Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2024 – 09:06 AM EST

PDB ID	:	3KO0
Title	:	Structure of the tfp-ca2+-bound activated form of the s100a4 Metastasis factor
Authors	:	Malashkevich, V.N.; Dulyaninova, N.G.; Knight, D.; Almo, S.C.; Bresnick, A.R.
Deposited on	:	2009-11-12
Resolution	:	2.30 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 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:

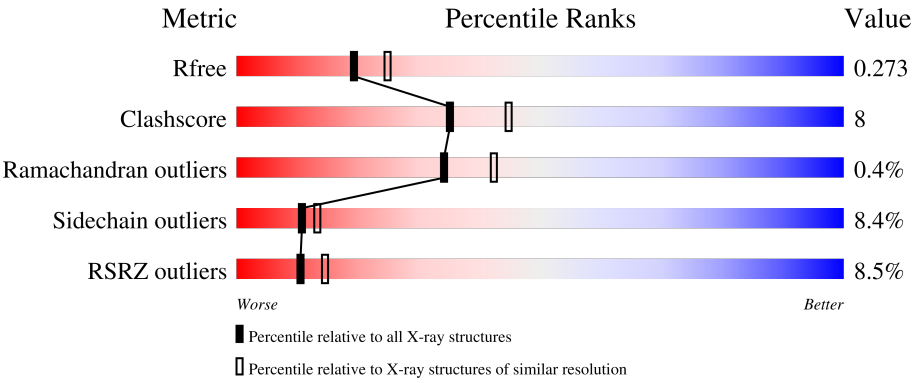
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 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 <=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	101	6% 72% 18% •• 8%
1	B	101	6% 73% 17% • 8%
1	C	101	3% 66% 24% • 8%
1	D	101	10% 67% 20% 5% 8%
1	E	101	5% 68% 19% • 9%

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Mol	Chain	Length	Quality of chain
1	F	101	10% 69% 20% 11%
1	G	101	12% 64% 24% 11%
1	H	101	27% 74% 18% 7%
1	I	101	5% 79% 9% 8%
1	J	101	2% 74% 15% 8%
1	K	101	5% 77% 14% 8%
1	L	101	5% 71% 20% 8%
1	M	101	7% 61% 27% 9%
1	N	101	4% 73% 15% 9%
1	O	101	9% 77% 14% 8%
1	P	101	6% 74% 17% 9%
1	Q	101	11% 63% 19% 5% 13%
1	R	101	7% 75% 12% 5% 8%
1	S	101	5% 71% 20% 8%
1	T	101	11% 79% 9% 8%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 16855 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 Protein S100-A4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	93	Total	C	N	O	S	0	1	0
			754	481	121	144	8			
1	B	93	Total	C	N	O	S	0	1	0
			740	471	118	142	9			
1	C	93	Total	C	N	O	S	0	1	0
			746	475	118	144	9			
1	D	93	Total	C	N	O	S	0	2	0
			752	479	119	144	10			
1	E	92	Total	C	N	O	S	0	0	0
			741	471	119	143	8			
1	F	90	Total	C	N	O	S	0	0	0
			709	451	110	140	8			
1	G	90	Total	C	N	O	S	0	0	0
			718	459	113	138	8			
1	H	94	Total	C	N	O	S	0	0	0
			752	477	120	147	8			
1	I	93	Total	C	N	O	S	0	0	0
			744	473	119	144	8			
1	J	93	Total	C	N	O	S	0	2	0
			756	482	120	144	10			
1	K	93	Total	C	N	O	S	0	0	0
			738	470	116	144	8			
1	L	93	Total	C	N	O	S	0	0	0
			744	473	119	144	8			
1	M	92	Total	C	N	O	S	0	0	0
			731	465	115	143	8			
1	N	92	Total	C	N	O	S	0	1	0
			743	473	118	143	9			
1	O	93	Total	C	N	O	S	0	0	0
			745	474	119	144	8			
1	P	92	Total	C	N	O	S	0	0	0
			733	465	117	143	8			

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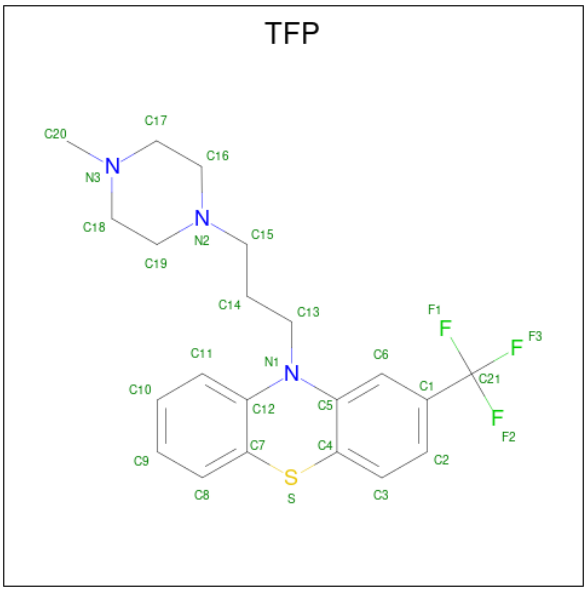
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	88	Total	C	N	O	S	0	1	0
			702	450	107	136	9			
1	R	93	Total	C	N	O	S	0	1	0
			745	474	118	144	9			
1	S	93	Total	C	N	O	S	0	0	0
			748	476	120	144	8			
1	T	93	Total	C	N	O	S	0	1	0
			744	475	116	144	9			

- Molecule 2 is 10-[3-(4-METHYL-PIPERAZIN-1-YL)-PROPYL]-2-TRIFLUOROMETHYL-10H-PHENOTHIAZINE (three-letter code: TFP) (formula: $C_{21}H_{24}F_3N_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	S	0	0
			28	21	3	3	1		
2	A	1	Total	C	F	N	S	0	0
			28	21	3	3	1		
2	B	1	Total	C	F	N	S	0	0
			28	21	3	3	1		
2	B	1	Total	C	F	N	S	0	0
			28	21	3	3	1		
2	C	1	Total	C	F	N	S	0	0
			28	21	3	3	1		
2	C	1	Total	C	F	N	S	0	0
			28	21	3	3	1		
2	D	1	Total	C	F	N	S	0	0
			28	21	3	3	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	D	1	Total	C	F	N	S	0	0
			28	21	3	3	1		
2	E	1	Total	C	F	N	S	0	0
			28	21	3	3	1		
2	E	1	Total	C	F	N	S	0	0
			28	21	3	3	1		
2	F	1	Total	C	F	N	S	0	0
			28	21	3	3	1		
2	F	1	Total	C	F	N	S	0	0
			28	21	3	3	1		
2	G	1	Total	C	F	N	S	0	0
			28	21	3	3	1		
2	G	1	Total	C	F	N	S	0	0
			28	21	3	3	1		
2	H	1	Total	C	F	N	S	0	0
			28	21	3	3	1		
2	H	1	Total	C	F	N	S	0	0
			28	21	3	3	1		
2	I	1	Total	C	F	N	S	0	0
			28	21	3	3	1		
2	I	1	Total	C	F	N	S	0	0
			28	21	3	3	1		
2	J	1	Total	C	F	N	S	0	0
			28	21	3	3	1		
2	J	1	Total	C	F	N	S	0	0
			28	21	3	3	1		
2	K	1	Total	C	F	N	S	0	0
			28	21	3	3	1		
2	K	1	Total	C	F	N	S	0	0
			28	21	3	3	1		
2	L	1	Total	C	F	N	S	0	0
			28	21	3	3	1		
2	L	1	Total	C	F	N	S	0	0
			28	21	3	3	1		
2	M	1	Total	C	F	N	S	0	0
			28	21	3	3	1		
2	M	1	Total	C	F	N	S	0	0
			28	21	3	3	1		
2	N	1	Total	C	F	N	S	0	0
			28	21	3	3	1		
2	N	1	Total	C	F	N	S	0	0
			28	21	3	3	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	O	1	Total	C	F	N	S	0	0
			28	21	3	3	1		
2	O	1	Total	C	F	N	S	0	0
			28	21	3	3	1		
2	P	1	Total	C	F	N	S	0	0
			28	21	3	3	1		
2	P	1	Total	C	F	N	S	0	0
			28	21	3	3	1		
2	Q	1	Total	C	F	N	S	0	0
			28	21	3	3	1		
2	Q	1	Total	C	F	N	S	0	0
			28	21	3	3	1		
2	R	1	Total	C	F	N	S	0	0
			28	21	3	3	1		
2	R	1	Total	C	F	N	S	0	0
			28	21	3	3	1		
2	S	1	Total	C	F	N	S	0	0
			28	21	3	3	1		
2	S	1	Total	C	F	N	S	0	0
			28	21	3	3	1		
2	T	1	Total	C	F	N	S	0	0
			28	21	3	3	1		
2	T	1	Total	C	F	N	S	0	0
			28	21	3	3	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Ca	0	0
			2	2		
3	B	2	Total	Ca	0	0
			2	2		
3	C	2	Total	Ca	0	0
			2	2		
3	D	2	Total	Ca	0	0
			2	2		
3	E	2	Total	Ca	0	0
			2	2		
3	F	2	Total	Ca	0	0
			2	2		
3	G	2	Total	Ca	0	0
			2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	H	2	Total Ca 2 2	0	0
3	I	2	Total Ca 2 2	0	0
3	J	2	Total Ca 2 2	0	0
3	K	2	Total Ca 2 2	0	0
3	L	2	Total Ca 2 2	0	0
3	M	2	Total Ca 2 2	0	0
3	N	2	Total Ca 2 2	0	0
3	O	2	Total Ca 2 2	0	0
3	P	2	Total Ca 2 2	0	0
3	Q	2	Total Ca 2 2	0	0
3	R	2	Total Ca 2 2	0	0
3	S	2	Total Ca 2 2	0	0
3	T	2	Total Ca 2 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	57	Total O 57 57	0	0
4	B	75	Total O 75 75	0	0
4	C	56	Total O 56 56	0	0
4	D	48	Total O 48 48	0	0
4	E	47	Total O 47 47	0	0
4	F	41	Total O 41 41	0	0

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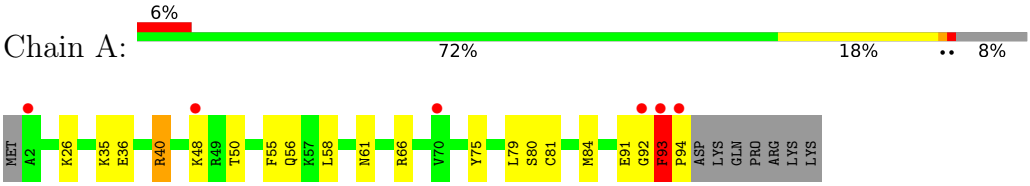
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	28	Total O 28 28	0	0
4	H	26	Total O 26 26	0	0
4	I	51	Total O 51 51	0	0
4	J	65	Total O 65 65	0	0
4	K	52	Total O 52 52	0	0
4	L	53	Total O 53 53	0	0
4	M	35	Total O 35 35	0	0
4	N	49	Total O 49 49	0	0
4	O	33	Total O 33 33	0	0
4	P	42	Total O 42 42	0	0
4	Q	28	Total O 28 28	0	0
4	R	32	Total O 32 32	0	0
4	S	60	Total O 60 60	0	0
4	T	32	Total O 32 32	0	0

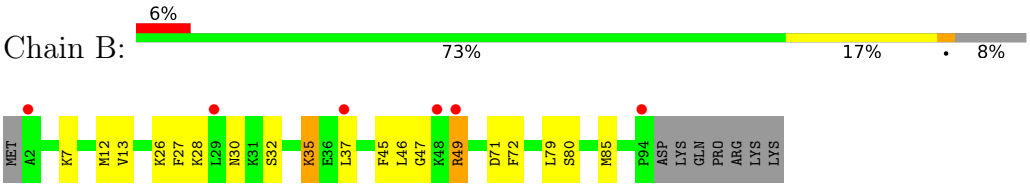
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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.

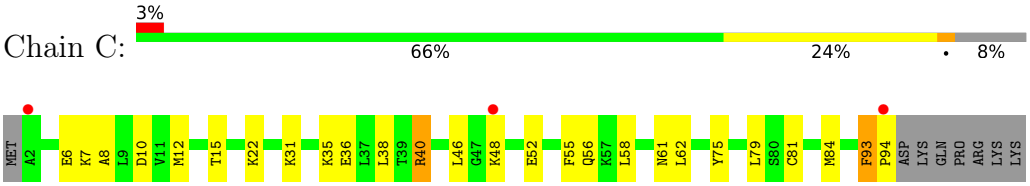
• Molecule 1: Protein S100-A4



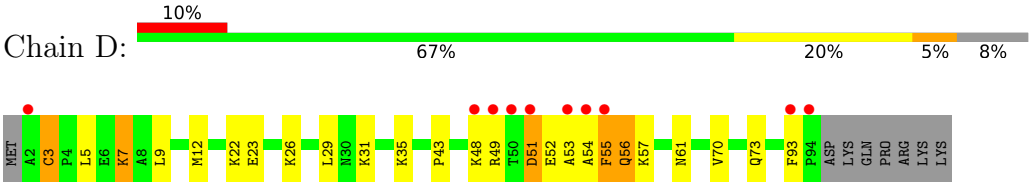
• Molecule 1: Protein S100-A4



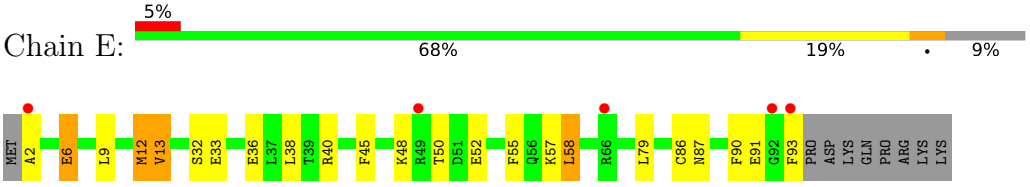
• Molecule 1: Protein S100-A4



• Molecule 1: Protein S100-A4

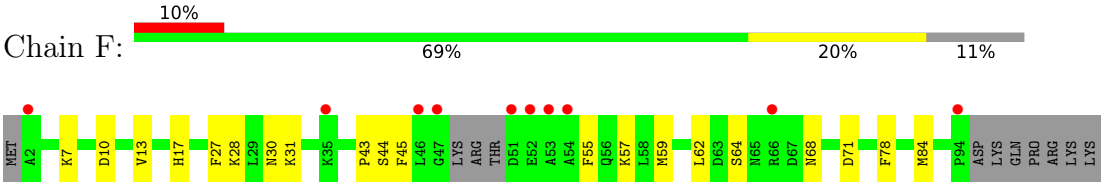


• Molecule 1: Protein S100-A4



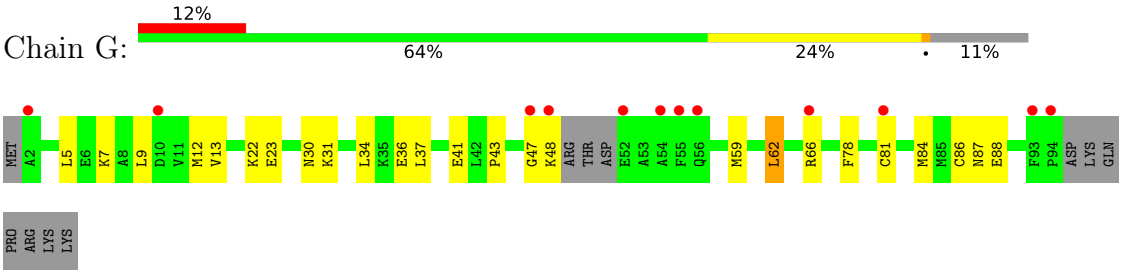
• Molecule 1: Protein S100-A4

Chain F:



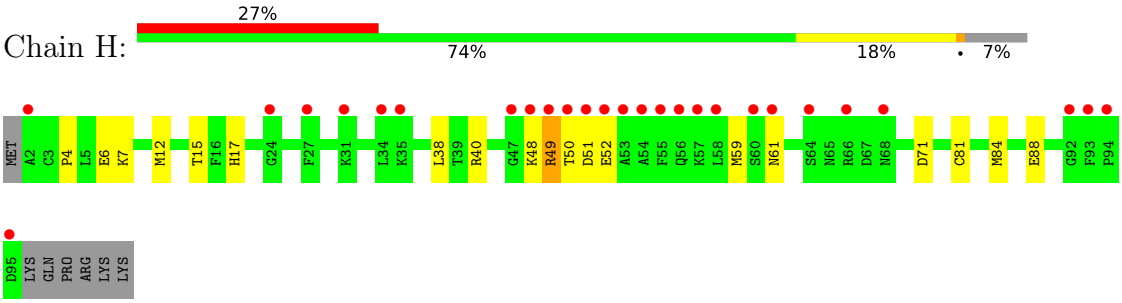
• Molecule 1: Protein S100-A4

Chain G:



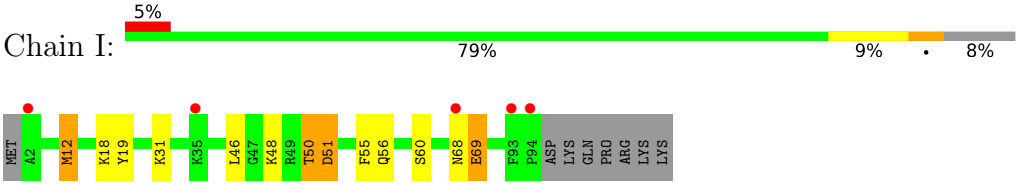
• Molecule 1: Protein S100-A4

Chain H:



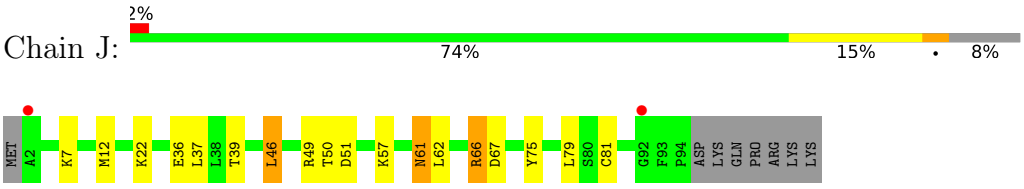
• Molecule 1: Protein S100-A4

Chain I:



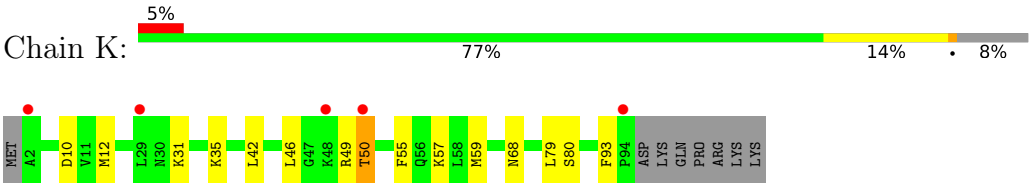
• Molecule 1: Protein S100-A4

Chain J:



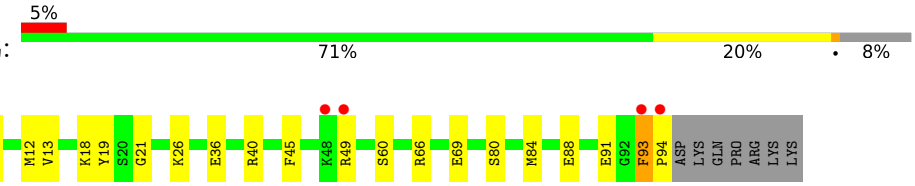
• Molecule 1: Protein S100-A4

Chain K:



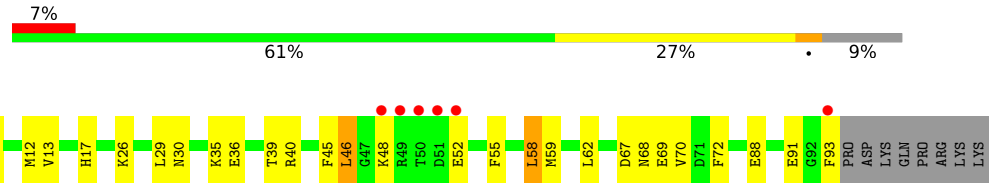
• Molecule 1: Protein S100-A4

Chain L:



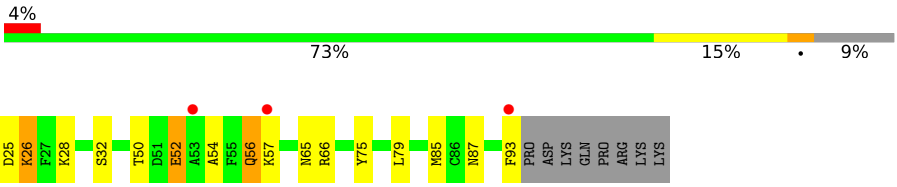
• Molecule 1: Protein S100-A4

Chain M:



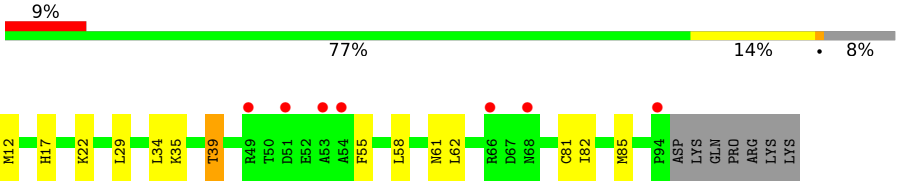
• Molecule 1: Protein S100-A4

Chain N:



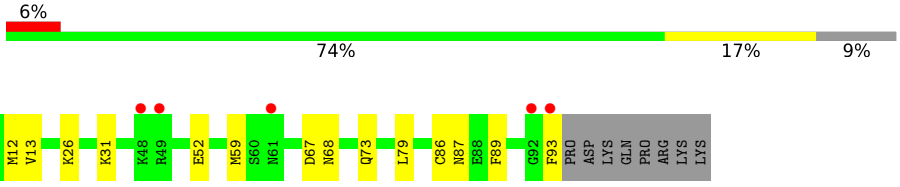
• Molecule 1: Protein S100-A4

Chain O:



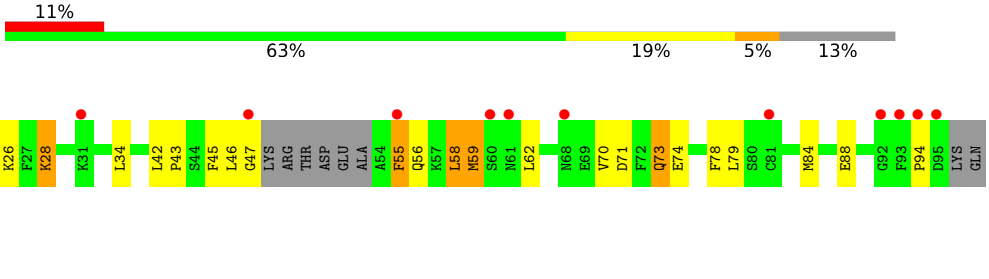
• Molecule 1: Protein S100-A4

Chain P:



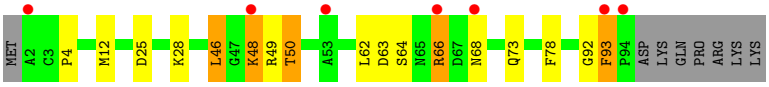
• Molecule 1: Protein S100-A4

Chain Q:

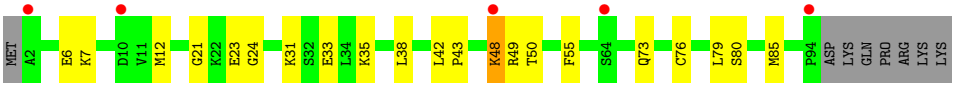


• Molecule 1: Protein S100-A4

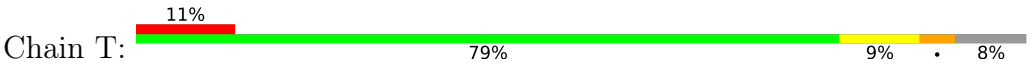
Chain R:

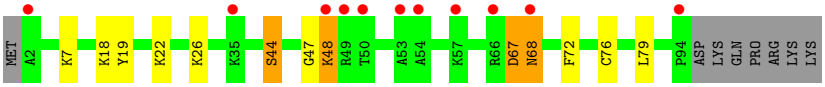


• Molecule 1: Protein S100-A4



• Molecule 1: Protein S100-A4





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	108.79Å 102.49Å 116.63Å 90.00° 92.59° 90.00°	Depositor
Resolution (Å)	19.94 – 2.30 19.88 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.7 (19.94-2.30) 97.7 (19.88-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	1.48 (at 2.30Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.206 , 0.259 0.226 , 0.273	Depositor DCC
R_{free} test set	5579 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	38.8	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 47.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.002 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	16855	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 66.75 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.7495e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: CA, TFP

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	1.01	0/771	0.90	1/1030 (0.1%)
1	B	0.92	0/757	0.74	0/1015
1	C	0.84	0/763	0.81	1/1022 (0.1%)
1	D	0.98	0/772	0.82	1/1033 (0.1%)
1	E	0.93	1/754 (0.1%)	0.78	0/1007
1	F	0.70	0/722	0.74	0/969
1	G	0.79	1/731 (0.1%)	0.72	0/977
1	H	0.66	0/766	0.69	0/1026
1	I	0.88	2/758 (0.3%)	0.82	1/1015 (0.1%)
1	J	0.80	0/776	0.85	1/1037 (0.1%)
1	K	0.90	0/752	0.80	0/1008
1	L	0.95	1/758 (0.1%)	0.86	1/1015 (0.1%)
1	M	0.72	0/744	0.74	0/996
1	N	0.81	0/759	0.78	0/1014
1	O	0.77	0/759	0.77	0/1016
1	P	0.79	1/746 (0.1%)	0.77	1/999 (0.1%)
1	Q	0.87	0/718	0.77	1/961 (0.1%)
1	R	0.73	0/762	0.70	0/1021
1	S	0.84	1/762 (0.1%)	0.80	0/1019
1	T	0.74	0/761	0.79	1/1019 (0.1%)
All	All	0.84	7/15091 (0.0%)	0.78	9/20199 (0.0%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	69	GLU	CD-OE2	-5.43	1.19	1.25
1	I	69	GLU	CG-CD	-5.39	1.43	1.51
1	E	33	GLU	CD-OE2	-5.31	1.19	1.25
1	G	86	CYS	CB-SG	-5.28	1.73	1.81
1	P	3	CYS	CB-SG	-5.22	1.73	1.81
1	S	76	CYS	CB-SG	-5.10	1.73	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	69	GLU	CD-OE1	-5.06	1.20	1.25

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	93	PHE	C-N-CD	-8.77	101.30	120.60
1	I	12	MET	CG-SD-CE	7.88	112.81	100.20
1	L	12	MET	CG-SD-CE	5.59	109.15	100.20
1	J	67	ASP	CB-CG-OD1	5.33	123.09	118.30
1	Q	58	LEU	CA-CB-CG	5.26	127.40	115.30
1	T	67	ASP	CB-CG-OD2	5.15	122.93	118.30
1	D	53	ALA	N-CA-C	-5.13	97.14	111.00
1	P	10	ASP	CB-CG-OD2	5.13	122.92	118.30
1	C	10	ASP	CB-CG-OD1	5.05	122.85	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	754	0	742	13	0
1	B	740	0	710	17	0
1	C	746	0	718	20	0
1	D	752	0	732	20	0
1	E	741	0	722	18	0
1	F	709	0	662	18	0
1	G	718	0	693	20	0
1	H	752	0	722	11	0
1	I	744	0	718	5	0
1	J	756	0	743	11	0
1	K	738	0	707	11	0
1	L	744	0	718	12	0
1	M	731	0	700	30	0
1	N	743	0	722	15	0
1	O	745	0	720	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	P	733	0	700	12	0
1	Q	702	0	671	19	0
1	R	745	0	716	9	0
1	S	748	0	729	14	0
1	T	744	0	718	10	0
2	A	56	0	48	0	0
2	B	56	0	48	4	0
2	C	56	0	48	0	0
2	D	56	0	48	0	0
2	E	56	0	48	2	0
2	F	56	0	48	2	0
2	G	56	0	48	2	0
2	H	56	0	48	0	0
2	I	56	0	48	0	0
2	J	56	0	48	0	0
2	K	56	0	48	0	0
2	L	56	0	48	1	0
2	M	56	0	48	3	0
2	N	56	0	48	2	0
2	O	56	0	48	1	0
2	P	56	0	48	2	0
2	Q	56	0	48	1	0
2	R	56	0	48	1	0
2	S	56	0	48	2	0
2	T	56	0	48	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0
3	I	2	0	0	0	0
3	J	2	0	0	0	0
3	K	2	0	0	0	0
3	L	2	0	0	0	0
3	M	2	0	0	0	0
3	N	2	0	0	0	0
3	O	2	0	0	0	0
3	P	2	0	0	0	0
3	Q	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	R	2	0	0	0	0
3	S	2	0	0	0	0
3	T	2	0	0	0	0
4	A	57	0	0	0	0
4	B	75	0	0	1	0
4	C	56	0	0	2	0
4	D	48	0	0	2	0
4	E	47	0	0	3	0
4	F	41	0	0	1	0
4	G	28	0	0	0	0
4	H	26	0	0	3	0
4	I	51	0	0	0	0
4	J	65	0	0	0	0
4	K	52	0	0	0	0
4	L	53	0	0	1	0
4	M	35	0	0	0	0
4	N	49	0	0	3	0
4	O	33	0	0	0	0
4	P	42	0	0	0	0
4	Q	28	0	0	0	0
4	R	32	0	0	4	0
4	S	60	0	0	1	0
4	T	32	0	0	1	0
All	All	16855	0	15223	256	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 8.

