



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 17, 2020 – 09:47 pm BST

PDB ID : 1HV5  
Title : CRYSTAL STRUCTURE OF THE STROMELYSIN-3 (MMP-11) CATALYTIC DOMAIN COMPLEXED WITH A PHOSPHINIC INHIBITOR  
Authors : Gall, A.L.; Ruff, M.; Kannan, R.; Cuniasse, P.; Yiotakis, A.; Dive, V.; Rio, M.C.; Basset, P.; Moras, D.  
Deposited on : 2001-01-08  
Resolution : 2.60 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](mailto: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.

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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

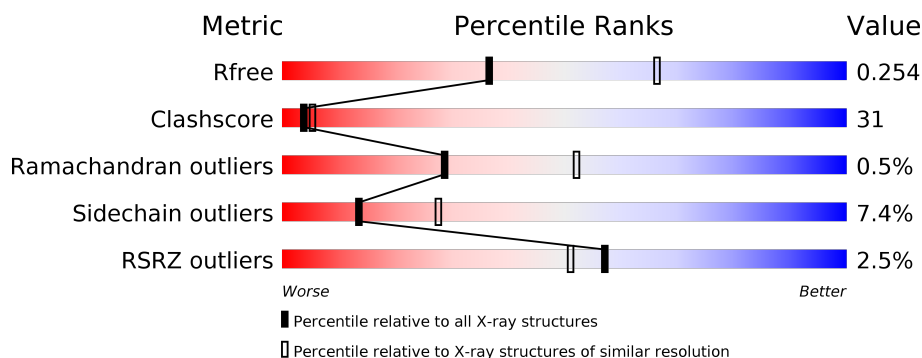
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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  $\geq 3$ , 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	165	<div> <div>0%</div> <div> <div></div> <div>63%</div> <div>31%</div> <div>0%</div> <div>0%</div> </div> <div>...</div> </div>
1	B	165	<div> <div>5%</div> <div> <div></div> <div>53%</div> <div>39%</div> <div>6%</div> <div>0%</div> </div> <div>..</div> </div>
1	C	165	<div> <div>2%</div> <div> <div></div> <div>64%</div> <div>30%</div> <div>0%</div> <div>0%</div> </div> <div>...</div> </div>
1	D	165	<div> <div>2%</div> <div> <div></div> <div>66%</div> <div>24%</div> <div>6%</div> <div>0%</div> </div> <div>..</div> </div>
1	E	165	<div> <div>2%</div> <div> <div></div> <div>58%</div> <div>34%</div> <div>6%</div> <div>0%</div> </div> <div>..</div> </div>
1	F	165	<div> <div>3%</div> <div> <div></div> <div>66%</div> <div>25%</div> <div>6%</div> <div>0%</div> </div> <div>..</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
4	CPS	F	5091	-	-	X	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 10772 atoms, of which 0 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 STROMELYSIN 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	162	Total	C	N	O	S	0	0	0
			1324	852	231	238	3			
1	B	164	Total	C	N	O	S	0	0	0
			1342	863	236	240	3			
1	C	162	Total	C	N	O	S	0	0	0
			1324	852	231	238	3			
1	D	162	Total	C	N	O	S	0	0	0
			1324	852	231	238	3			
1	E	165	Total	C	N	O	S	0	0	0
			1352	868	238	243	3			
1	F	162	Total	C	N	O	S	0	0	0
			1324	852	231	238	3			

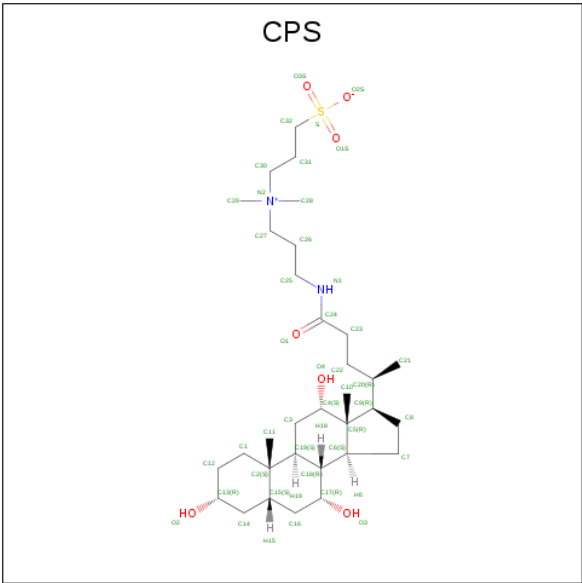
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	2	Total	Zn	0	0
			2	2		
2	E	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		
2	C	2	Total	Zn	0	0
			2	2		
2	A	2	Total	Zn	0	0
			2	2		
2	F	2	Total	Zn	0	0
			2	2		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total Ca 1 1	0	0
3	E	1	Total Ca 1 1	0	0
3	B	1	Total Ca 1 1	0	0
3	C	1	Total Ca 1 1	0	0
3	A	1	Total Ca 1 1	0	0
3	F	1	Total Ca 1 1	0	0

- Molecule 4 is 3-[(3-CHOLAMIDOPROPYL)DIMETHYLAMMONIO]-1-PROPANESULFO NATE (three-letter code: CPS) (formula: C<sub>32</sub>H<sub>58</sub>N<sub>2</sub>O<sub>7</sub>S).



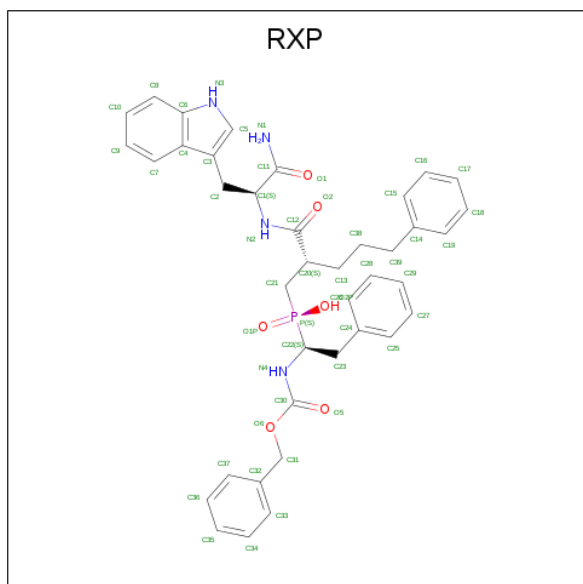
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 26 23 3	4	0
4	A	1	Total C O 26 23 3	4	0
4	B	1	Total C O 26 23 3	4	0
4	B	1	Total C O 26 23 3	4	0
4	C	1	Total C O 26 23 3	4	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	C	O			4	0
			26	23	3				
4	D	1	Total	C	O			4	0
			26	23	3				
4	D	1	Total	C	O			4	0
			26	23	3				
4	E	1	Total	C	O			4	0
			26	23	3				
4	E	1	Total	C	O			4	0
			26	23	3				
4	F	1	Total	C	O			4	0
			26	23	3				
4	F	1	Total	C	N	O	S	0	0
			42	32	2	7	1		

- Molecule 5 is 1-BENZYLOXYCARBONYLAMINO-2-PHENYL-ETHYL)-{2-[1-CARBAMOYL-2-(1H-INDOL-3-YL)-ETHYLCARBAMOYL]-5-PHENYL-PENTYL}-PHOSPHINIC ACID (three-letter code: RXP) (formula: C<sub>39</sub>H<sub>43</sub>N<sub>4</sub>O<sub>6</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			50	39	4	6	1		
5	B	1	Total	C	N	O	P	0	0
			50	39	4	6	1		
5	C	1	Total	C	N	O	P	0	0
			50	39	4	6	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	D	1	Total	C	N	O	P	0	0
			50	39	4	6	1		
5	E	1	Total	C	N	O	P	0	0
			50	39	4	6	1		
5	F	1	Total	C	N	O	P	0	0
			50	39	4	6	1		

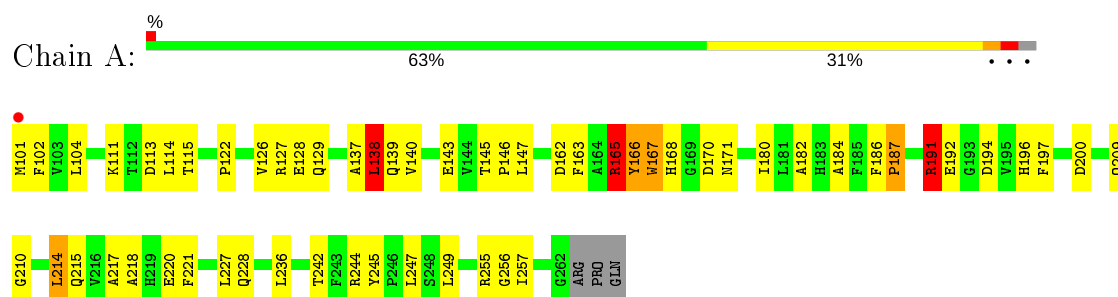
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	376	Total	O	0	0
			376	376		
6	B	318	Total	O	0	0
			318	318		
6	C	367	Total	O	0	0
			367	367		
6	D	341	Total	O	0	0
			341	341		
6	E	353	Total	O	0	0
			353	353		
6	F	381	Total	O	0	0
			381	381		

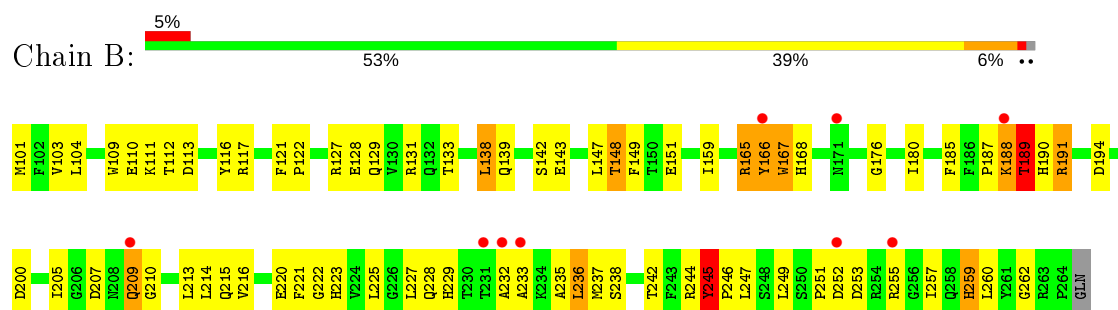
### 3 Residue-property plots

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.

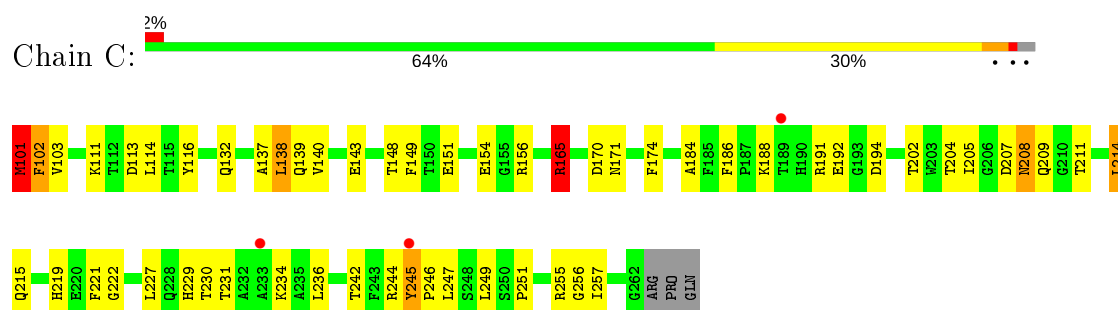
#### • Molecule 1: STROMELYSIN 3



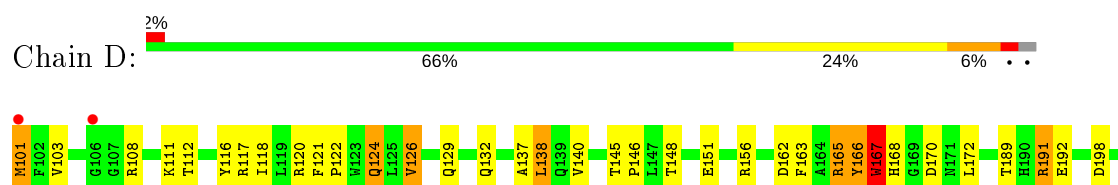
#### • Molecule 1: STROMELYSIN 3



#### • Molecule 1: STROMELYSIN 3



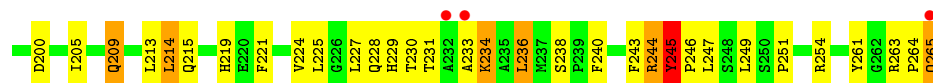
#### • Molecule 1: STROMELYSIN 3



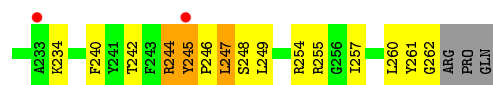




• Molecule 1: STROMELYSIN 3



• Molecule 1: STROMELYSIN 3



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	140.10 Å   148.50 Å   91.40 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	19.89 – 2.60 19.89 – 2.59	Depositor EDS
% Data completeness (in resolution range)	96.9 (19.89-2.60) 96.7 (19.89-2.59)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.50 (at 2.59 Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.218   ,   0.262 0.209   ,   0.254	Depositor DCC
$R_{free}$ test set	6042 reflections (10.14%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.1	Xtriage
Anisotropy	0.517	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 57.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	10772	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.55% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: RXP, ZN, CPS, CA

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	0.70	1/1367 (0.1%)	0.87	5/1861 (0.3%)
1	B	0.70	3/1386 (0.2%)	0.99	11/1887 (0.6%)
1	C	0.63	0/1367	0.94	9/1861 (0.5%)
1	D	0.79	3/1367 (0.2%)	0.97	11/1861 (0.6%)
1	E	0.66	1/1396 (0.1%)	0.88	5/1899 (0.3%)
1	F	0.75	3/1367 (0.2%)	0.94	7/1861 (0.4%)
All	All	0.70	11/8250 (0.1%)	0.93	48/11230 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	3
1	E	0	1
1	F	0	1
All	All	0	6

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	166	TYR	C-N	-15.08	0.99	1.34
1	E	167	TRP	N-CA	11.29	1.69	1.46
1	A	167	TRP	N-CA	9.55	1.65	1.46
1	F	165	ARG	C-N	-9.54	1.12	1.34
1	F	168	HIS	C-N	-7.49	1.19	1.33

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	188	LYS	CB-CA-C	12.47	135.34	110.40
1	F	245	TYR	C-N-CD	10.84	151.17	128.40
1	C	245	TYR	C-N-CD	10.81	151.10	128.40
1	D	101	MET	N-CA-C	8.98	135.24	111.00
1	C	102	PHE	O-C-N	-8.87	108.51	122.70

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	166	TYR	Peptide
1	D	166	TYR	Mainchain,Peptide
1	D	245	TYR	Sidechain
1	E	166	TYR	Peptide
1	F	165	ARG	Mainchain

## 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	1324	0	1253	70	0
1	B	1342	0	1272	77	0
1	C	1324	0	1253	77	0
1	D	1324	0	1252	58	0
1	E	1352	0	1281	85	0
1	F	1324	0	1252	68	1
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	52	0	70	16	0
4	B	52	0	70	15	0
4	C	52	0	70	15	0
4	D	52	0	70	9	0
4	E	52	0	70	16	0
4	F	68	0	91	30	0
5	A	50	0	42	5	0
5	B	50	0	42	4	0
5	C	50	0	42	1	0
5	D	50	0	42	1	0
5	E	50	0	42	9	0
5	F	50	0	42	2	0
6	A	376	0	0	35	0
6	B	318	0	0	30	0
6	C	367	0	0	31	0
6	D	341	0	0	28	0
6	E	353	0	0	31	1
6	F	381	0	0	34	0
All	All	10772	0	8256	517	1

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 31.

