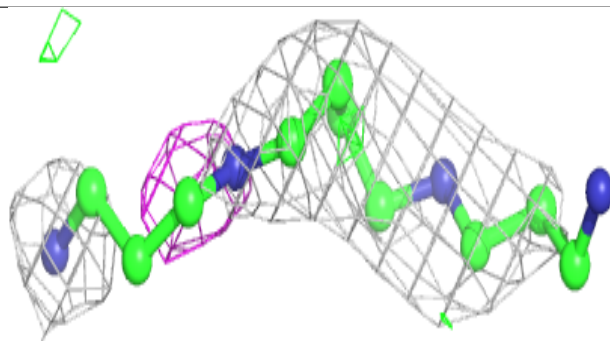
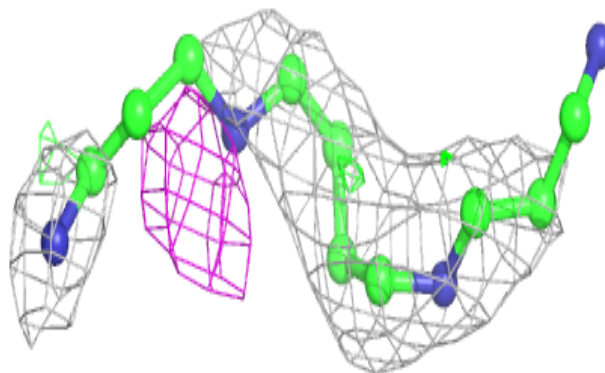
**Electron density around SPM B 210:**

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

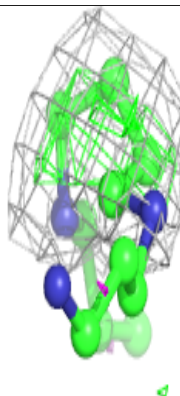
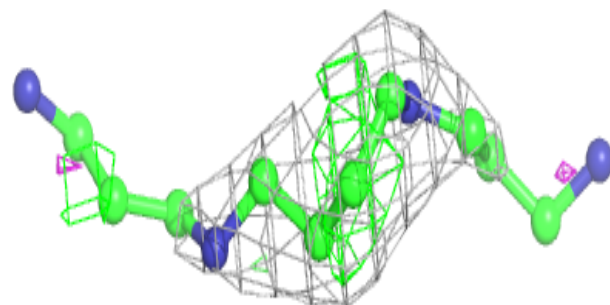
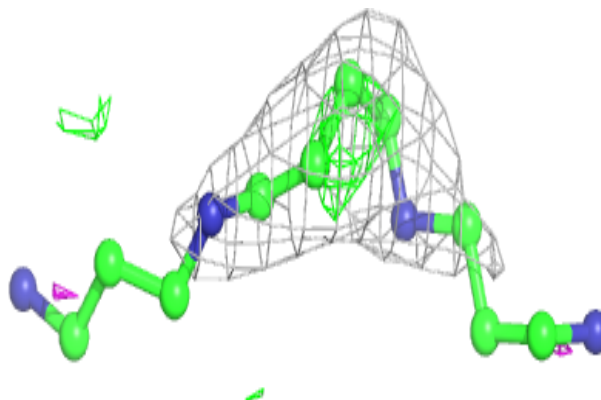


Electron density around SPM A 211:

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

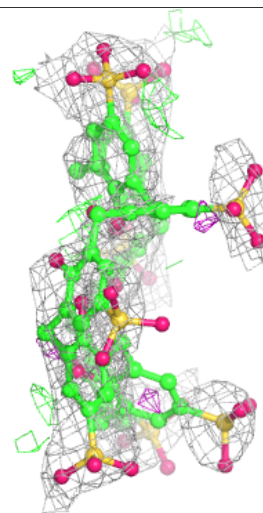
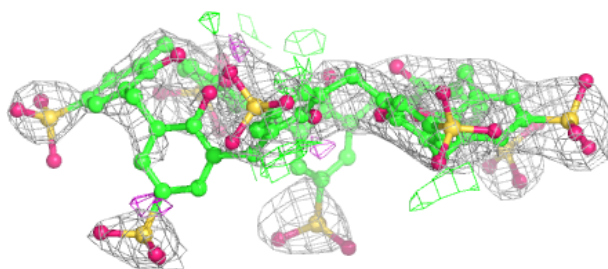
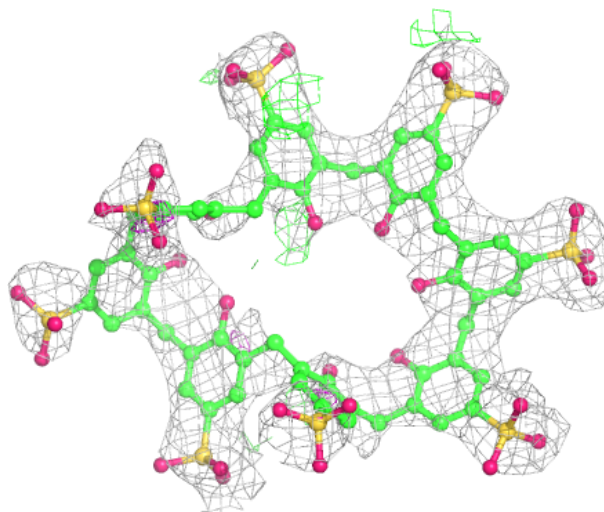
**Electron density around SPM A 212:**

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



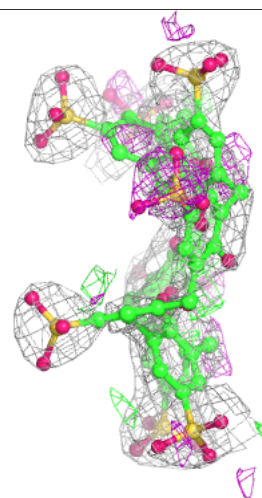
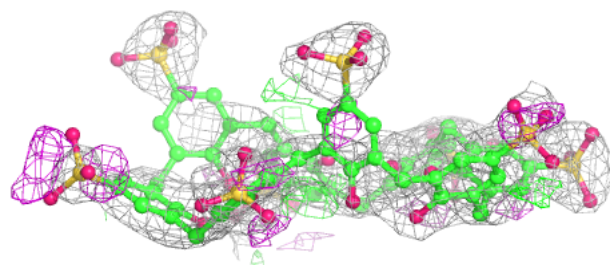
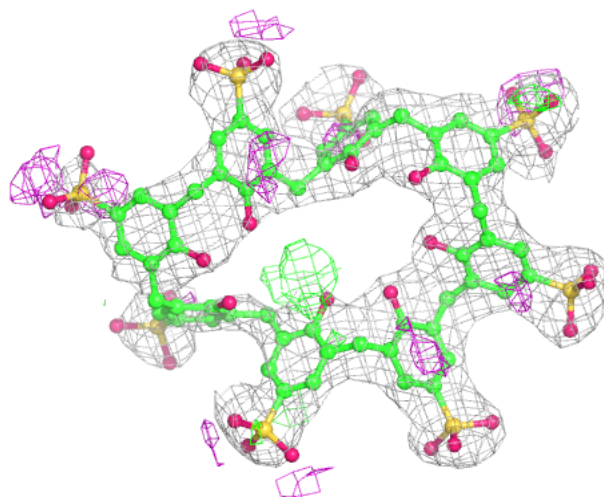
Electron density around EVB B 203:

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



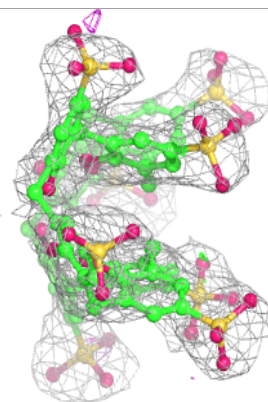
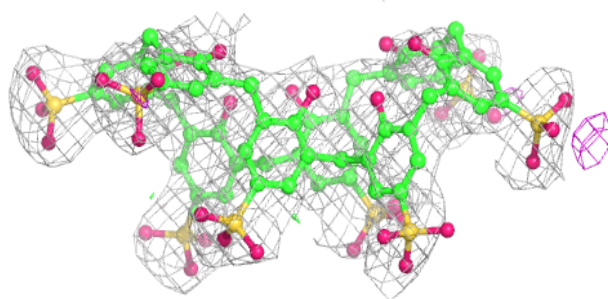
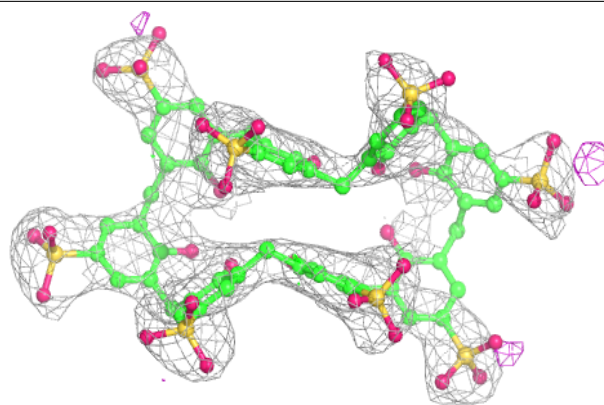
Electron density around EVB A 204:

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



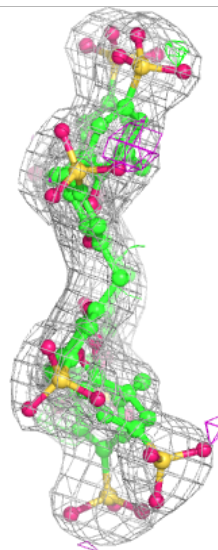
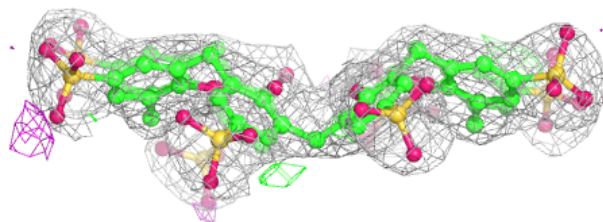
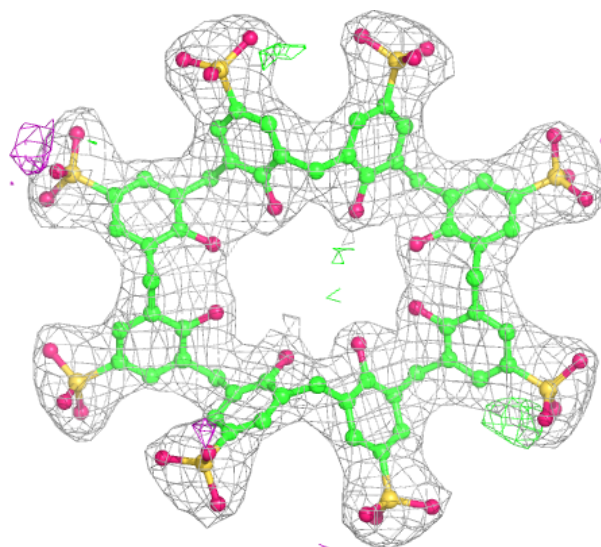
Electron density around EVB B 204:

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



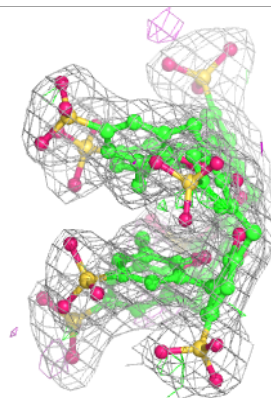
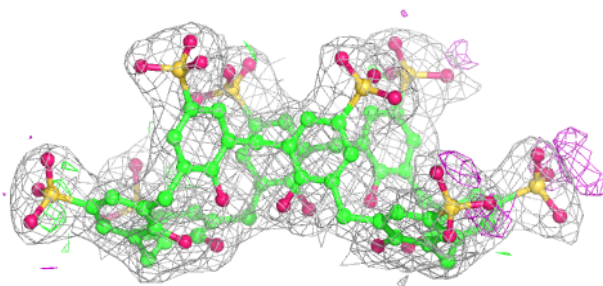
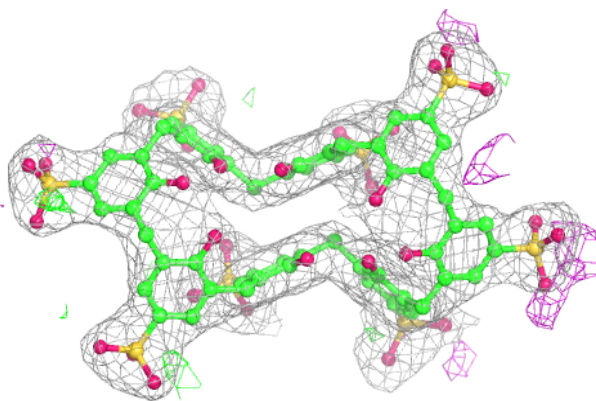
Electron density around EVB B 202:

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



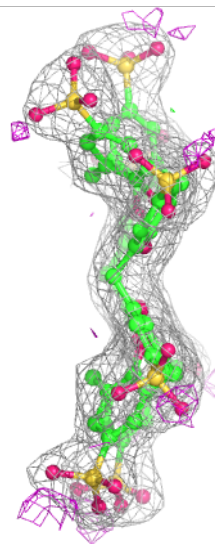
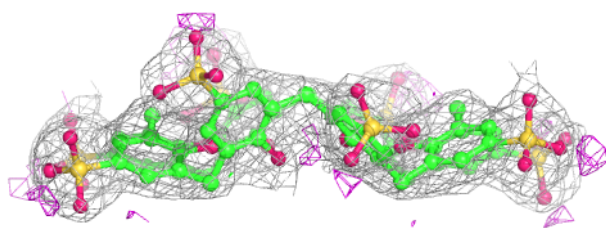
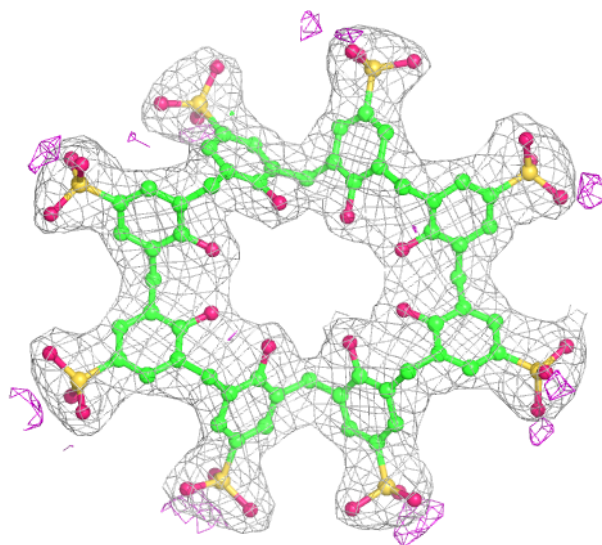
Electron density around EVB A 203:

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



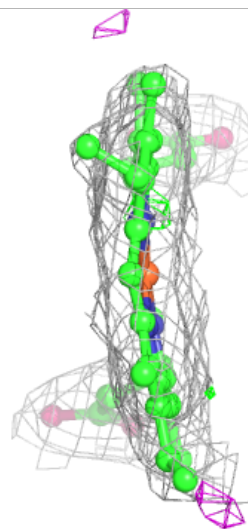
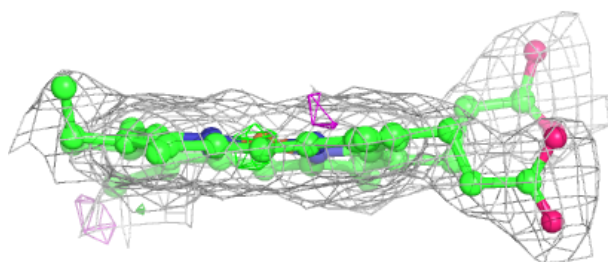
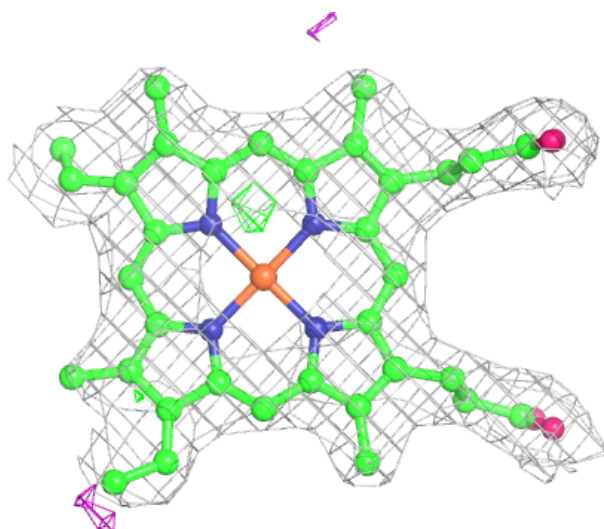
Electron density around EVB A 202:

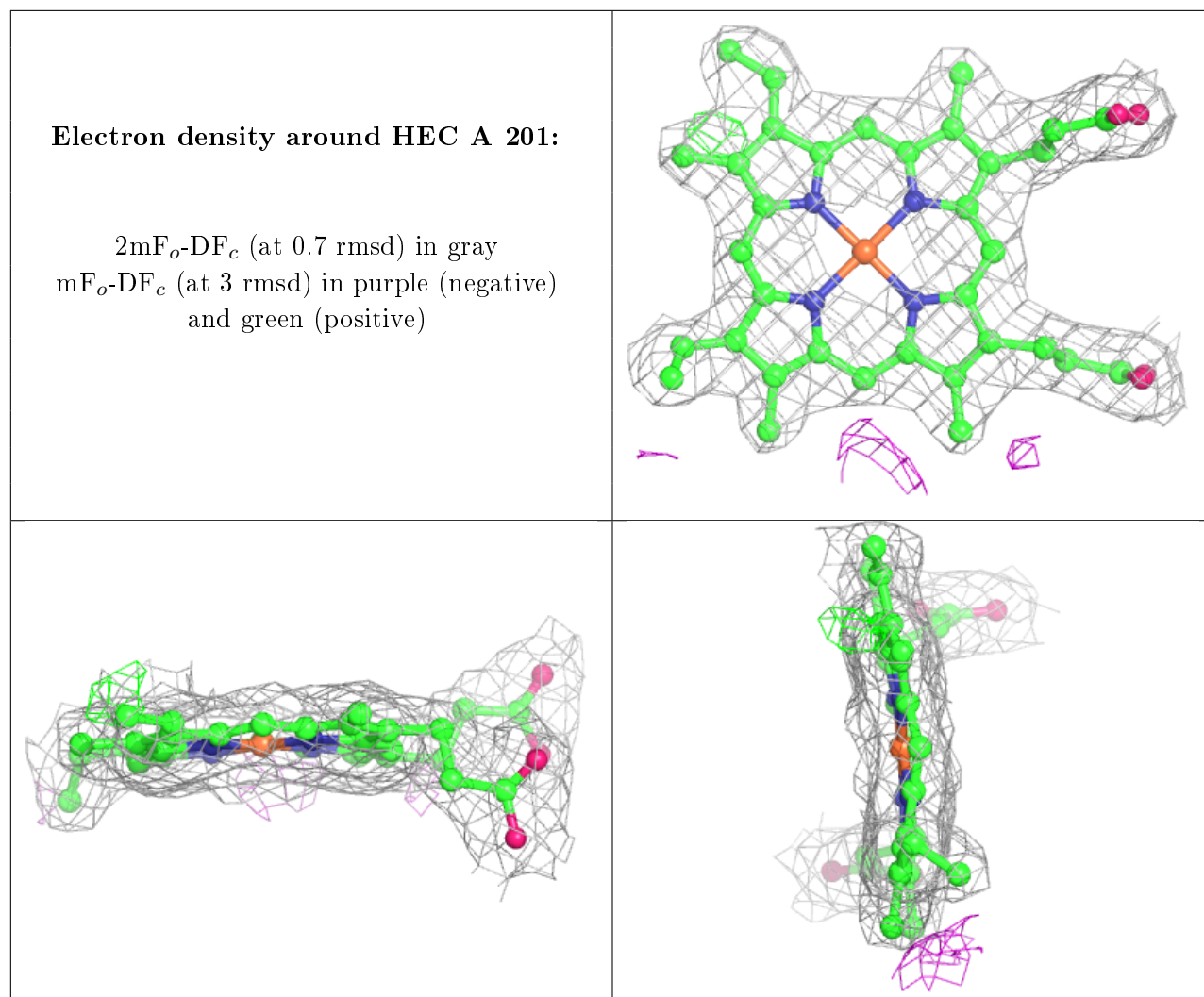
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEC B 201:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.