All (256) 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)
1:Q:12[A]:MET:HE1	4:R:1326:HOH:O	1.52	1.08
1:A:93:PHE:N	1:A:94:PRO:CD	2.16	1.04
1:A:92:GLY:O	1:A:93:PHE:HB2	1.59	1.00
1:M:12:MET:SD	1:N:12[A]:MET:SD	2.59	0.99
1:A:93:PHE:N	1:A:94:PRO:HD2	1.82	0.94
1:G:12:MET:HE1	4:H:1515:HOH:O	1.68	0.93
1:I:12:MET:SD	1:J:12[A]:MET:SD	2.69	0.91
1:M:29:LEU:HB2	1:M:70:VAL:CG2	2.03	0.89
1:E:87:ASN:HD22	1:F:17:HIS:HE1	1.18	0.87
1:O:12:MET:SD	1:P:12:MET:CE	2.64	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:ARG:HB3	1:B:49:ARG:NH1	1.92	0.85
1:A:93:PHE:H	1:A:94:PRO:HD2	1.37	0.84
1:N:52:GLU:HA	1:N:52:GLU:OE1	1.77	0.83
1:O:35:LYS:O	1:O:39:THR:HG23	1.78	0.83
1:E:6:GLU:OE1	1:F:44:SER:HB2	1.80	0.81
1:G:34:LEU:HD23	1:G:59:MET:HG2	1.64	0.80
1:C:8:ALA:O	1:C:12[A]:MET:HG3	1.81	0.80
1:O:12:MET:SD	1:P:12:MET:SD	2.81	0.79
1:M:2:ALA:HB3	1:M:7:LYS:NZ	1.99	0.77
1:D:52:GLU:O	1:D:52:GLU:HG2	1.83	0.76
1:C:6:GLU:OE2	1:D:43:PRO:HD2	1.86	0.76
1:N:52:GLU:O	1:N:56:GLN:HB2	1.87	0.75
1:T:67:ASP:O	1:T:68:ASN:CB	2.30	0.75
1:Q:46:LEU:O	1:Q:47:GLY:C	2.23	0.74
1:Q:71:ASP:OD1	1:Q:73:GLN:HG2	1.87	0.74
1:A:93:PHE:H	1:A:94:PRO:CD	1.88	0.73
1:E:87:ASN:ND2	1:F:17:HIS:HE1	1.87	0.73
1:H:4:PRO:HA	1:H:7:LYS:HE2	1.69	0.73
1:E:87:ASN:HD22	1:F:17:HIS:CE1	2.06	0.72
1:M:30:ASN:HA	1:M:69:GLU:HG2	1.72	0.72
1:M:29:LEU:HB2	1:M:70:VAL:HG22	1.72	0.71
1:E:87:ASN:ND2	1:F:17:HIS:CE1	2.60	0.69
1:J:66:ARG:HH11	1:J:66:ARG:CG	2.05	0.69
1:B:47:GLY:HA3	2:B:201:TFP:H201	1.73	0.69
1:M:67:ASP:O	1:M:68:ASN:HB2	1.93	0.69
1:T:67:ASP:O	1:T:68:ASN:HB2	1.93	0.69
1:M:12:MET:HE3	4:N:1099:HOH:O	1.92	0.68
1:M:39:THR:HG22	1:M:46:LEU:HD12	1.75	0.68
1:M:2:ALA:HB3	1:M:7:LYS:HZ1	1.58	0.68
1:K:49:ARG:CB	1:T:26:LYS:HE2	2.24	0.67
1:L:40:ARG:NH1	4:L:2343:HOH:O	2.24	0.67
4:C:1146:HOH:O	1:D:3:CYS:HB2	1.93	0.66
1:O:85:MET:CE	1:O:85:MET:HA	2.24	0.66
1:O:35:LYS:HA	1:O:55:PHE:CZ	2.31	0.66
1:C:93:PHE:CB	1:C:94:PRO:HD3	2.26	0.66
1:D:51:ASP:OD1	1:D:51:ASP:N	2.29	0.66
1:N:25:ASP:OD2	1:N:28:LYS:HE2	1.95	0.65
1:B:49:ARG:HB3	1:B:49:ARG:HH11	1.60	0.65
1:H:49:ARG:HH11	1:H:49:ARG:HB2	1.62	0.65
1:Q:55:PHE:CD1	1:Q:55:PHE:C	2.70	0.63
1:A:26:LYS:HG2	1:J:49:ARG:NH1	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:LYS:HD3	1:B:71:ASP:HB3	1.79	0.63
1:M:12:MET:CE	1:N:12[A]:MET:SD	2.87	0.63
1:E:6:GLU:OE1	1:F:44:SER:CB	2.47	0.62
1:O:12:MET:SD	1:P:12:MET:HE1	2.37	0.62
1:E:36:GLU:OE1	1:E:40:ARG:NH1	2.32	0.62
1:G:34:LEU:CD2	1:G:59:MET:HG2	2.30	0.62
1:O:85:MET:HA	1:O:85:MET:HE3	1.81	0.61
1:K:46:LEU:HD13	1:K:50:THR:HG21	1.82	0.61
1:O:35:LYS:HA	1:O:55:PHE:HZ	1.65	0.61
1:R:68:ASN:ND2	4:R:1832:HOH:O	2.33	0.61
1:A:92:GLY:O	1:A:93:PHE:CB	2.40	0.60
1:Q:43:PRO:O	1:Q:47:GLY:N	2.33	0.60
1:J:66:ARG:HH11	1:J:66:ARG:HG2	1.67	0.59
1:N:52:GLU:OE1	1:N:52:GLU:CA	2.50	0.59
1:S:12:MET:HG3	1:S:79:LEU:CD1	2.32	0.59
1:L:36:GLU:O	1:L:40:ARG:HG2	2.03	0.58
1:K:49:ARG:CB	1:T:26:LYS:CE	2.81	0.58
1:C:84:MET:CE	1:D:73:GLN:HG3	2.34	0.58
1:D:7:LYS:NZ	4:D:709:HOH:O	2.37	0.57
1:C:93:PHE:HB2	1:C:94:PRO:HD3	1.86	0.57
1:A:50:THR:HG23	1:A:55:PHE:CE2	2.40	0.57
1:Q:62:LEU:HD22	1:Q:78:PHE:HB2	1.86	0.57
1:M:45:PHE:HE1	2:M:201:TFP:C8	2.19	0.56
1:G:87:ASN:OD1	1:H:17:HIS:HE1	1.88	0.56
1:L:21:GLY:HA3	1:S:48:LYS:HG2	1.87	0.56
1:M:17:HIS:HE1	1:N:87:ASN:OD1	1.89	0.56
1:Q:28:LYS:HE2	1:Q:71:ASP:HB3	1.89	0.55
1:G:87:ASN:OD1	1:H:17:HIS:CE1	2.59	0.54
1:A:91:GLU:HG3	1:B:27:PHE:CD1	2.42	0.54
1:S:6:GLU:OE1	1:T:44:SER:OG	2.24	0.54
1:E:9:LEU:O	1:E:13:VAL:HG12	2.07	0.54
1:Q:26:LYS:HE3	4:T:1968:HOH:O	2.08	0.54
1:M:2:ALA:HB3	1:M:7:LYS:HZ2	1.72	0.54
1:M:58:LEU:O	1:M:62:LEU:HG	2.08	0.54
1:M:3:CYS:H	1:M:7:LYS:NZ	2.06	0.54
1:G:22:LYS:NZ	1:G:36:GLU:OE2	2.36	0.54
1:D:9:LEU:HD23	1:D:12[B]:MET:CE	2.37	0.53
1:F:45:PHE:HE1	2:F:201:TFP:C8	2.21	0.53
1:G:62:LEU:HD11	1:G:78:PHE:CG	2.43	0.53
1:M:46:LEU:HD11	1:M:55:PHE:CE1	2.44	0.53
1:C:22:LYS:NZ	1:C:36:GLU:OE1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:90:PHE:CE1	1:F:13:VAL:HG12	2.43	0.53
1:K:12:MET:HG3	1:K:79:LEU:HD12	1.91	0.53
1:F:31:LYS:HA	1:F:59:MET:CE	2.38	0.53
1:G:47:GLY:HA3	2:G:201:TFP:H201	1.91	0.53
1:I:18:LYS:HD3	1:I:19:TYR:CE2	2.44	0.52
1:E:50:THR:HB	1:E:55:PHE:CE1	2.45	0.52
1:G:62:LEU:CD1	1:G:78:PHE:HB2	2.40	0.52
1:J:39:THR:HA	1:J:46:LEU:HD12	1.91	0.52
1:R:25:ASP:OD2	1:R:28:LYS:HD2	2.09	0.52
1:G:62:LEU:HD11	1:G:78:PHE:HB2	1.92	0.52
1:G:12:MET:SD	1:H:12:MET:HE1	2.49	0.52
1:A:75:TYR:CZ	1:A:79:LEU:HD11	2.46	0.51
1:B:26:LYS:HE2	1:C:48:LYS:O	2.10	0.51
1:M:70:VAL:HG23	1:M:70:VAL:O	2.09	0.51
1:E:45:PHE:O	2:E:201:TFP:H171	2.11	0.51
1:C:93:PHE:CB	1:C:94:PRO:CD	2.88	0.51
1:D:52:GLU:O	1:D:52:GLU:CG	2.55	0.51
1:M:3:CYS:H	1:M:7:LYS:HZ2	1.59	0.51
1:T:18:LYS:HD3	1:T:19:TYR:CE2	2.45	0.51
1:B:49:ARG:HB3	1:B:49:ARG:CZ	2.40	0.51
1:C:84:MET:HE1	1:D:73:GLN:HG3	1.93	0.50
1:R:46:LEU:HD13	1:R:50:THR:HG21	1.92	0.50
1:H:71:ASP:HB2	4:H:1259:HOH:O	2.10	0.50
1:E:91:GLU:HG2	1:F:27:PHE:CD1	2.47	0.50
1:N:75:TYR:CZ	1:N:79:LEU:HD11	2.47	0.50
1:J:61:ASN:C	1:J:61:ASN:ND2	2.64	0.50
1:G:62:LEU:HD11	1:G:78:PHE:CB	2.42	0.50
1:S:35:LYS:HG3	1:S:55:PHE:CZ	2.47	0.49
1:R:49:ARG:NH2	1:S:24:GLY:O	2.41	0.49
1:N:93:PHE:C	4:N:1615:HOH:O	2.50	0.49
1:D:51:ASP:OD1	1:D:54:ALA:HB3	2.12	0.49
1:H:84:MET:O	1:H:88:GLU:HG2	2.13	0.49
1:G:43:PRO:HD2	1:H:6:GLU:OE2	2.13	0.49
1:I:68:ASN:O	1:I:69:GLU:HG3	2.12	0.49
1:K:12:MET:HG3	1:K:79:LEU:CD1	2.44	0.48
1:O:29:LEU:HD13	1:O:34:LEU:HD12	1.94	0.48
1:E:58:LEU:HD23	4:E:932:HOH:O	2.13	0.48
1:Q:34:LEU:CD2	1:Q:59:MET:HG2	2.43	0.48
1:A:80:SER:O	1:A:84:MET:HG3	2.14	0.48
1:Q:21:GLY:HA2	1:Q:26:LYS:HG3	1.96	0.48
1:Q:59:MET:O	1:Q:59:MET:SD	2.72	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:MET:HG3	2:B:201:TFP:C11	2.44	0.47
1:R:62:LEU:HD21	1:R:78:PHE:CD1	2.49	0.47
1:B:35:LYS:HD3	4:B:439:HOH:O	2.13	0.47
1:M:17:HIS:CE1	1:N:87:ASN:OD1	2.67	0.47
1:I:51:ASP:OD1	1:I:51:ASP:N	2.31	0.47
1:C:93:PHE:HB3	1:C:94:PRO:HD3	1.95	0.47
1:E:2:ALA:HB3	4:E:2123:HOH:O	2.14	0.47
1:L:18:LYS:HD3	1:L:19:TYR:CE2	2.50	0.46
2:M:201:TFP:H6	1:P:93:PHE:HE2	1.81	0.46
1:O:17:HIS:HE1	1:P:87:ASN:OD1	1.98	0.46
1:P:9:LEU:O	1:P:13:VAL:HG23	2.16	0.46
1:D:51:ASP:O	1:D:52:GLU:HB3	2.16	0.46
1:M:35:LYS:HB2	1:M:35:LYS:HE3	1.63	0.46
1:J:22:LYS:HE2	1:J:36:GLU:OE1	2.15	0.46
1:O:12:MET:SD	1:P:12:MET:HE3	2.51	0.46
1:L:45:PHE:HE1	2:L:201:TFP:C8	2.29	0.46
1:M:29:LEU:HD12	1:M:70:VAL:CG2	2.46	0.46
1:J:66:ARG:CG	1:J:66:ARG:NH1	2.70	0.45
2:S:202:TFP:H6	2:S:202:TFP:H131	1.73	0.45
1:A:36:GLU:O	1:A:40:ARG:HG3	2.16	0.45
1:R:92:GLY:O	1:R:93:PHE:O	2.33	0.45
1:B:37:LEU:HD23	1:B:37:LEU:C	2.37	0.45
1:F:7:LYS:NZ	4:F:1050:HOH:O	2.34	0.45
4:C:1838:HOH:O	1:D:12[A]:MET:CE	2.63	0.45
1:Q:45:PHE:HE1	2:Q:201:TFP:C8	2.30	0.45
1:G:12:MET:SD	1:H:12:MET:CE	3.05	0.45
1:M:12:MET:HE1	1:N:12[A]:MET:SD	2.57	0.45
1:Q:12[A]:MET:CE	4:R:1326:HOH:O	2.34	0.45
1:D:93:PHE:HE2	2:E:201:TFP:H6	1.82	0.45
1:D:57:LYS:O	1:D:61:ASN:HB2	2.17	0.45
1:E:12:MET:HE2	1:E:79:LEU:HD12	1.98	0.45
1:E:86:CYS:HB2	1:F:13:VAL:HG21	1.98	0.45
1:F:28:LYS:HG2	1:F:71:ASP:HB3	1.98	0.45
1:I:50:THR:HB	1:I:55:PHE:CE2	2.52	0.44
1:S:12:MET:HG3	1:S:79:LEU:HD12	1.98	0.44
1:C:12[A]:MET:HE1	1:D:12[A]:MET:HB2	1.99	0.44
1:M:36:GLU:O	1:M:40:ARG:HG3	2.17	0.44
1:M:39:THR:HG22	1:M:46:LEU:CD1	2.44	0.44
1:R:63:ASP:OD2	1:R:66:ARG:HA	2.17	0.44
1:B:46:LEU:HA	1:B:46:LEU:HD12	1.69	0.44
1:S:85:MET:HG3	2:S:201:TFP:C12	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:79:LEU:HD23	1:T:79:LEU:HA	1.85	0.44
1:R:12[B]:MET:HE2	4:R:1847:HOH:O	2.17	0.44
1:S:23:GLU:N	1:S:33:GLU:OE2	2.50	0.44
1:B:12:MET:HG3	1:B:79:LEU:HD12	1.98	0.44
1:L:9:LEU:O	1:L:13:VAL:HG23	2.18	0.44
1:K:10:ASP:OD1	2:N:202:TFP:N3	2.51	0.44
1:C:12[B]:MET:HE1	4:D:1422:HOH:O	2.17	0.44
1:F:30:ASN:OD1	1:F:30:ASN:C	2.56	0.44
1:G:12:MET:CE	4:H:1515:HOH:O	2.45	0.44
1:P:12:MET:HG2	1:P:79:LEU:HD13	2.00	0.44
1:T:67:ASP:O	1:T:68:ASN:HB3	2.14	0.44
1:R:48:LYS:HG2	1:S:21:GLY:HA3	1.99	0.44
1:O:58:LEU:O	1:O:62:LEU:HG	2.18	0.43
1:G:9:LEU:O	1:G:13:VAL:HG23	2.19	0.43
1:L:80:SER:O	1:L:84:MET:HG2	2.19	0.43
1:J:75:TYR:CZ	1:J:79:LEU:HD11	2.53	0.43
1:Q:59:MET:SD	1:Q:59:MET:C	2.97	0.43
1:P:86:CYS:O	1:P:89:PHE:HB3	2.17	0.43
1:F:45:PHE:HE1	2:F:201:TFP:H8	1.83	0.43
2:G:201:TFP:H142	2:G:201:TFP:H162	1.63	0.43
1:L:26:LYS:HE2	1:S:49:ARG:HB2	2.01	0.43
1:C:36:GLU:O	1:C:40:ARG:CG	2.67	0.43
1:K:46:LEU:HD22	1:K:50:THR:CG2	2.48	0.43
1:D:56:GLN:HE21	1:D:56:GLN:HA	1.84	0.43
1:B:13:VAL:HG22	1:B:72:PHE:HZ	1.84	0.43
1:E:40:ARG:NH2	4:E:1729:HOH:O	2.50	0.43
1:G:9:LEU:HD23	1:H:12:MET:HE1	2.01	0.43
1:J:61:ASN:C	1:J:61:ASN:HD22	2.23	0.43
1:S:73:GLN:HG3	4:S:265:HOH:O	2.17	0.43
1:M:93:PHE:HD1	2:P:201:TFP:H131	1.84	0.42
2:O:202:TFP:H6	2:O:202:TFP:H131	1.79	0.42
1:C:58:LEU:O	1:C:62:LEU:HG	2.19	0.42
1:D:29:LEU:HB2	1:D:70:VAL:HB	2.01	0.42
1:Q:70:VAL:HA	1:Q:74:GLU:OE1	2.18	0.42
2:P:202:TFP:H6	2:P:202:TFP:H131	1.81	0.42
1:D:35:LYS:HG2	1:D:55:PHE:CZ	2.54	0.42
1:G:5:LEU:HD22	1:H:15:THR:HG21	2.00	0.42
1:K:35:LYS:HG3	1:K:55:PHE:CZ	2.55	0.42
1:L:93:PHE:HA	1:L:94:PRO:HD2	1.87	0.42
1:B:45:PHE:HE1	2:B:201:TFP:C8	2.32	0.42
1:M:9:LEU:HD23	1:M:12:MET:HE2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:26:LYS:HD3	1:T:48:LYS:HG2	2.01	0.42
1:G:23:GLU:HG3	1:G:30:ASN:HD21	1.84	0.42
1:M:46:LEU:HD23	1:M:46:LEU:HA	1.74	0.42
1:Q:84:MET:O	1:Q:88:GLU:HG2	2.19	0.42
1:C:35:LYS:HG3	1:C:55:PHE:CZ	2.55	0.42
1:E:6:GLU:OE2	1:F:43:PRO:HD2	2.20	0.42
1:C:31:LYS:HE2	1:C:35:LYS:NZ	2.35	0.42
1:Q:79:LEU:HD23	1:Q:79:LEU:HA	1.85	0.42
1:S:12:MET:CG	1:S:79:LEU:HD12	2.49	0.41
1:C:35:LYS:HE3	1:C:35:LYS:HB2	1.89	0.41
1:L:26:LYS:HG3	1:S:49:ARG:NH2	2.36	0.41
1:T:72:PHE:CE2	1:T:76:CYS:SG	3.14	0.41
1:D:51:ASP:OD1	1:D:54:ALA:CB	2.69	0.41
1:O:17:HIS:CE1	1:P:87:ASN:OD1	2.74	0.41
1:C:46:LEU:HD21	1:C:55:PHE:CZ	2.56	0.41
2:M:202:TFP:C6	2:M:202:TFP:H141	2.51	0.41
1:B:85:MET:HG3	2:B:201:TFP:C12	2.51	0.41
1:F:62:LEU:HD22	1:F:78:PHE:HB2	2.03	0.41
1:G:37:LEU:O	1:G:41:GLU:HB2	2.20	0.41
1:O:82:ILE:HG21	1:P:9:LEU:HD13	2.01	0.41
1:N:85:MET:HG3	2:N:201:TFP:C12	2.51	0.41
1:Q:42:LEU:N	1:Q:43:PRO:CD	2.83	0.41
1:B:12:MET:HG3	1:B:79:LEU:CD1	2.51	0.41
1:F:7:LYS:O	1:F:10:ASP:HB3	2.21	0.41
1:K:46:LEU:HD23	1:K:46:LEU:HA	1.60	0.41
1:N:50:THR:CG2	1:N:54:ALA:HB3	2.51	0.41
1:P:67:ASP:O	1:P:68:ASN:HB2	2.20	0.41
1:B:30:ASN:C	1:B:30:ASN:OD1	2.59	0.40
1:C:15:THR:HG21	1:D:5:LEU:HD22	2.03	0.40
1:K:59:MET:CE	1:K:68:ASN:C	2.90	0.40
1:L:49:ARG:NH1	1:M:26:LYS:HG2	2.36	0.40
1:N:26:LYS:NZ	1:N:26:LYS:H	2.19	0.40
2:R:202:TFP:H141	2:R:202:TFP:C6	2.51	0.40
1:J:37:LEU:C	1:J:37:LEU:HD23	2.42	0.40
1:K:42:LEU:HD23	1:L:6:GLU:HG2	2.02	0.40
1:M:13:VAL:HG22	1:M:72:PHE:HZ	1.86	0.40
1:S:42:LEU:N	1:S:43:PRO:CD	2.84	0.40
1:C:75:TYR:CZ	1:C:79:LEU:HD11	2.56	0.40
1:M:29:LEU:HD12	1:M:70:VAL:HG23	2.03	0.40
1:N:18:LYS:HE3	4:N:2273:HOH:O	2.22	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	92/101 (91%)	91 (99%)	0	1 (1%)	14	15
1	B	92/101 (91%)	91 (99%)	1 (1%)	0	100	100
1	C	92/101 (91%)	90 (98%)	1 (1%)	1 (1%)	14	15
1	D	93/101 (92%)	92 (99%)	1 (1%)	0	100	100
1	E	90/101 (89%)	88 (98%)	2 (2%)	0	100	100
1	F	86/101 (85%)	83 (96%)	3 (4%)	0	100	100
1	G	86/101 (85%)	85 (99%)	1 (1%)	0	100	100
1	H	92/101 (91%)	87 (95%)	5 (5%)	0	100	100
1	I	91/101 (90%)	90 (99%)	1 (1%)	0	100	100
1	J	93/101 (92%)	92 (99%)	1 (1%)	0	100	100
1	K	91/101 (90%)	90 (99%)	0	1 (1%)	14	15
1	L	91/101 (90%)	88 (97%)	2 (2%)	1 (1%)	14	15
1	M	90/101 (89%)	90 (100%)	0	0	100	100
1	N	91/101 (90%)	91 (100%)	0	0	100	100
1	O	91/101 (90%)	87 (96%)	4 (4%)	0	100	100
1	P	90/101 (89%)	89 (99%)	1 (1%)	0	100	100
1	Q	85/101 (84%)	82 (96%)	2 (2%)	1 (1%)	13	14
1	R	92/101 (91%)	89 (97%)	2 (2%)	1 (1%)	14	15
1	S	91/101 (90%)	88 (97%)	3 (3%)	0	100	100
1	T	92/101 (91%)	87 (95%)	4 (4%)	1 (1%)	14	15
All	All	1811/2020 (90%)	1770 (98%)	34 (2%)	7 (0%)	34	42

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	93	PHE

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Mol	Chain	Res	Type
1	C	93	PHE
1	T	47	GLY
1	R	93	PHE
1	Q	94	PRO
1	K	93	PHE
1	L	93	PHE

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	85/92 (92%)	77 (91%)	8 (9%)	8 10
1	B	82/92 (89%)	77 (94%)	5 (6%)	18 25
1	C	83/92 (90%)	76 (92%)	7 (8%)	11 13
1	D	85/92 (92%)	74 (87%)	11 (13%)	4 4
1	E	83/92 (90%)	73 (88%)	10 (12%)	5 5
1	F	78/92 (85%)	73 (94%)	5 (6%)	17 23
1	G	80/92 (87%)	72 (90%)	8 (10%)	7 9
1	H	84/92 (91%)	74 (88%)	10 (12%)	5 5
1	I	83/92 (90%)	76 (92%)	7 (8%)	11 13
1	J	86/92 (94%)	76 (88%)	10 (12%)	5 6
1	K	82/92 (89%)	78 (95%)	4 (5%)	25 35
1	L	83/92 (90%)	79 (95%)	4 (5%)	25 36
1	M	81/92 (88%)	73 (90%)	8 (10%)	8 9
1	N	83/92 (90%)	76 (92%)	7 (8%)	11 13
1	O	83/92 (90%)	78 (94%)	5 (6%)	19 26
1	P	81/92 (88%)	76 (94%)	5 (6%)	18 25
1	Q	79/92 (86%)	73 (92%)	6 (8%)	13 16
1	R	83/92 (90%)	76 (92%)	7 (8%)	11 13
1	S	84/92 (91%)	78 (93%)	6 (7%)	14 19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	T	83/92 (90%)	78 (94%)	5 (6%)	19 26
All	All	1651/1840 (90%)	1513 (92%)	138 (8%)	11 13

All (138) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	48	LYS
1	A	56	GLN
1	A	58	LEU
1	A	61	ASN
1	A	66	ARG
1	A	81	CYS
1	A	93	PHE
1	B	7	LYS
1	B	32	SER
1	B	35	LYS
1	B	49	ARG
1	B	80	SER
1	C	7	LYS
1	C	38	LEU
1	C	40	ARG
1	C	52	GLU
1	C	56	GLN
1	C	61	ASN
1	C	81	CYS
1	D	3	CYS
1	D	7	LYS
1	D	22	LYS
1	D	23	GLU
1	D	26	LYS
1	D	31	LYS
1	D	48	LYS
1	D	49	ARG
1	D	51	ASP
1	D	55	PHE
1	D	56	GLN
1	E	6	GLU
1	E	12	MET
1	E	13	VAL
1	E	32	SER
1	E	38	LEU

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Mol	Chain	Res	Type
1	E	48	LYS
1	E	52	GLU
1	E	57	LYS
1	E	58	LEU
1	E	93	PHE
1	F	55	PHE
1	F	57	LYS
1	F	64	SER
1	F	68	ASN
1	F	84	MET
1	G	7	LYS
1	G	31	LYS
1	G	48	LYS
1	G	62	LEU
1	G	66	ARG
1	G	81	CYS
1	G	84	MET
1	G	88	GLU
1	H	38	LEU
1	H	40	ARG
1	H	48	LYS
1	H	49	ARG
1	H	50	THR
1	H	51	ASP
1	H	52	GLU
1	H	59	MET
1	H	61	ASN
1	H	81	CYS
1	I	31	LYS
1	I	46	LEU
1	I	48	LYS
1	I	50	THR
1	I	51	ASP
1	I	56	GLN
1	I	60	SER
1	J	7	LYS
1	J	46	LEU
1	J	50	THR
1	J	51	ASP
1	J	57	LYS
1	J	61	ASN
1	J	62	LEU

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Mol	Chain	Res	Type
1	J	66	ARG
1	J	81[A]	CYS
1	J	81[B]	CYS
1	K	31	LYS
1	K	50	THR
1	K	57	LYS
1	K	80	SER
1	L	60	SER
1	L	66	ARG
1	L	88	GLU
1	L	91	GLU
1	M	7	LYS
1	M	46	LEU
1	M	48	LYS
1	M	52	GLU
1	M	58	LEU
1	M	59	MET
1	M	88	GLU
1	M	91	GLU
1	N	26	LYS
1	N	32	SER
1	N	52	GLU
1	N	56	GLN
1	N	57	LYS
1	N	65	ASN
1	N	66	ARG
1	O	7	LYS
1	O	22	LYS
1	O	39	THR
1	O	61	ASN
1	O	81	CYS
1	P	26	LYS
1	P	31	LYS
1	P	52	GLU
1	P	59	MET
1	P	73	GLN
1	Q	28	LYS
1	Q	55	PHE
1	Q	56	GLN
1	Q	58	LEU
1	Q	59	MET
1	Q	73	GLN

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Mol	Chain	Res	Type
1	R	4	PRO
1	R	46	LEU
1	R	48	LYS
1	R	50	THR
1	R	64	SER
1	R	66	ARG
1	R	73	GLN
1	S	7	LYS
1	S	31	LYS
1	S	38	LEU
1	S	48	LYS
1	S	50	THR
1	S	80	SER
1	T	7	LYS
1	T	22	LYS
1	T	44	SER
1	T	48	LYS
1	T	68	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	GLN
1	B	68	ASN
1	C	61	ASN
1	C	73	GLN
1	D	56	GLN
1	E	61	ASN
1	E	87	ASN
1	F	17	HIS
1	F	68	ASN
1	H	17	HIS
1	H	73	GLN
1	J	61	ASN
1	K	61	ASN
1	M	17	HIS
1	M	73	GLN
1	O	17	HIS
1	P	17	HIS
1	Q	17	HIS
1	R	87	ASN
1	T	68	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 80 ligands modelled in this entry, 40 are monoatomic - leaving 40 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	$\#\|Z\| > 2$
2	TFP	H	201	-	31,31,31	2.42	6 (19%)	45,45,45	1.43	8 (17%)
2	TFP	A	202	-	31,31,31	1.78	5 (16%)	45,45,45	1.61	10 (22%)
2	TFP	D	202	-	31,31,31	2.04	4 (12%)	45,45,45	1.38	4 (8%)
2	TFP	E	201	-	31,31,31	2.39	4 (12%)	45,45,45	1.81	10 (22%)
2	TFP	P	201	-	31,31,31	2.27	6 (19%)	45,45,45	1.77	13 (28%)
2	TFP	T	201	-	31,31,31	2.28	5 (16%)	45,45,45	1.58	6 (13%)
2	TFP	C	201	-	31,31,31	2.44	5 (16%)	45,45,45	1.80	13 (28%)
2	TFP	R	202	-	31,31,31	2.10	4 (12%)	45,45,45	1.57	6 (13%)
2	TFP	L	201	-	31,31,31	2.17	4 (12%)	45,45,45	1.98	13 (28%)
2	TFP	G	202	-	31,31,31	1.99	5 (16%)	45,45,45	1.66	11 (24%)
2	TFP	I	202	-	31,31,31	1.72	4 (12%)	45,45,45	1.62	7 (15%)
2	TFP	T	202	-	31,31,31	2.02	4 (12%)	45,45,45	1.94	12 (26%)
2	TFP	N	202	-	31,31,31	1.91	4 (12%)	45,45,45	1.53	9 (20%)
2	TFP	C	202	-	31,31,31	1.71	4 (12%)	45,45,45	1.36	8 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	TFP	H	202	-	31,31,31	1.95	4 (12%)	45,45,45	1.25	4 (8%)
2	TFP	K	202	-	31,31,31	1.77	4 (12%)	45,45,45	1.61	11 (24%)
2	TFP	Q	202	-	31,31,31	2.06	5 (16%)	45,45,45	1.54	10 (22%)
2	TFP	M	201	-	31,31,31	2.32	4 (12%)	45,45,45	1.52	9 (20%)
2	TFP	P	202	-	31,31,31	1.76	4 (12%)	45,45,45	1.56	9 (20%)
2	TFP	O	202	-	31,31,31	1.79	4 (12%)	45,45,45	1.33	5 (11%)
2	TFP	M	202	-	31,31,31	2.14	4 (12%)	45,45,45	1.44	8 (17%)
2	TFP	G	201	-	31,31,31	2.33	4 (12%)	45,45,45	1.41	9 (20%)
2	TFP	J	201	-	31,31,31	2.23	5 (16%)	45,45,45	2.11	14 (31%)
2	TFP	B	201	-	31,31,31	2.30	6 (19%)	45,45,45	1.80	9 (20%)
2	TFP	N	201	-	31,31,31	2.29	6 (19%)	45,45,45	1.35	7 (15%)
2	TFP	R	201	-	31,31,31	2.04	4 (12%)	45,45,45	1.66	10 (22%)
2	TFP	S	201	-	31,31,31	2.25	4 (12%)	45,45,45	1.74	11 (24%)
2	TFP	E	202	-	31,31,31	1.81	4 (12%)	45,45,45	1.41	5 (11%)
2	TFP	B	202	-	31,31,31	1.87	4 (12%)	45,45,45	1.60	11 (24%)
2	TFP	F	202	-	31,31,31	1.65	3 (9%)	45,45,45	1.42	7 (15%)
2	TFP	F	201	-	31,31,31	2.29	4 (12%)	45,45,45	1.34	8 (17%)
2	TFP	K	201	-	31,31,31	2.17	5 (16%)	45,45,45	1.87	13 (28%)
2	TFP	Q	201	-	31,31,31	2.31	4 (12%)	45,45,45	1.35	5 (11%)
2	TFP	D	201	-	31,31,31	2.32	5 (16%)	45,45,45	1.72	14 (31%)
2	TFP	J	202	-	31,31,31	2.02	4 (12%)	45,45,45	1.38	5 (11%)
2	TFP	O	201	-	31,31,31	2.31	4 (12%)	45,45,45	2.07	13 (28%)
2	TFP	A	201	-	31,31,31	2.20	4 (12%)	45,45,45	2.13	14 (31%)
2	TFP	L	202	-	31,31,31	1.94	4 (12%)	45,45,45	1.62	10 (22%)
2	TFP	I	201	-	31,31,31	2.08	4 (12%)	45,45,45	1.69	7 (15%)
2	TFP	S	202	-	31,31,31	1.86	4 (12%)	45,45,45	1.53	10 (22%)