The worst 5 of 517 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)
4:D:5004:CPS:C10	4:D:5004:CPS:C5	1.75	1.65
4:B:5007:CPS:C10	4:B:5007:CPS:C5	1.74	1.64
4:A:5006:CPS:C10	4:A:5006:CPS:C5	1.75	1.63
4:F:5091:CPS:C19	4:F:5091:CPS:C18	1.75	1.63
4:F:5011:CPS:C5	4:F:5011:CPS:C10	1.76	1.61

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:101:MET:CE	6:E:6062:HOH:O[2_665]	1.33	0.87

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	160/165 (97%)	155 (97%)	5 (3%)	0	100	100
1	B	162/165 (98%)	148 (91%)	12 (7%)	2 (1%)	13	27
1	C	160/165 (97%)	151 (94%)	9 (6%)	0	100	100
1	D	160/165 (97%)	151 (94%)	7 (4%)	2 (1%)	12	24
1	E	163/165 (99%)	152 (93%)	10 (6%)	1 (1%)	25	47
1	F	160/165 (97%)	153 (96%)	7 (4%)	0	100	100
All	All	965/990 (98%)	910 (94%)	50 (5%)	5 (0%)	29	52

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	188	LYS
1	B	189	THR
1	D	167	TRP
1	E	167	TRP
1	D	245	TYR

### 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 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	137/140 (98%)	132 (96%)	5 (4%)	35	61
1	B	139/140 (99%)	126 (91%)	13 (9%)	8	17
1	C	137/140 (98%)	131 (96%)	6 (4%)	28	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	137/140 (98%)	125 (91%)	12 (9%)	10	19
1	E	140/140 (100%)	127 (91%)	13 (9%)	9	17
1	F	137/140 (98%)	125 (91%)	12 (9%)	10	19
All	All	827/840 (98%)	766 (93%)	61 (7%)	13	28

5 of 61 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	165	ARG
1	D	249	LEU
1	F	209	GLN
1	D	170	ASP
1	D	208	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	124	GLN
1	D	208	ASN
1	E	259	HIS
1	D	129	GLN
1	D	132	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 36 ligands modelled in this entry, 18 are monoatomic - leaving 18 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
5	RXP	A	6001	2	50,54,54	4.97	37 (74%)	61,73,73	2.62	27 (44%)
4	CPS	C	5003	-	29,29,45	4.83	15 (51%)	47,47,70	4.08	29 (61%)
4	CPS	F	5011	-	29,29,45	4.96	17 (58%)	47,47,70	3.86	26 (55%)
4	CPS	A	5006	-	29,29,45	4.77	17 (58%)	47,47,70	4.02	25 (53%)
5	RXP	B	6002	2	50,54,54	5.90	36 (72%)	61,73,73	2.88	21 (34%)
4	CPS	D	5004	-	29,29,45	4.87	16 (55%)	47,47,70	3.97	28 (59%)
4	CPS	E	5010	-	29,29,45	4.92	16 (55%)	47,47,70	3.96	25 (53%)
5	RXP	F	6006	2	50,54,54	4.94	32 (64%)	61,73,73	2.35	24 (39%)
5	RXP	C	6003	2	50,54,54	4.89	37 (74%)	61,73,73	2.95	25 (40%)
4	CPS	E	5005	-	29,29,45	4.86	15 (51%)	47,47,70	4.16	28 (59%)
4	CPS	A	5001	-	29,29,45	4.98	17 (58%)	47,47,70	4.08	27 (57%)
5	RXP	E	6005	2	50,54,54	4.94	32 (64%)	61,73,73	2.35	24 (39%)
4	CPS	B	5007	-	29,29,45	4.89	18 (62%)	47,47,70	3.94	27 (57%)
5	RXP	D	6004	2	50,54,54	4.98	34 (68%)	61,73,73	2.59	22 (36%)
4	CPS	B	5002	-	29,29,45	4.85	17 (58%)	47,47,70	3.97	28 (59%)
4	CPS	C	5008	-	29,29,45	4.89	17 (58%)	47,47,70	3.96	24 (51%)
4	CPS	F	5091	-	45,45,45	4.75	23 (51%)	69,70,70	3.26	35 (50%)
4	CPS	D	5009	-	29,29,45	5.05	16 (55%)	47,47,70	3.91	27 (57%)

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
5	RXP	A	6001	2	-	6/40/46/46	0/5/5/5
4	CPS	C	5003	-	-	0/6/71/90	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CPS	F	5011	-	-	0/6/71/90	0/4/4/4
4	CPS	A	5006	-	-	0/6/71/90	0/4/4/4
5	RXP	B	6002	2	-	5/40/46/46	0/5/5/5
4	CPS	D	5004	-	-	0/6/71/90	0/4/4/4
4	CPS	E	5010	-	-	0/6/71/90	0/4/4/4
5	RXP	F	6006	2	-	5/40/46/46	0/5/5/5
5	RXP	C	6003	2	-	5/40/46/46	0/5/5/5
4	CPS	E	5005	-	-	0/6/71/90	0/4/4/4
4	CPS	A	5001	-	-	0/6/71/90	0/4/4/4
5	RXP	E	6005	2	-	5/40/46/46	0/5/5/5
4	CPS	B	5007	-	-	0/6/71/90	0/4/4/4
5	RXP	D	6004	2	-	4/40/46/46	0/5/5/5
4	CPS	B	5002	-	-	0/6/71/90	0/4/4/4
4	CPS	C	5008	-	-	0/6/71/90	0/4/4/4
4	CPS	F	5091	-	-	14/25/90/90	0/4/4/4
4	CPS	D	5009	-	-	0/6/71/90	0/4/4/4

The worst 5 of 412 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	5091	CPS	C10-C5	18.26	1.84	1.54
4	F	5011	CPS	C10-C5	13.60	1.76	1.54
4	E	5005	CPS	C10-C5	13.57	1.76	1.54
4	A	5001	CPS	C10-C5	13.53	1.76	1.54
4	D	5009	CPS	O4-C4	-13.53	1.21	1.43

The worst 5 of 472 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	6002	RXP	O6-C31-C32	11.70	137.51	109.39
4	E	5005	CPS	C6-C18-C17	11.34	126.85	111.81
4	C	5008	CPS	C6-C18-C17	11.14	126.58	111.81
4	B	5007	CPS	C6-C18-C17	11.10	126.53	111.81
4	E	5010	CPS	C6-C18-C17	11.01	126.41	111.81

There are no chirality outliers.

5 of 44 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	6001	RXP	C32-C31-O6-C30

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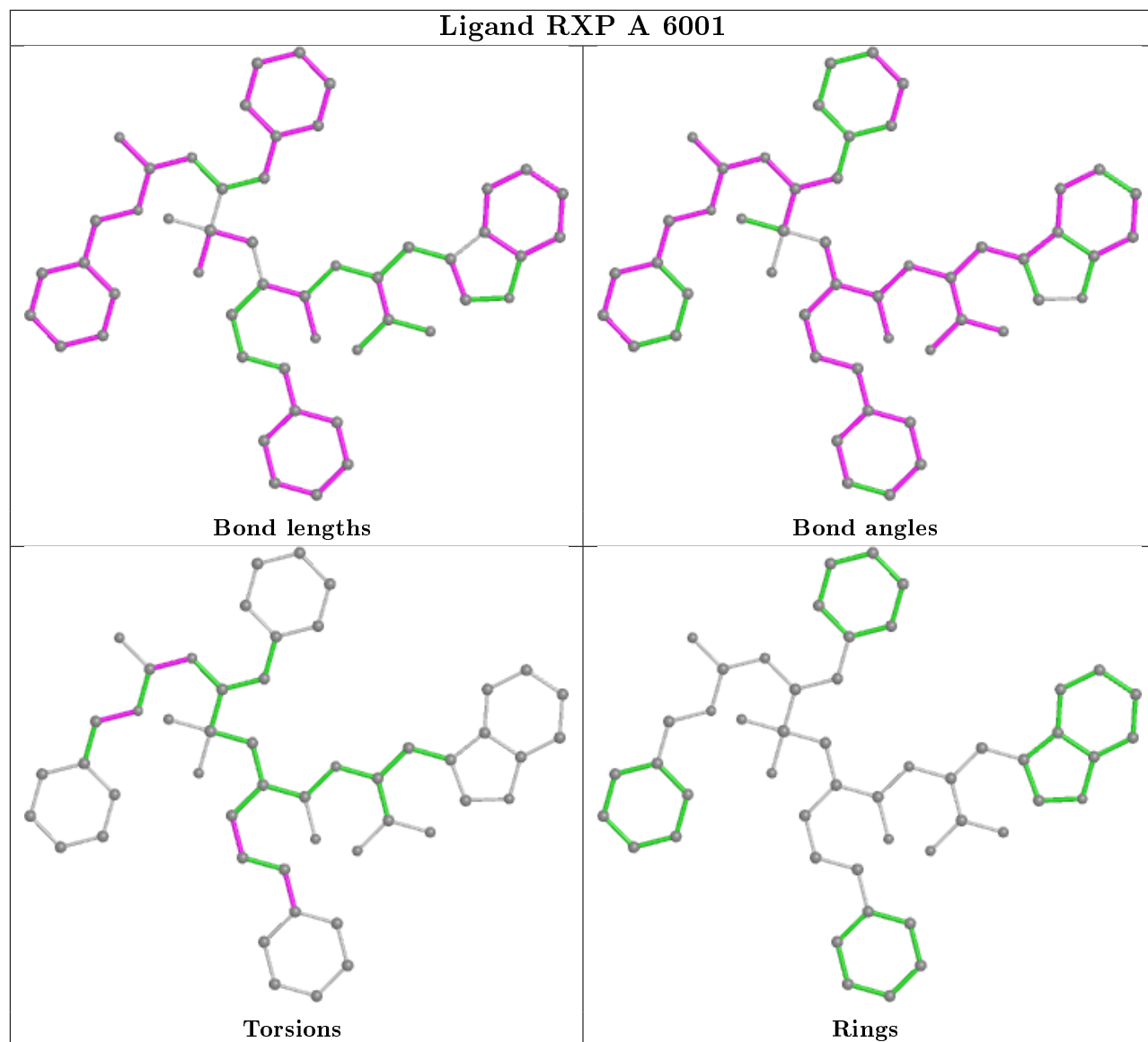
Mol	Chain	Res	Type	Atoms
5	B	6002	RXP	O5-C30-N4-C22
5	B	6002	RXP	O6-C30-N4-C22
5	F	6006	RXP	C32-C31-O6-C30
5	E	6005	RXP	C32-C31-O6-C30

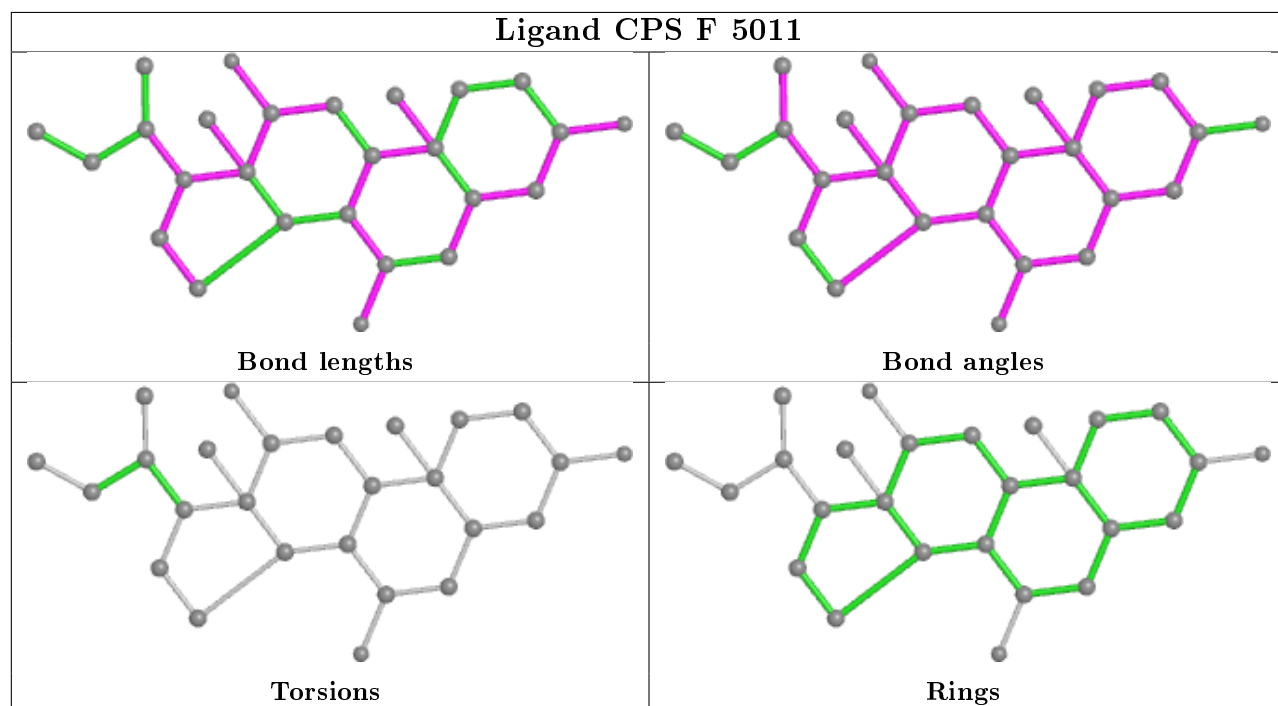
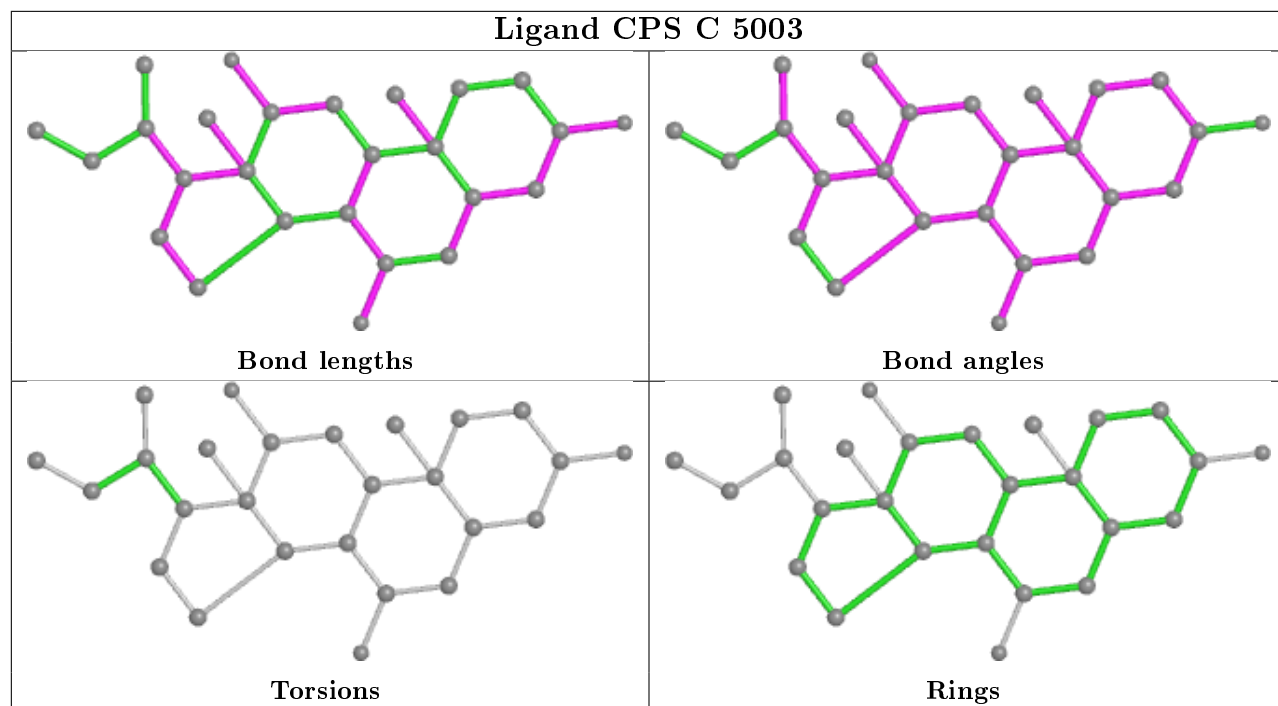
There are no ring outliers.