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	TFP	H	201	-	-	2/12/34/34	0/4/4/4
2	TFP	A	202	-	-	0/12/34/34	0/4/4/4
2	TFP	D	202	-	-	1/12/34/34	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TFP	E	201	-	-	4/12/34/34	0/3/4/4
2	TFP	P	201	-	-	3/12/34/34	0/3/4/4
2	TFP	T	201	-	-	2/12/34/34	0/4/4/4
2	TFP	C	201	-	-	4/12/34/34	0/4/4/4
2	TFP	R	202	-	-	0/12/34/34	0/4/4/4
2	TFP	L	201	-	-	4/12/34/34	0/4/4/4
2	TFP	G	202	-	-	0/12/34/34	0/4/4/4
2	TFP	I	202	-	-	0/12/34/34	0/3/4/4
2	TFP	T	202	-	-	0/12/34/34	0/4/4/4
2	TFP	N	202	-	-	0/12/34/34	0/3/4/4
2	TFP	C	202	-	-	0/12/34/34	0/4/4/4
2	TFP	H	202	-	-	0/12/34/34	0/4/4/4
2	TFP	K	202	-	-	0/12/34/34	0/4/4/4
2	TFP	Q	202	-	-	0/12/34/34	0/3/4/4
2	TFP	M	201	-	-	2/12/34/34	0/3/4/4
2	TFP	P	202	-	-	1/12/34/34	0/3/4/4
2	TFP	O	202	-	-	2/12/34/34	0/4/4/4
2	TFP	M	202	-	-	0/12/34/34	0/4/4/4
2	TFP	G	201	-	-	5/12/34/34	0/3/4/4
2	TFP	J	201	-	-	3/12/34/34	0/3/4/4
2	TFP	B	201	-	-	5/12/34/34	0/4/4/4
2	TFP	N	201	-	-	3/12/34/34	0/4/4/4
2	TFP	R	201	-	-	3/12/34/34	0/4/4/4
2	TFP	S	201	-	-	2/12/34/34	0/4/4/4
2	TFP	E	202	-	-	0/12/34/34	0/3/4/4
2	TFP	B	202	-	-	0/12/34/34	0/4/4/4
2	TFP	F	202	-	-	0/12/34/34	0/4/4/4
2	TFP	F	201	-	-	3/12/34/34	0/3/4/4
2	TFP	K	201	-	-	5/12/34/34	0/4/4/4
2	TFP	Q	201	-	-	2/12/34/34	0/4/4/4
2	TFP	D	201	-	-	1/12/34/34	0/4/4/4
2	TFP	J	202	-	-	1/12/34/34	0/3/4/4
2	TFP	O	201	-	-	5/12/34/34	0/4/4/4
2	TFP	A	201	-	-	4/12/34/34	0/4/4/4
2	TFP	L	202	-	-	1/12/34/34	0/3/4/4
2	TFP	I	201	-	-	1/12/34/34	0/4/4/4
2	TFP	S	202	-	-	3/12/34/34	0/3/4/4

All (175) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	201	TFP	C12-C7	8.86	1.51	1.40
2	M	202	TFP	C12-C7	8.53	1.50	1.40
2	D	201	TFP	C5-C4	8.47	1.50	1.40
2	G	201	TFP	C12-C7	8.45	1.50	1.40
2	E	201	TFP	C12-C7	8.21	1.50	1.40
2	C	201	TFP	C12-C7	8.18	1.50	1.40
2	E	201	TFP	C5-C4	8.18	1.50	1.40
2	H	201	TFP	C12-C7	8.05	1.50	1.40
2	S	201	TFP	C12-C7	8.04	1.50	1.40
2	F	201	TFP	C12-C7	8.03	1.50	1.40
2	P	201	TFP	C12-C7	8.02	1.50	1.40
2	R	202	TFP	C5-C4	7.91	1.50	1.40
2	K	201	TFP	C5-C4	7.89	1.50	1.40
2	B	201	TFP	C12-C7	7.81	1.49	1.40
2	Q	201	TFP	C12-C7	7.75	1.49	1.40
2	T	201	TFP	C12-C7	7.74	1.49	1.40
2	C	201	TFP	C5-C4	7.64	1.49	1.40
2	T	201	TFP	C5-C4	7.64	1.49	1.40
2	B	201	TFP	C5-C4	7.63	1.49	1.40
2	D	202	TFP	C5-C4	7.54	1.49	1.40
2	A	201	TFP	C12-C7	7.52	1.49	1.40
2	N	201	TFP	C12-C7	7.49	1.49	1.40
2	O	201	TFP	C5-C4	7.45	1.49	1.40
2	J	201	TFP	C12-C7	7.45	1.49	1.40
2	H	201	TFP	C5-C4	7.38	1.49	1.40
2	A	201	TFP	C5-C4	7.37	1.49	1.40
2	Q	202	TFP	C12-C7	7.36	1.49	1.40
2	M	201	TFP	C12-C7	7.36	1.49	1.40
2	Q	201	TFP	C5-C4	7.35	1.49	1.40
2	M	201	TFP	C5-C4	7.32	1.49	1.40
2	P	201	TFP	C5-C4	7.31	1.49	1.40
2	D	201	TFP	C12-C7	7.30	1.49	1.40
2	J	201	TFP	C5-C4	7.29	1.49	1.40
2	G	201	TFP	C5-C4	7.27	1.49	1.40
2	L	201	TFP	C12-C7	7.25	1.49	1.40
2	S	201	TFP	C5-C4	7.23	1.49	1.40
2	N	201	TFP	C5-C4	7.17	1.49	1.40
2	L	201	TFP	C5-C4	7.11	1.49	1.40
2	N	202	TFP	C5-C4	7.07	1.49	1.40
2	F	201	TFP	C5-C4	7.01	1.48	1.40
2	K	201	TFP	C12-C7	6.94	1.48	1.40
2	R	201	TFP	C5-C4	6.93	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	202	TFP	C12-C7	6.86	1.48	1.40
2	L	202	TFP	C5-C4	6.86	1.48	1.40
2	H	202	TFP	C12-C7	6.84	1.48	1.40
2	H	202	TFP	C5-C4	6.83	1.48	1.40
2	T	202	TFP	C5-C4	6.80	1.48	1.40
2	T	202	TFP	C12-C7	6.80	1.48	1.40
2	K	202	TFP	C5-C4	6.75	1.48	1.40
2	E	202	TFP	C5-C4	6.73	1.48	1.40
2	I	201	TFP	C5-C4	6.72	1.48	1.40
2	G	202	TFP	C5-C4	6.64	1.48	1.40
2	I	201	TFP	C12-C7	6.59	1.48	1.40
2	J	202	TFP	C5-C4	6.58	1.48	1.40
2	Q	202	TFP	C5-C4	6.57	1.48	1.40
2	C	202	TFP	C12-C7	6.52	1.48	1.40
2	J	202	TFP	C12-C7	6.42	1.48	1.40
2	M	202	TFP	C5-C4	6.41	1.48	1.40
2	R	201	TFP	C12-C7	6.34	1.48	1.40
2	O	202	TFP	C12-C7	6.31	1.48	1.40
2	D	202	TFP	C12-C7	6.19	1.47	1.40
2	S	202	TFP	C12-C7	6.18	1.47	1.40
2	L	202	TFP	C12-C7	6.04	1.47	1.40
2	E	202	TFP	C12-C7	6.03	1.47	1.40
2	B	202	TFP	C5-C4	6.03	1.47	1.40
2	G	202	TFP	C12-C7	6.02	1.47	1.40
2	I	202	TFP	C12-C7	5.98	1.47	1.40
2	P	202	TFP	C5-C4	5.90	1.47	1.40
2	A	202	TFP	C12-C7	5.87	1.47	1.40
2	N	202	TFP	C12-C7	5.81	1.47	1.40
2	O	202	TFP	C5-C4	5.77	1.47	1.40
2	B	202	TFP	C12-C7	5.57	1.47	1.40
2	F	202	TFP	C5-C4	5.47	1.47	1.40
2	K	202	TFP	C12-C7	5.46	1.47	1.40
2	M	201	TFP	C4-S	-5.38	1.67	1.76
2	P	202	TFP	C12-C7	5.15	1.46	1.40
2	I	202	TFP	C5-C4	5.14	1.46	1.40
2	C	202	TFP	C5-C4	4.87	1.46	1.40
2	S	202	TFP	C5-C4	4.85	1.46	1.40
2	Q	201	TFP	C7-S	-4.84	1.67	1.76
2	F	202	TFP	C12-C7	4.79	1.46	1.40
2	D	201	TFP	C4-S	-4.62	1.68	1.76
2	S	202	TFP	C7-S	-4.61	1.68	1.76
2	G	201	TFP	C4-S	-4.53	1.68	1.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	202	TFP	C7-S	-4.53	1.68	1.76
2	A	202	TFP	C5-C4	4.52	1.45	1.40
2	F	201	TFP	C4-S	-4.46	1.68	1.76
2	L	202	TFP	C7-S	-4.42	1.68	1.76
2	H	201	TFP	C4-S	-4.21	1.69	1.76
2	G	202	TFP	C7-S	-4.19	1.69	1.76
2	H	201	TFP	C7-S	-4.17	1.69	1.76
2	E	201	TFP	C4-S	-4.15	1.69	1.76
2	B	202	TFP	C7-S	-4.13	1.69	1.76
2	M	201	TFP	C7-S	-4.11	1.69	1.76
2	I	201	TFP	C7-S	-4.09	1.69	1.76
2	R	201	TFP	C4-S	-4.06	1.69	1.76
2	C	201	TFP	C7-S	-4.03	1.69	1.76
2	A	201	TFP	C4-S	-4.01	1.69	1.76
2	C	201	TFP	C4-S	-4.00	1.69	1.76
2	D	202	TFP	C7-S	-3.99	1.69	1.76
2	Q	201	TFP	C4-S	-3.97	1.69	1.76
2	T	202	TFP	C7-S	-3.97	1.69	1.76
2	B	201	TFP	C4-S	-3.94	1.69	1.76
2	N	201	TFP	C4-S	-3.94	1.69	1.76
2	R	201	TFP	C7-S	-3.85	1.69	1.76
2	K	201	TFP	C4-S	-3.85	1.69	1.76
2	J	202	TFP	C4-S	-3.84	1.69	1.76
2	P	201	TFP	C7-S	-3.84	1.69	1.76
2	P	201	TFP	C4-S	-3.78	1.69	1.76
2	I	201	TFP	C4-S	-3.78	1.69	1.76
2	T	201	TFP	C4-S	-3.74	1.69	1.76
2	Q	202	TFP	C7-S	-3.69	1.69	1.76
2	F	201	TFP	C7-S	-3.67	1.70	1.76
2	L	201	TFP	C4-S	-3.66	1.70	1.76
2	E	201	TFP	C7-S	-3.61	1.70	1.76
2	J	201	TFP	C4-S	-3.54	1.70	1.76
2	P	202	TFP	C4-S	-3.54	1.70	1.76
2	J	202	TFP	C7-S	-3.50	1.70	1.76
2	S	201	TFP	C4-S	-3.43	1.70	1.76
2	L	201	TFP	C7-S	-3.40	1.70	1.76
2	N	201	TFP	C7-S	-3.32	1.70	1.76
2	J	201	TFP	C7-S	-3.30	1.70	1.76
2	M	202	TFP	C7-S	-3.30	1.70	1.76
2	T	201	TFP	C7-S	-3.29	1.70	1.76
2	G	201	TFP	C7-S	-3.24	1.70	1.76
2	S	202	TFP	C4-S	-3.17	1.70	1.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	202	TFP	C7-S	-3.13	1.70	1.76
2	I	202	TFP	C4-S	-3.13	1.70	1.76
2	B	201	TFP	C7-S	-3.13	1.70	1.76
2	S	201	TFP	C7-S	-3.10	1.71	1.76
2	R	202	TFP	C4-S	-3.09	1.71	1.76
2	I	202	TFP	C7-S	-3.07	1.71	1.76
2	O	201	TFP	C7-S	-3.04	1.71	1.76
2	A	202	TFP	C4-S	-3.01	1.71	1.76
2	H	201	TFP	C5-N1	2.99	1.45	1.40
2	F	202	TFP	C7-S	-2.95	1.71	1.76
2	C	201	TFP	C12-N1	2.87	1.45	1.40
2	N	201	TFP	C12-N1	2.86	1.45	1.40
2	N	202	TFP	C7-S	-2.81	1.71	1.76
2	B	201	TFP	C5-N1	2.80	1.45	1.40
2	K	201	TFP	C7-S	-2.80	1.71	1.76
2	O	202	TFP	C4-S	-2.80	1.71	1.76
2	G	202	TFP	C4-S	-2.78	1.71	1.76
2	K	202	TFP	C7-S	-2.70	1.71	1.76
2	C	202	TFP	C4-S	-2.69	1.71	1.76
2	N	202	TFP	C4-S	-2.69	1.71	1.76
2	H	202	TFP	C7-S	-2.66	1.71	1.76
2	O	202	TFP	C7-S	-2.66	1.71	1.76
2	J	201	TFP	C5-N1	2.65	1.44	1.40
2	T	201	TFP	C12-N1	2.58	1.44	1.40
2	D	201	TFP	C7-S	-2.57	1.71	1.76
2	P	202	TFP	C7-S	-2.56	1.71	1.76
2	T	202	TFP	C3-C2	2.55	1.43	1.38
2	O	201	TFP	C4-S	-2.55	1.71	1.76
2	L	202	TFP	C4-S	-2.55	1.71	1.76
2	H	202	TFP	C4-S	-2.53	1.71	1.76
2	D	201	TFP	C5-N1	2.51	1.44	1.40
2	N	201	TFP	C5-N1	2.50	1.44	1.40
2	E	202	TFP	C4-S	-2.48	1.72	1.76
2	A	201	TFP	C7-S	-2.43	1.72	1.76
2	B	202	TFP	C4-S	-2.38	1.72	1.76
2	R	202	TFP	C7-S	-2.35	1.72	1.76
2	G	202	TFP	C12-N1	2.25	1.44	1.40
2	Q	202	TFP	C4-S	-2.24	1.72	1.76
2	K	202	TFP	C4-S	-2.24	1.72	1.76
2	Q	202	TFP	C12-N1	2.21	1.44	1.40
2	A	202	TFP	C3-C2	2.17	1.42	1.38
2	P	201	TFP	C12-N1	2.16	1.44	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	202	TFP	C4-S	-2.15	1.72	1.76
2	H	201	TFP	C12-N1	2.11	1.43	1.40
2	M	202	TFP	C12-N1	2.09	1.43	1.40
2	K	201	TFP	C12-N1	2.09	1.43	1.40
2	E	202	TFP	C7-S	-2.07	1.72	1.76
2	B	201	TFP	C12-N1	2.06	1.43	1.40
2	P	201	TFP	C5-N1	2.04	1.43	1.40

All (368) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	201	TFP	C13-N1-C12	6.51	127.52	119.03
2	J	201	TFP	C13-N1-C12	-6.14	111.03	119.03
2	P	201	TFP	C13-N1-C5	-6.01	111.21	119.03
2	O	201	TFP	C6-C5-N1	-6.00	114.33	121.72
2	B	201	TFP	C13-N1-C5	5.98	126.82	119.03
2	I	201	TFP	C16-C17-N3	-5.90	104.13	110.80
2	R	202	TFP	C16-C17-N3	-5.70	104.37	110.80
2	A	201	TFP	C13-N1-C5	-5.54	111.81	119.03
2	J	201	TFP	C13-N1-C5	5.43	126.10	119.03
2	E	202	TFP	C13-N1-C5	-5.33	112.08	119.03
2	L	201	TFP	C13-N1-C5	-5.15	112.32	119.03
2	J	202	TFP	C13-N1-C5	-5.03	112.47	119.03
2	T	201	TFP	C16-C17-N3	-4.99	105.17	110.80
2	L	201	TFP	C13-N1-C12	4.97	125.50	119.03
2	T	202	TFP	C16-C17-N3	-4.88	105.29	110.80
2	C	201	TFP	C17-C16-N2	-4.80	100.80	110.64
2	T	202	TFP	C3-C4-C5	-4.74	114.26	119.91
2	O	201	TFP	C4-C5-N1	4.74	126.86	119.94
2	I	202	TFP	C13-N1-C5	-4.72	112.88	119.03
2	R	201	TFP	C16-C17-N3	-4.69	105.50	110.80
2	P	202	TFP	C13-N1-C5	-4.61	113.03	119.03
2	E	201	TFP	C6-C5-N1	-4.57	116.09	121.72
2	L	201	TFP	C6-C5-N1	-4.53	116.13	121.72
2	K	201	TFP	C6-C5-N1	-4.52	116.14	121.72
2	S	202	TFP	C13-N1-C5	-4.46	113.22	119.03
2	S	201	TFP	C13-N1-C5	4.42	124.79	119.03
2	I	201	TFP	C19-C18-N3	-4.34	105.90	110.80
2	O	202	TFP	C13-N1-C5	-4.24	113.50	119.03
2	Q	202	TFP	C13-N1-C5	-4.19	113.56	119.03
2	D	201	TFP	C13-N1-C12	-4.19	113.57	119.03
2	A	201	TFP	C19-C18-N3	-4.17	106.09	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	S	201	TFP	C19-C18-N3	-4.15	106.11	110.80
2	O	201	TFP	C13-N1-C5	-4.12	113.67	119.03
2	E	201	TFP	C4-C5-N1	4.08	125.90	119.94
2	T	202	TFP	C13-N1-C5	-4.06	113.75	119.03
2	L	202	TFP	C13-N1-C5	-4.02	113.80	119.03
2	C	201	TFP	C18-N3-C17	4.01	115.13	109.52
2	K	201	TFP	C13-N1-C5	-4.00	113.82	119.03
2	B	201	TFP	C13-N1-C12	-4.00	113.82	119.03
2	L	201	TFP	C4-C5-N1	3.97	125.73	119.94
2	E	201	TFP	C13-N1-C5	-3.95	113.89	119.03
2	H	201	TFP	C19-C18-N3	-3.90	106.39	110.80
2	A	201	TFP	C6-C5-N1	-3.90	116.91	121.72
2	L	202	TFP	C19-C18-N3	-3.90	106.40	110.80
2	T	202	TFP	C3-C4-S	3.88	126.45	118.47
2	T	202	TFP	C4-C5-N1	-3.87	114.29	119.94
2	F	202	TFP	C4-C5-N1	-3.86	114.30	119.94
2	J	201	TFP	C4-C5-N1	3.86	125.57	119.94
2	G	202	TFP	C11-C12-N1	3.85	126.80	121.77
2	P	201	TFP	C16-C17-N3	-3.82	106.49	110.80
2	S	201	TFP	C4-C5-N1	3.78	125.47	119.94
2	O	201	TFP	C6-C1-C21	-3.78	114.47	119.58
2	R	201	TFP	C13-N1-C12	-3.73	114.17	119.03
2	H	201	TFP	C16-C17-N3	-3.70	106.62	110.80
2	N	202	TFP	F1-C21-C1	-3.69	104.82	112.93
2	I	202	TFP	C16-C17-N3	-3.69	106.64	110.80
2	J	201	TFP	C19-C18-N3	-3.63	106.71	110.80
2	K	201	TFP	C13-N1-C12	3.63	123.75	119.03
2	B	202	TFP	C11-C12-N1	3.62	126.51	121.77
2	C	201	TFP	C18-C19-N2	-3.60	103.25	110.64
2	B	202	TFP	C6-C5-N1	3.60	126.15	121.72
2	E	201	TFP	C16-C17-N3	3.58	114.85	110.80
2	C	202	TFP	C16-C17-N3	-3.57	106.77	110.80
2	C	201	TFP	C13-N1-C5	-3.53	114.42	119.03
2	M	202	TFP	C3-C4-C5	-3.53	115.70	119.91
2	G	202	TFP	C16-C17-N3	-3.51	106.84	110.80
2	D	202	TFP	C4-C5-N1	-3.50	114.83	119.94
2	A	201	TFP	C16-C17-N3	-3.50	106.86	110.80
2	B	202	TFP	C4-C5-N1	-3.49	114.85	119.94
2	T	202	TFP	C6-C5-C4	3.48	122.85	118.99
2	I	201	TFP	C6-C5-N1	-3.48	117.43	121.72
2	R	202	TFP	C7-C12-N1	-3.43	114.93	119.94
2	K	202	TFP	C7-C12-N1	-3.43	114.93	119.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	O	201	TFP	C2-C1-C21	3.42	125.41	119.97
2	R	201	TFP	C11-C12-N1	-3.42	117.29	121.77
2	K	201	TFP	C4-C5-N1	3.41	124.92	119.94
2	A	202	TFP	C4-C5-N1	-3.36	115.03	119.94
2	T	201	TFP	C19-C18-N3	-3.35	107.02	110.80
2	L	202	TFP	C16-C17-N3	-3.34	107.03	110.80
2	A	202	TFP	C7-C12-N1	-3.33	115.08	119.94
2	I	202	TFP	C11-C12-N1	3.31	126.10	121.77
2	K	202	TFP	C4-C5-N1	-3.31	115.11	119.94
2	O	201	TFP	C13-N1-C12	3.31	123.33	119.03
2	M	202	TFP	C4-C5-N1	-3.30	115.11	119.94
2	D	201	TFP	C4-C5-N1	3.30	124.75	119.94
2	J	201	TFP	C12-N1-C5	-3.29	112.70	120.15
2	S	202	TFP	C11-C12-N1	3.29	126.07	121.77
2	H	202	TFP	F2-C21-C1	-3.27	105.75	112.93
2	E	201	TFP	C12-N1-C5	-3.26	112.77	120.15
2	E	202	TFP	C14-C13-N1	-3.25	102.84	112.99
2	A	202	TFP	C11-C12-N1	3.24	126.01	121.77
2	A	202	TFP	C19-C18-N3	-3.23	107.15	110.80
2	H	202	TFP	C16-C17-N3	-3.23	107.16	110.80
2	M	201	TFP	C13-N1-C12	-3.23	114.82	119.03
2	K	201	TFP	C12-N1-C5	-3.22	112.86	120.15
2	F	202	TFP	C11-C12-N1	3.22	125.98	121.77
2	D	202	TFP	C19-C18-N3	-3.22	107.17	110.80
2	K	202	TFP	F2-C21-C1	-3.21	105.87	112.93
2	B	202	TFP	C7-C12-N1	-3.14	115.36	119.94
2	J	201	TFP	C19-N2-C16	3.12	115.86	108.83
2	N	202	TFP	C13-N1-C5	-3.12	114.96	119.03
2	Q	201	TFP	C7-C12-N1	3.12	124.50	119.94
2	S	201	TFP	C11-C12-N1	-3.12	117.68	121.77
2	M	201	TFP	C4-C5-N1	3.12	124.49	119.94
2	L	201	TFP	C16-C17-N3	-3.10	107.30	110.80
2	T	201	TFP	C18-C19-N2	-3.09	104.30	110.64
2	K	201	TFP	C7-C12-N1	3.07	124.42	119.94
2	Q	201	TFP	C13-N1-C12	-3.06	115.04	119.03
2	P	202	TFP	F3-C21-F2	3.06	116.94	105.72
2	F	202	TFP	C7-C12-N1	-3.06	115.48	119.94
2	N	202	TFP	C7-C12-N1	-3.06	115.48	119.94
2	O	202	TFP	C16-C17-N3	-3.06	107.35	110.80
2	A	201	TFP	C14-C13-N1	3.04	122.46	112.99
2	G	202	TFP	F2-C21-C1	-3.03	106.26	112.93
2	C	202	TFP	C7-C12-N1	-3.03	115.52	119.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	201	TFP	C7-C12-N1	3.02	124.35	119.94
2	O	202	TFP	C7-C12-N1	-3.02	115.53	119.94
2	Q	202	TFP	C11-C12-N1	2.99	125.68	121.77
2	S	202	TFP	C4-C5-N1	-2.98	115.59	119.94
2	J	201	TFP	C11-C12-N1	-2.97	117.88	121.77
2	A	201	TFP	C4-C5-N1	2.94	124.23	119.94
2	D	202	TFP	C16-C17-N3	-2.93	107.49	110.80
2	S	201	TFP	C6-C5-N1	-2.93	118.10	121.72
2	L	202	TFP	C4-C5-N1	-2.92	115.68	119.94
2	J	201	TFP	C6-C5-N1	-2.92	118.12	121.72
2	A	202	TFP	C13-N1-C5	-2.91	115.23	119.03
2	P	202	TFP	C7-C12-N1	-2.91	115.69	119.94
2	O	201	TFP	C12-N1-C5	-2.90	113.59	120.15
2	F	202	TFP	C6-C5-N1	2.90	125.29	121.72
2	E	201	TFP	C19-C18-N3	-2.89	107.54	110.80
2	R	201	TFP	C15-N2-C16	-2.89	103.84	111.23
2	F	201	TFP	C19-C18-N3	-2.89	107.54	110.80
2	K	202	TFP	C3-C4-S	2.89	124.41	118.47
2	B	201	TFP	C12-N1-C5	-2.88	113.63	120.15
2	G	201	TFP	C19-C18-N3	-2.88	107.55	110.80
2	D	201	TFP	C6-C5-C4	-2.87	115.81	118.99
2	M	201	TFP	C12-N1-C5	-2.87	113.65	120.15
2	M	201	TFP	C7-C12-N1	2.87	124.13	119.94
2	P	201	TFP	F3-C21-C1	-2.87	106.63	112.93
2	S	201	TFP	C12-N1-C5	-2.85	113.70	120.15
2	R	202	TFP	F1-C21-C1	-2.84	106.69	112.93
2	B	201	TFP	C16-C17-N3	-2.84	107.60	110.80
2	G	202	TFP	C7-C12-N1	-2.83	115.80	119.94
2	A	201	TFP	C15-N2-C16	-2.83	103.99	111.23
2	C	201	TFP	C7-C12-N1	2.83	124.07	119.94
2	P	201	TFP	C12-N1-C5	-2.83	113.75	120.15
2	A	201	TFP	C15-C14-C13	-2.83	103.40	112.86
2	M	202	TFP	C14-C13-N1	-2.78	104.32	112.99
2	Q	201	TFP	F3-C21-C1	-2.78	106.83	112.93
2	D	201	TFP	F2-C21-C1	-2.77	106.84	112.93
2	I	202	TFP	C19-C18-N3	-2.77	107.67	110.80
2	R	201	TFP	C6-C5-N1	-2.76	118.32	121.72
2	A	202	TFP	F2-C21-C1	-2.76	106.87	112.93
2	N	201	TFP	C20-N3-C18	-2.75	106.55	110.66
2	K	201	TFP	C20-N3-C17	-2.75	106.55	110.66
2	G	201	TFP	C17-C16-N2	-2.75	105.01	110.64
2	N	202	TFP	C12-N1-C5	-2.73	113.97	120.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	202	TFP	C4-C5-N1	-2.73	115.96	119.94
2	M	201	TFP	C6-C5-N1	-2.73	118.36	121.72
2	F	201	TFP	C4-C5-N1	2.72	123.92	119.94
2	S	201	TFP	C14-C13-N1	2.72	121.48	112.99
2	M	201	TFP	C11-C12-N1	-2.72	118.21	121.77
2	F	201	TFP	C6-C5-N1	-2.72	118.37	121.72
2	A	202	TFP	C3-C4-S	2.71	124.05	118.47
2	F	202	TFP	C13-N1-C5	-2.71	115.50	119.03
2	L	201	TFP	C6-C1-C21	-2.71	115.92	119.58
2	T	202	TFP	C7-C12-N1	-2.71	115.99	119.94
2	S	201	TFP	C6-C5-C4	-2.69	116.01	118.99
2	D	201	TFP	C13-N1-C5	2.69	122.53	119.03
2	Q	202	TFP	C4-C5-N1	-2.69	116.02	119.94
2	N	202	TFP	C19-C18-N3	-2.68	107.78	110.80
2	P	201	TFP	C4-C5-N1	2.68	123.85	119.94
2	N	201	TFP	C7-C12-N1	2.68	123.85	119.94
2	O	201	TFP	F3-C21-C1	-2.68	107.05	112.93
2	J	201	TFP	C6-C5-C4	-2.66	116.04	118.99
2	P	201	TFP	C15-N2-C16	-2.66	104.44	111.23
2	D	201	TFP	C11-C12-N1	-2.66	118.28	121.77
2	R	201	TFP	C7-C12-N1	2.66	123.82	119.94
2	B	201	TFP	C11-C12-N1	-2.65	118.29	121.77
2	S	201	TFP	C14-C15-N2	-2.64	107.18	113.84
2	P	201	TFP	C15-C14-C13	-2.64	104.02	112.86
2	F	202	TFP	C3-C4-S	2.64	123.89	118.47
2	Q	202	TFP	C6-C5-N1	2.64	124.97	121.72
2	H	202	TFP	C7-C12-N1	-2.64	116.09	119.94
2	C	201	TFP	C15-C14-C13	-2.63	104.06	112.86
2	B	202	TFP	C19-N2-C16	2.62	114.72	108.83
2	O	201	TFP	C11-C12-N1	-2.61	118.34	121.77
2	N	202	TFP	C19-N2-C16	2.61	114.71	108.83
2	G	201	TFP	C4-C5-N1	2.60	123.74	119.94
2	P	202	TFP	C4-C5-N1	-2.60	116.14	119.94
2	M	201	TFP	F3-C21-C1	-2.60	107.22	112.93
2	R	201	TFP	C4-C5-N1	2.60	123.73	119.94
2	J	201	TFP	C20-N3-C18	-2.60	106.78	110.66
2	K	201	TFP	C18-N3-C17	2.60	113.15	109.52
2	B	202	TFP	C20-N3-C17	-2.60	106.78	110.66
2	T	202	TFP	F2-C21-C1	-2.58	107.25	112.93
2	H	201	TFP	C4-C5-N1	2.58	123.70	119.94
2	G	202	TFP	C3-C4-S	2.57	123.76	118.47
2	Q	202	TFP	F2-C21-C1	-2.57	107.28	112.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	202	TFP	C13-N1-C5	-2.57	115.69	119.03
2	K	202	TFP	C14-C13-N1	-2.56	105.01	112.99
2	E	201	TFP	C7-C12-N1	2.55	123.67	119.94
2	M	202	TFP	C7-C12-N1	-2.55	116.21	119.94
2	N	201	TFP	C15-N2-C19	-2.55	104.72	111.23
2	K	201	TFP	C11-C12-N1	-2.54	118.44	121.77
2	I	202	TFP	C7-C12-N1	-2.53	116.25	119.94
2	B	202	TFP	C19-C18-N3	2.52	113.66	110.80
2	A	201	TFP	C12-N1-C5	-2.52	114.44	120.15
2	I	201	TFP	C4-C5-N1	2.52	123.61	119.94
2	L	201	TFP	C11-C12-N1	-2.51	118.47	121.77
2	C	201	TFP	C4-C5-N1	2.51	123.60	119.94
2	N	202	TFP	C16-C17-N3	-2.50	107.98	110.80
2	K	202	TFP	C11-C12-N1	2.50	125.04	121.77
2	T	201	TFP	C7-C12-N1	2.50	123.59	119.94
2	P	202	TFP	C16-C17-N3	-2.50	107.98	110.80
2	O	202	TFP	C11-C12-N1	2.50	125.03	121.77
2	H	201	TFP	C6-C5-C4	-2.47	116.25	118.99
2	A	202	TFP	C14-C15-N2	-2.47	107.61	113.84
2	K	201	TFP	C20-N3-C18	-2.47	106.96	110.66
2	P	201	TFP	C6-C5-N1	-2.47	118.67	121.72
2	F	201	TFP	C13-N1-C5	-2.46	115.82	119.03
2	B	201	TFP	F3-C21-C1	-2.46	107.52	112.93
2	M	202	TFP	C11-C12-N1	2.46	124.99	121.77
2	L	201	TFP	C14-C13-N1	2.46	120.65	112.99
2	F	201	TFP	C7-C12-N1	2.45	123.52	119.94
2	C	201	TFP	C19-C18-N3	2.45	113.58	110.80
2	L	202	TFP	C3-C4-S	2.45	123.50	118.47
2	L	201	TFP	C19-C18-N3	-2.45	108.04	110.80
2	P	202	TFP	F2-C21-C1	-2.45	107.56	112.93
2	S	202	TFP	F2-C21-C1	-2.44	107.56	112.93
2	B	202	TFP	C3-C4-S	2.44	123.48	118.47
2	N	202	TFP	C4-C5-N1	-2.44	116.38	119.94
2	G	201	TFP	C6-C5-N1	-2.43	118.72	121.72
2	P	201	TFP	C14-C13-N1	2.43	120.58	112.99
2	D	201	TFP	C19-C18-N3	-2.43	108.06	110.80
2	D	201	TFP	C12-N1-C5	-2.43	114.66	120.15
2	L	202	TFP	C7-C12-N1	-2.43	116.40	119.94
2	D	201	TFP	C7-C12-N1	2.42	123.48	119.94
2	T	202	TFP	C11-C12-N1	2.42	124.94	121.77
2	T	201	TFP	C4-C5-N1	2.40	123.44	119.94
2	R	202	TFP	C18-N3-C17	2.40	112.88	109.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	202	TFP	C17-C16-N2	-2.39	105.73	110.64
2	E	202	TFP	C4-C5-N1	-2.39	116.45	119.94
2	F	201	TFP	C11-C12-N1	-2.39	118.64	121.77
2	L	201	TFP	C15-N2-C19	-2.39	105.14	111.23
2	L	202	TFP	C18-C19-N2	-2.38	105.75	110.64
2	J	202	TFP	C7-C12-N1	-2.38	116.47	119.94
2	M	201	TFP	C2-C1-C6	2.37	122.34	117.76
2	G	201	TFP	C7-C12-N1	2.37	123.40	119.94
2	B	201	TFP	C4-C5-N1	2.37	123.40	119.94
2	O	201	TFP	C7-C12-N1	2.35	123.38	119.94
2	G	202	TFP	C14-C15-N2	-2.35	107.91	113.84
2	A	201	TFP	C11-C12-N1	-2.35	118.69	121.77
2	T	202	TFP	F3-C21-C1	2.34	118.06	112.93
2	N	202	TFP	C11-C12-N1	2.34	124.82	121.77
2	Q	201	TFP	C11-C12-N1	-2.34	118.71	121.77
2	C	201	TFP	C11-C12-C7	-2.33	115.38	118.65
2	H	201	TFP	C7-C12-N1	2.33	123.34	119.94
2	K	201	TFP	C10-C11-C12	2.33	123.15	118.26
2	R	201	TFP	C19-N2-C16	2.33	114.07	108.83
2	C	201	TFP	F3-C21-C1	-2.33	107.82	112.93
2	D	201	TFP	C14-C13-N1	2.32	120.24	112.99
2	P	202	TFP	C11-C12-N1	2.32	124.80	121.77
2	T	201	TFP	C6-C5-N1	-2.32	118.86	121.72
2	S	202	TFP	C7-C12-N1	-2.32	116.56	119.94
2	G	202	TFP	C5-C4-S	-2.31	116.61	120.30
2	G	202	TFP	C2-C1-C6	2.31	122.21	117.76
2	T	202	TFP	C18-C19-N2	-2.30	105.92	110.64
2	S	202	TFP	C12-C7-S	-2.30	116.62	120.30
2	J	201	TFP	C8-C7-C12	-2.30	117.17	119.91
2	E	202	TFP	C3-C4-S	2.30	123.19	118.47
2	S	202	TFP	F1-C21-C1	-2.29	107.89	112.93
2	D	201	TFP	C14-C15-N2	-2.29	108.06	113.84
2	G	201	TFP	C15-C14-C13	-2.29	105.19	112.86
2	D	202	TFP	C6-C5-N1	2.29	124.54	121.72
2	C	201	TFP	C15-N2-C16	2.28	117.07	111.23
2	M	202	TFP	C3-C4-S	2.27	123.14	118.47
2	E	201	TFP	C11-C12-N1	-2.27	118.80	121.77
2	C	202	TFP	C4-C5-N1	-2.26	116.64	119.94
2	R	202	TFP	C4-C5-N1	-2.26	116.64	119.94
2	L	201	TFP	C2-C1-C21	2.26	123.55	119.97
2	K	202	TFP	C3-C4-C5	-2.26	117.22	119.91
2	F	201	TFP	C17-C16-N2	-2.26	106.02	110.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	202	TFP	C18-C19-N2	-2.25	106.02	110.64
2	O	202	TFP	C14-C13-N1	-2.24	105.99	112.99
2	M	202	TFP	C13-N1-C5	-2.24	116.12	119.03
2	I	202	TFP	C12-N1-C5	-2.23	115.10	120.15
2	A	201	TFP	C17-C16-N2	-2.23	106.07	110.64
2	A	202	TFP	C6-C5-C4	2.23	121.46	118.99
2	N	201	TFP	C11-C12-N1	-2.23	118.85	121.77
2	C	202	TFP	C11-C12-N1	2.23	124.68	121.77
2	G	201	TFP	C16-C17-N3	-2.22	108.29	110.80
2	I	201	TFP	C14-C15-N2	-2.22	108.24	113.84
2	A	202	TFP	C3-C4-C5	-2.21	117.27	119.91
2	J	201	TFP	C7-C12-N1	2.21	123.17	119.94
2	P	201	TFP	C19-C18-N3	-2.21	108.31	110.80
2	L	201	TFP	C14-C15-N2	-2.20	108.29	113.84
2	E	201	TFP	C18-N3-C17	2.19	112.59	109.52
2	E	202	TFP	C7-C12-N1	-2.19	116.74	119.94
2	T	202	TFP	F3-C21-F1	-2.19	97.69	105.72
2	R	201	TFP	C12-N1-C5	-2.18	115.22	120.15
2	A	201	TFP	C7-C12-N1	2.18	123.12	119.94
2	I	201	TFP	F2-C21-C1	-2.18	108.15	112.93
2	B	202	TFP	C18-N3-C17	2.18	112.56	109.52
2	G	202	TFP	F1-C21-C1	-2.18	108.15	112.93
2	G	201	TFP	C11-C12-N1	-2.17	118.92	121.77
2	D	201	TFP	C2-C1-C6	2.17	121.94	117.76
2	C	202	TFP	C6-C5-N1	2.17	124.39	121.72
2	C	201	TFP	C12-N1-C5	-2.17	115.25	120.15
2	H	201	TFP	C12-N1-C5	-2.16	115.25	120.15
2	C	202	TFP	C13-N1-C5	-2.16	116.22	119.03
2	K	201	TFP	C15-N2-C16	-2.16	105.72	111.23
2	D	201	TFP	C6-C5-N1	-2.15	119.07	121.72
2	N	201	TFP	C10-C11-C12	2.15	122.76	118.26
2	P	202	TFP	C5-C6-C1	-2.14	117.48	120.57
2	B	202	TFP	C14-C13-N1	-2.14	106.32	112.99
2	H	201	TFP	C14-C13-N1	2.13	119.63	112.99
2	B	201	TFP	C6-C5-C4	-2.13	116.63	118.99
2	G	201	TFP	C18-N3-C17	2.13	112.50	109.52
2	L	202	TFP	C20-N3-C18	-2.12	107.48	110.66
2	H	201	TFP	C17-C16-N2	-2.12	106.29	110.64
2	Q	202	TFP	C6-C1-C21	2.12	122.44	119.58
2	J	201	TFP	C6-C1-C21	-2.12	116.72	119.58
2	S	202	TFP	C8-C7-C12	2.12	122.43	119.91
2	G	202	TFP	C6-C5-N1	2.12	124.33	121.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	201	TFP	C14-C15-N2	-2.11	108.52	113.84
2	H	202	TFP	C2-C1-C6	2.11	121.83	117.76
2	S	202	TFP	C2-C1-C6	2.11	121.82	117.76
2	N	201	TFP	C19-C18-N3	-2.11	108.42	110.80
2	I	202	TFP	C19-N2-C16	2.10	113.56	108.83
2	S	201	TFP	C7-C12-N1	2.10	123.01	119.94
2	J	201	TFP	C14-C15-N2	-2.10	108.55	113.84
2	Q	201	TFP	C6-C1-C21	2.10	122.41	119.58
2	F	201	TFP	C12-N1-C5	-2.09	115.41	120.15
2	Q	202	TFP	C19-C18-N3	-2.09	108.44	110.80
2	D	201	TFP	C8-C7-C12	-2.09	117.42	119.91
2	P	201	TFP	C19-N2-C16	2.09	113.52	108.83
2	O	201	TFP	C12-C7-S	2.09	123.64	120.30
2	L	202	TFP	C20-N3-C17	2.08	113.78	110.66
2	L	201	TFP	C12-N1-C5	-2.08	115.44	120.15
2	S	201	TFP	C19-N2-C16	2.08	113.51	108.83
2	P	201	TFP	C15-N2-C19	-2.08	105.92	111.23
2	Q	202	TFP	C12-N1-C5	-2.08	115.45	120.15
2	Q	202	TFP	C3-C4-S	2.08	122.74	118.47
2	C	201	TFP	C13-N1-C12	2.08	121.73	119.03
2	I	201	TFP	C13-N1-C5	2.07	121.73	119.03
2	C	202	TFP	F1-C21-C1	-2.07	108.38	112.93
2	J	202	TFP	C3-C2-C1	2.07	123.98	121.22
2	P	201	TFP	C7-C12-N1	2.07	122.96	119.94
2	Q	202	TFP	C14-C13-N1	-2.07	106.53	112.99
2	P	202	TFP	C2-C3-C4	-2.06	116.52	120.01
2	S	202	TFP	C3-C4-S	2.06	122.71	118.47
2	J	202	TFP	C4-C5-N1	-2.06	116.94	119.94
2	M	201	TFP	F1-C21-C1	-2.05	108.43	112.93
2	F	202	TFP	C8-C7-S	2.05	122.68	118.47
2	N	201	TFP	C6-C1-C21	2.05	122.34	119.58
2	R	202	TFP	C2-C1-C6	2.04	121.70	117.76
2	K	202	TFP	C6-C5-C4	2.04	121.26	118.99
2	C	202	TFP	C19-C18-N3	-2.04	108.50	110.80
2	M	202	TFP	C13-N1-C12	2.04	121.68	119.03
2	R	201	TFP	C14-C15-N2	-2.03	108.73	113.84
2	L	202	TFP	C11-C12-N1	2.03	124.42	121.77
2	J	202	TFP	C14-C15-N2	-2.02	108.74	113.84
2	A	201	TFP	C20-N3-C17	-2.02	107.65	110.66
2	E	201	TFP	C6-C1-C21	-2.02	116.86	119.58
2	O	201	TFP	C16-C17-N3	-2.01	108.53	110.80
2	B	202	TFP	C17-C16-N2	-2.01	106.52	110.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	O	201	TFP	C14-C15-N2	-2.00	108.79	113.84

There are no chirality outliers.

All (72) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	201	TFP	C14-C13-N1-C12
2	E	201	TFP	C14-C13-N1-C12
2	K	201	TFP	C14-C13-N1-C12
2	L	201	TFP	C14-C13-N1-C12
2	O	201	TFP	C14-C13-N1-C12
2	P	201	TFP	C14-C13-N1-C12
2	C	201	TFP	C14-C15-N2-C16
2	B	201	TFP	C14-C13-N1-C5
2	C	201	TFP	C14-C13-N1-C12
2	T	201	TFP	C14-C15-N2-C19
2	G	201	TFP	N1-C13-C14-C15
2	K	201	TFP	C13-C14-C15-N2
2	F	201	TFP	C14-C15-N2-C16
2	G	201	TFP	C14-C15-N2-C16
2	F	201	TFP	C14-C13-N1-C12
2	J	201	TFP	C14-C13-N1-C5
2	N	201	TFP	C14-C13-N1-C12
2	A	201	TFP	C13-C14-C15-N2
2	C	201	TFP	N1-C13-C14-C15
2	P	201	TFP	C13-C14-C15-N2
2	E	201	TFP	C13-C14-C15-N2
2	G	201	TFP	C14-C13-N1-C12
2	H	201	TFP	C14-C13-N1-C12
2	J	201	TFP	C13-C14-C15-N2
2	S	202	TFP	N1-C13-C14-C15
2	T	201	TFP	N1-C13-C14-C15
2	B	201	TFP	C13-C14-C15-N2
2	L	201	TFP	C13-C14-C15-N2
2	R	201	TFP	C13-C14-C15-N2
2	A	201	TFP	C14-C15-N2-C19
2	L	201	TFP	C14-C15-N2-C19
2	F	201	TFP	N1-C13-C14-C15
2	O	201	TFP	C13-C14-C15-N2
2	A	201	TFP	C14-C15-N2-C16
2	B	201	TFP	C14-C15-N2-C19
2	C	201	TFP	C14-C15-N2-C19

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Mol	Chain	Res	Type	Atoms
2	L	201	TFP	C14-C15-N2-C16
2	B	201	TFP	C14-C15-N2-C16
2	G	201	TFP	C14-C15-N2-C19
2	O	201	TFP	C14-C15-N2-C16
2	P	201	TFP	N1-C13-C14-C15
2	O	201	TFP	C14-C15-N2-C19
2	S	201	TFP	C14-C15-N2-C16
2	M	201	TFP	N1-C13-C14-C15
2	S	201	TFP	C14-C15-N2-C19
2	J	201	TFP	N1-C13-C14-C15
2	Q	201	TFP	N1-C13-C14-C15
2	S	202	TFP	C13-C14-C15-N2
2	M	201	TFP	C13-C14-C15-N2
2	P	202	TFP	N1-C13-C14-C15
2	O	202	TFP	N1-C13-C14-C15
2	K	201	TFP	C14-C15-N2-C16
2	E	201	TFP	N1-C13-C14-C15
2	I	201	TFP	N1-C13-C14-C15
2	D	201	TFP	C14-C13-N1-C5
2	N	201	TFP	C13-C14-C15-N2
2	Q	201	TFP	C13-C14-C15-N2
2	R	201	TFP	N1-C13-C14-C15
2	O	202	TFP	C14-C15-N2-C19
2	G	201	TFP	C13-C14-C15-N2
2	J	202	TFP	N1-C13-C14-C15
2	K	201	TFP	C14-C15-N2-C19
2	B	201	TFP	C14-C13-N1-C12
2	O	201	TFP	C14-C13-N1-C5
2	N	201	TFP	C14-C13-N1-C5
2	S	202	TFP	C14-C13-N1-C12
2	K	201	TFP	C14-C13-N1-C5
2	R	201	TFP	C14-C13-N1-C5
2	E	201	TFP	C14-C13-N1-C5
2	D	202	TFP	C14-C13-N1-C12
2	H	201	TFP	C14-C13-N1-C5
2	L	202	TFP	C13-C14-C15-N2

There are no ring outliers.

16 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	201	TFP	2	0

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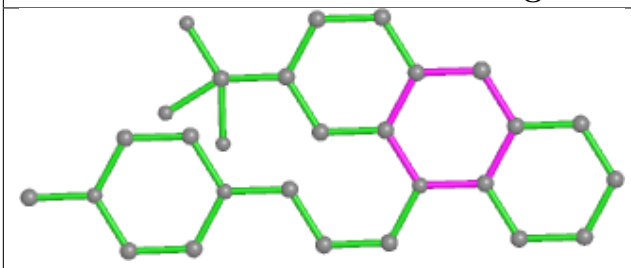
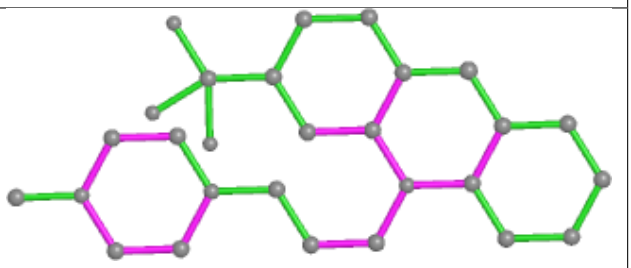
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	P	201	TFP	1	0
2	R	202	TFP	1	0
2	L	201	TFP	1	0
2	N	202	TFP	1	0
2	M	201	TFP	2	0
2	P	202	TFP	1	0
2	O	202	TFP	1	0
2	M	202	TFP	1	0
2	G	201	TFP	2	0
2	B	201	TFP	4	0
2	N	201	TFP	1	0
2	S	201	TFP	1	0
2	F	201	TFP	2	0
2	Q	201	TFP	1	0
2	S	202	TFP	1	0

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 then 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.

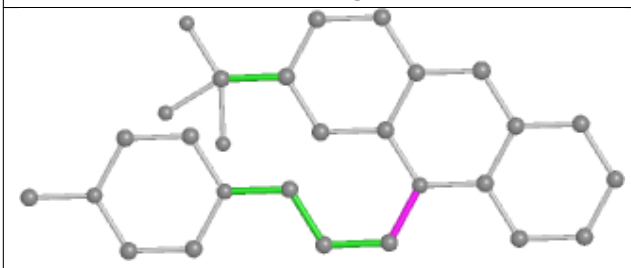
Ligand TFP H 201



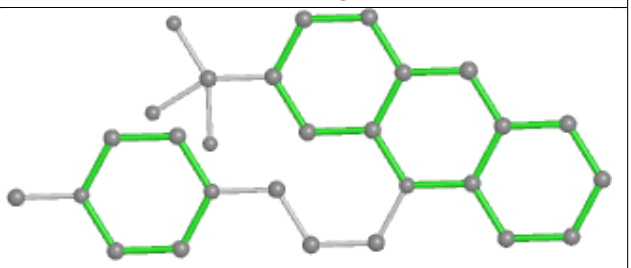
Bond lengths



Bond angles

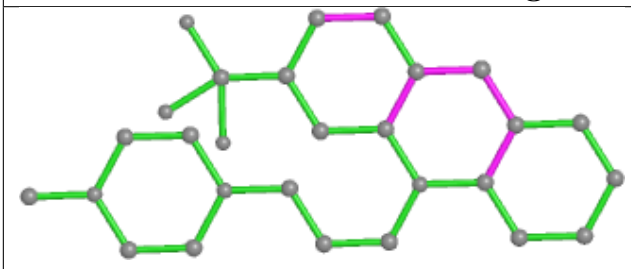


Torsions

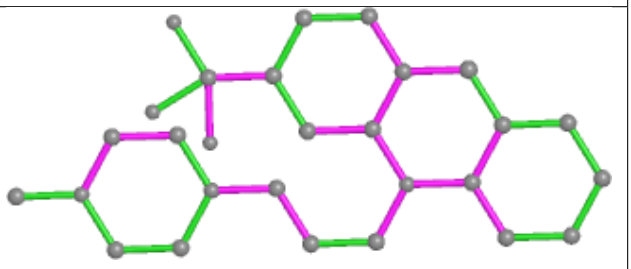


Rings

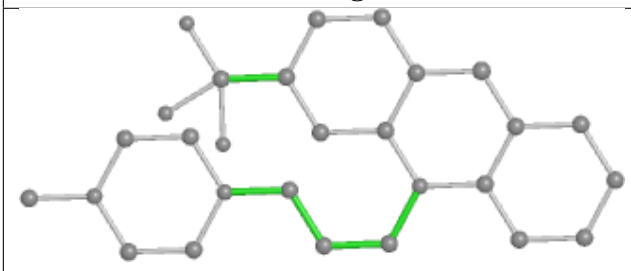
Ligand TFP A 202



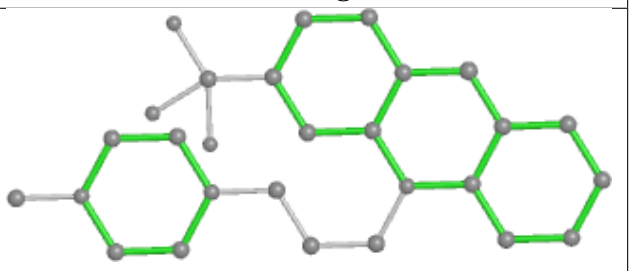
Bond lengths



Bond angles

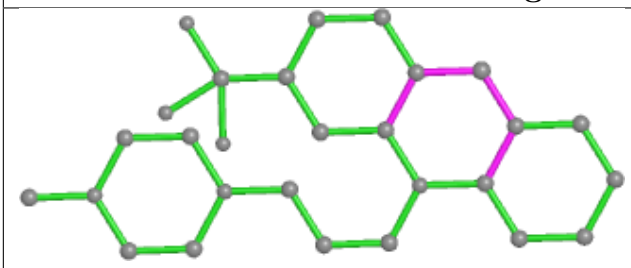


Torsions

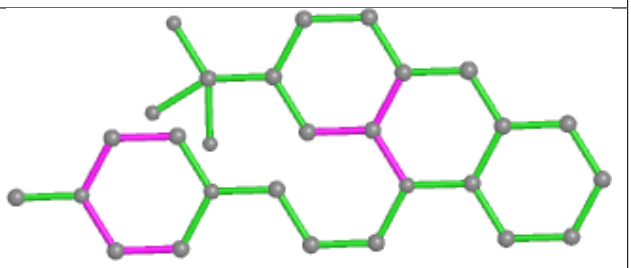


Rings

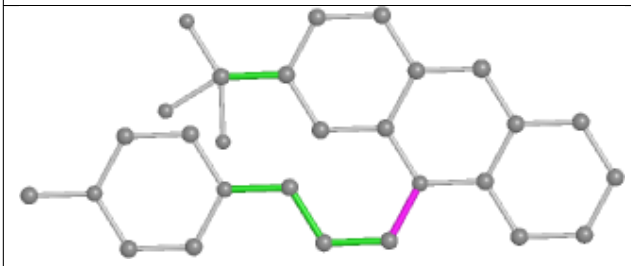
Ligand TFP D 202



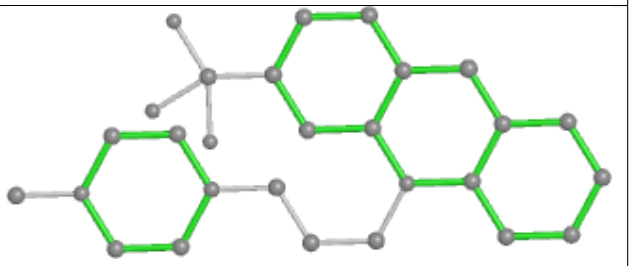
Bond lengths



Bond angles

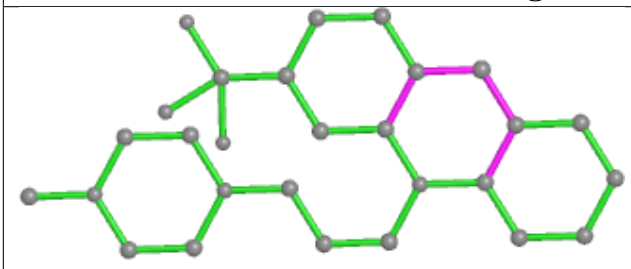


Torsions

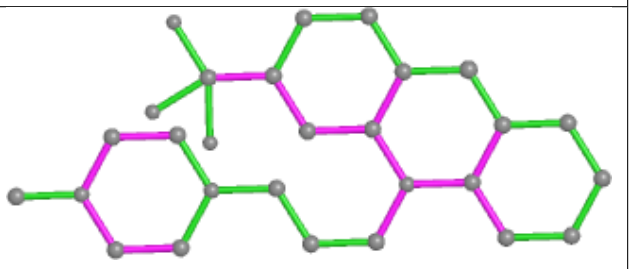


Rings

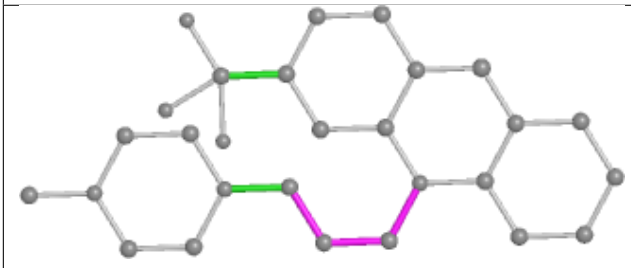
Ligand TFP E 201



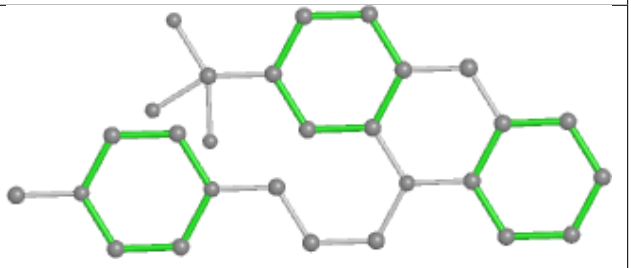
Bond lengths



Bond angles

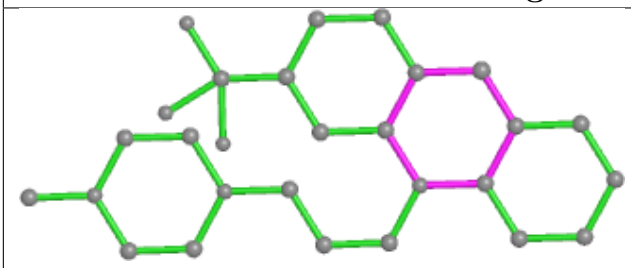


Torsions

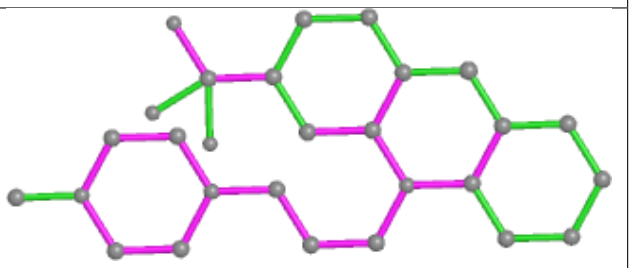


Rings

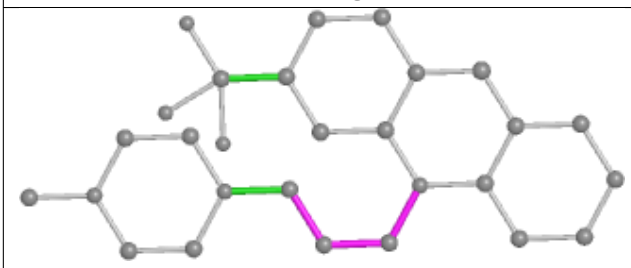
Ligand TFP P 201



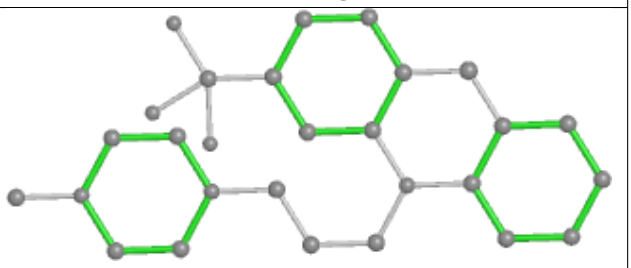
Bond lengths



Bond angles

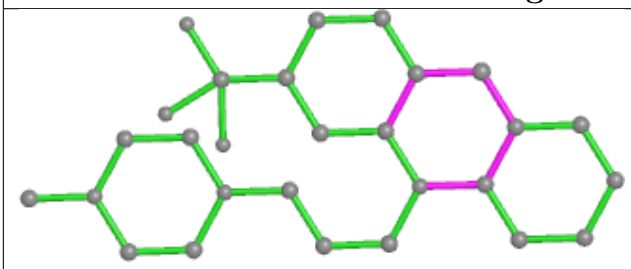


Torsions



Rings

Ligand TFP T 201



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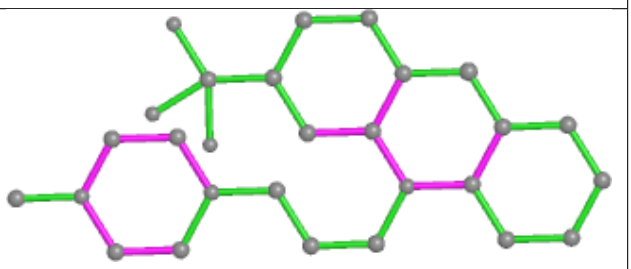

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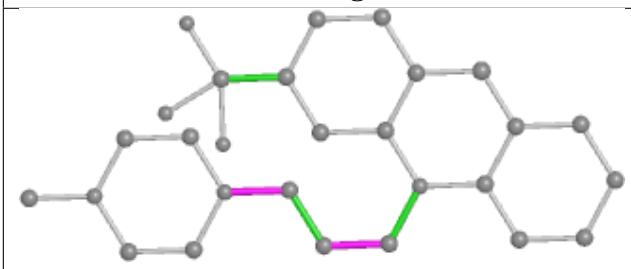
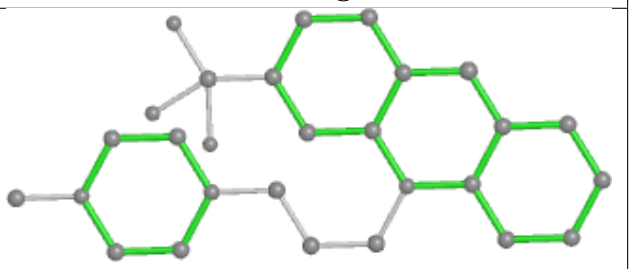
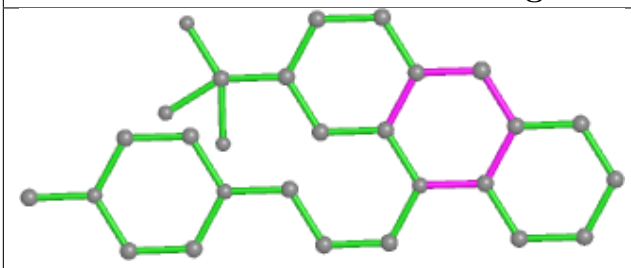


Torsions



Rings

Ligand TFP C 201



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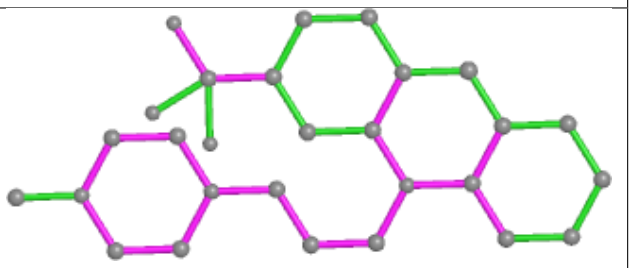

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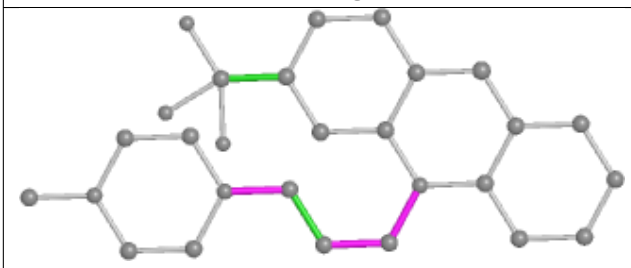

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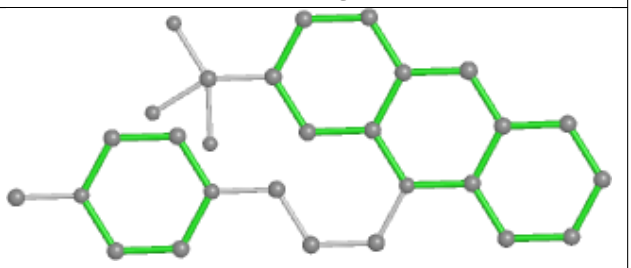

Rings

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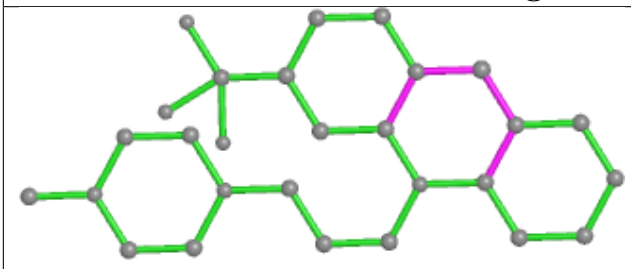

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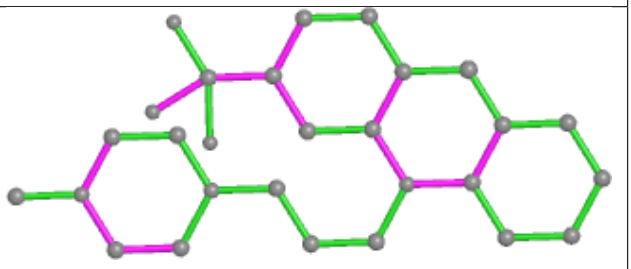

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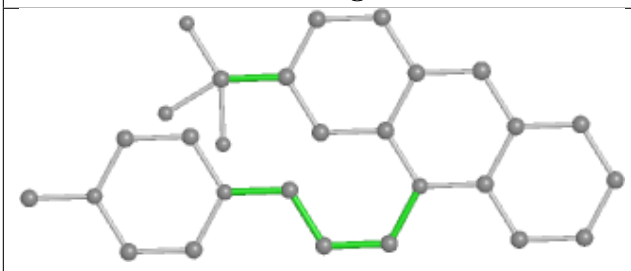

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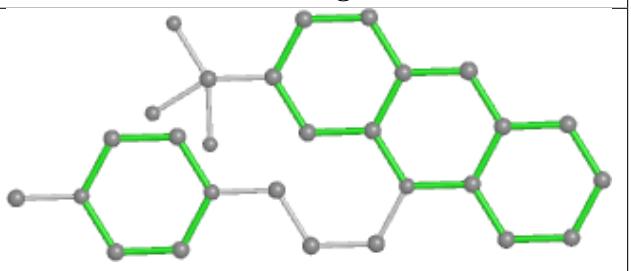