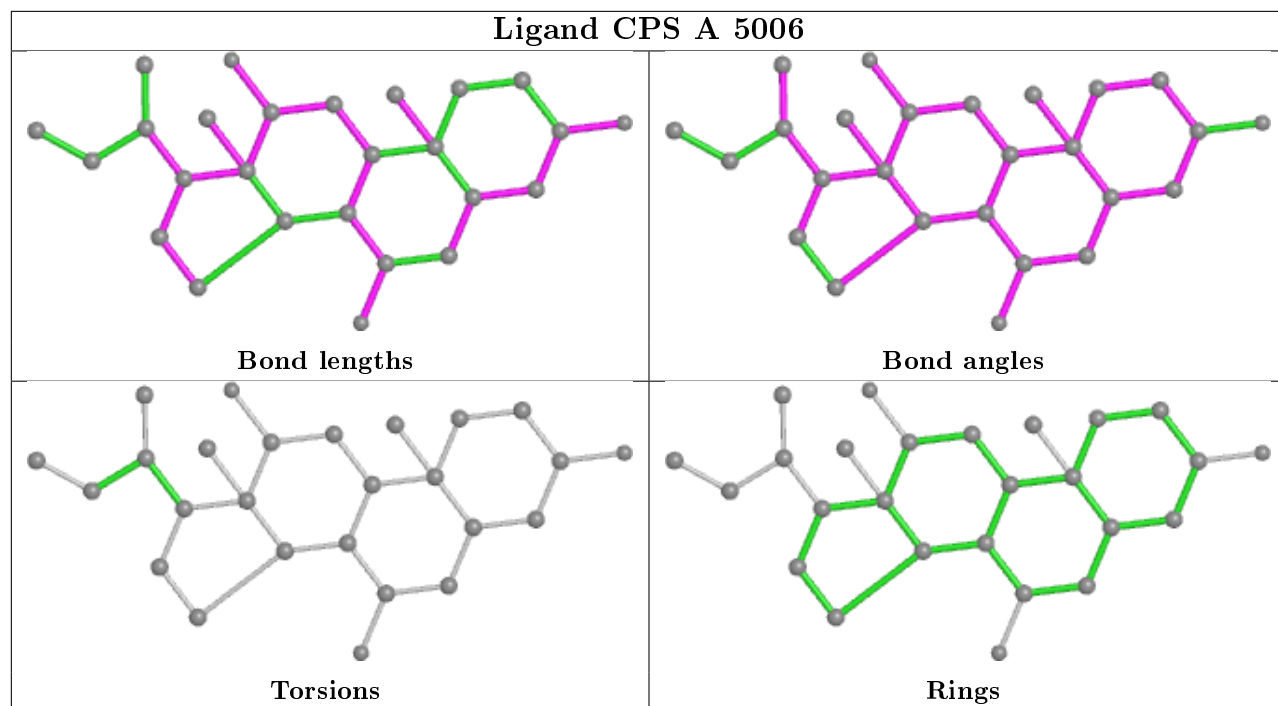
18 monomers are involved in 122 short contacts:

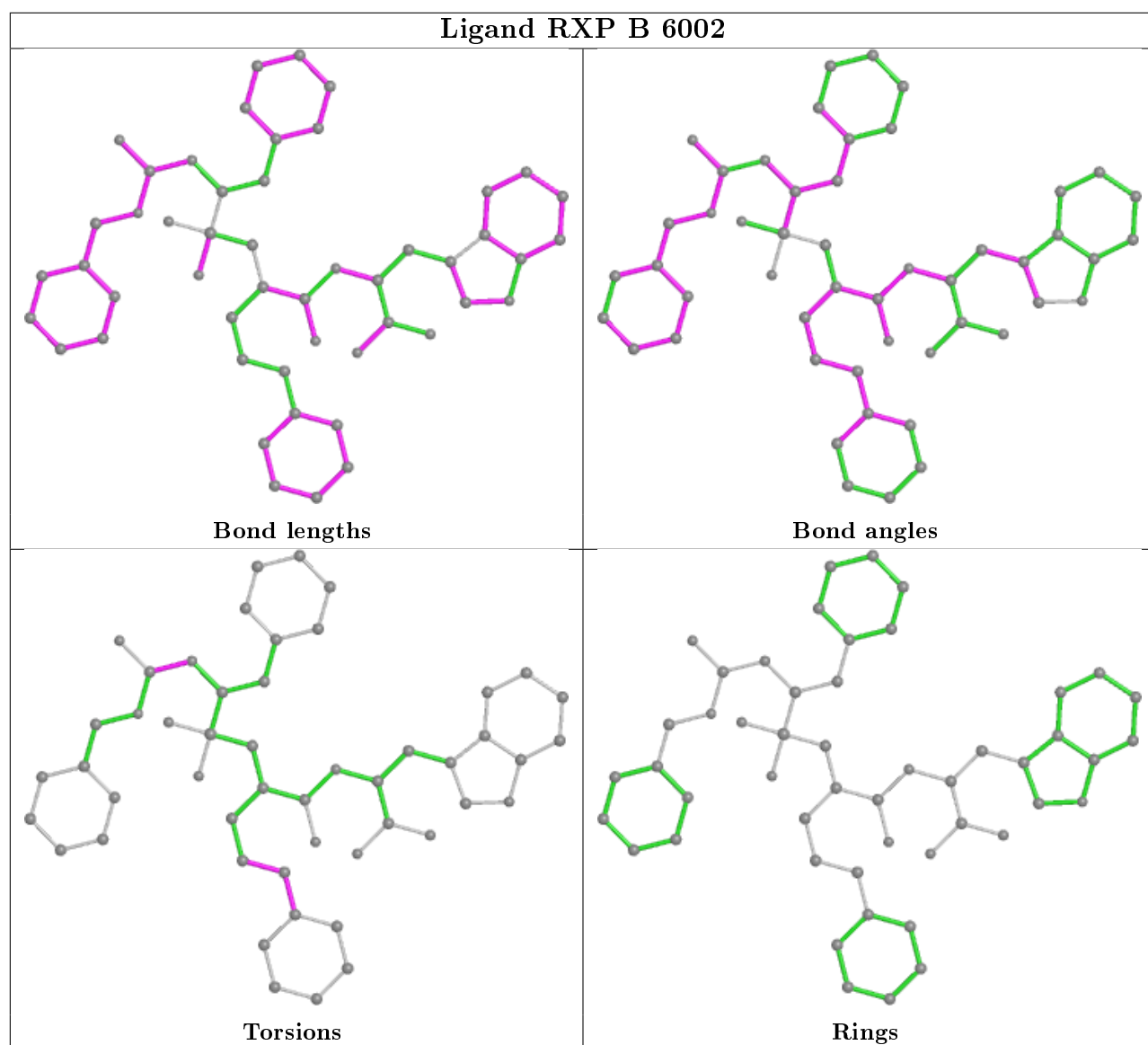
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	6001	RXP	5	0
4	C	5003	CPS	6	0
4	F	5011	CPS	7	0
4	A	5006	CPS	9	0
5	B	6002	RXP	4	0
4	D	5004	CPS	5	0
4	E	5010	CPS	6	0
5	F	6006	RXP	2	0
5	C	6003	RXP	1	0
4	E	5005	CPS	10	0
4	A	5001	CPS	7	0
5	E	6005	RXP	9	0
4	B	5007	CPS	7	0
5	D	6004	RXP	1	0
4	B	5002	CPS	8	0
4	C	5008	CPS	9	0
4	F	5091	CPS	23	0
4	D	5009	CPS	4	0

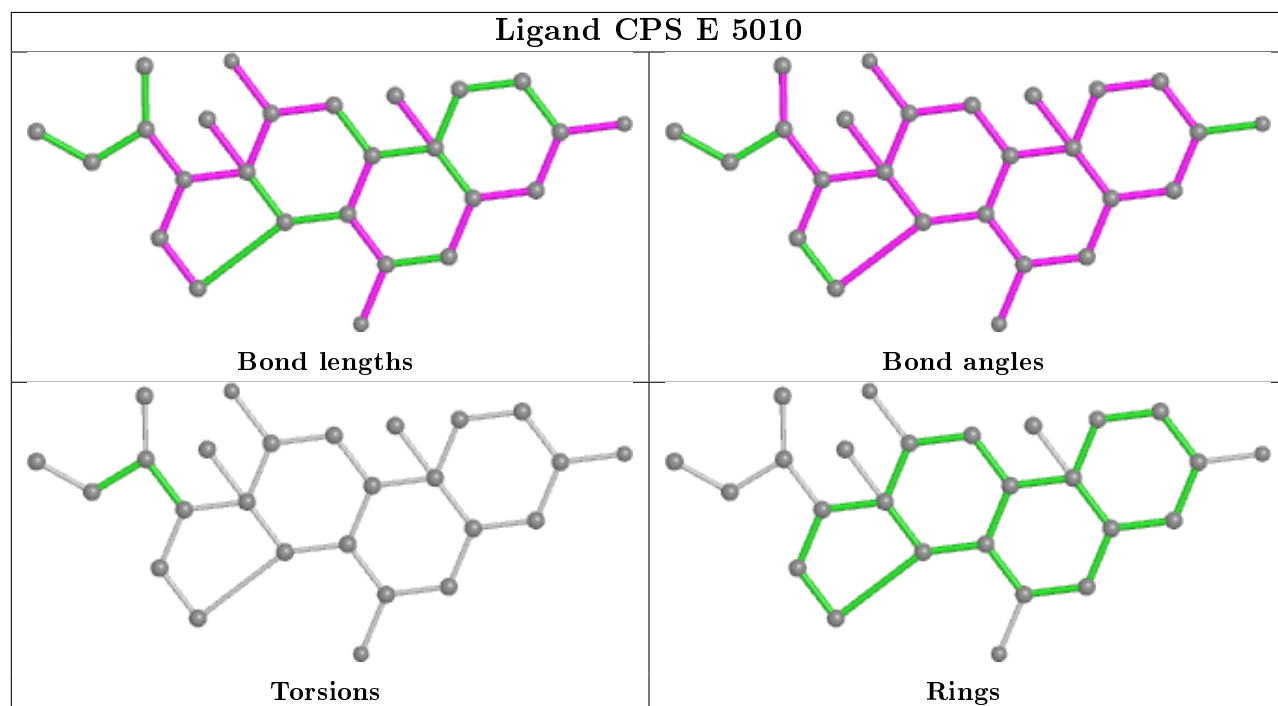
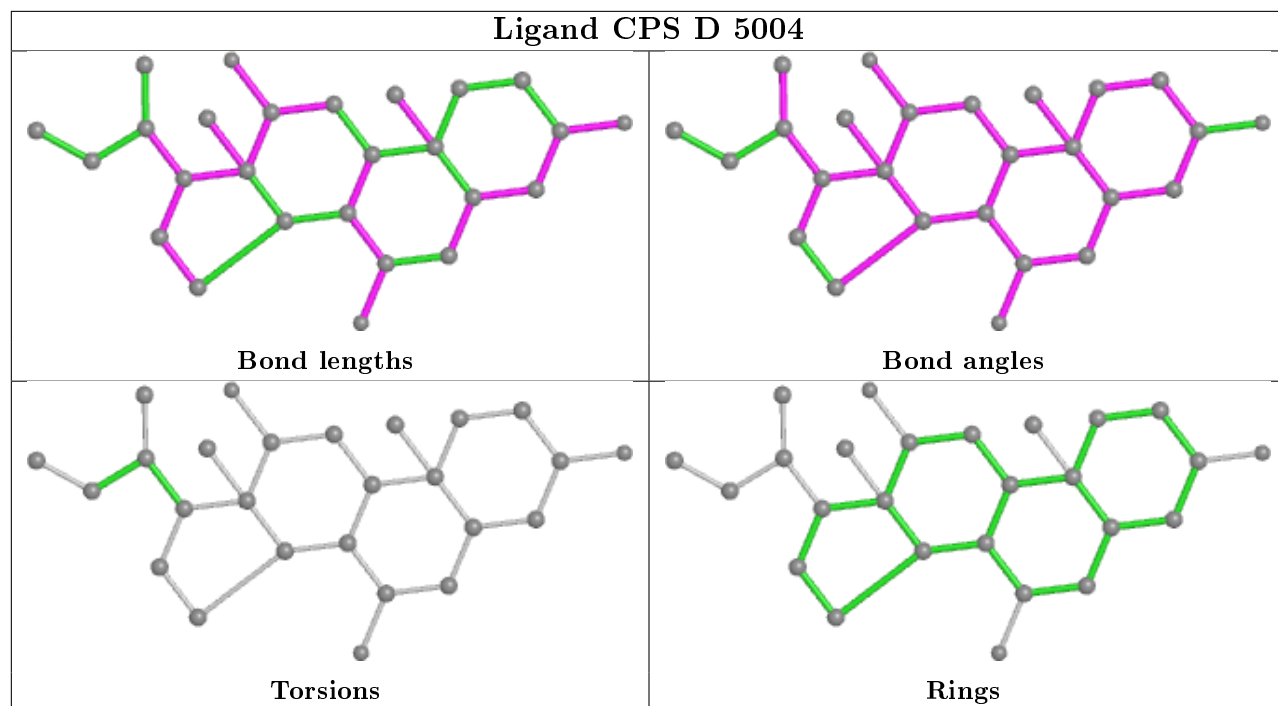
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