Rings

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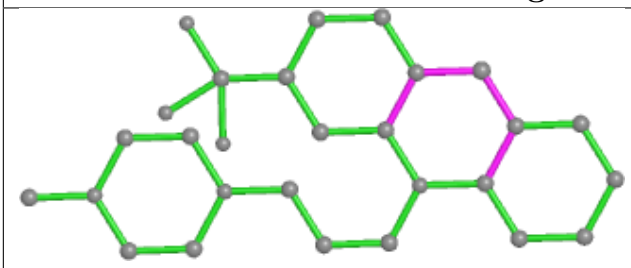

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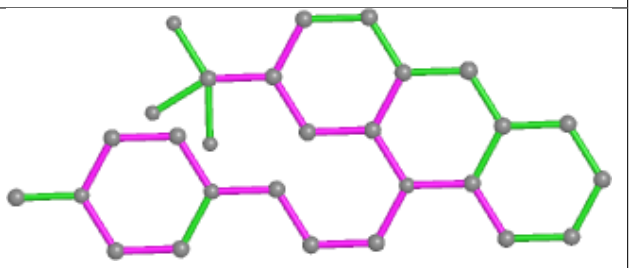

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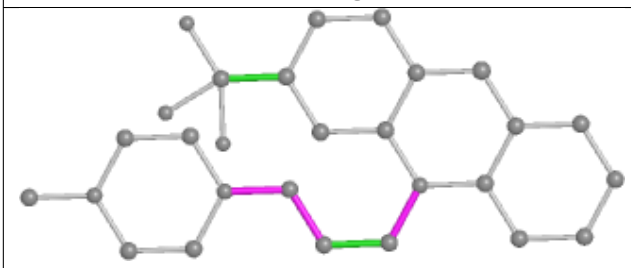

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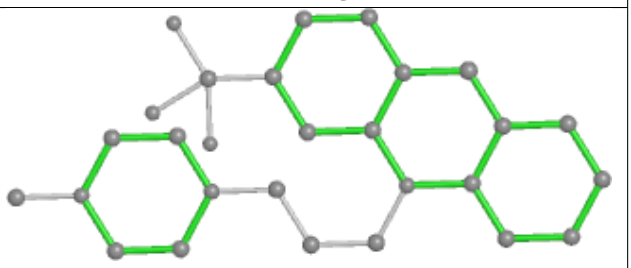

Rings

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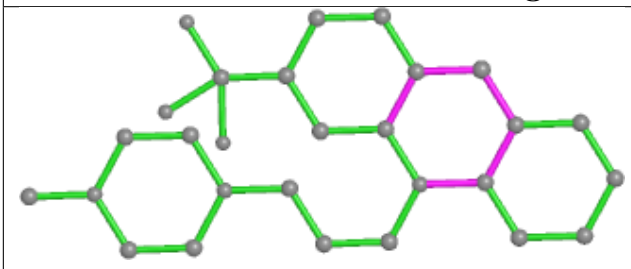

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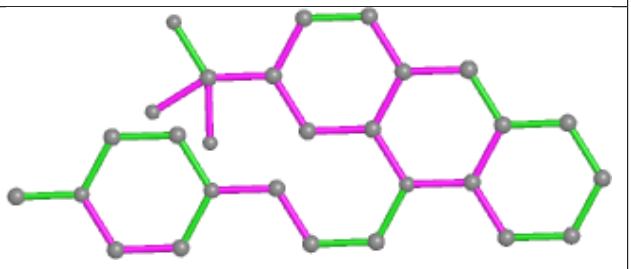

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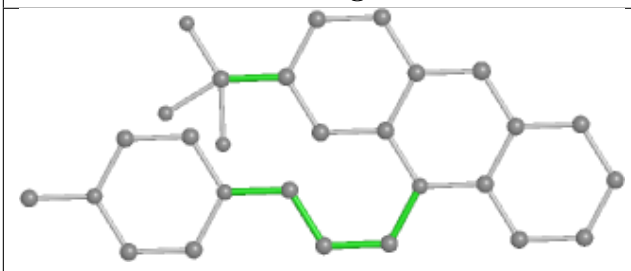

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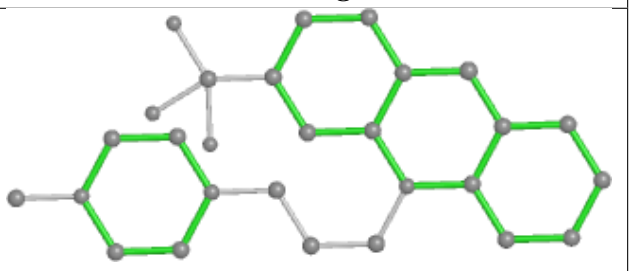

Rings

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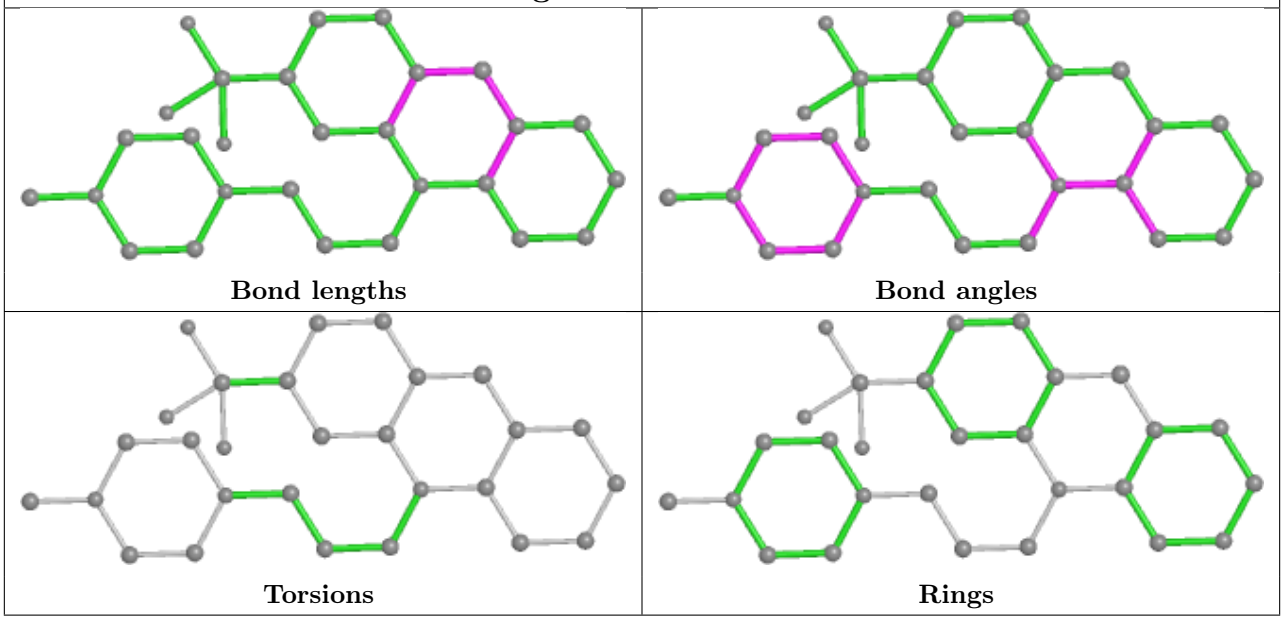

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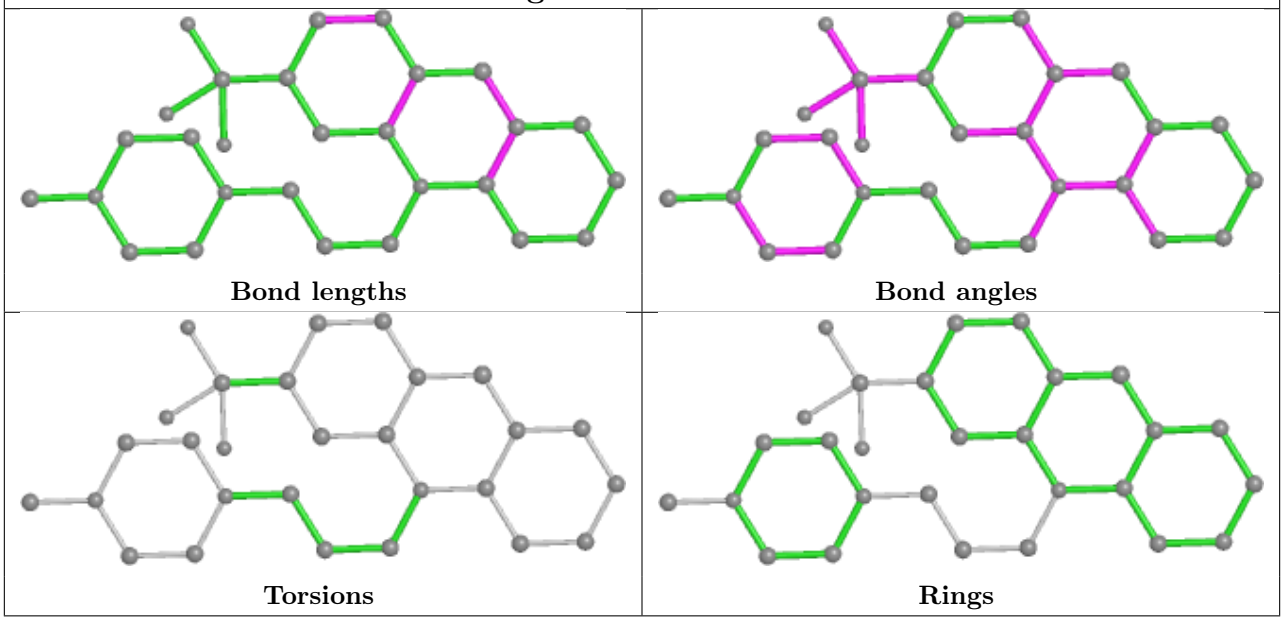

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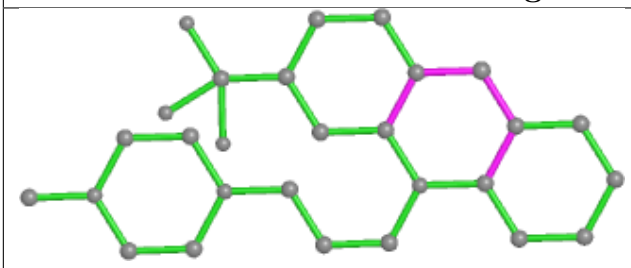

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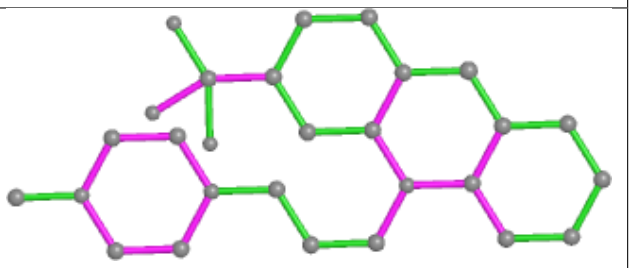

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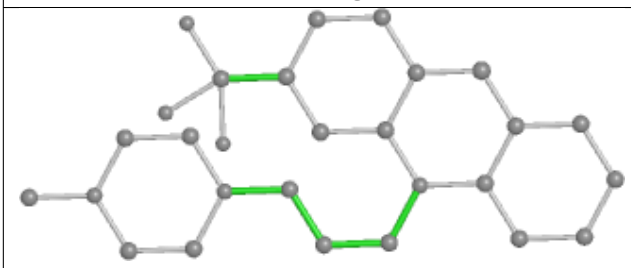

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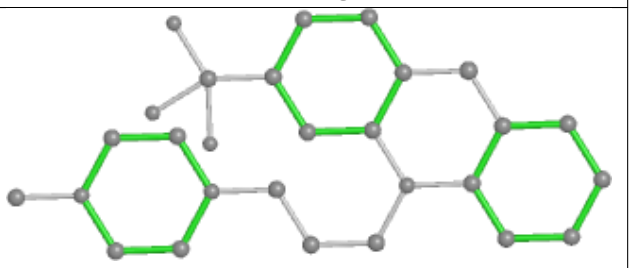

Rings

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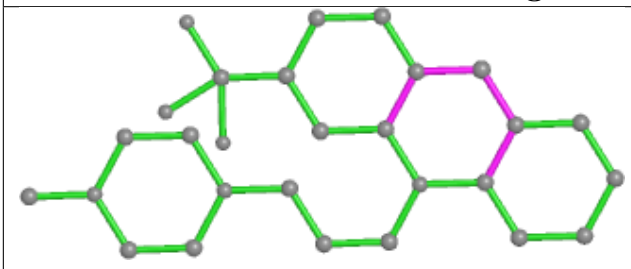

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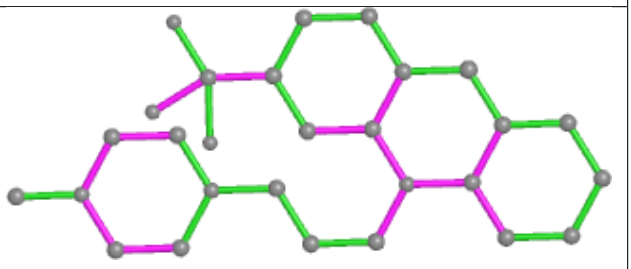

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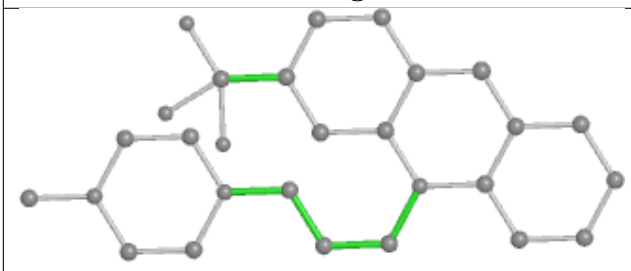

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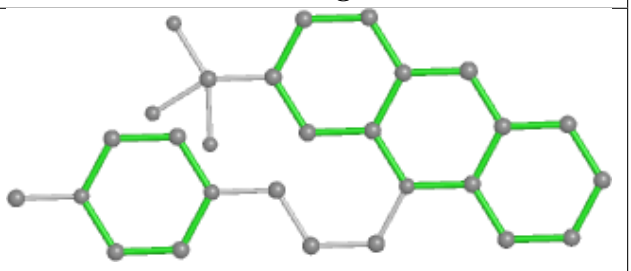

Rings

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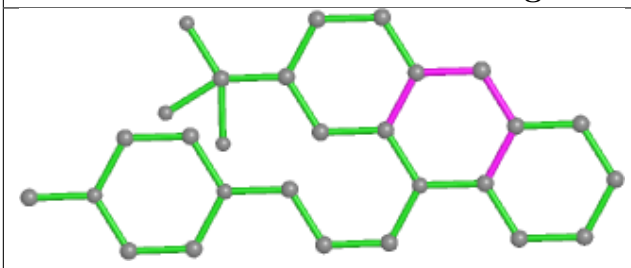

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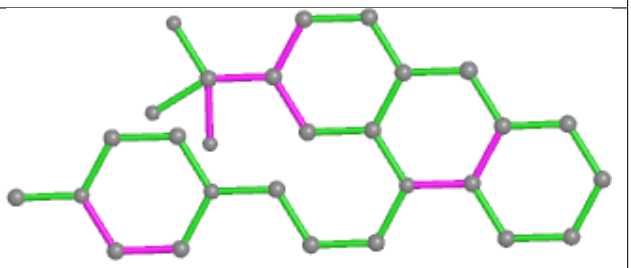

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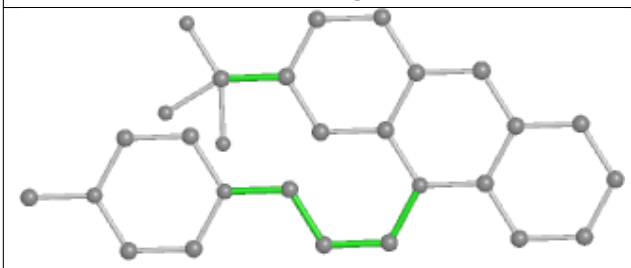

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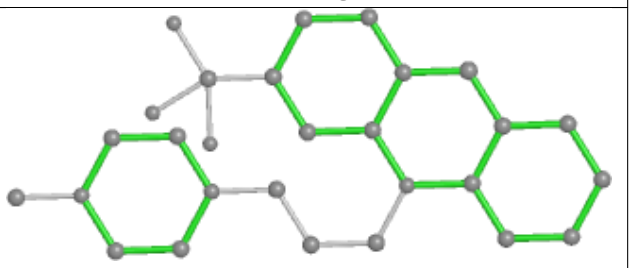

Rings

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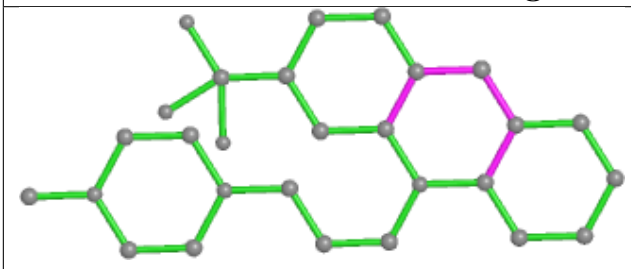

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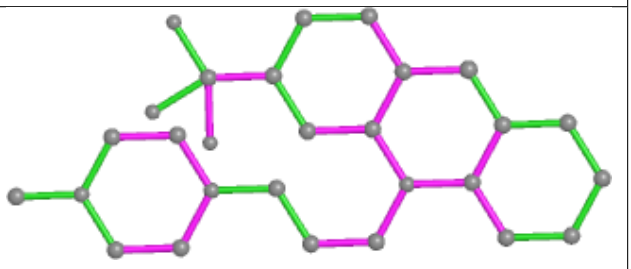

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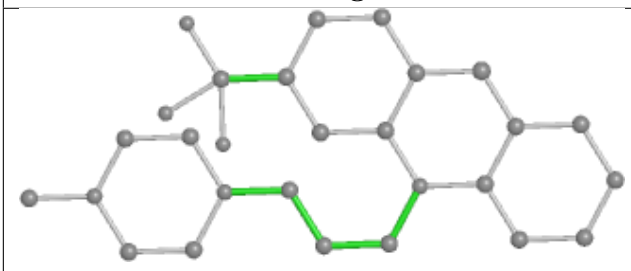

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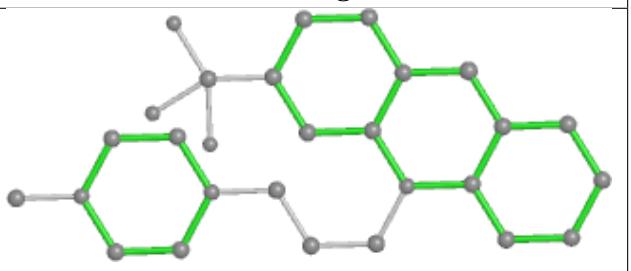

Rings

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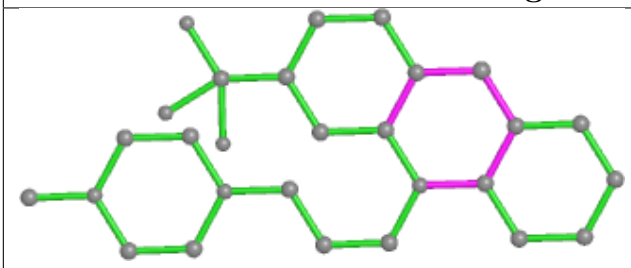

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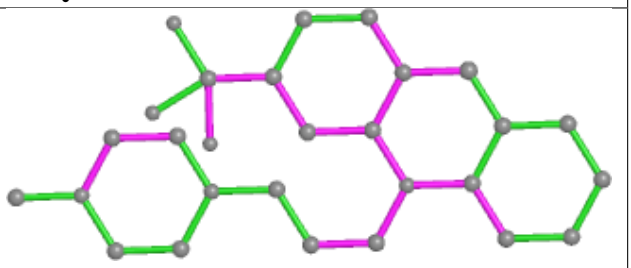

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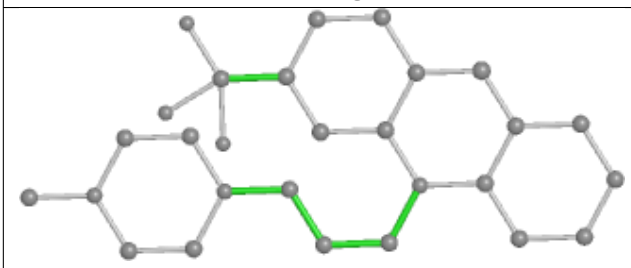

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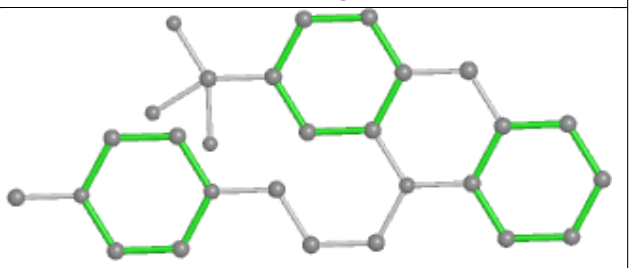
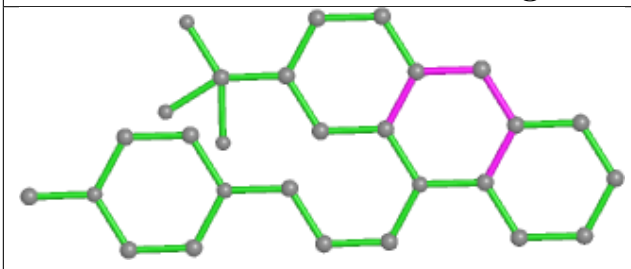


Rings

Ligand TFP M 201



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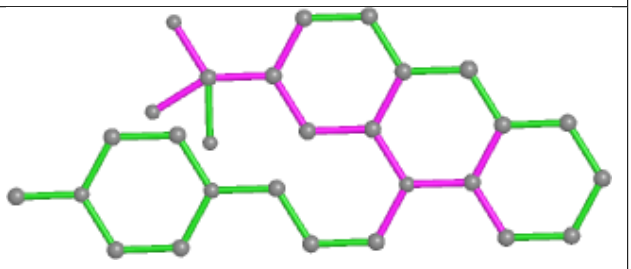

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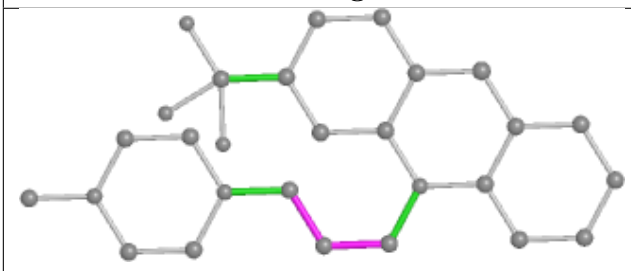

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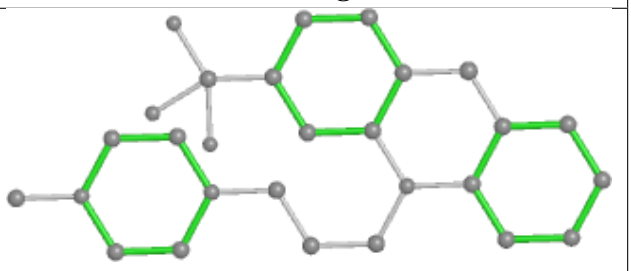

Rings

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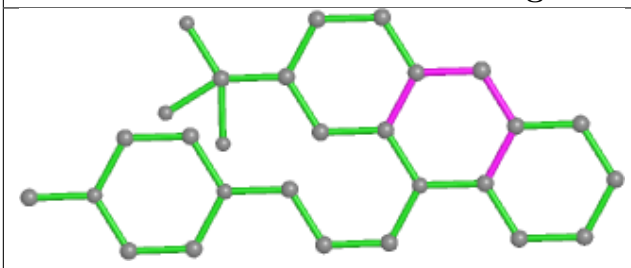

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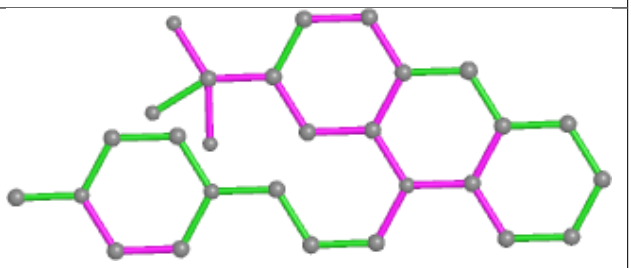
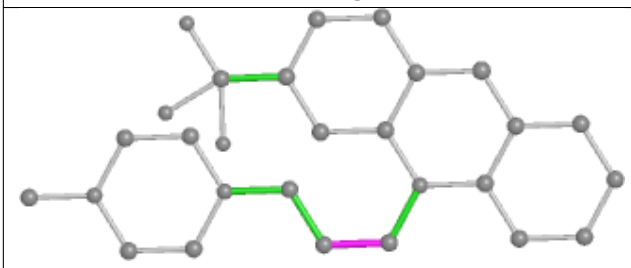


Bond angles



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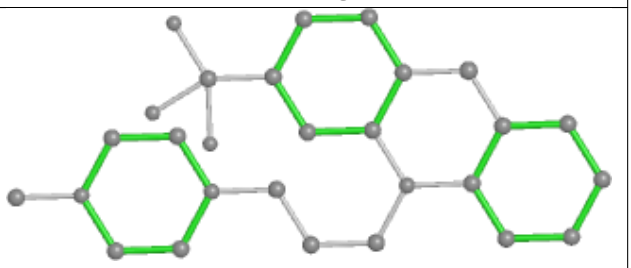

Rings

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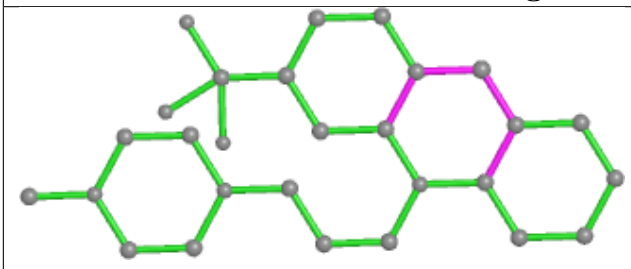

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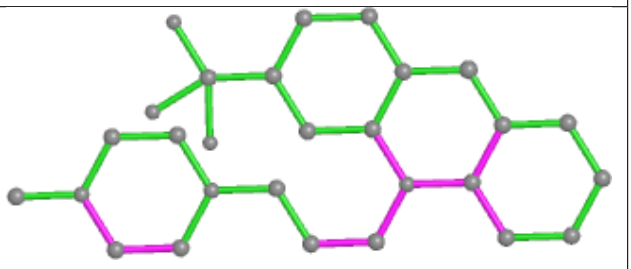

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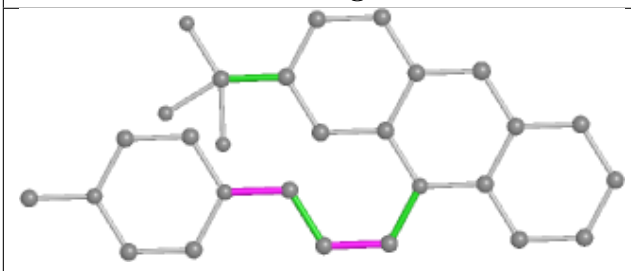

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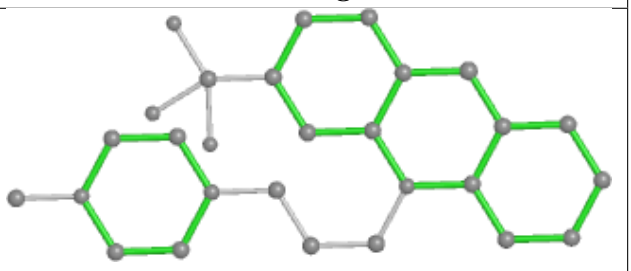
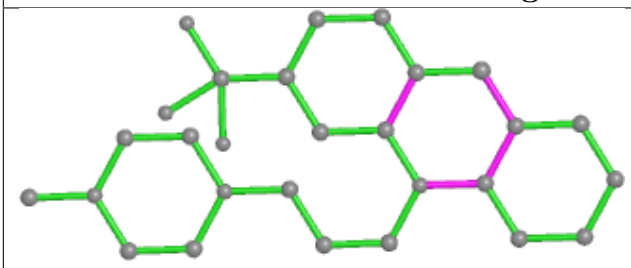


Rings

Ligand TFP M 202



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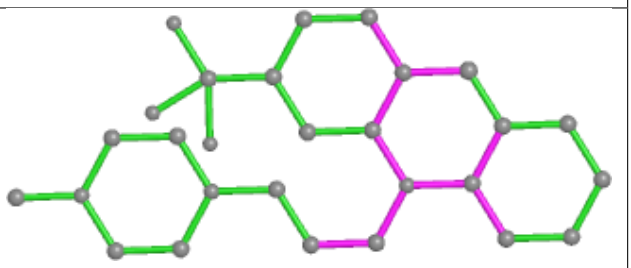
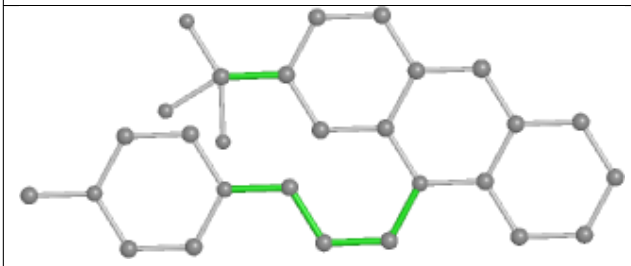


Bond angles



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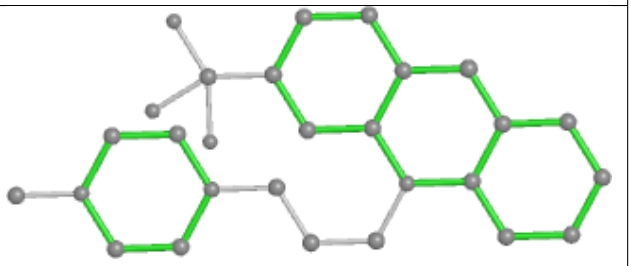
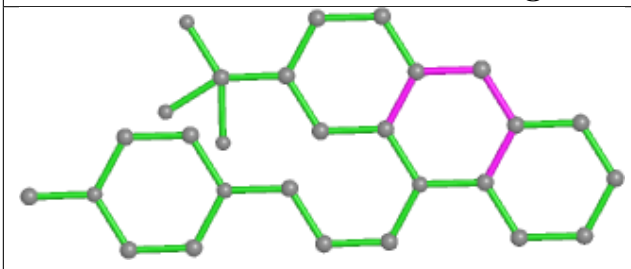
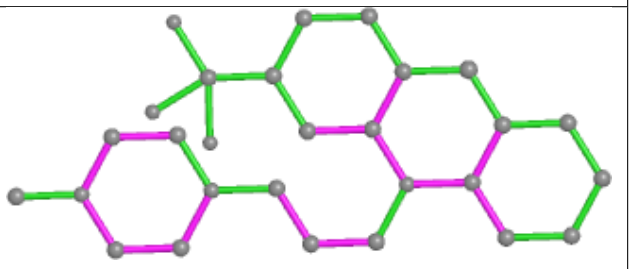


Rings

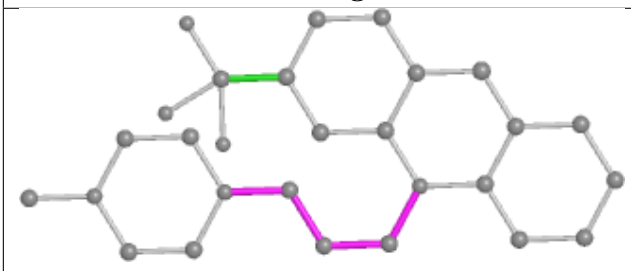
Ligand TFP G 201



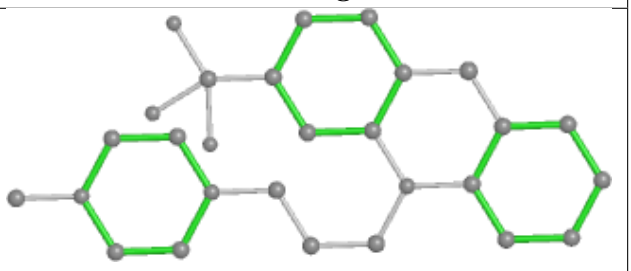
Bond lengths



Bond angles

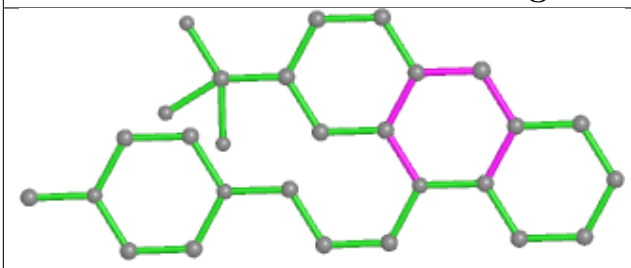


Torsions



Rings

Ligand TFP J 201



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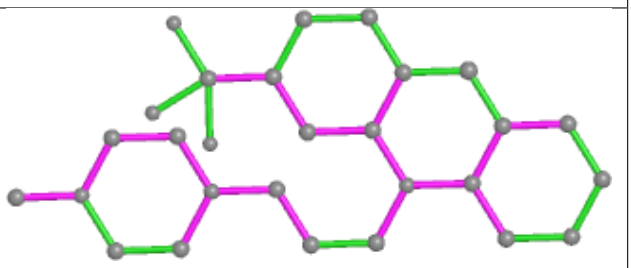

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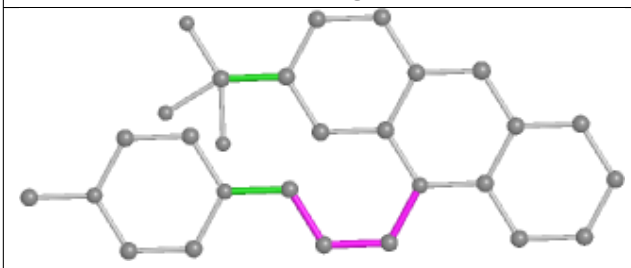

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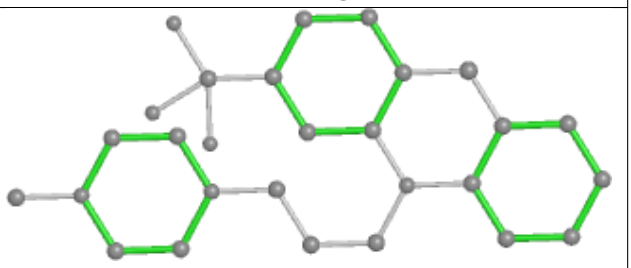

Rings

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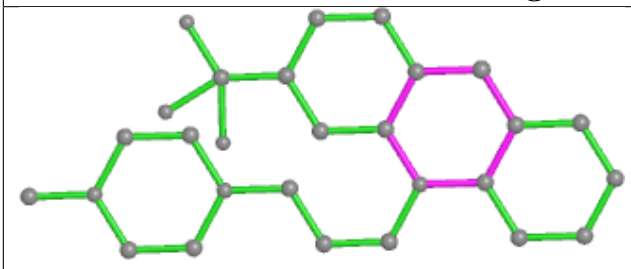

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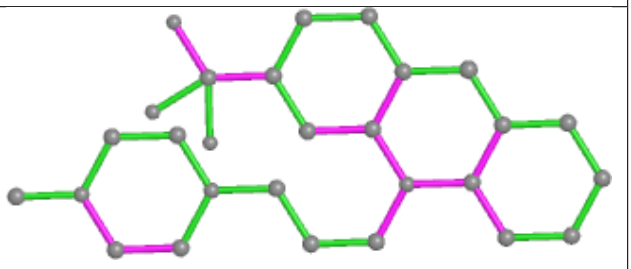

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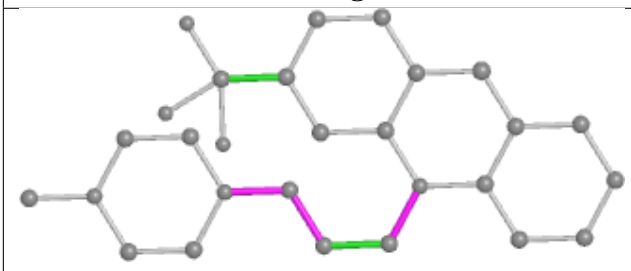

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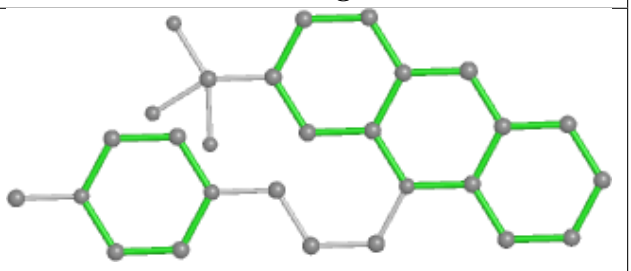

Rings

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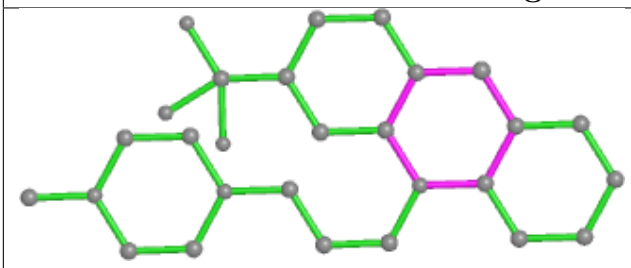

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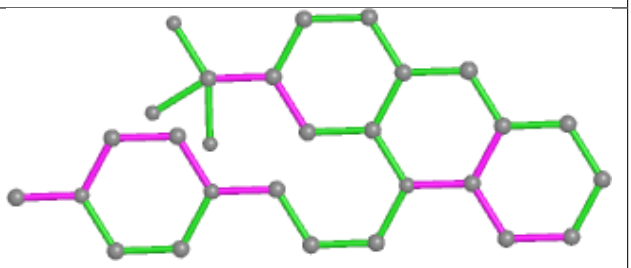

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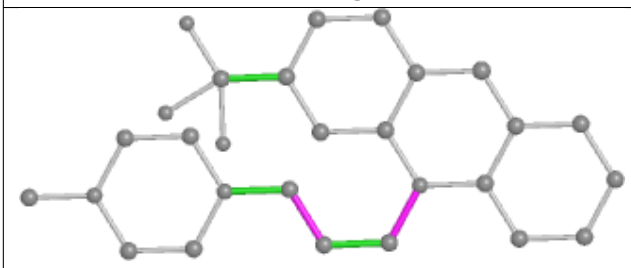

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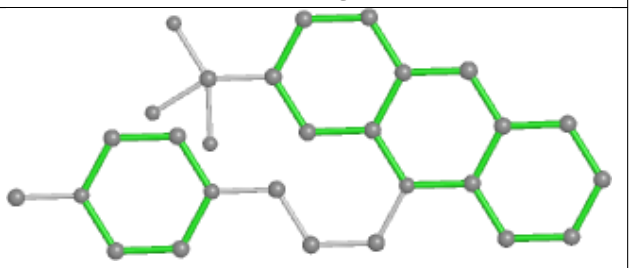
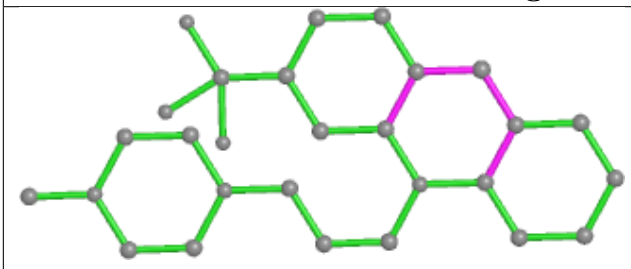


Rings

Ligand TFP R 201



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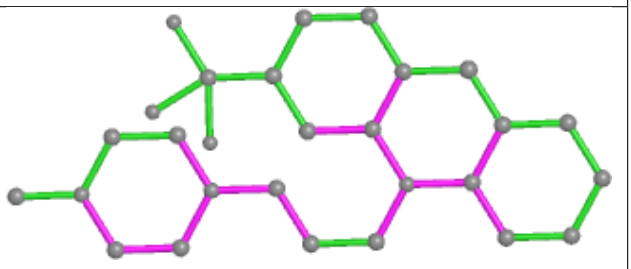

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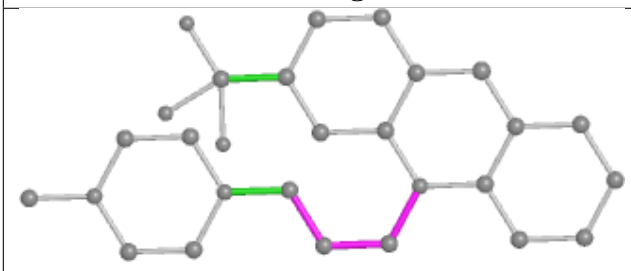

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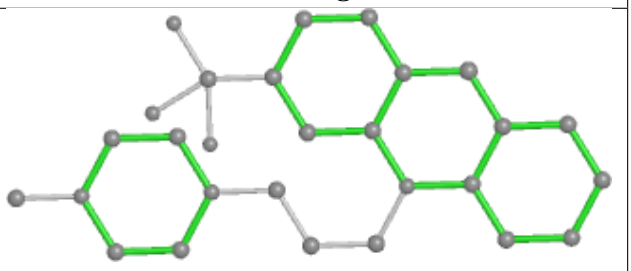
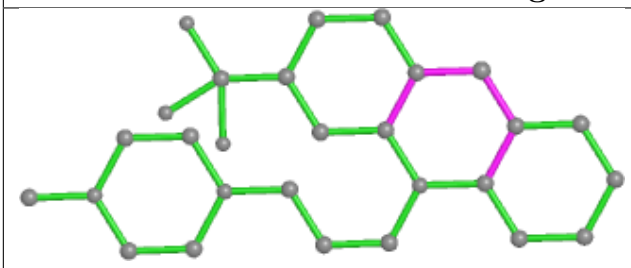


Rings

Ligand TFP S 201



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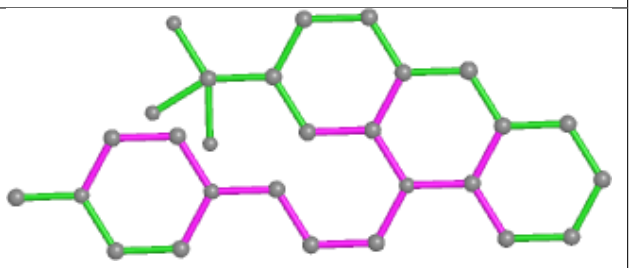
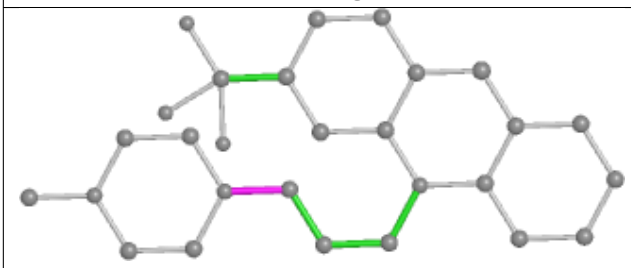


Bond angles



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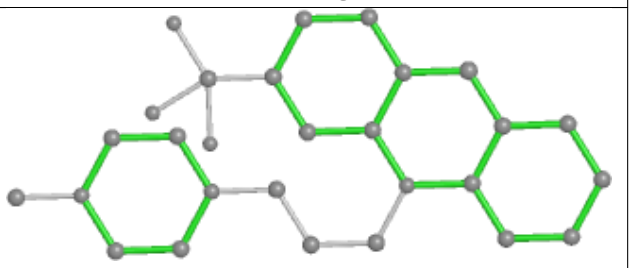
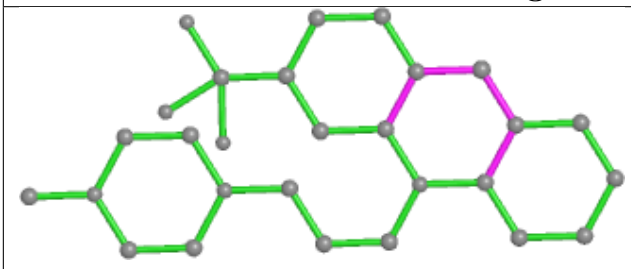


Rings

Ligand TFP E 202



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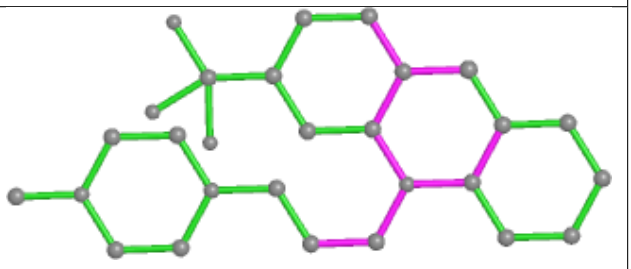

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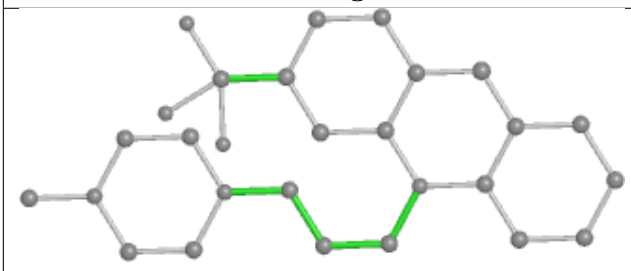

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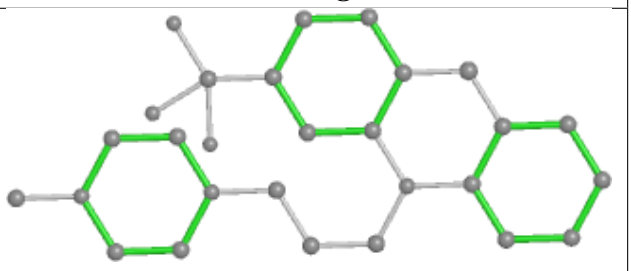
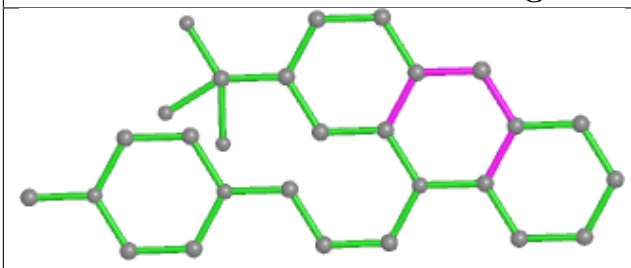


Rings

Ligand TFP B 202



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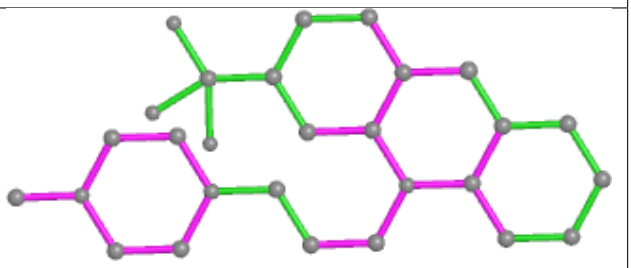
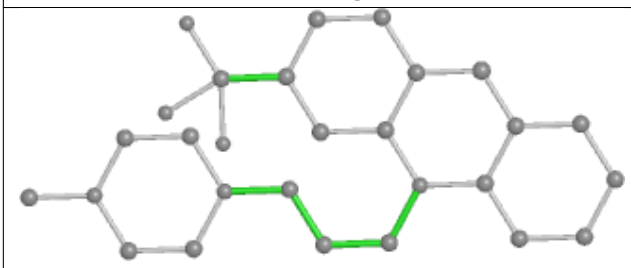


Bond angles



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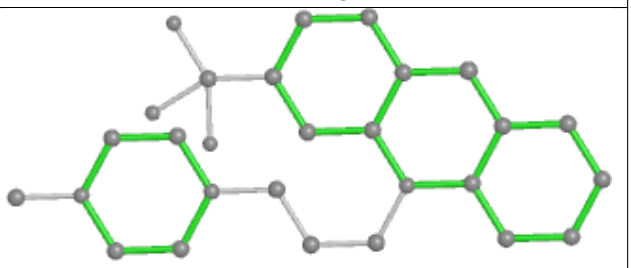
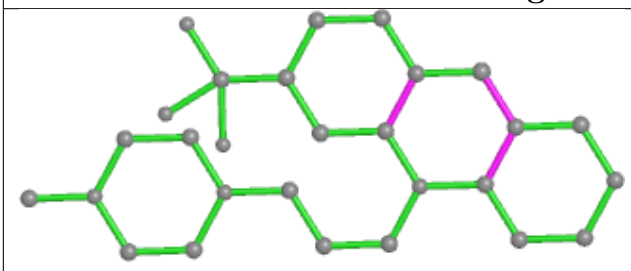


Rings

Ligand TFP F 202



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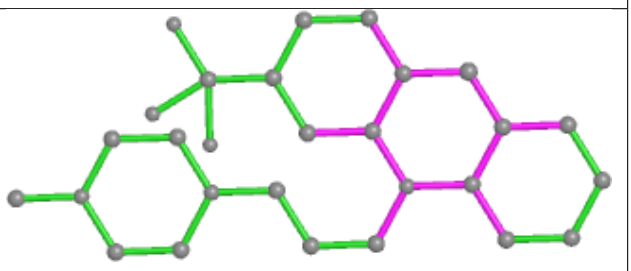

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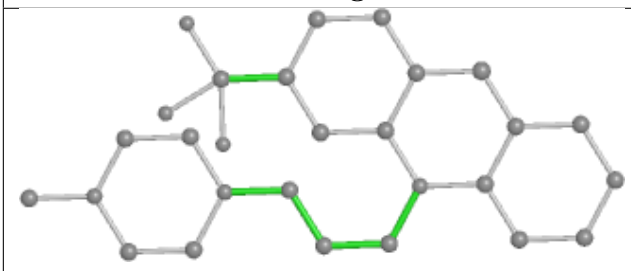

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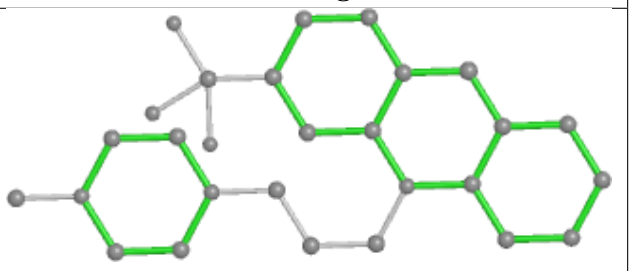
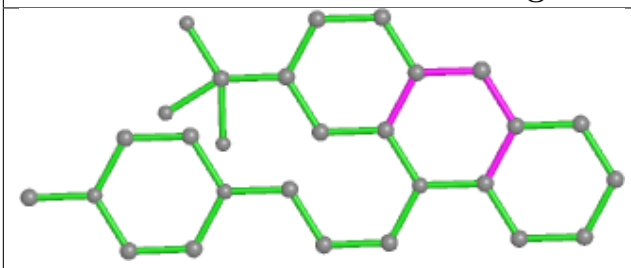


Rings

Ligand TFP F 201



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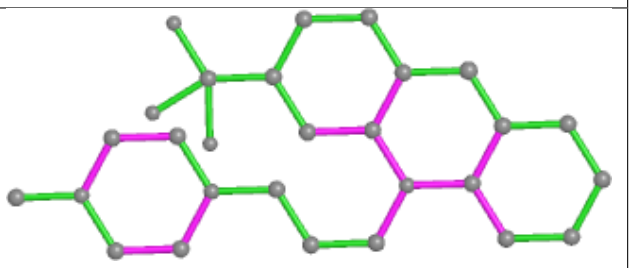
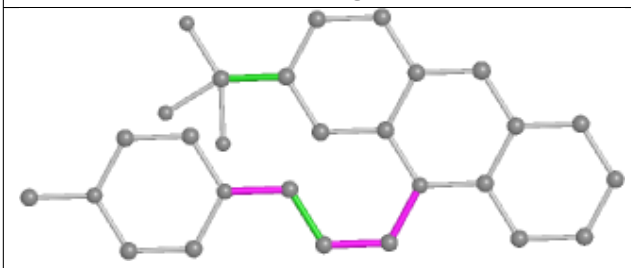


Bond angles



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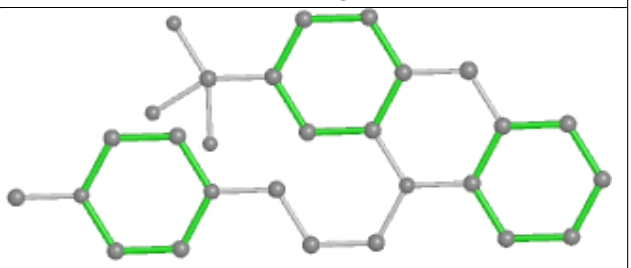
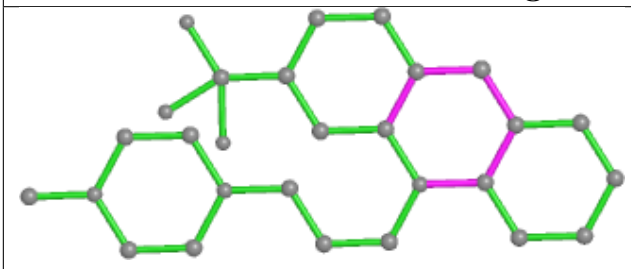


Rings

Ligand TFP K 201



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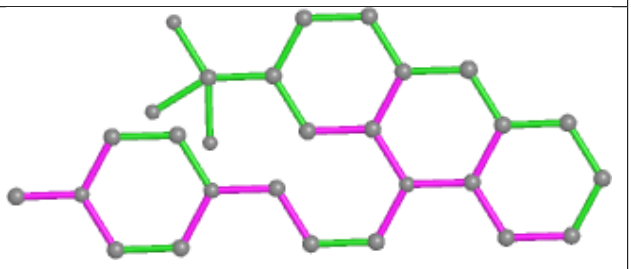
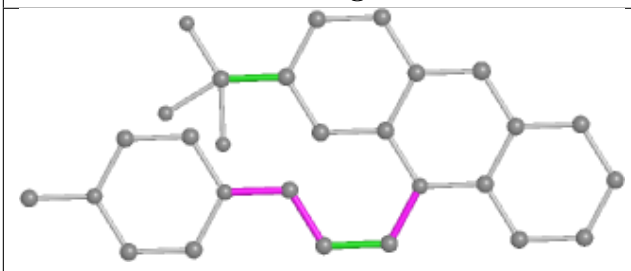


Bond angles



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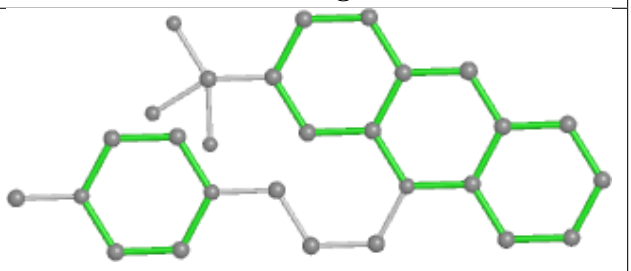
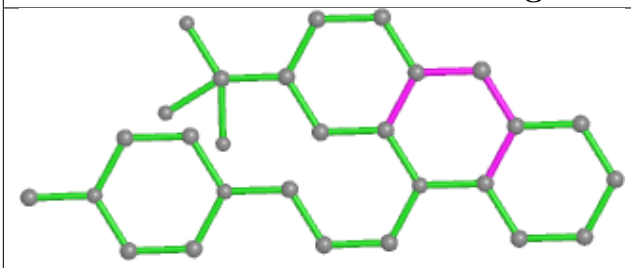


Rings

Ligand TFP Q 201



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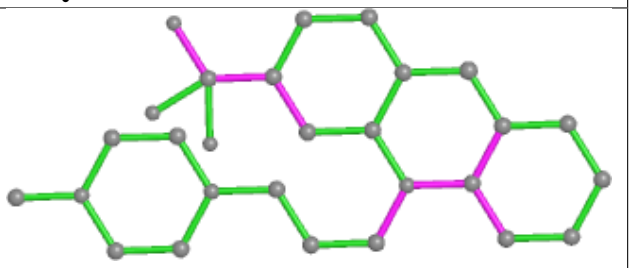
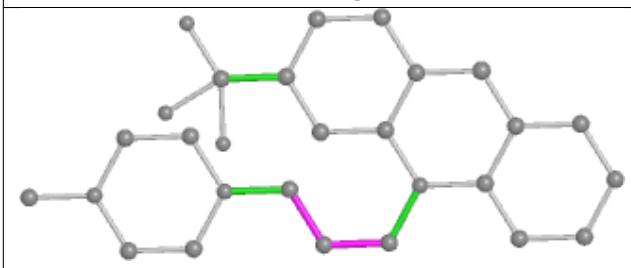


Bond angles



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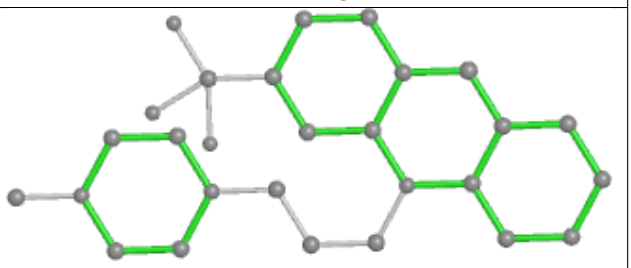
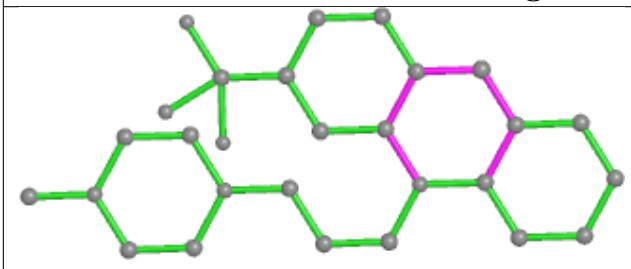
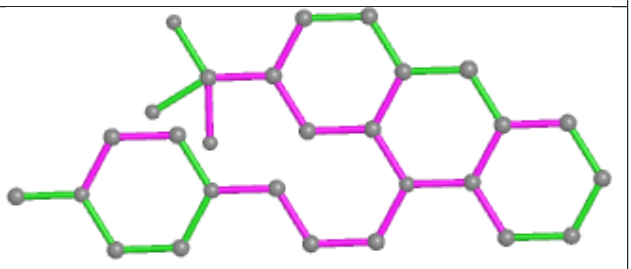


Rings

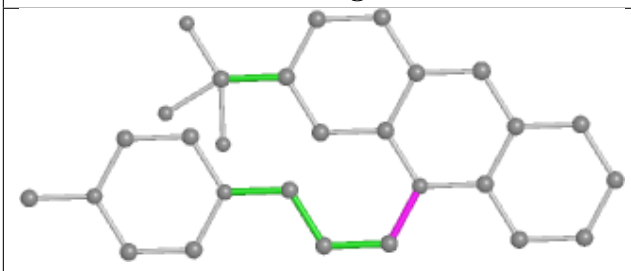
Ligand TFP D 201



Bond lengths



Bond angles



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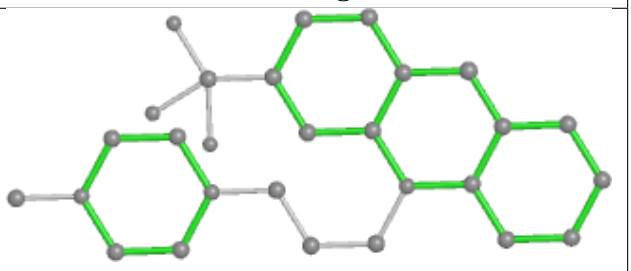
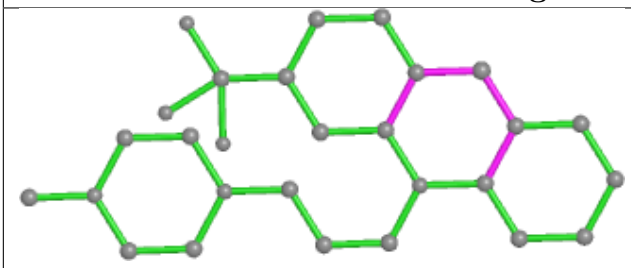


Rings

Ligand TFP J 202



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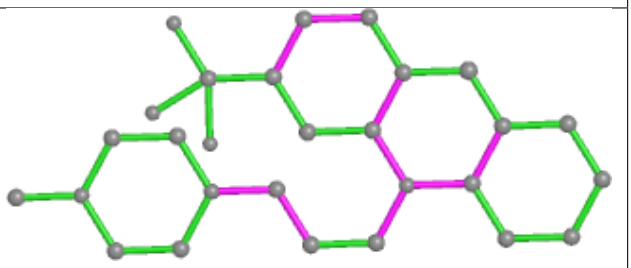
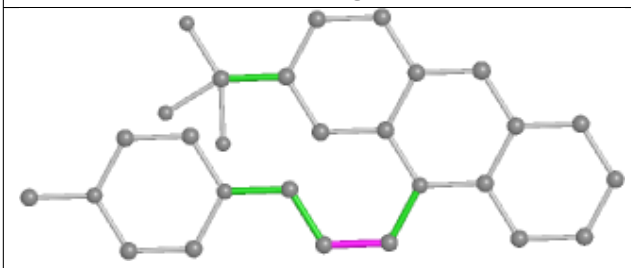


Bond angles



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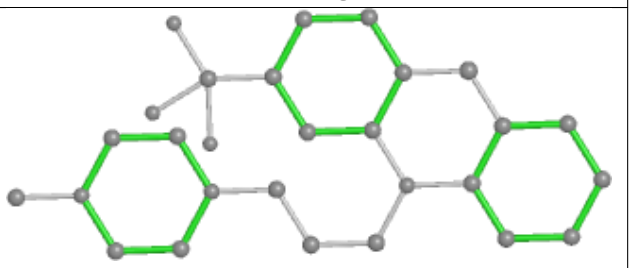
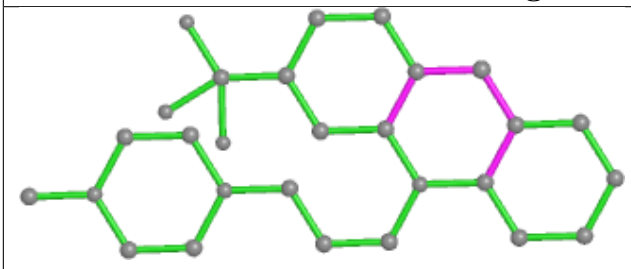


Rings

Ligand TFP O 201



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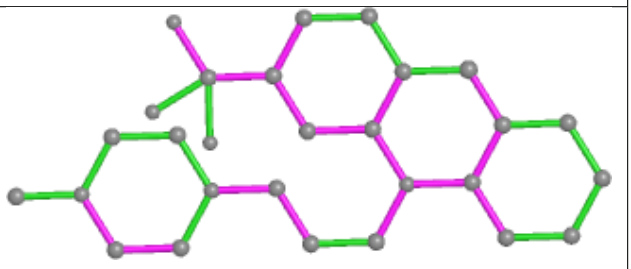
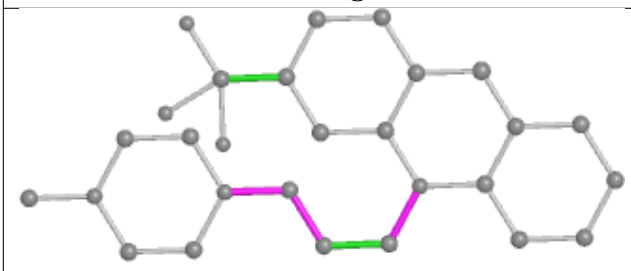
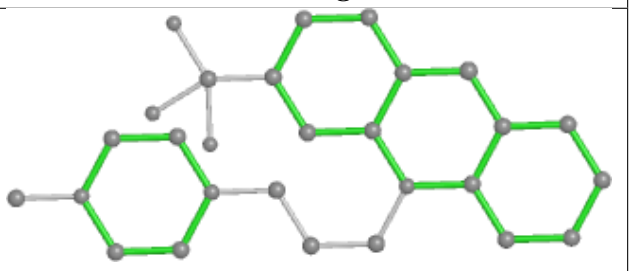