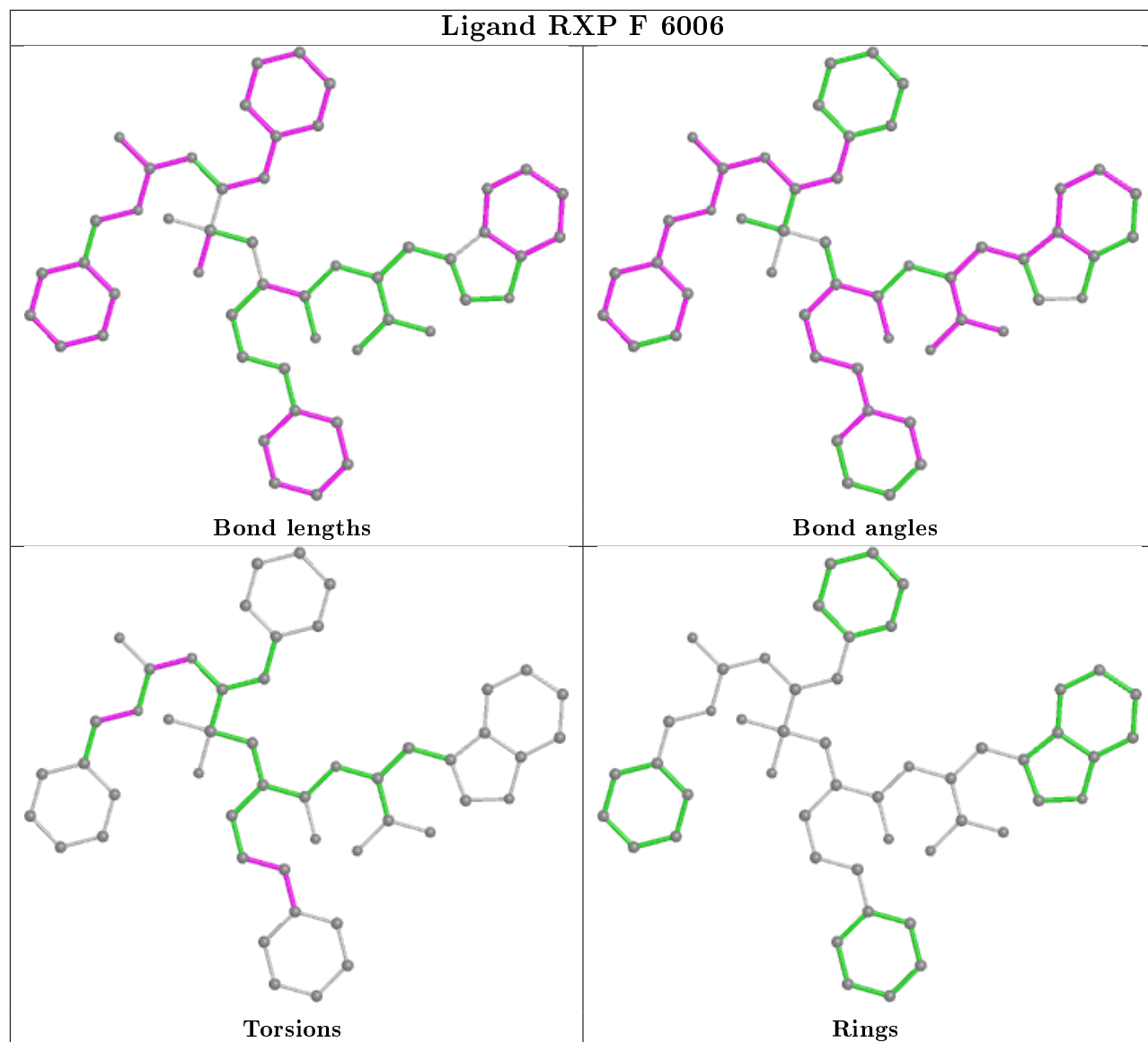






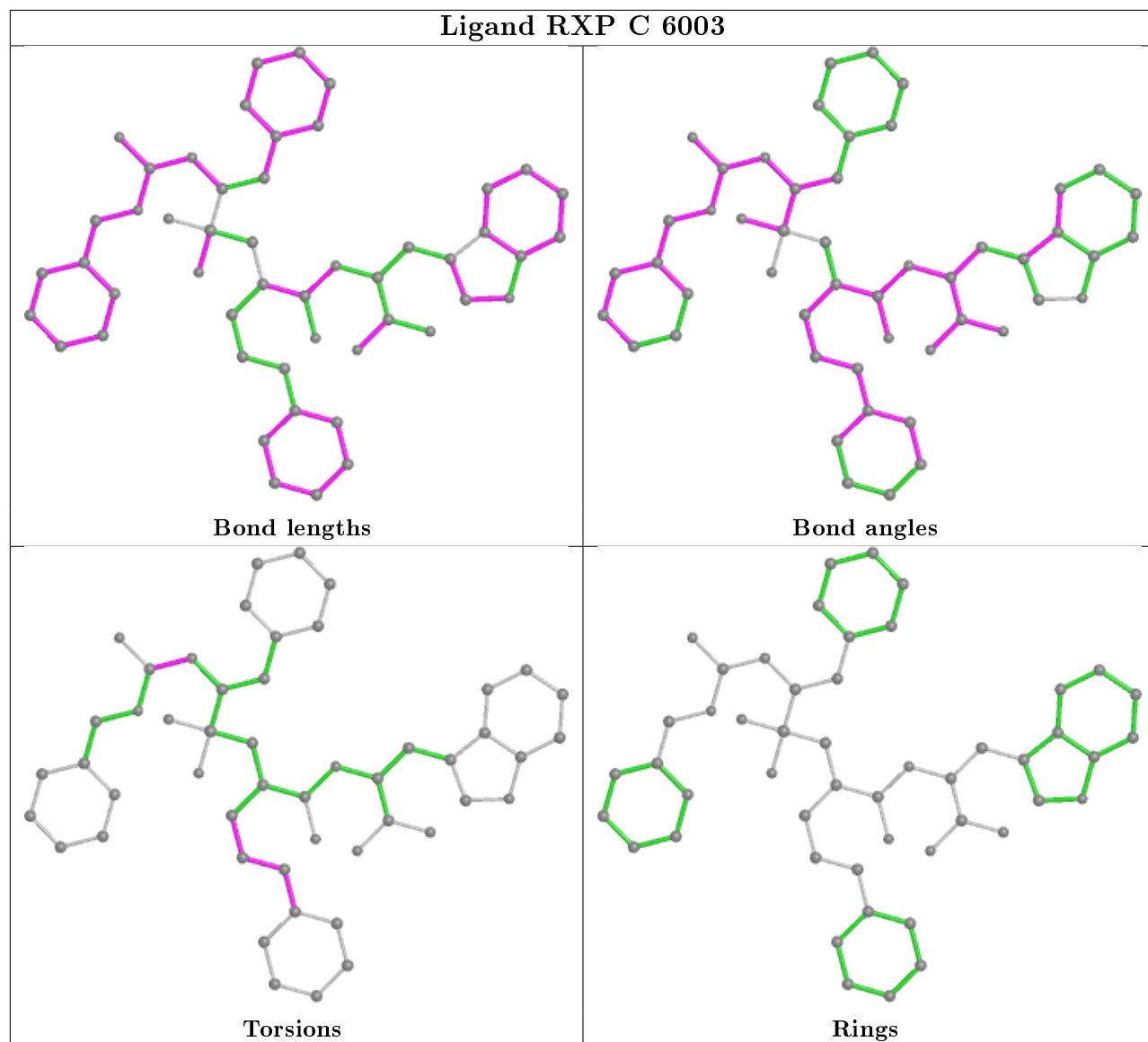


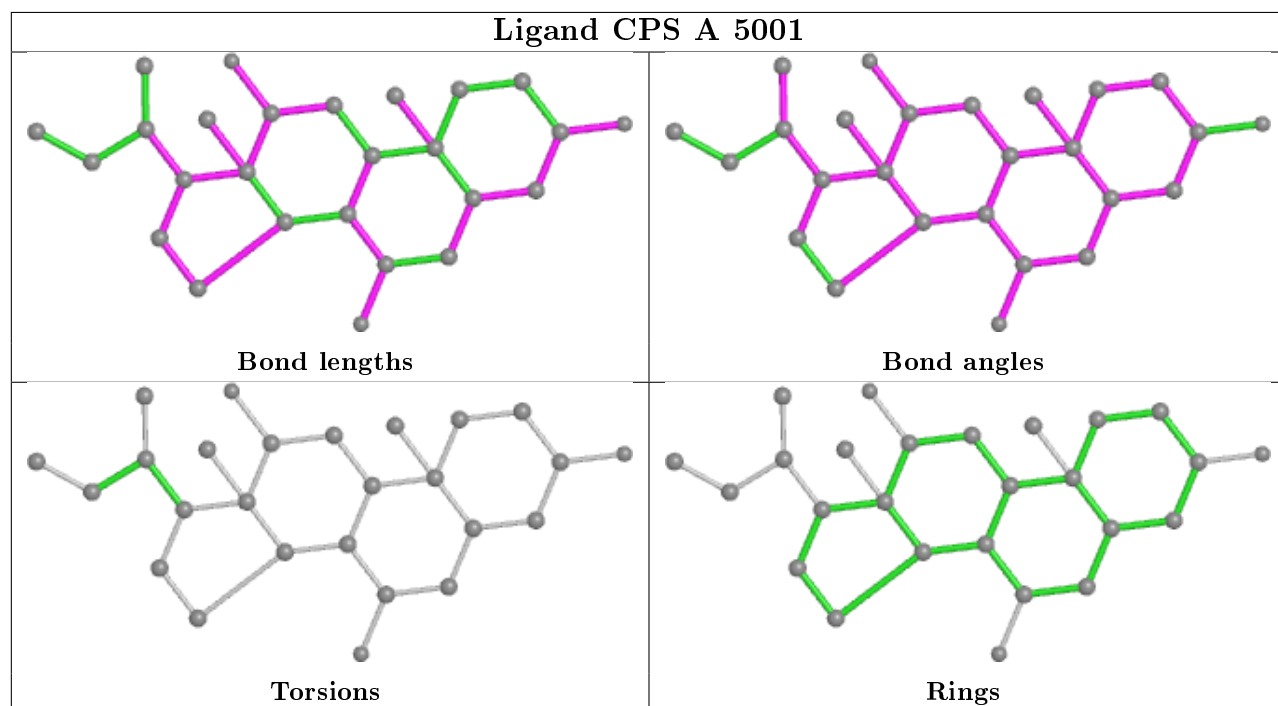
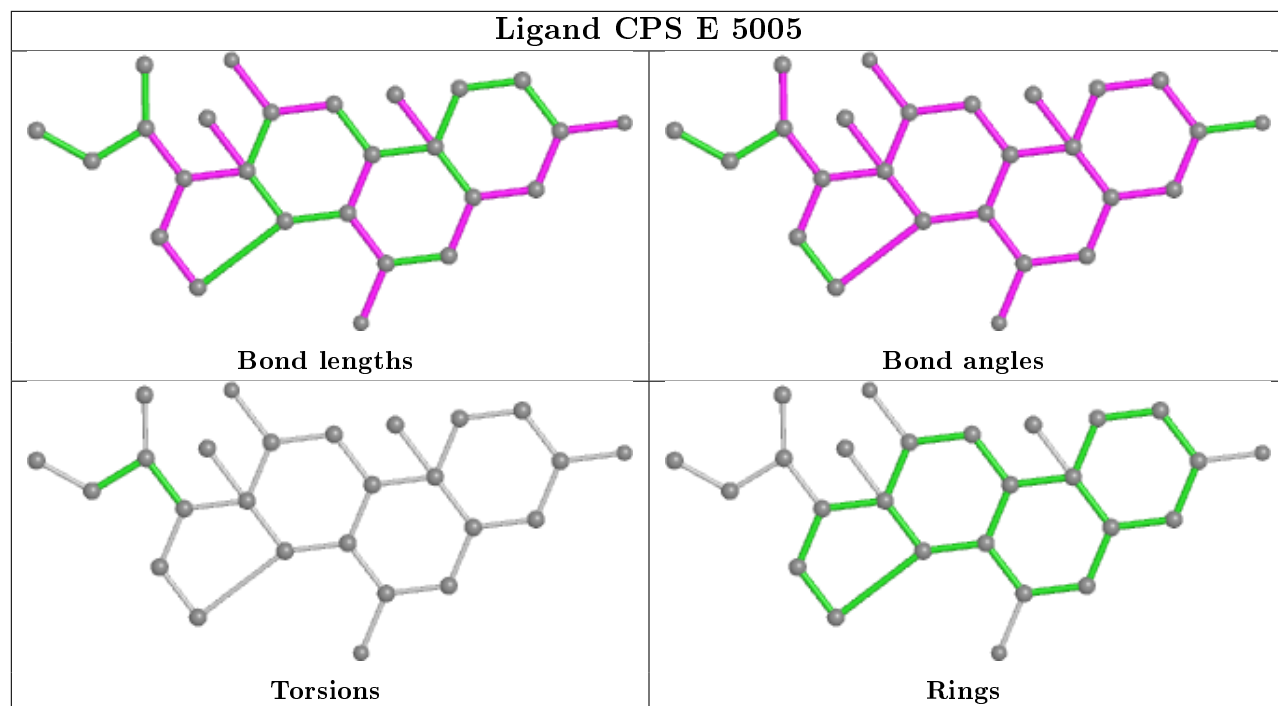




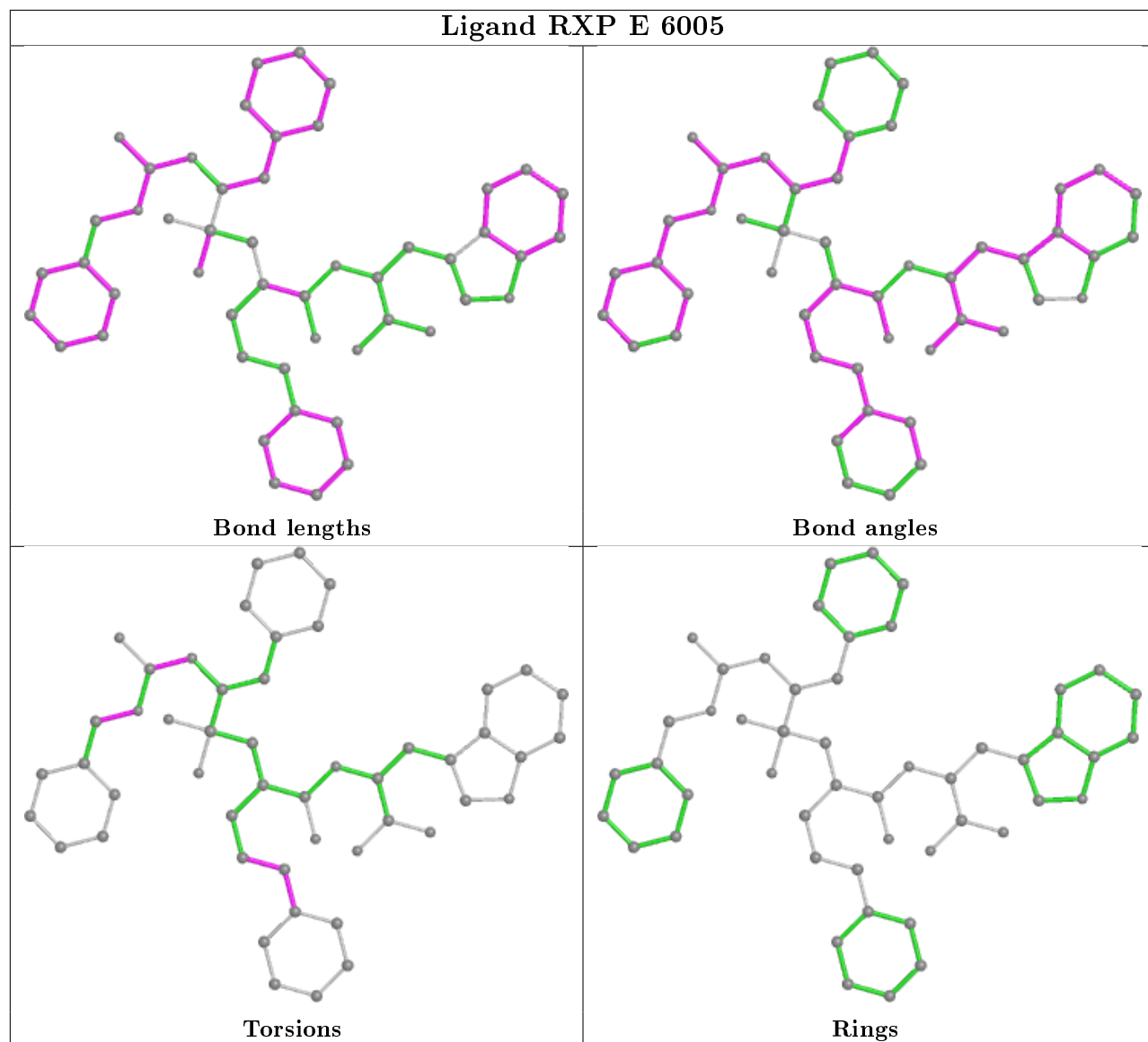


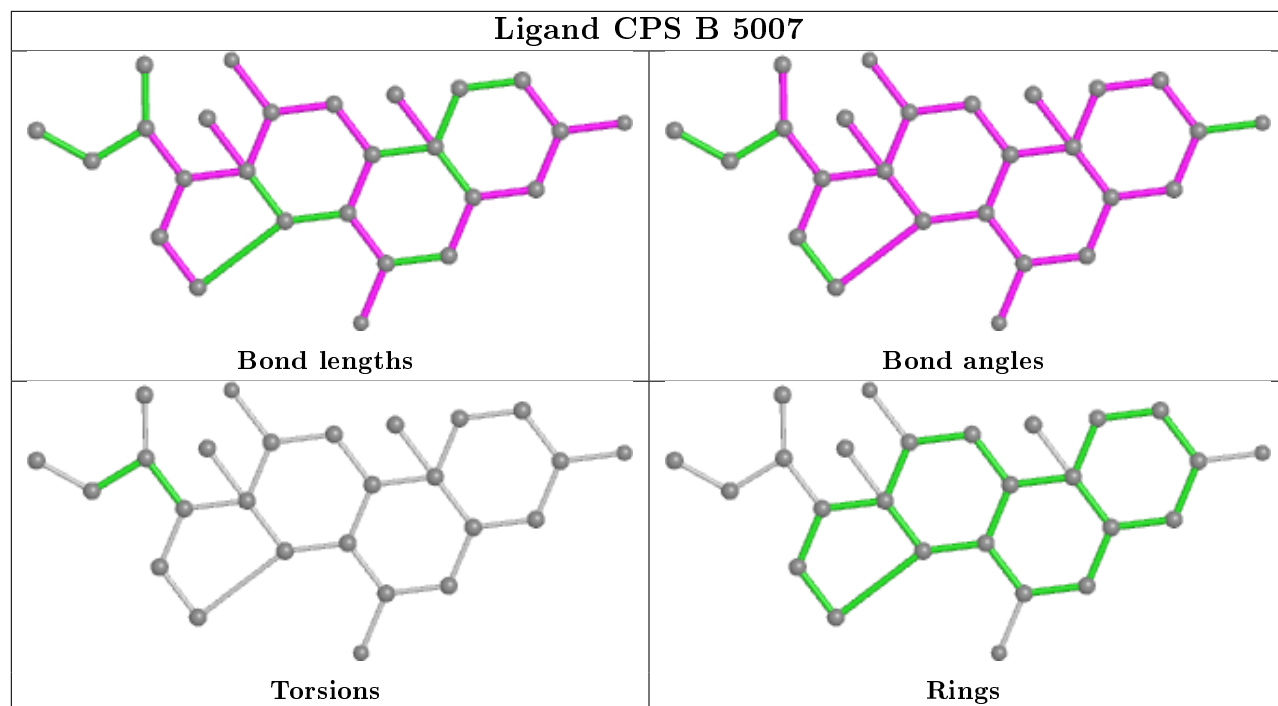
## Ligand RXP C 6003



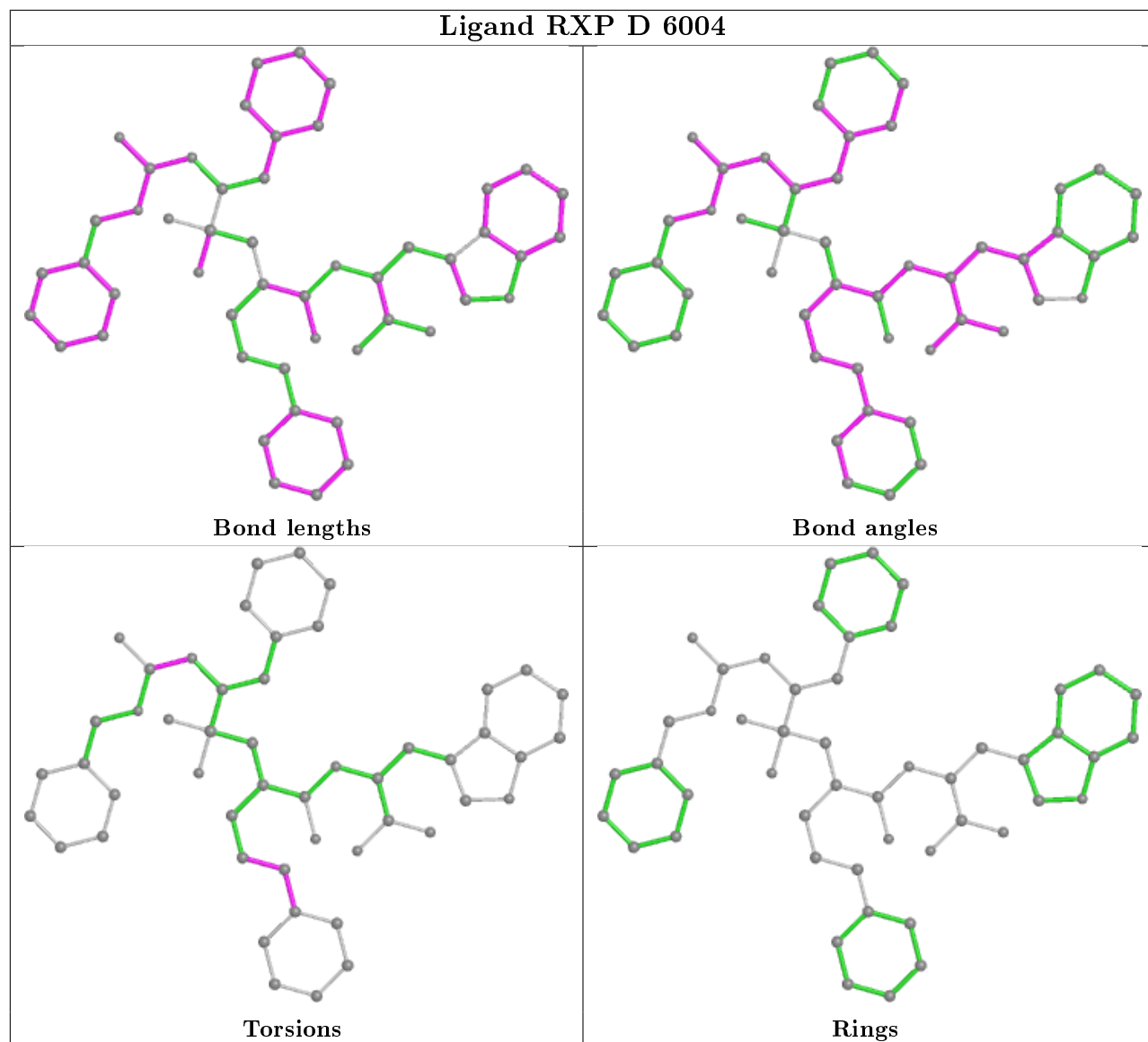


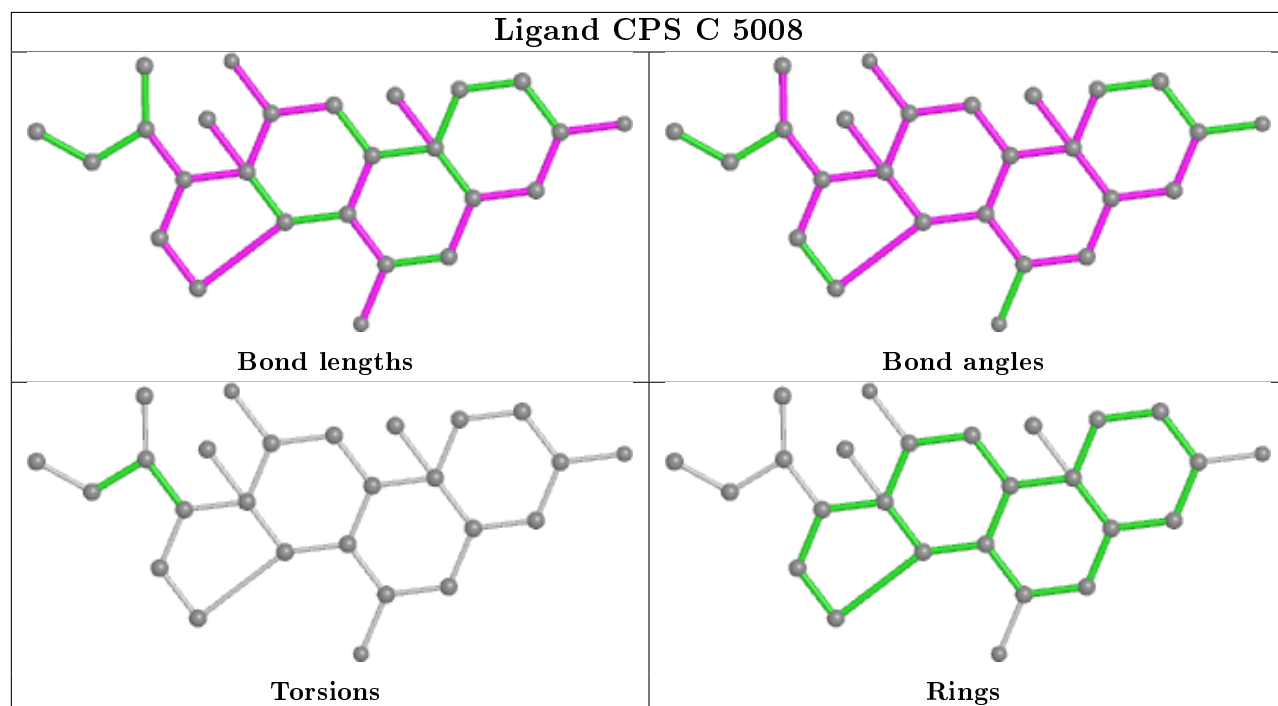
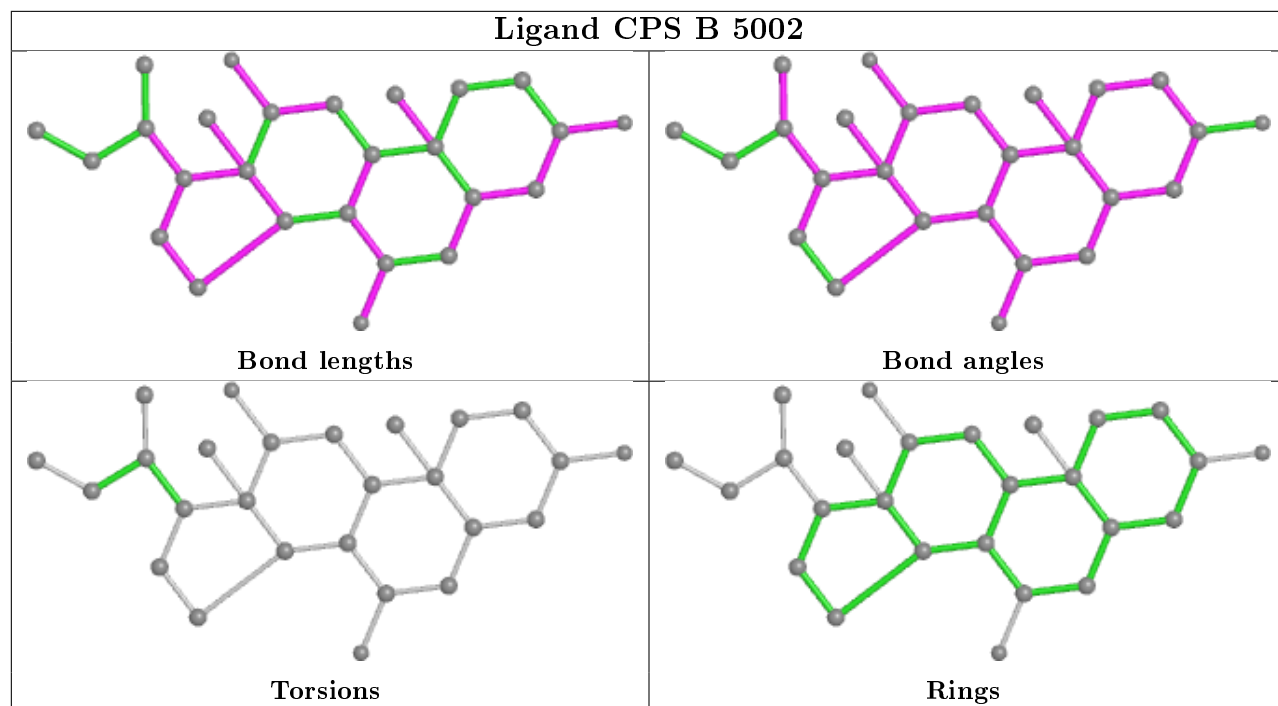
## Ligand RXP E 6005

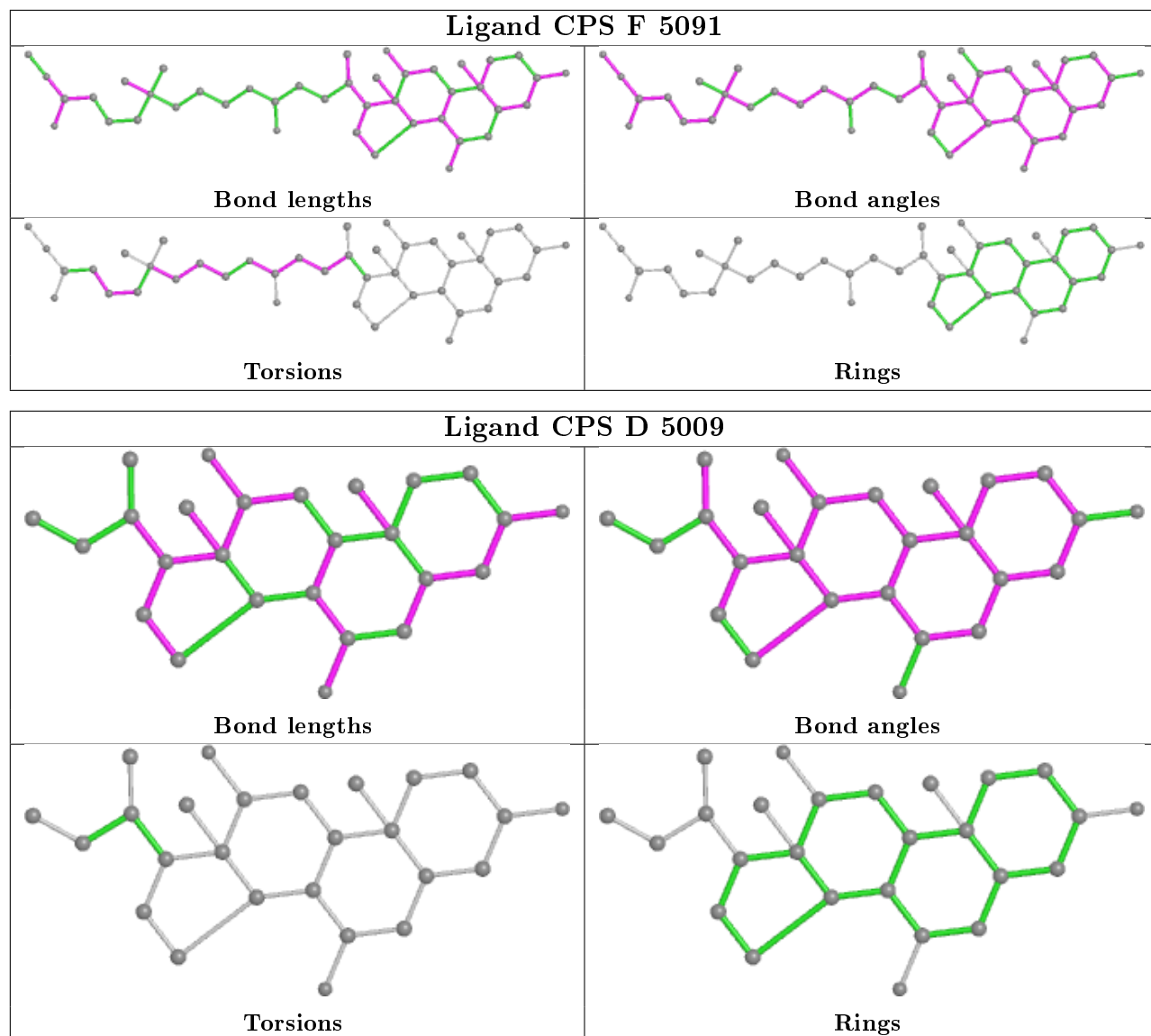




## Ligand RXP D 6004







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	F	2
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	F	168:HIS	C	169:GLY	N	1.19
1	F	165:ARG	C	166:TYR	N	1.12
1	D	166:TYR	C	167:TRP	N	0.99



## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	162/165 (98%)	-0.51	1 (0%) 89 88	15, 26, 38, 50	0
1	B	164/165 (99%)	-0.18	9 (5%) 25 19	20, 36, 53, 60	0
1	C	162/165 (98%)	-0.42	3 (1%) 66 62	19, 30, 44, 53	0
1	D	162/165 (98%)	-0.39	3 (1%) 66 62	16, 29, 45, 55	0
1	E	165/165 (100%)	-0.33	3 (1%) 68 64	14, 31, 48, 56	0
1	F	162/165 (98%)	-0.34	5 (3%) 49 42	17, 31, 43, 56	0
All	All	977/990 (98%)	-0.36	24 (2%) 57 51	14, 30, 47, 60	0

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	233	ALA	6.6
1	C	245	TYR	4.7
1	E	233	ALA	4.5
1	F	245	TYR	4.4
1	F	233	ALA	4.4

### 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](#)

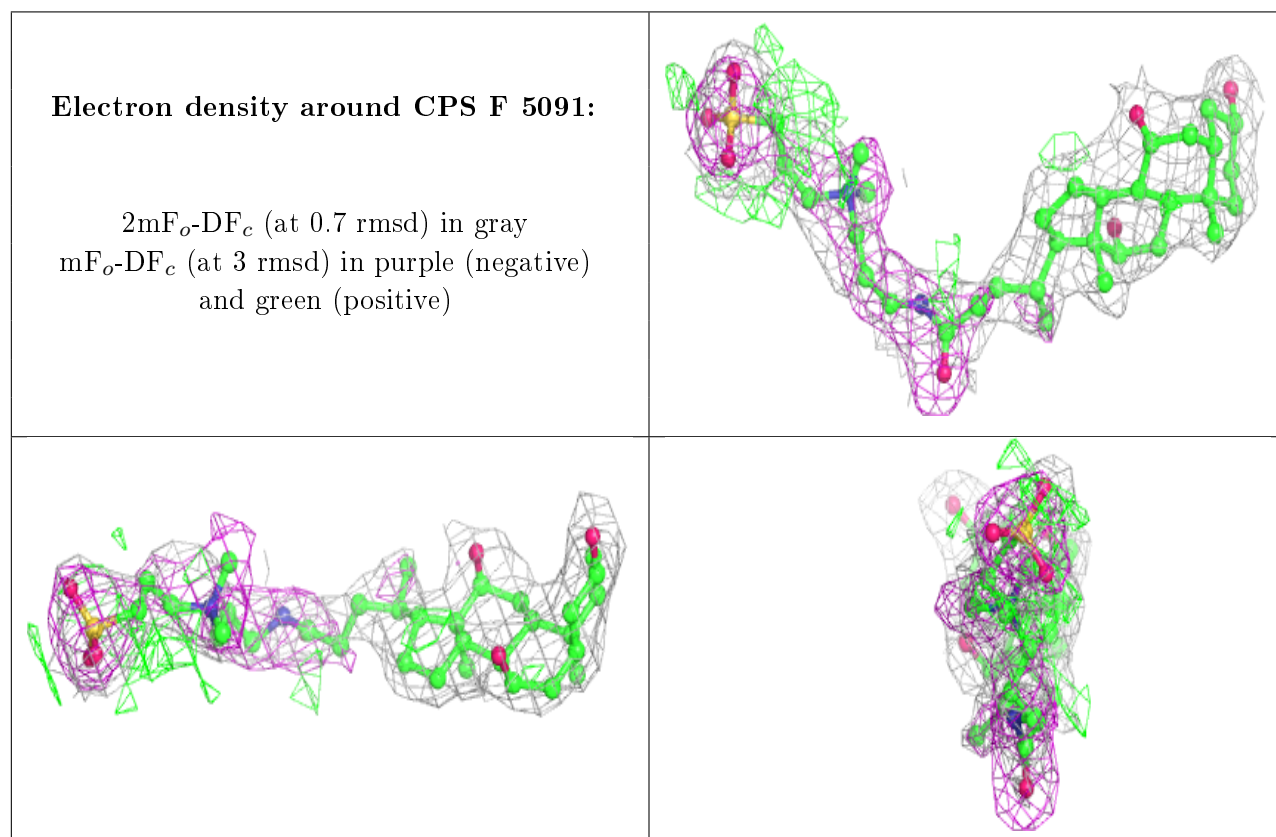
There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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, 95<sup>th</sup> 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.

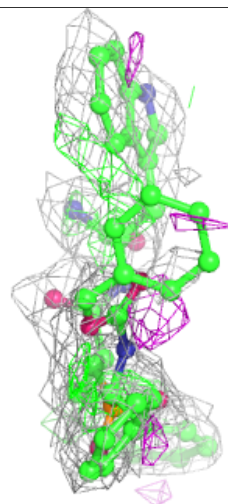
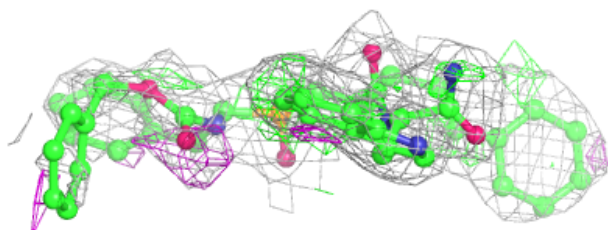
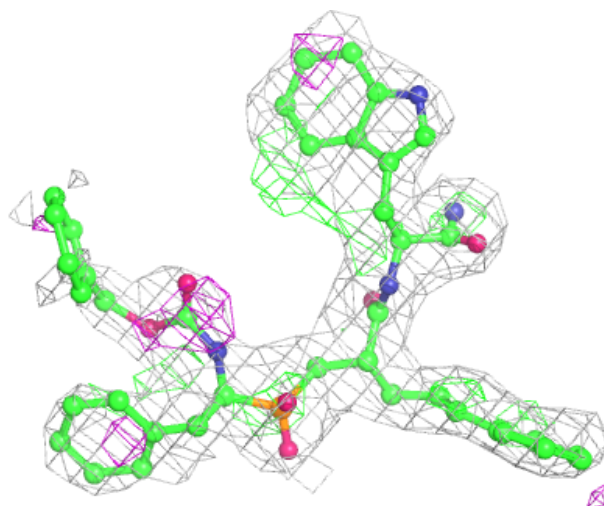
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	CPS	F	5091	42/42	0.69	0.35	17,17,17,17	0
5	RXP	E	6005	50/50	0.81	0.32	32,41,62,62	0
4	CPS	F	5011	26/42	0.82	0.24	53,54,55,55	4
4	CPS	C	5008	26/42	0.83	0.20	48,49,50,50	4
4	CPS	B	5002	26/42	0.85	0.29	50,51,52,53	4
4	CPS	D	5009	26/42	0.85	0.19	58,59,59,60	4
4	CPS	E	5005	26/42	0.85	0.34	46,48,49,50	4
4	CPS	D	5004	26/42	0.86	0.20	35,37,38,39	4
4	CPS	A	5006	26/42	0.86	0.18	49,50,51,51	4
4	CPS	C	5003	26/42	0.87	0.20	34,36,38,38	4
5	RXP	B	6002	50/50	0.88	0.26	36,44,63,64	0
5	RXP	A	6001	50/50	0.90	0.22	22,29,50,51	0
5	RXP	C	6003	50/50	0.91	0.21	25,34,53,54	0
4	CPS	A	5001	26/42	0.91	0.16	34,36,37,39	4
4	CPS	B	5007	26/42	0.94	0.13	33,34,35,37	4
5	RXP	F	6006	50/50	0.94	0.18	20,25,52,53	0
4	CPS	E	5010	26/42	0.94	0.14	30,32,34,34	4
5	RXP	D	6004	50/50	0.94	0.18	21,27,42,43	0
3	CA	B	5506	1/1	0.96	0.06	26,26,26,26	0
3	CA	D	5512	1/1	0.97	0.11	15,15,15,15	0
3	CA	C	5509	1/1	0.98	0.04	24,24,24,24	0
2	ZN	B	5505	1/1	0.98	0.06	26,26,26,26	0
3	CA	E	5515	1/1	0.98	0.04	28,28,28,28	0
3	CA	A	5503	1/1	0.98	0.05	18,18,18,18	0
2	ZN	A	5501	1/1	0.98	0.07	24,24,24,24	0
3	CA	F	5518	1/1	0.98	0.06	18,18,18,18	0
2	ZN	B	5504	1/1	0.99	0.09	25,25,25,25	0
2	ZN	E	5513	1/1	0.99	0.06	24,24,24,24	0
2	ZN	C	5507	1/1	0.99	0.09	23,23,23,23	0
2	ZN	E	5514	1/1	0.99	0.04	21,21,21,21	0
2	ZN	D	5510	1/1	0.99	0.08	22,22,22,22	0
2	ZN	D	5511	1/1	0.99	0.08	18,18,18,18	0
2	ZN	F	5516	1/1	0.99	0.09	26,26,26,26	0
2	ZN	A	5502	1/1	0.99	0.07	19,19,19,19	0
2	ZN	C	5508	1/1	1.00	0.05	16,16,16,16	0
2	ZN	F	5517	1/1	1.00	0.07	23,23,23,23	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.



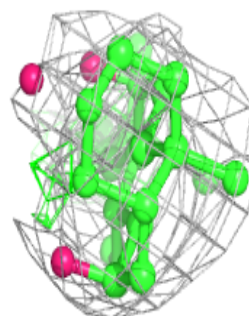
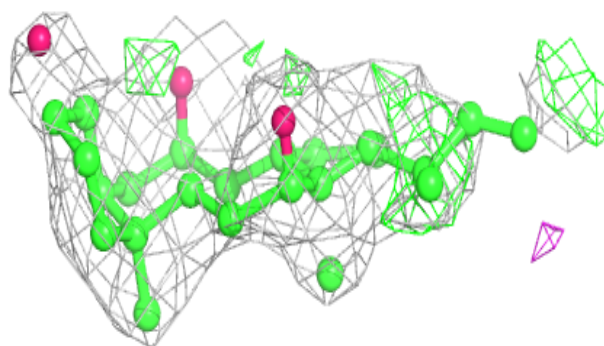
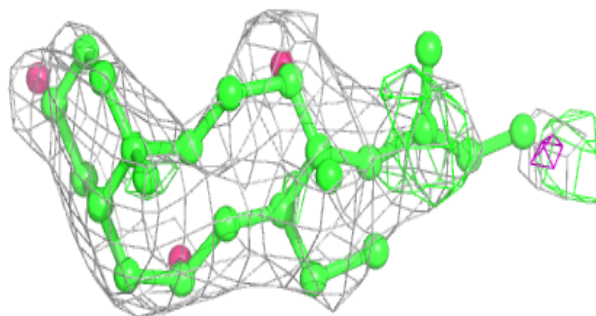
**Electron density around RXP E 6005:**

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

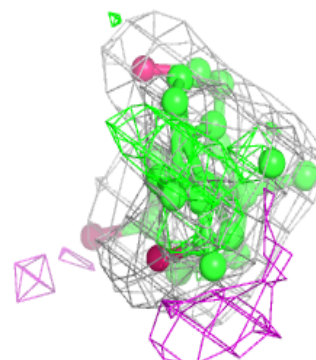
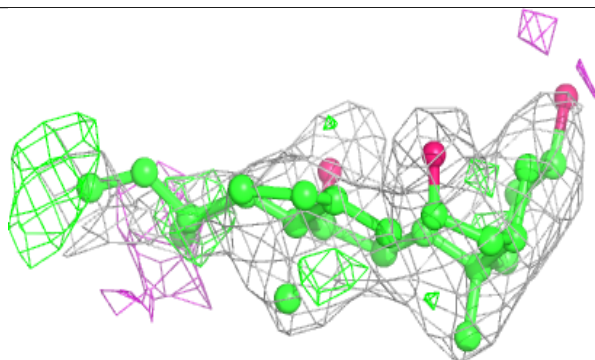
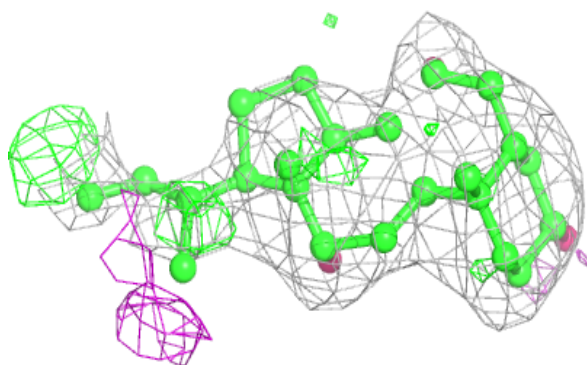


**Electron density around CPS F 5011:**

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and green (positive)

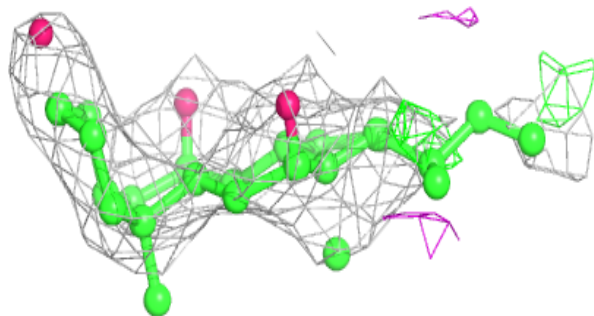
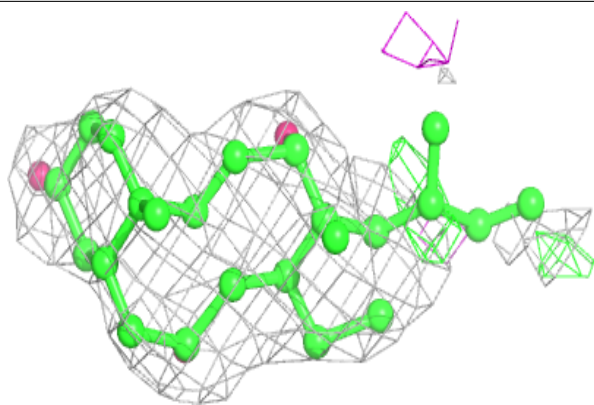
**Electron density around CPS C 5008:**

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and green (positive)

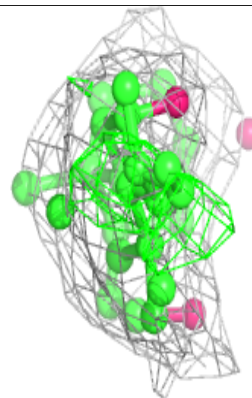
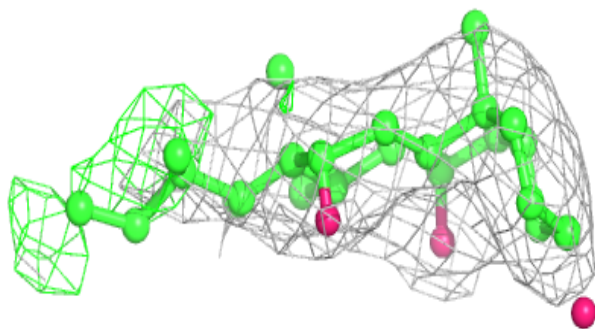
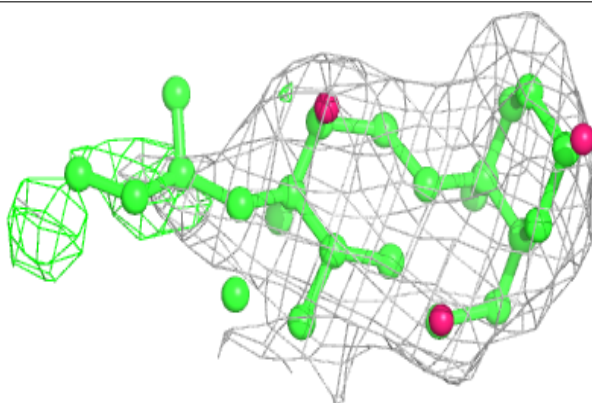


**Electron density around CPS B 5002:**

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and green (positive)

**Electron density around CPS D 5009:**

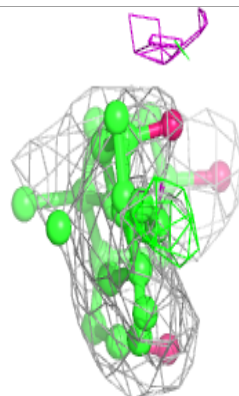
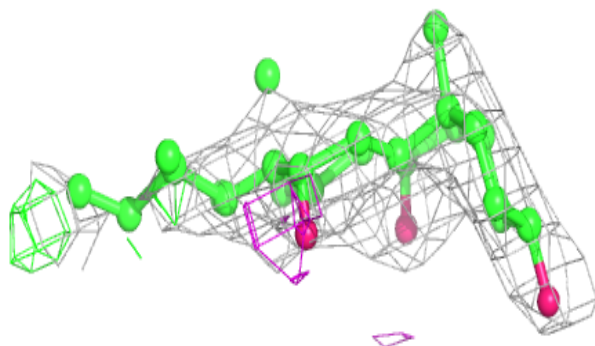
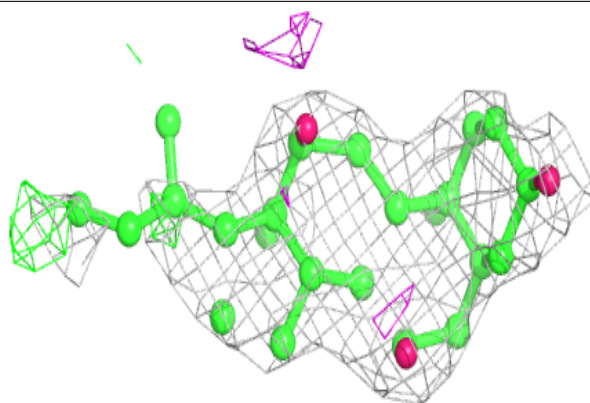
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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



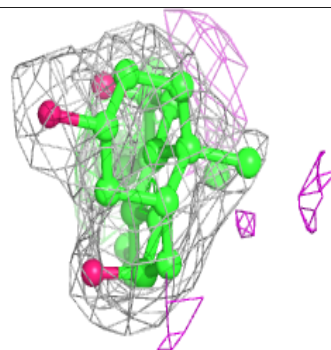
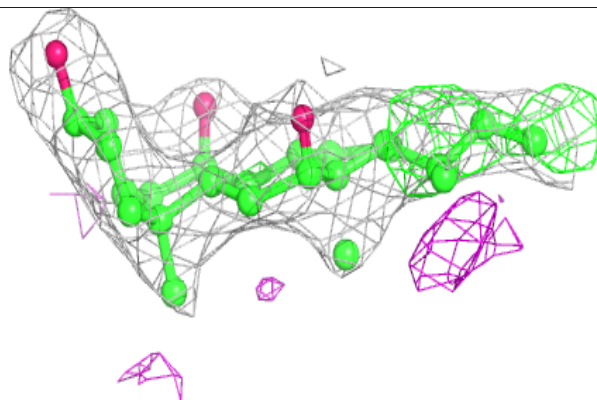
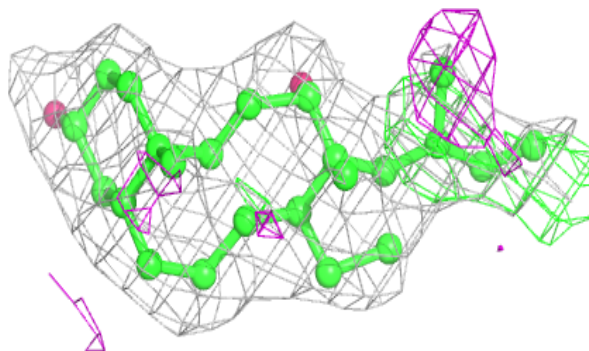


**Electron density around CPS E 5005:**

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

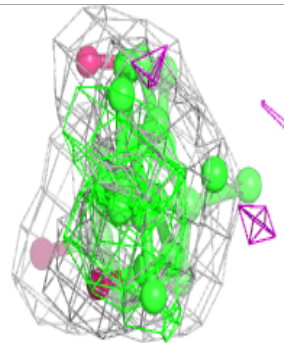
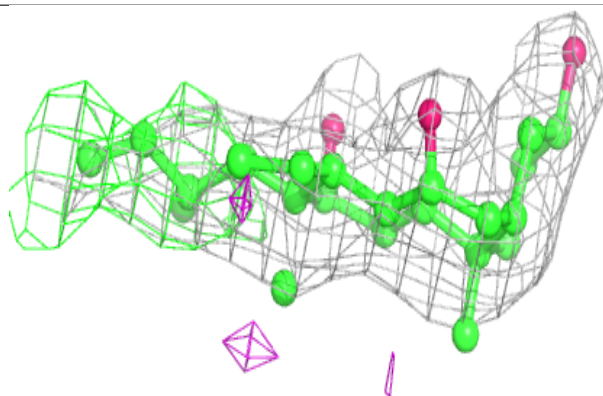
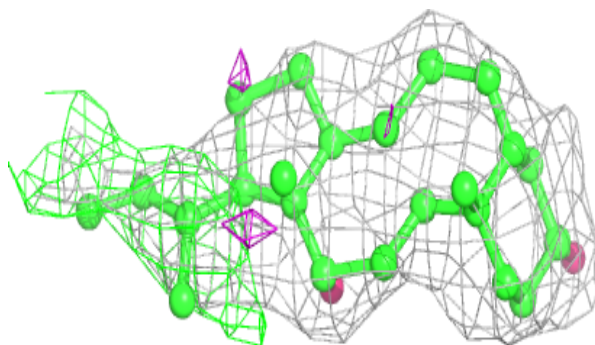
**Electron density around CPS D 5004:**

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

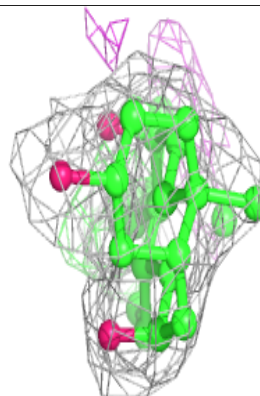
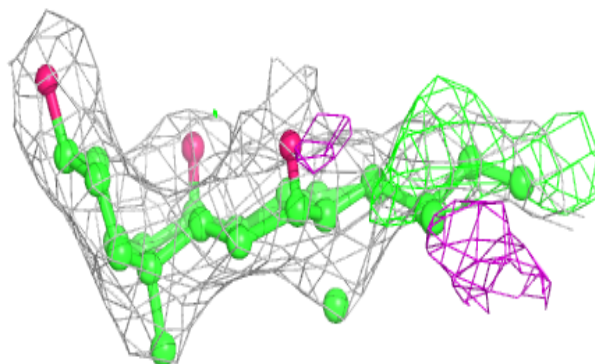
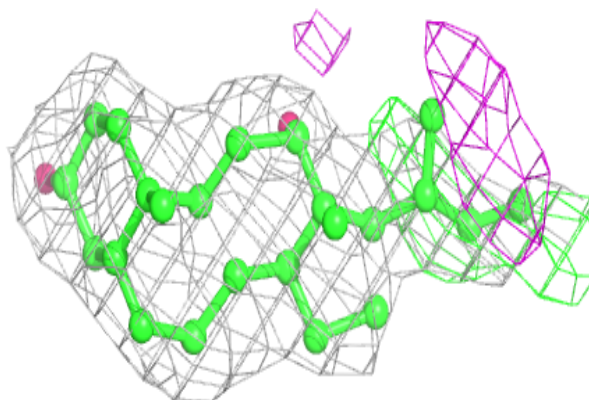


**Electron density around CPS A 5006:**

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

**Electron density around CPS C 5003:**

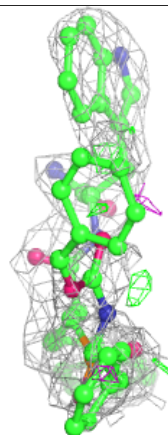
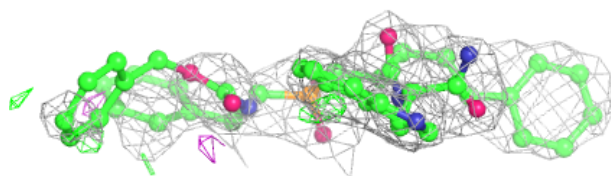
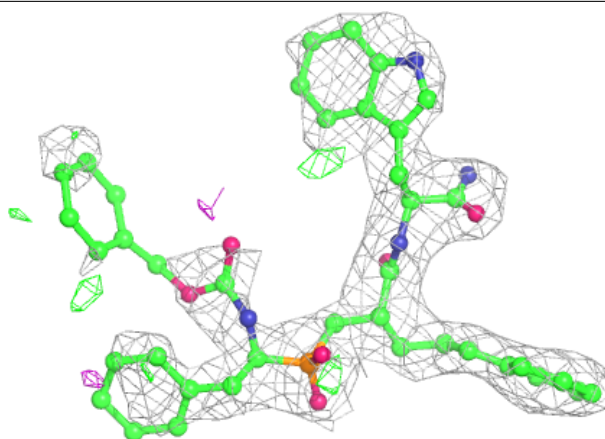
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





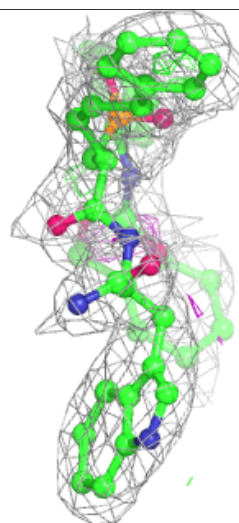
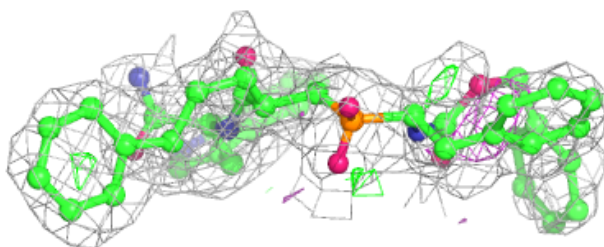
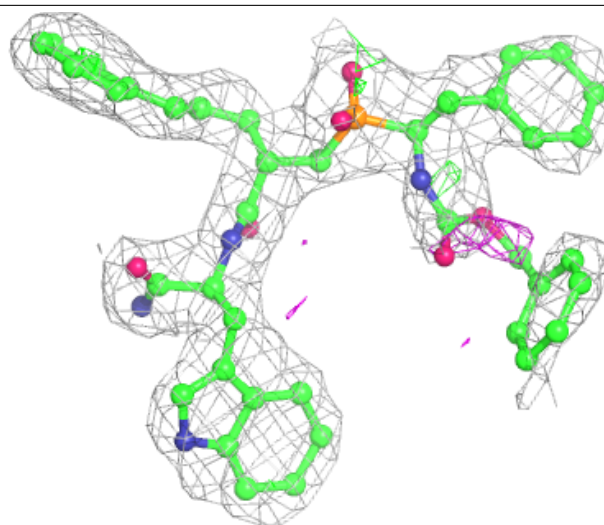
**Electron density around RXP B 6002:**

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



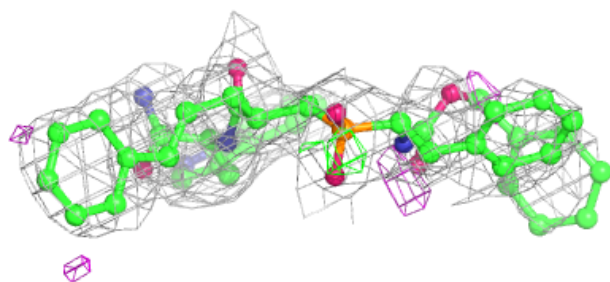
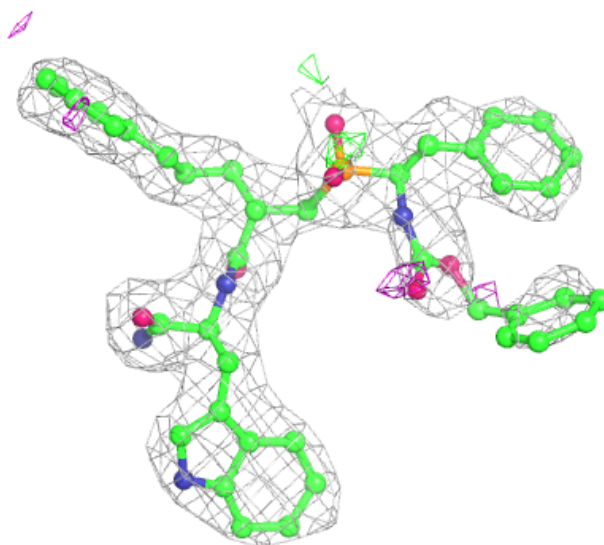
**Electron density around RXP A 6001:**

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



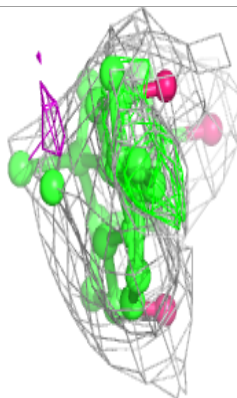
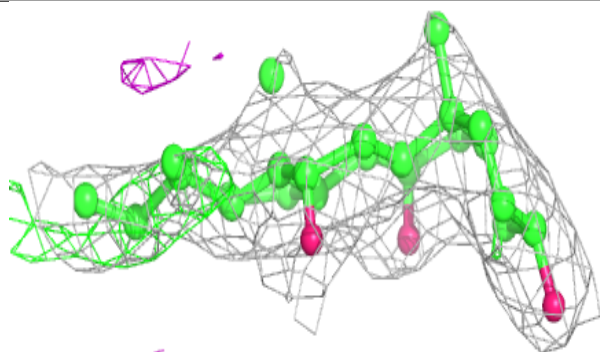
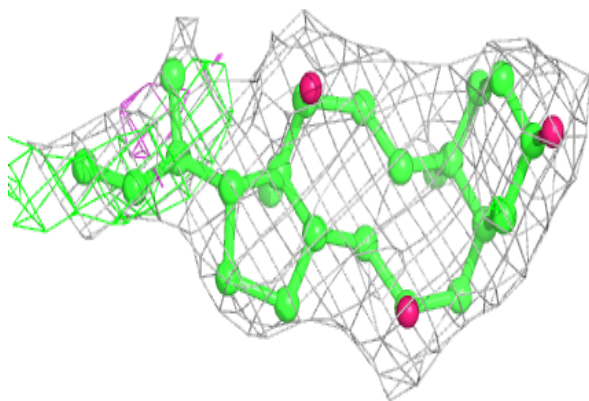
**Electron density around RXP C 6003:**

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

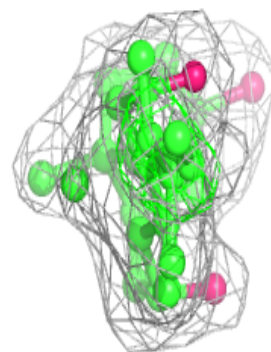
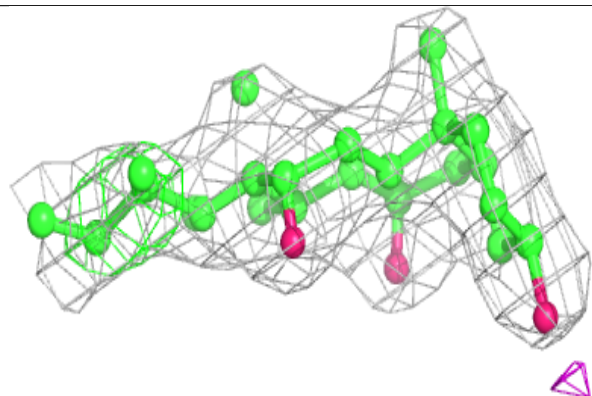
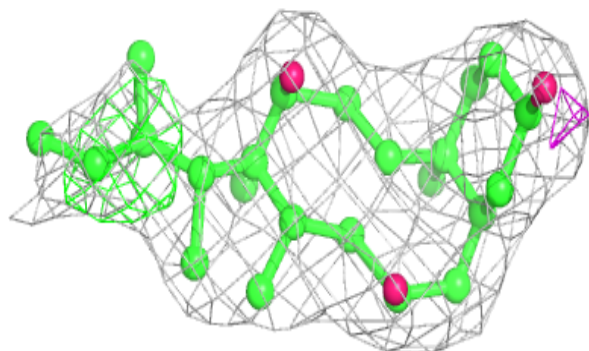


**Electron density around CPS A 5001:**

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

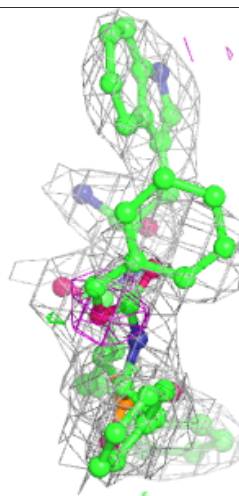
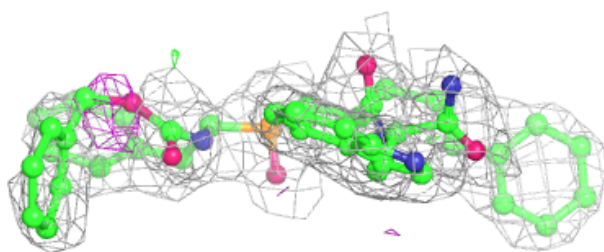
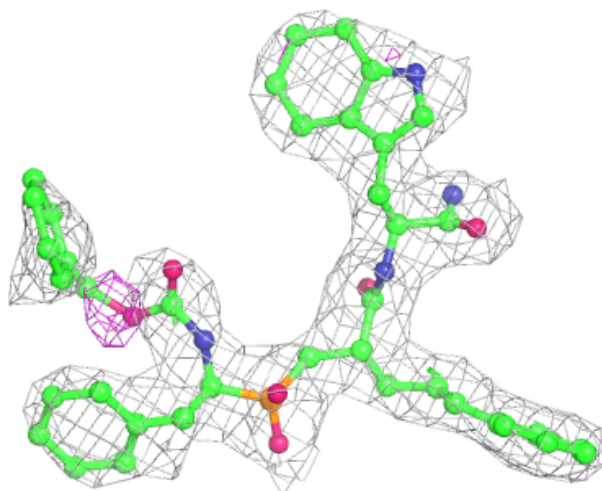
**Electron density around CPS B 5007:**

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



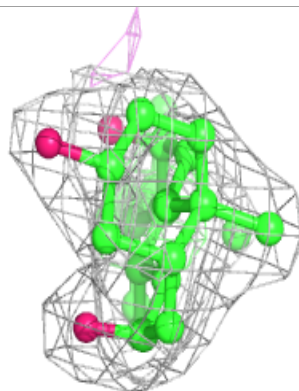
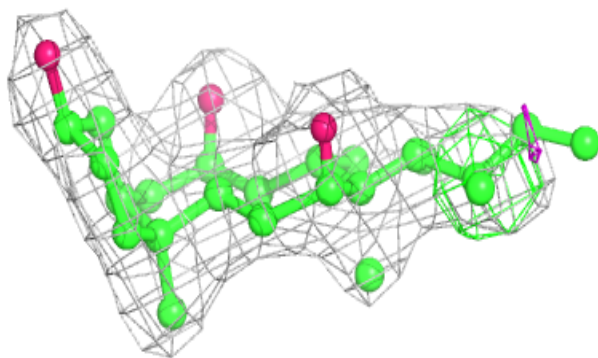
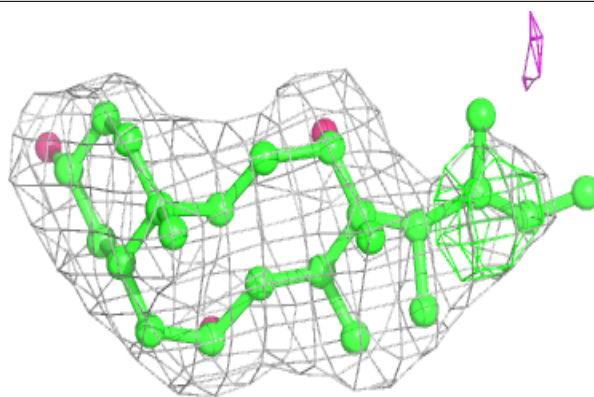
**Electron density around RXP F 6006:**

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



**Electron density around CPS E 5010:**

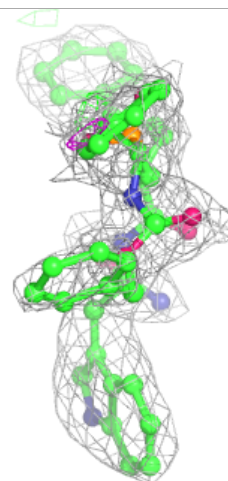
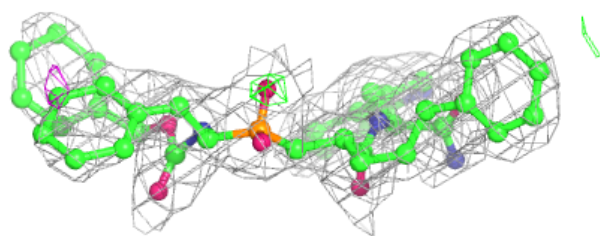
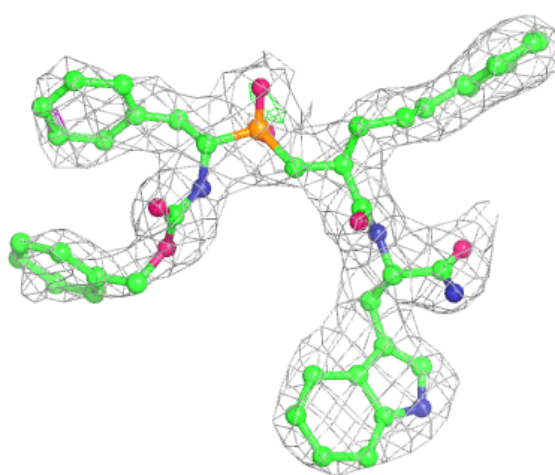
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around RXP D 6004:**

$2mF_o-DF_c$  (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.