Bond angles

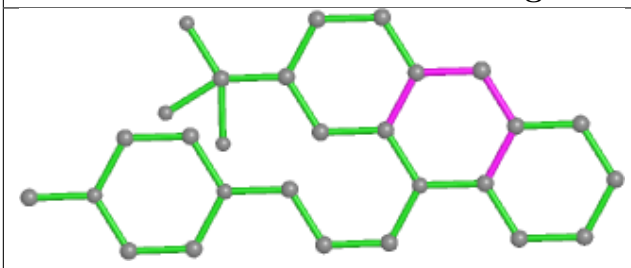


Torsions

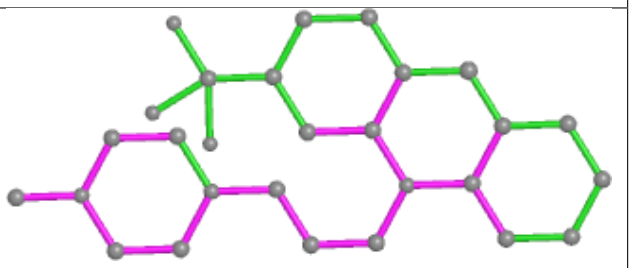


Rings

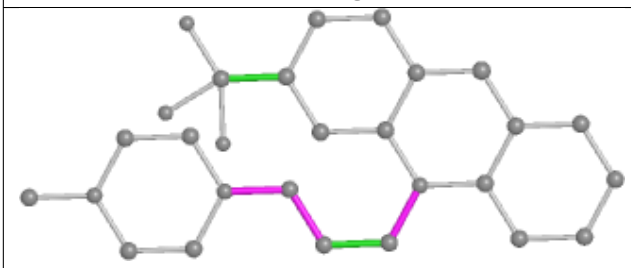
Ligand TFP A 201



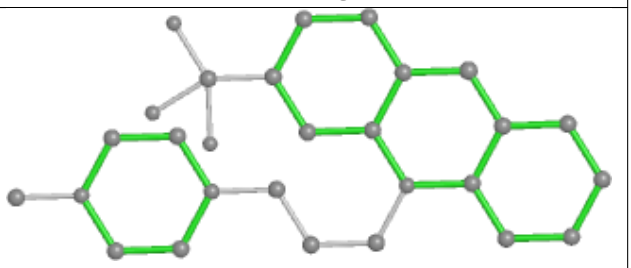
Bond lengths



Bond angles

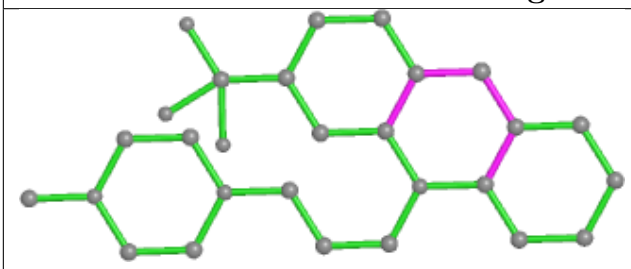


Torsions

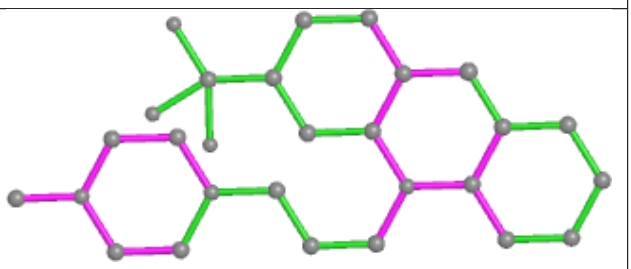


Rings

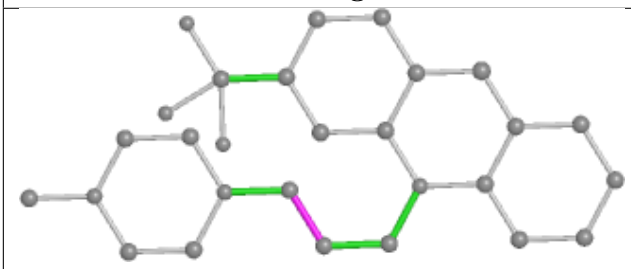
Ligand TFP L 202



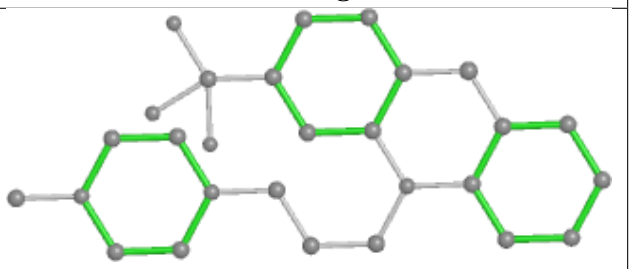
Bond lengths



Bond angles

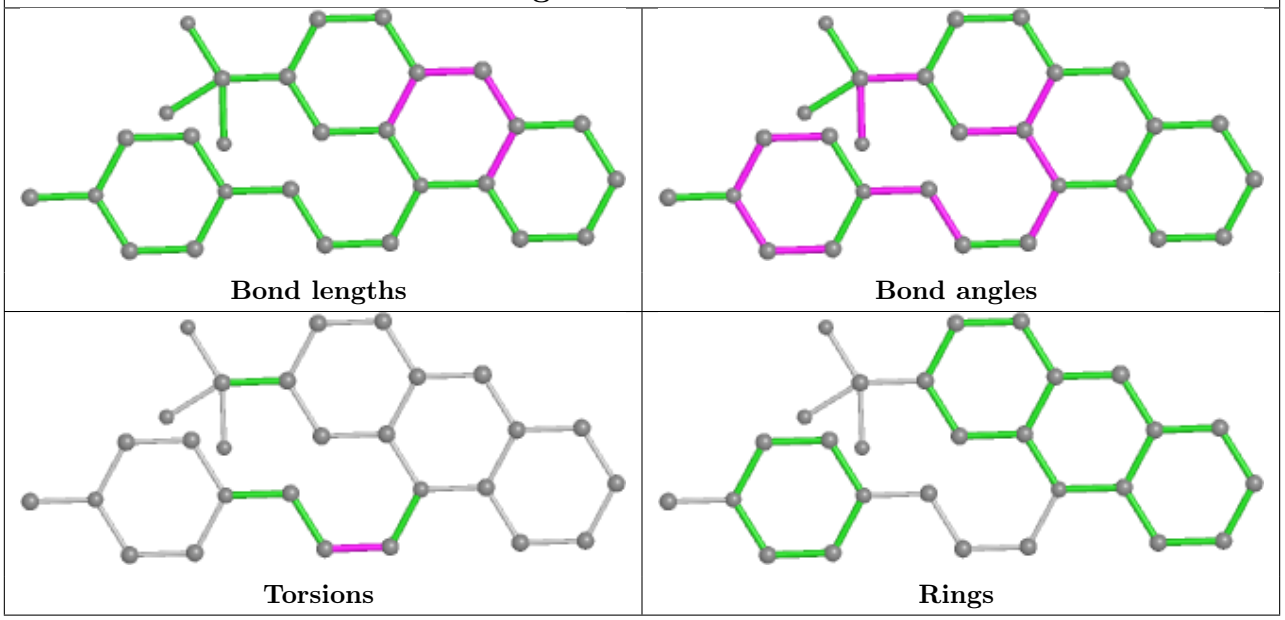


Torsions

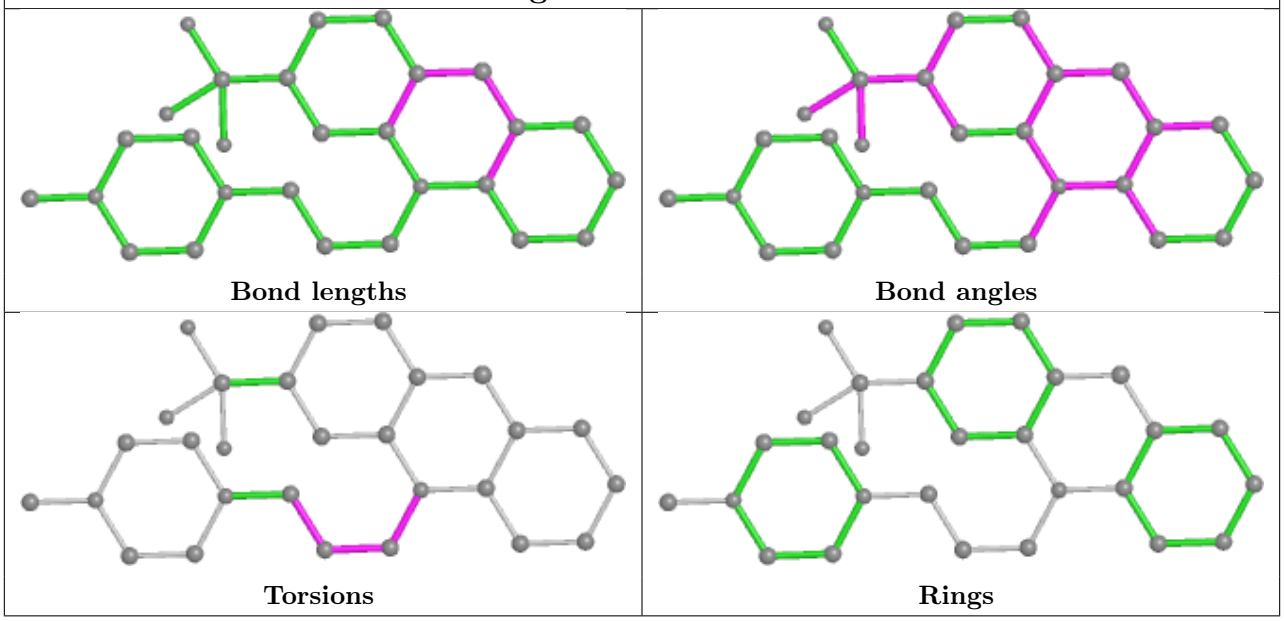


Rings

Ligand TFP I 201



Ligand TFP S 202



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

6.1 Protein, DNA and RNA chains

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^{th} 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	93/101 (92%)	0.34	6 (6%) 18 24	13, 20, 47, 57	0
1	B	93/101 (92%)	0.22	6 (6%) 18 24	14, 22, 48, 66	0
1	C	93/101 (92%)	0.13	3 (3%) 47 54	11, 21, 37, 48	0
1	D	93/101 (92%)	0.55	10 (10%) 5 8	17, 25, 70, 77	0
1	E	92/101 (91%)	0.15	5 (5%) 25 32	14, 24, 45, 51	0
1	F	90/101 (89%)	0.48	10 (11%) 5 7	15, 27, 51, 69	1 (1%)
1	G	90/101 (89%)	0.57	12 (13%) 3 4	7, 27, 49, 56	3 (3%)
1	H	94/101 (93%)	1.13	27 (28%) 0 0	20, 33, 63, 67	1 (1%)
1	I	93/101 (92%)	0.32	5 (5%) 25 32	15, 27, 42, 49	1 (1%)
1	J	93/101 (92%)	0.15	2 (2%) 62 69	13, 22, 39, 49	0
1	K	93/101 (92%)	0.26	5 (5%) 25 32	13, 23, 48, 54	0
1	L	93/101 (92%)	0.17	5 (5%) 25 32	15, 22, 46, 60	0
1	M	92/101 (91%)	0.37	7 (7%) 13 18	17, 28, 53, 60	2 (2%)
1	N	92/101 (91%)	0.17	4 (4%) 35 42	12, 21, 45, 52	1 (1%)
1	O	93/101 (92%)	0.39	9 (9%) 7 10	11, 29, 43, 49	2 (2%)
1	P	92/101 (91%)	0.21	6 (6%) 18 24	15, 26, 44, 50	0
1	Q	88/101 (87%)	0.63	11 (12%) 3 5	22, 33, 56, 58	2 (2%)
1	R	93/101 (92%)	0.32	7 (7%) 14 19	21, 30, 49, 56	0
1	S	93/101 (92%)	0.15	5 (5%) 25 32	5, 21, 39, 45	2 (2%)
1	T	93/101 (92%)	0.61	11 (11%) 4 6	12, 27, 58, 64	1 (1%)
All	All	1846/2020 (91%)	0.36	156 (8%) 10 14	5, 26, 49, 77	16 (0%)

All (156) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	53	ALA	7.2
1	H	54	ALA	6.6
1	C	94	PRO	5.9
1	F	53	ALA	5.6
1	K	2	ALA	5.5
1	P	2	ALA	5.5
1	G	48	LYS	5.4
1	D	50	THR	5.1
1	M	2	ALA	5.0
1	A	92	GLY	4.9
1	H	95	ASP	4.8
1	D	49	ARG	4.8
1	T	49	ARG	4.8
1	F	47	GLY	4.7
1	E	93	PHE	4.6
1	A	93	PHE	4.5
1	H	94	PRO	4.5
1	D	53	ALA	4.4
1	T	48	LYS	4.3
1	B	2	ALA	4.3
1	D	2	ALA	4.3
1	D	54	ALA	4.3
1	S	10	ASP	4.2
1	H	58	LEU	4.2
1	D	51	ASP	4.2
1	I	94	PRO	4.2
1	S	2	ALA	4.2
1	M	93	PHE	4.2
1	Q	94	PRO	4.1
1	P	93	PHE	4.1
1	F	51	ASP	4.1
1	F	94	PRO	4.1
1	D	48	LYS	4.1
1	F	2	ALA	4.0
1	H	31	LYS	4.0
1	Q	61	ASN	3.9
1	G	81	CYS	3.8
1	D	94	PRO	3.8
1	E	2	ALA	3.8
1	A	94	PRO	3.7
1	G	10	ASP	3.7
1	Q	81	CYS	3.6
1	T	54	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	H	56	GLN	3.6
1	R	93	PHE	3.6
1	Q	31	LYS	3.6
1	B	48	LYS	3.5
1	F	54	ALA	3.5
1	J	2	ALA	3.5
1	T	50	THR	3.5
1	T	2	ALA	3.5
1	O	2	ALA	3.5
1	Q	95	ASP	3.4
1	O	53	ALA	3.4
1	K	50	THR	3.3
1	C	48	LYS	3.3
1	O	51	ASP	3.3
1	H	2	ALA	3.3
1	H	64	SER	3.3
1	N	93	PHE	3.1
1	Q	93	PHE	3.1
1	I	2	ALA	3.1
1	T	35	LYS	3.1
1	L	2	ALA	3.1
1	L	94	PRO	3.0
1	H	66	ARG	3.0
1	E	49	ARG	3.0
1	Q	92	GLY	3.0
1	B	94	PRO	3.0
1	N	2	ALA	3.0
1	T	57	LYS	3.0
1	F	66	ARG	3.0
1	T	66	ARG	3.0
1	H	51	ASP	2.9
1	O	10	ASP	2.9
1	G	54	ALA	2.9
1	S	64	SER	2.9
1	G	52	GLU	2.9
1	O	54	ALA	2.9
1	K	48	LYS	2.9
1	G	66	ARG	2.9
1	H	55	PHE	2.9
1	R	53	ALA	2.8
1	R	94	PRO	2.8
1	H	49	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	R	2	ALA	2.8
1	F	35	LYS	2.8
1	I	35	LYS	2.8
1	R	66	ARG	2.8
1	L	48	LYS	2.8
1	G	93	PHE	2.8
1	G	94	PRO	2.8
1	H	68	ASN	2.8
1	R	48	LYS	2.7
1	P	48	LYS	2.7
1	T	94	PRO	2.7
1	G	55	PHE	2.6
1	H	34	LEU	2.6
1	E	66	ARG	2.6
1	I	68	ASN	2.6
1	B	49	ARG	2.5
1	H	52	GLU	2.5
1	H	47	GLY	2.5
1	Q	60	SER	2.5
1	H	57	LYS	2.4
1	R	68	ASN	2.4
1	M	49	ARG	2.4
1	G	47	GLY	2.4
1	C	2	ALA	2.4
1	G	56	GLN	2.4
1	M	52	GLU	2.4
1	K	94	PRO	2.4
1	F	46	LEU	2.3
1	S	48	LYS	2.3
1	S	94	PRO	2.3
1	A	70	VAL	2.3
1	N	53	ALA	2.3
1	D	55	PHE	2.3
1	N	57	LYS	2.3
1	B	29	LEU	2.3
1	O	49	ARG	2.3
1	H	61	ASN	2.3
1	T	68	ASN	2.2
1	Q	55	PHE	2.2
1	P	61	ASN	2.2
1	H	60	SER	2.2
1	P	92	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	T	53	ALA	2.2
1	J	92	GLY	2.2
1	O	68	ASN	2.2
1	I	93	PHE	2.2
1	K	29	LEU	2.2
1	O	94	PRO	2.2
1	Q	47	GLY	2.2
1	P	49	ARG	2.1
1	M	50	THR	2.1
1	H	35	LYS	2.1
1	H	24	GLY	2.1
1	H	48	LYS	2.1
1	Q	68	ASN	2.1
1	M	48	LYS	2.1
1	G	2	ALA	2.1
1	A	48	LYS	2.1
1	B	37	LEU	2.1
1	M	51	ASP	2.1
1	E	92	GLY	2.1
1	F	52	GLU	2.1
1	D	93	PHE	2.1
1	A	2	ALA	2.0
1	H	93	PHE	2.0
1	L	93	PHE	2.0
1	H	50	THR	2.0
1	L	49	ARG	2.0
1	O	66	ARG	2.0
1	H	27	PHE	2.0
1	H	92	GLY	2.0

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 monosaccharides 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, 95^{th} 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
2	TFP	F	201	28/28	0.85	0.18	40,42,49,49	0
2	TFP	H	201	28/28	0.85	0.17	27,30,31,31	0
2	TFP	G	201	28/28	0.88	0.16	44,45,47,47	0
2	TFP	O	201	28/28	0.89	0.17	31,37,39,39	0
2	TFP	Q	201	28/28	0.89	0.14	44,47,50,50	0
3	CA	H	302	1/1	0.89	0.05	32,32,32,32	0
3	CA	M	302	1/1	0.89	0.04	28,28,28,28	0
2	TFP	J	201	28/28	0.90	0.15	31,34,40,40	0
3	CA	G	302	1/1	0.90	0.05	26,26,26,26	0
2	TFP	B	201	28/28	0.90	0.16	37,39,40,41	0
2	TFP	P	201	28/28	0.90	0.17	36,40,44,44	0
2	TFP	T	201	28/28	0.91	0.13	27,30,33,33	0
2	TFP	D	201	28/28	0.91	0.15	37,40,45,46	0
2	TFP	E	201	28/28	0.92	0.16	37,38,40,40	0
2	TFP	M	201	28/28	0.92	0.15	41,45,49,50	0
2	TFP	I	201	28/28	0.92	0.14	25,29,33,34	0
2	TFP	K	201	28/28	0.93	0.14	32,34,38,39	0
2	TFP	R	201	28/28	0.93	0.15	30,32,36,37	0
3	CA	T	301	1/1	0.93	0.04	21,21,21,21	0
2	TFP	M	202	28/28	0.94	0.16	15,24,28,29	0
2	TFP	N	201	28/28	0.94	0.11	26,27,32,33	0
2	TFP	S	201	28/28	0.94	0.12	22,26,32,33	0
2	TFP	L	201	28/28	0.94	0.13	28,31,34,34	0
2	TFP	O	202	28/28	0.94	0.17	14,27,31,33	0
2	TFP	P	202	28/28	0.94	0.15	11,20,27,29	0
2	TFP	F	202	28/28	0.94	0.15	19,26,29,30	0
3	CA	P	302	1/1	0.94	0.05	20,20,20,20	0
3	CA	Q	302	1/1	0.94	0.04	48,48,48,48	0
2	TFP	Q	202	28/28	0.94	0.16	24,31,35,36	0
3	CA	T	302	1/1	0.94	0.04	33,33,33,33	0
2	TFP	C	201	28/28	0.95	0.11	24,26,31,32	0
2	TFP	C	202	28/28	0.95	0.17	12,16,24,25	0
2	TFP	H	202	28/28	0.95	0.16	14,21,29,30	0
2	TFP	I	202	28/28	0.95	0.19	16,22,32,32	0
2	TFP	E	202	28/28	0.95	0.14	13,21,26,27	0
3	CA	S	302	1/1	0.95	0.11	13,13,13,13	0
3	CA	C	302	1/1	0.95	0.11	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CA	F	302	1/1	0.95	0.03	28,28,28,28	0
2	TFP	K	202	28/28	0.96	0.19	9,18,27,27	0
3	CA	H	301	1/1	0.96	0.04	38,38,38,38	0
2	TFP	T	202	28/28	0.96	0.14	12,18,26,27	0
3	CA	L	301	1/1	0.96	0.11	17,17,17,17	0
3	CA	M	301	1/1	0.96	0.09	32,32,32,32	0
2	TFP	A	202	28/28	0.96	0.17	6,14,24,26	0
3	CA	O	301	1/1	0.96	0.03	31,31,31,31	0
3	CA	A	302	1/1	0.96	0.09	12,12,12,12	0
3	CA	Q	301	1/1	0.96	0.04	30,30,30,30	0
3	CA	B	301	1/1	0.96	0.09	14,14,14,14	0
3	CA	R	302	1/1	0.96	0.03	37,37,37,37	0
2	TFP	G	202	28/28	0.96	0.15	14,24,32,33	0
3	CA	D	301	1/1	0.96	0.08	23,23,23,23	0
2	TFP	A	201	28/28	0.96	0.10	20,24,25,26	0
2	TFP	D	202	28/28	0.97	0.11	10,21,29,30	0
2	TFP	R	202	28/28	0.97	0.17	17,28,33,34	0
2	TFP	S	202	28/28	0.97	0.17	10,14,21,22	0
3	CA	N	301	1/1	0.97	0.06	18,18,18,18	0
3	CA	N	302	1/1	0.97	0.05	14,14,14,14	0
3	CA	D	302	1/1	0.97	0.04	19,19,19,19	0
3	CA	F	301	1/1	0.97	0.04	23,23,23,23	0
2	TFP	J	202	28/28	0.97	0.18	10,13,24,25	0
3	CA	G	301	1/1	0.97	0.03	24,24,24,24	0
2	TFP	N	202	28/28	0.97	0.14	12,14,22,24	0
2	TFP	B	202	28/28	0.97	0.19	13,16,27,27	0
2	TFP	L	202	28/28	0.97	0.16	14,17,26,27	0
3	CA	I	301	1/1	0.97	0.07	24,24,24,24	0
3	CA	K	302	1/1	0.98	0.13	20,20,20,20	0
3	CA	C	301	1/1	0.98	0.05	17,17,17,17	0
3	CA	E	301	1/1	0.98	0.03	19,19,19,19	0
3	CA	E	302	1/1	0.98	0.09	23,23,23,23	0
3	CA	A	301	1/1	0.98	0.09	15,15,15,15	0
3	CA	B	302	1/1	0.98	0.09	18,18,18,18	0
3	CA	I	302	1/1	0.98	0.02	27,27,27,27	0
3	CA	L	302	1/1	0.99	0.08	18,18,18,18	0
3	CA	R	301	1/1	0.99	0.06	27,27,27,27	0
3	CA	K	301	1/1	0.99	0.10	17,17,17,17	0
3	CA	S	301	1/1	0.99	0.08	14,14,14,14	0
3	CA	O	302	1/1	0.99	0.04	25,25,25,25	0
3	CA	J	301	1/1	0.99	0.07	13,13,13,13	0
3	CA	J	302	1/1	0.99	0.09	14,14,14,14	0

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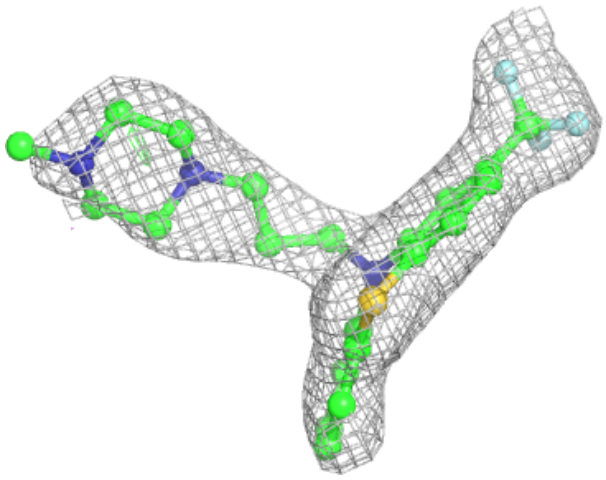
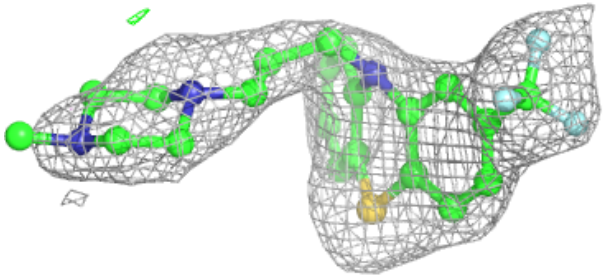
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CA	P	301	1/1	1.00	0.03	16,16,16,16	0

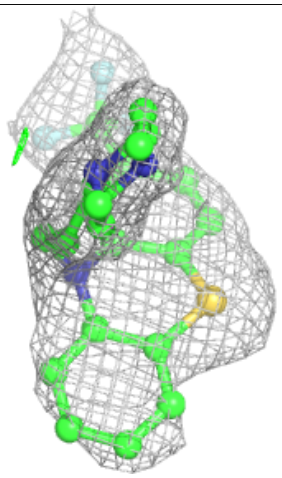
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TFP 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)

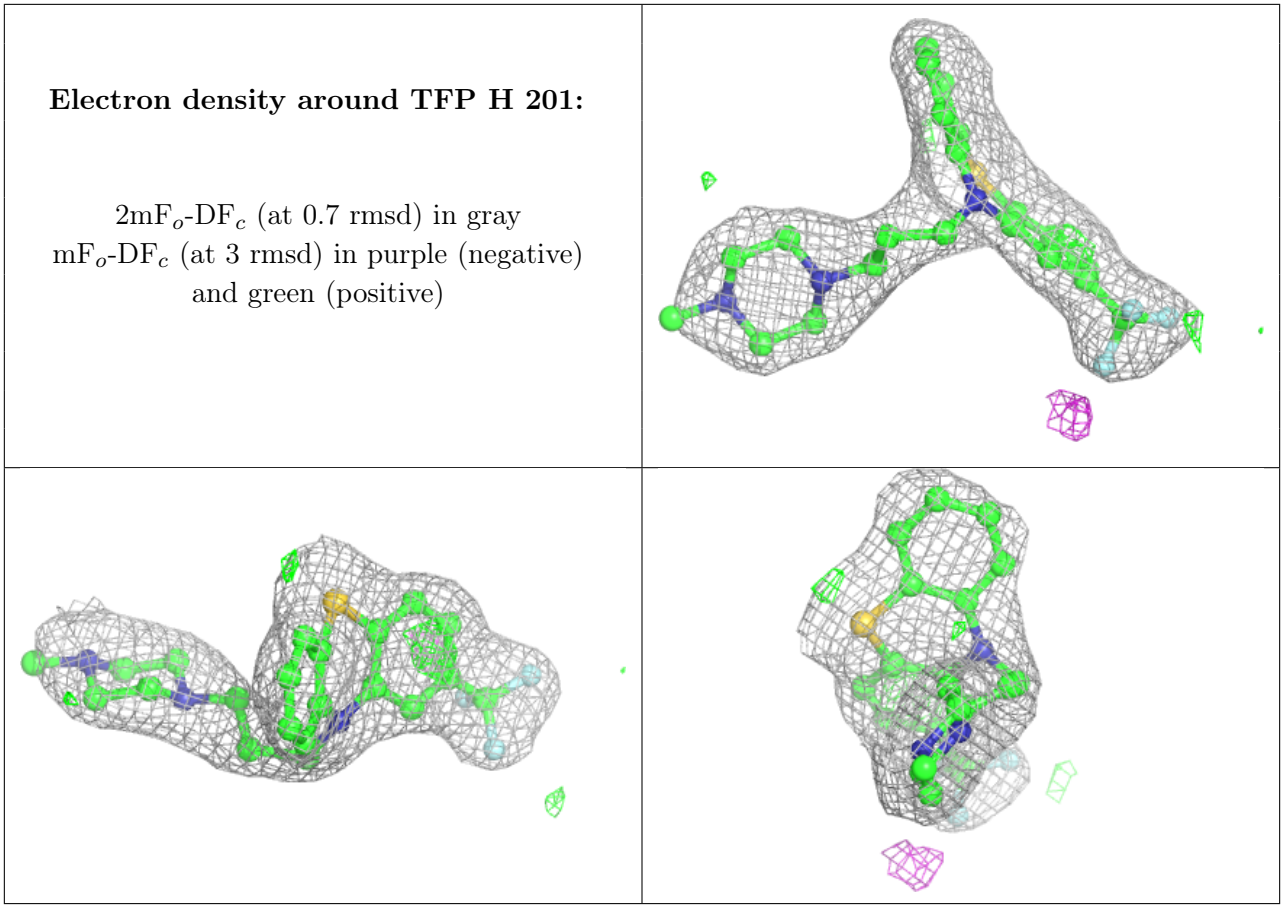






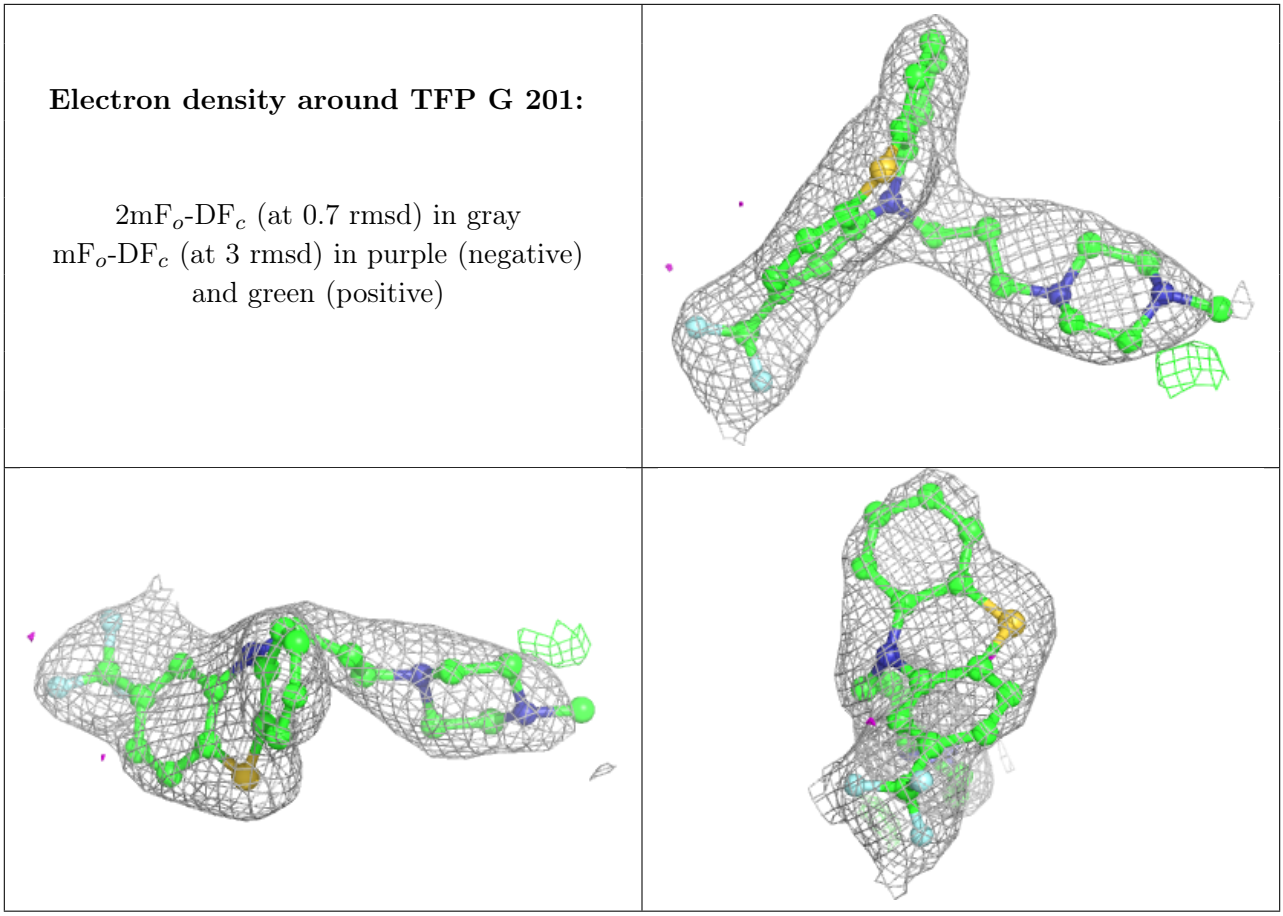
Electron density around TFP H 201:

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



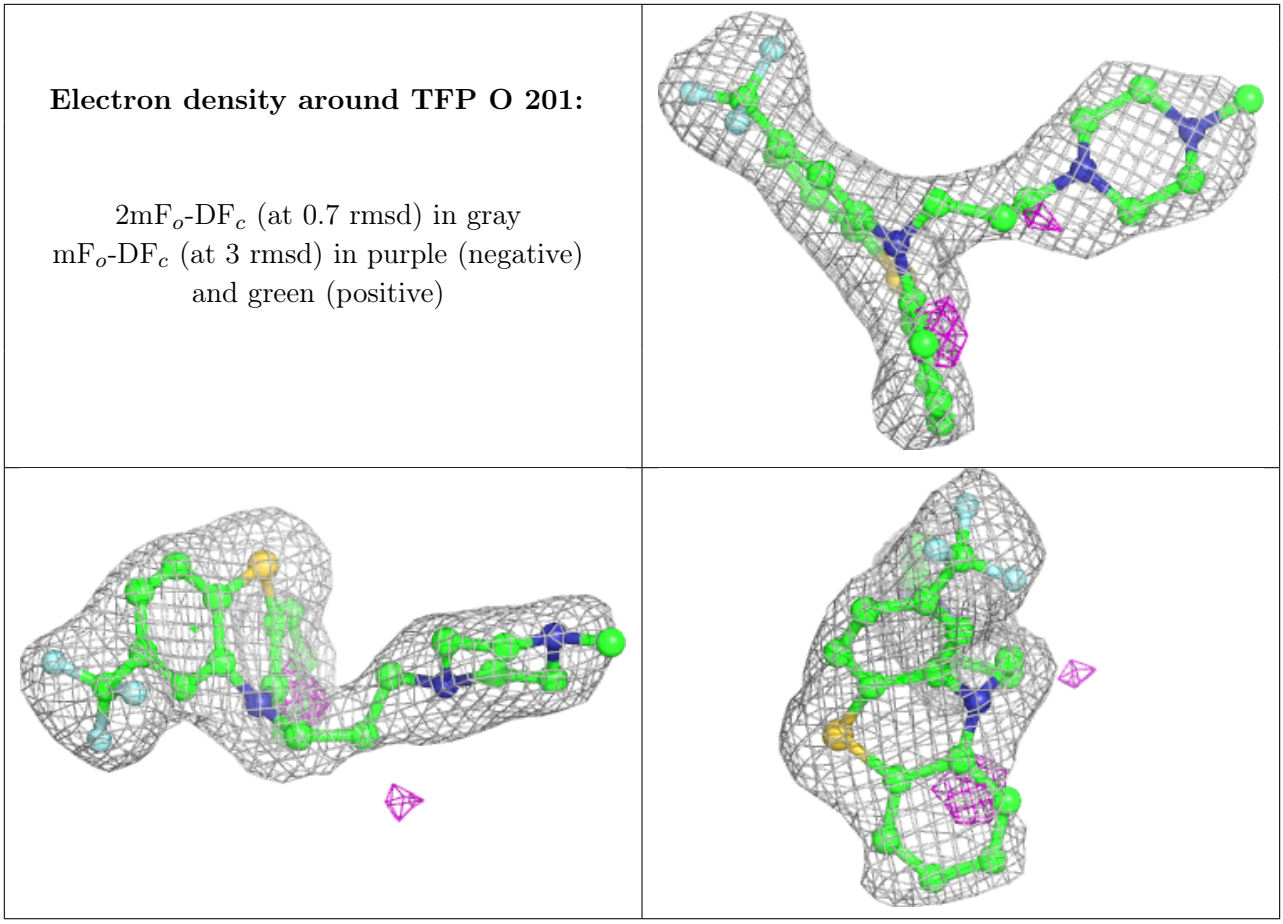
Electron density around TFP G 201:

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



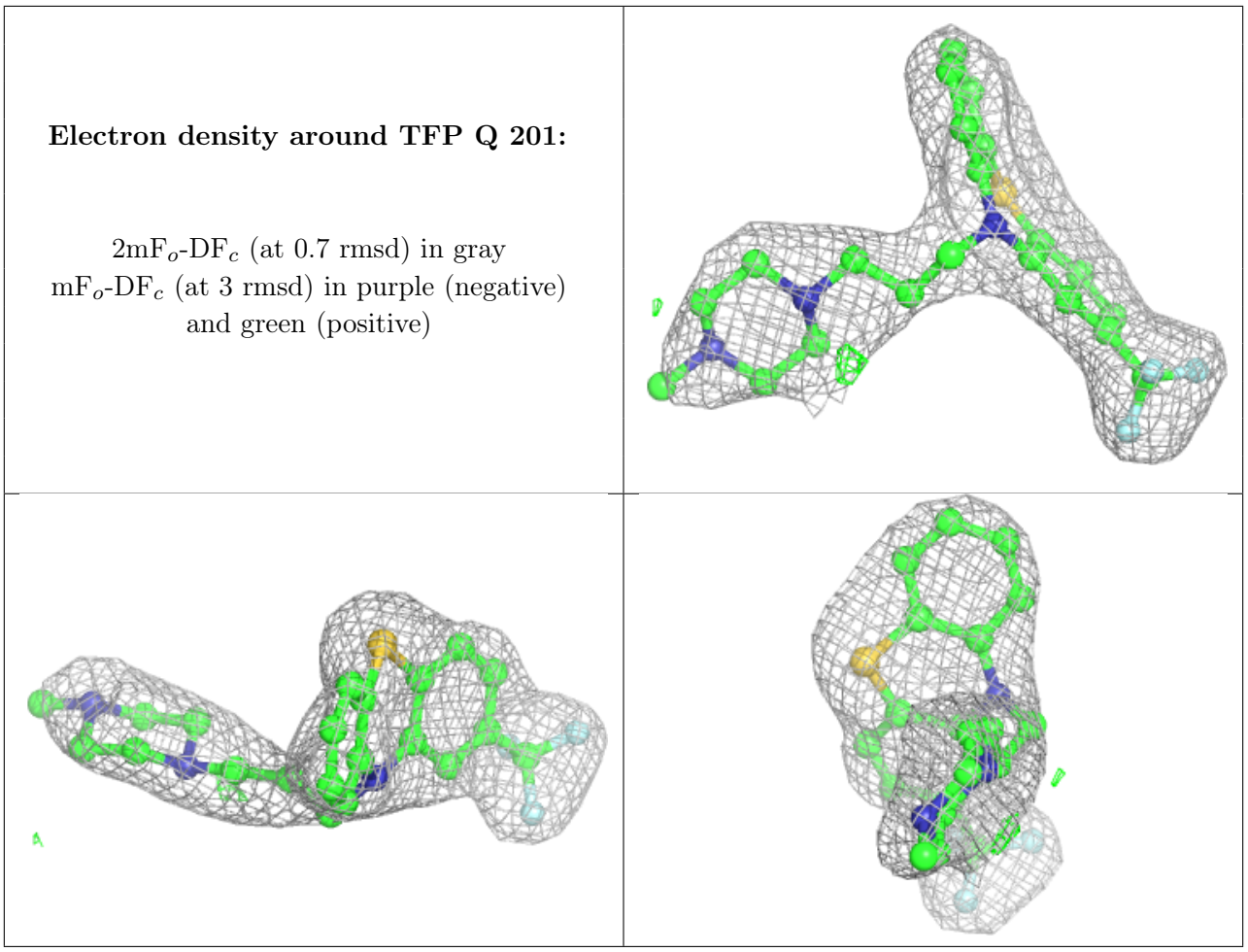
Electron density around TFP O 201:

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



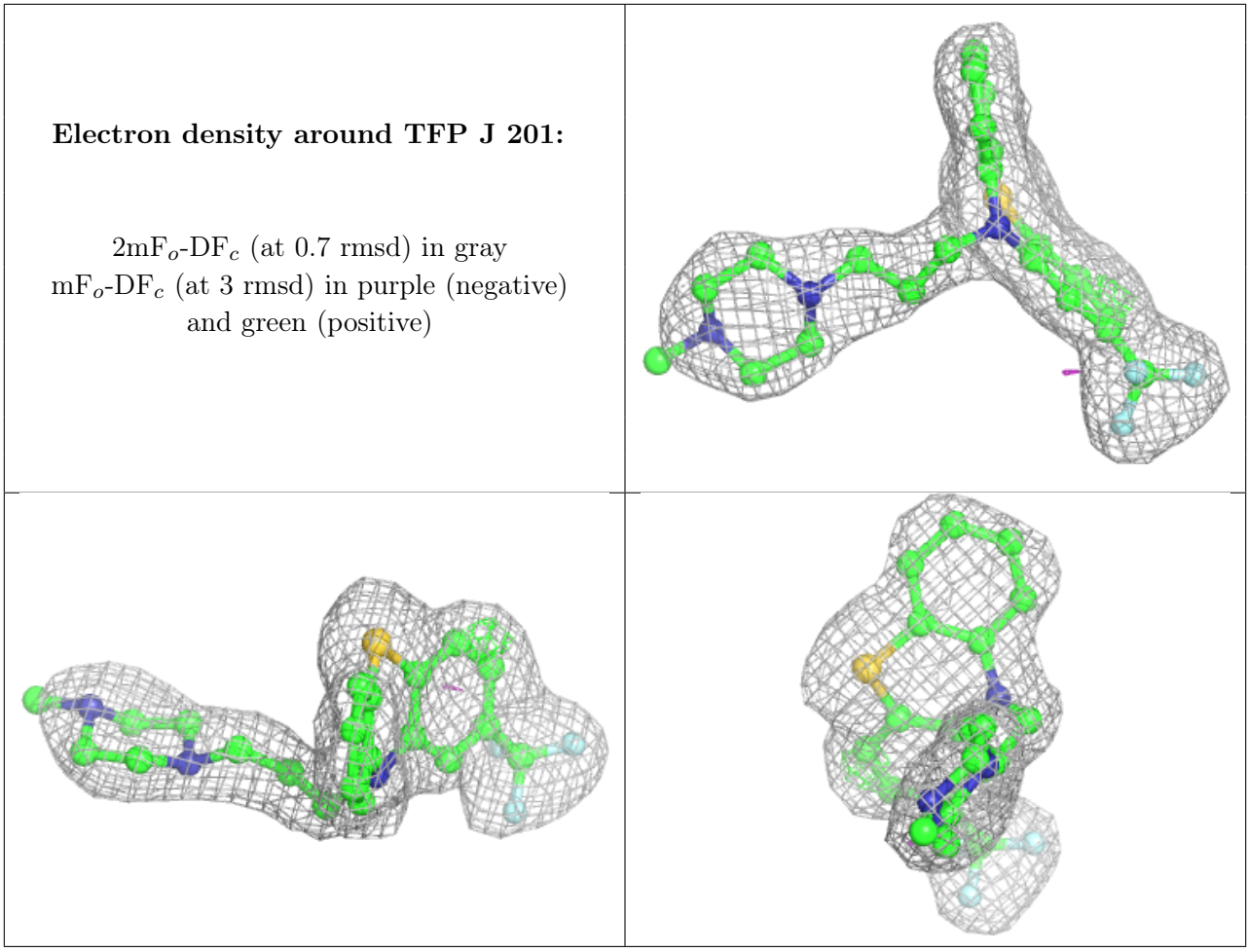
Electron density around TFP Q 201:

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



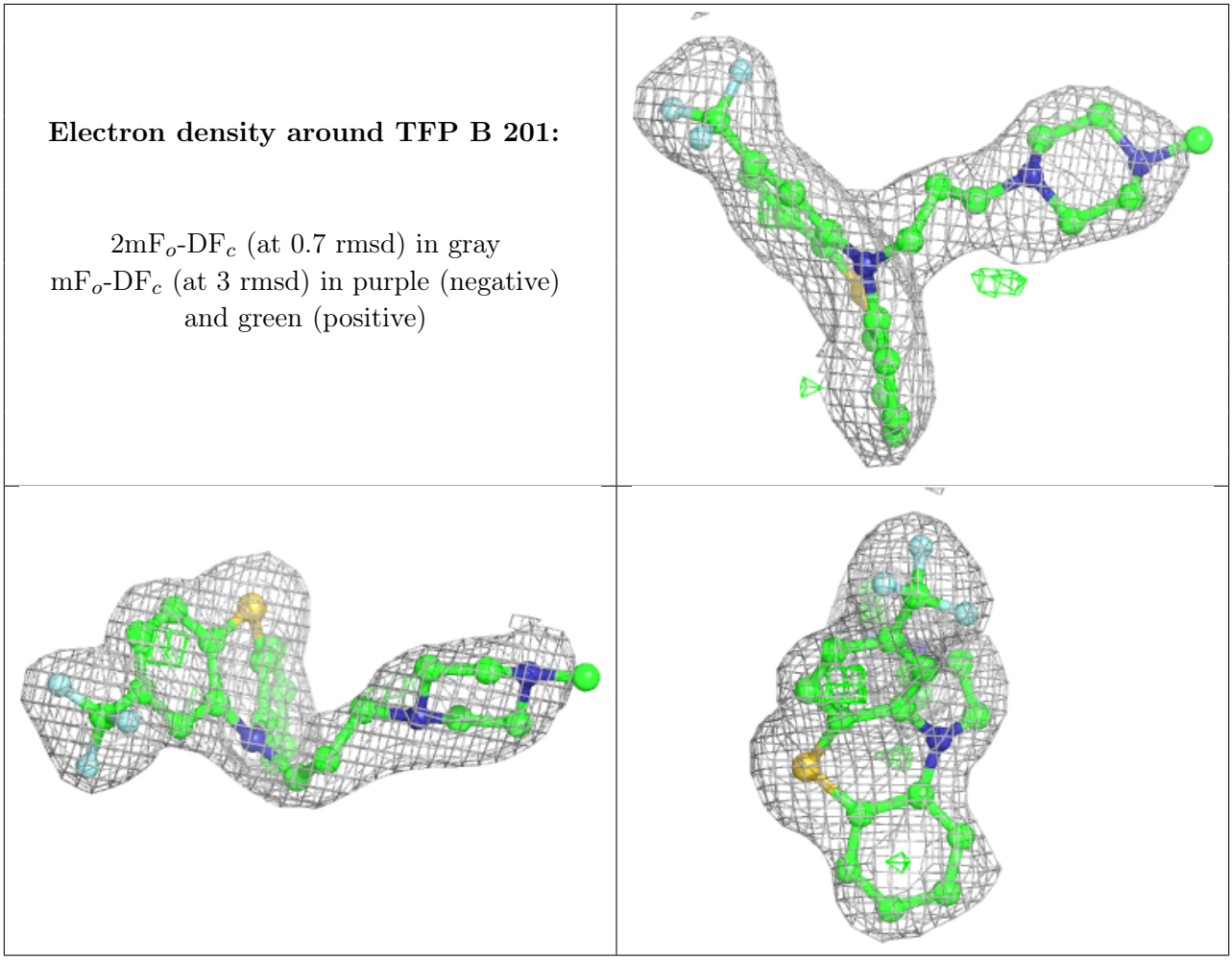
Electron density around TFP J 201:

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



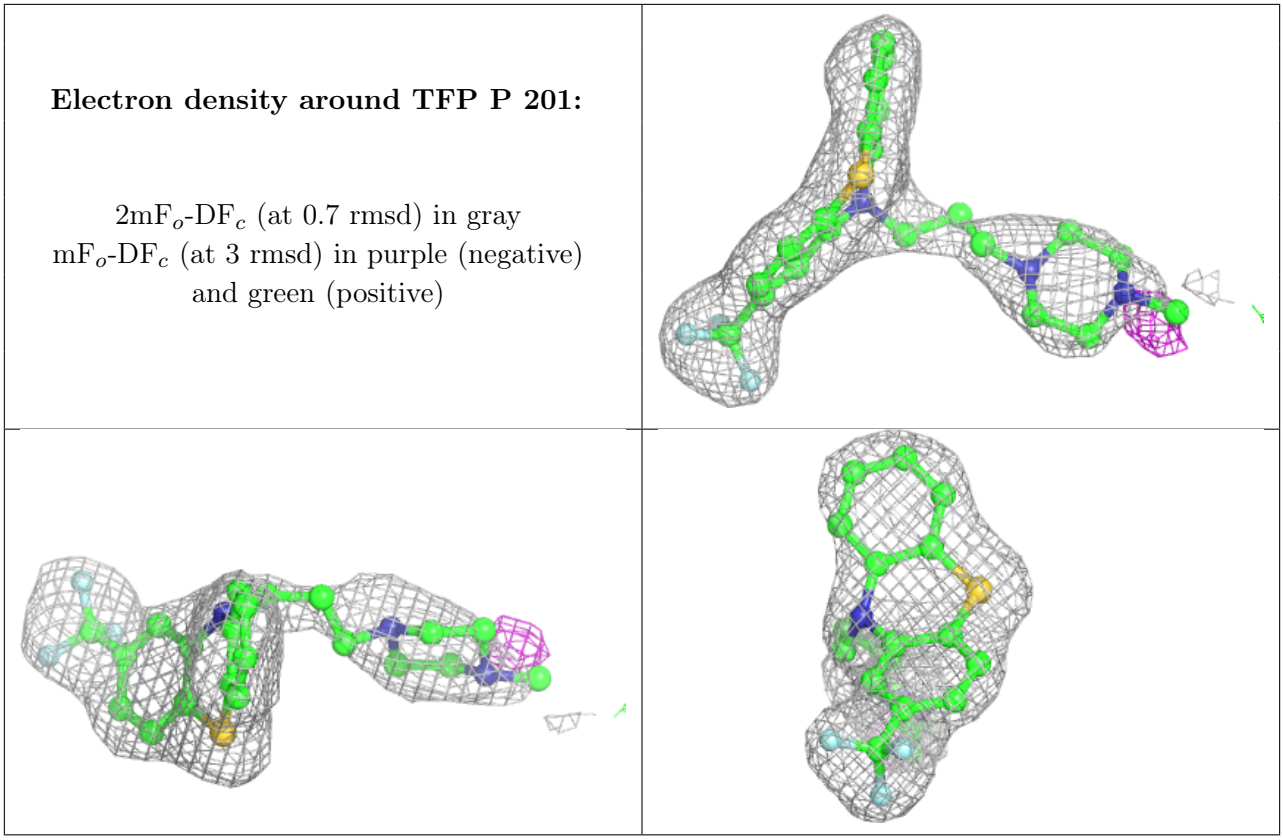
Electron density around TFP B 201:

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



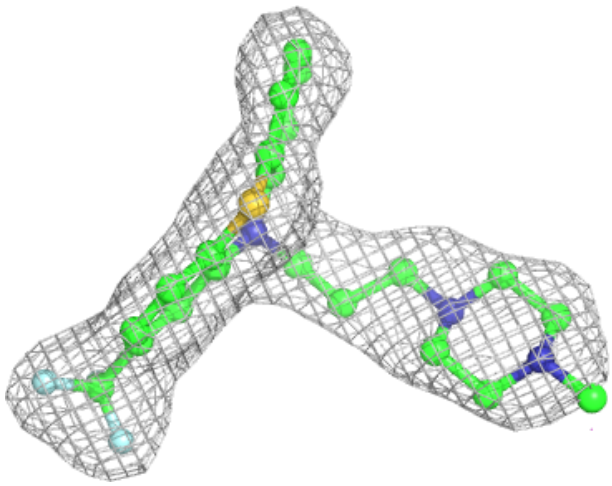
Electron density around TFP P 201:

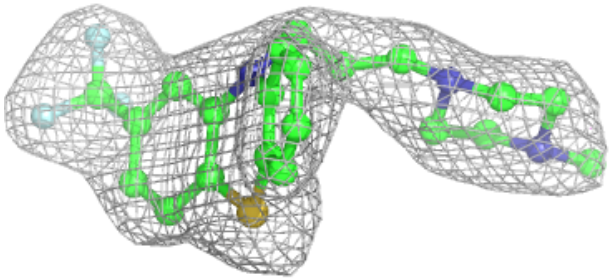
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

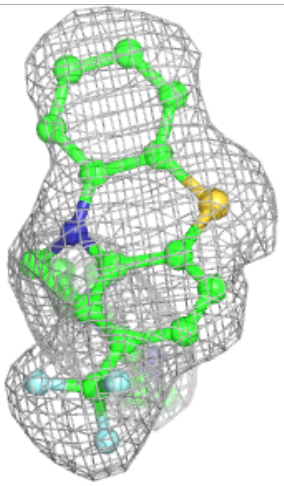


Electron density around TFP T 201:

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

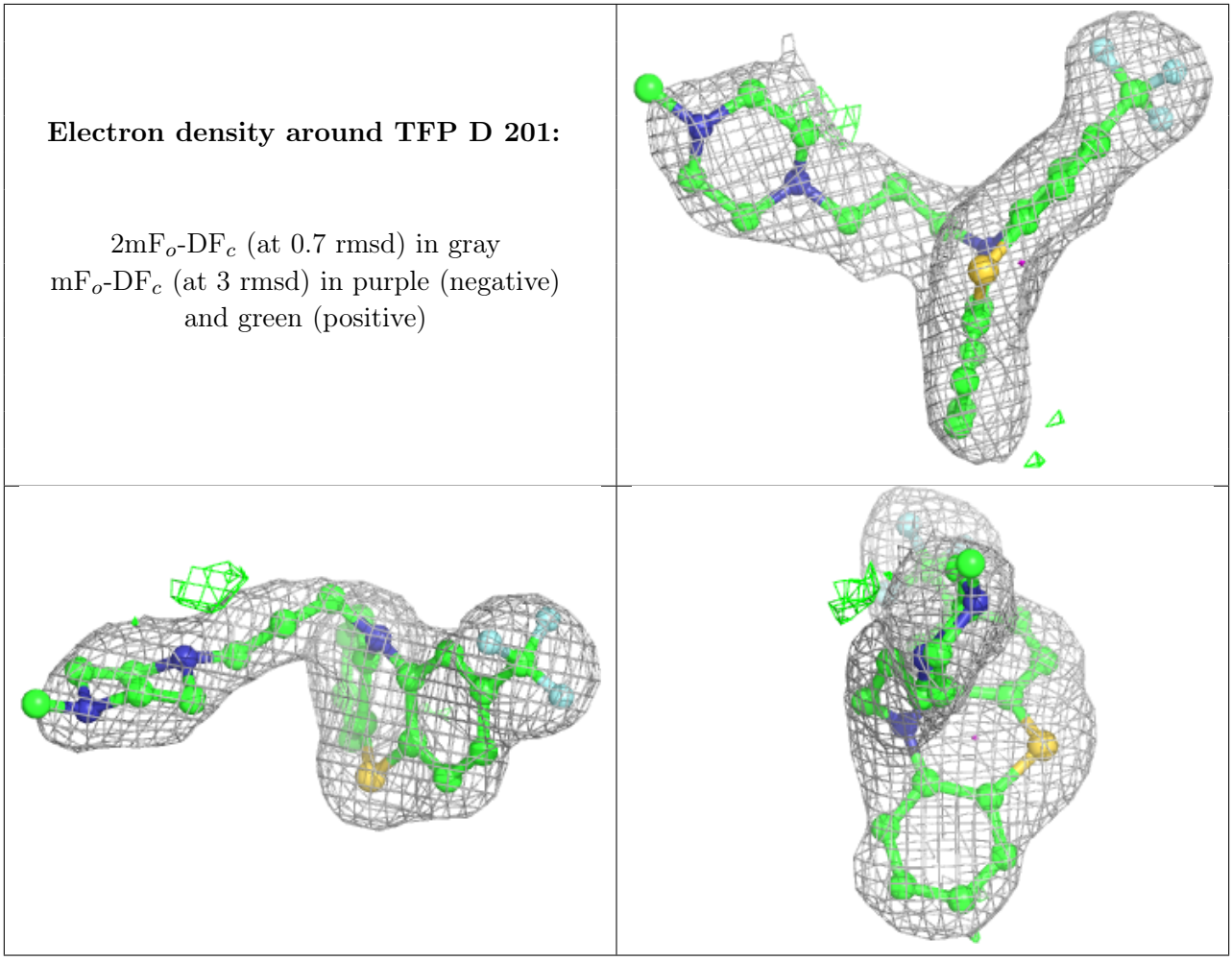






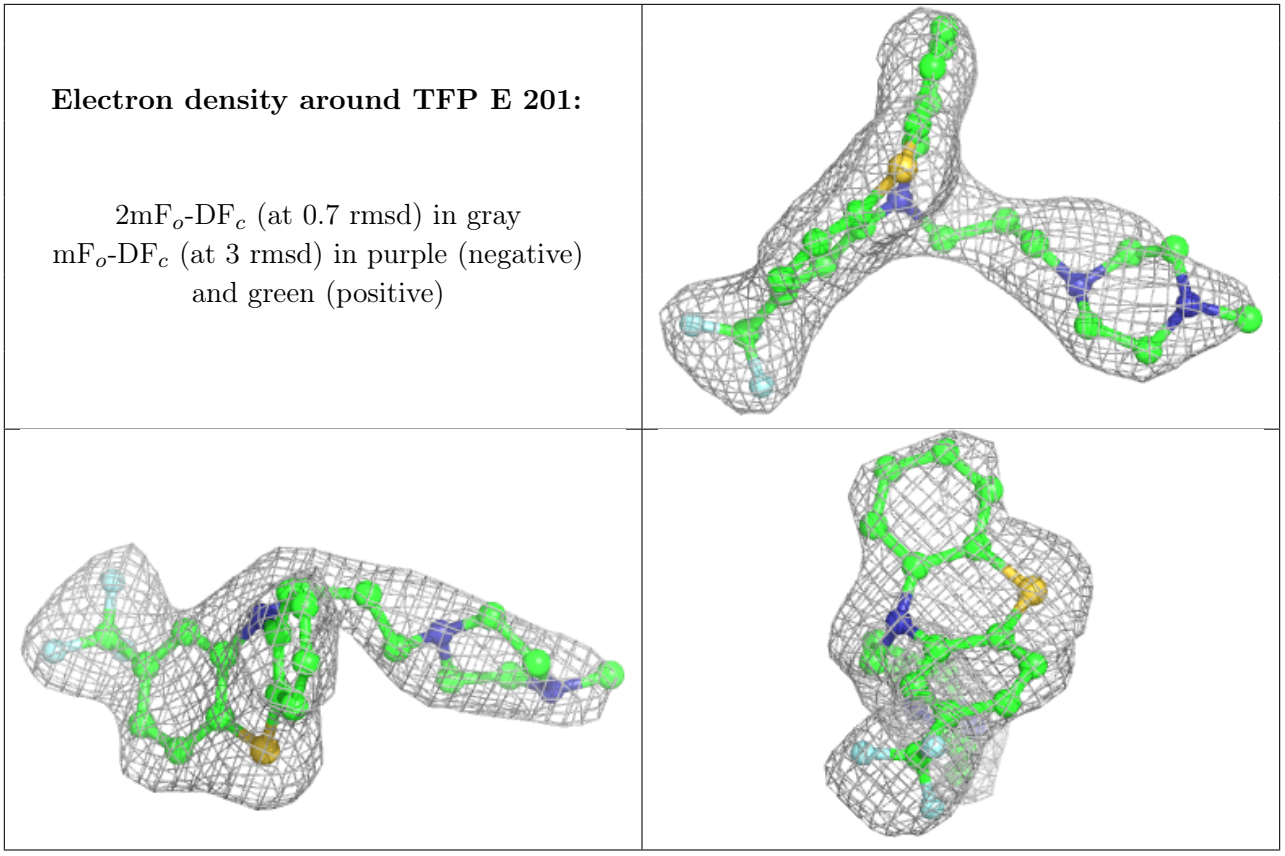
Electron density around TFP D 201:

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



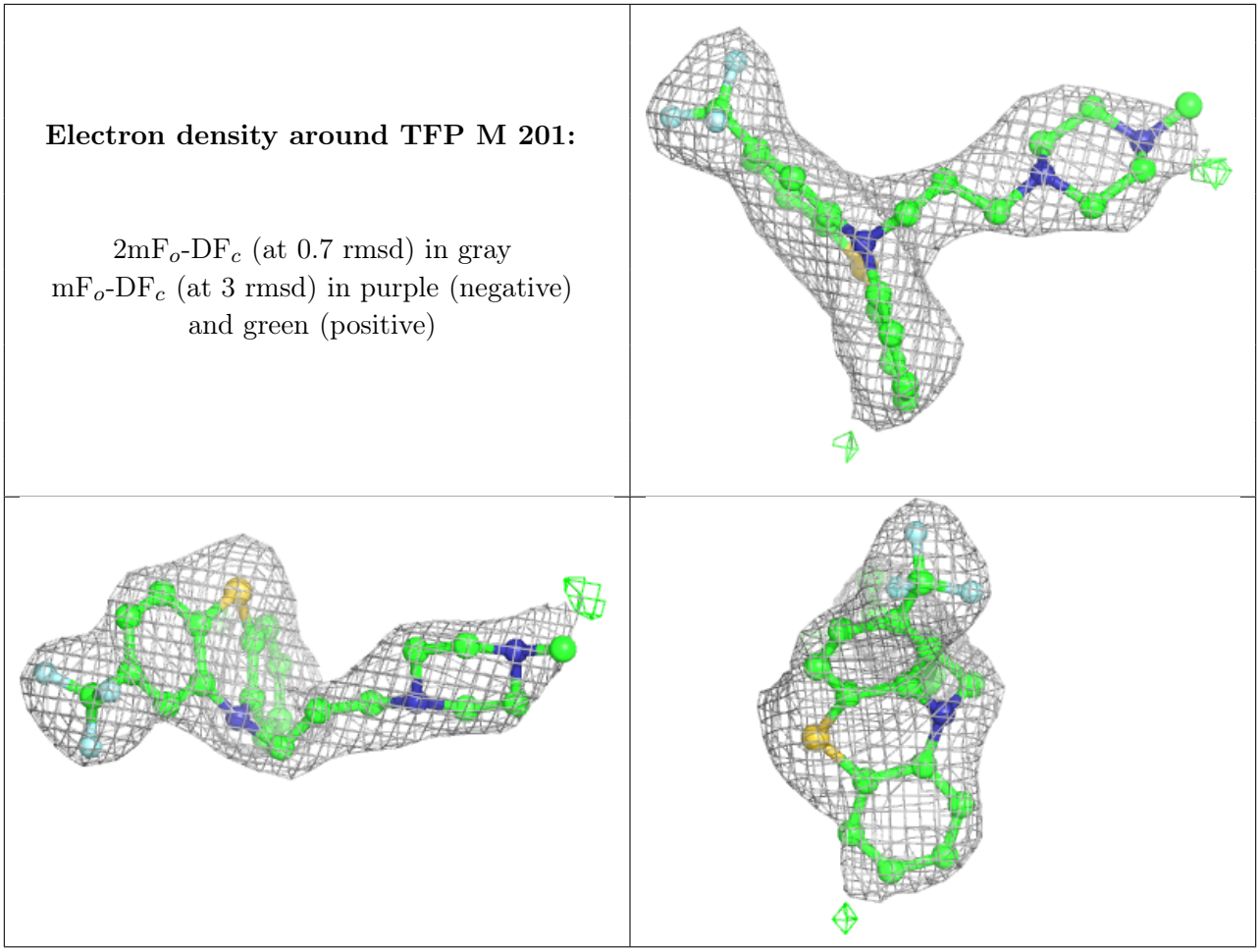
Electron density around TFP E 201:

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



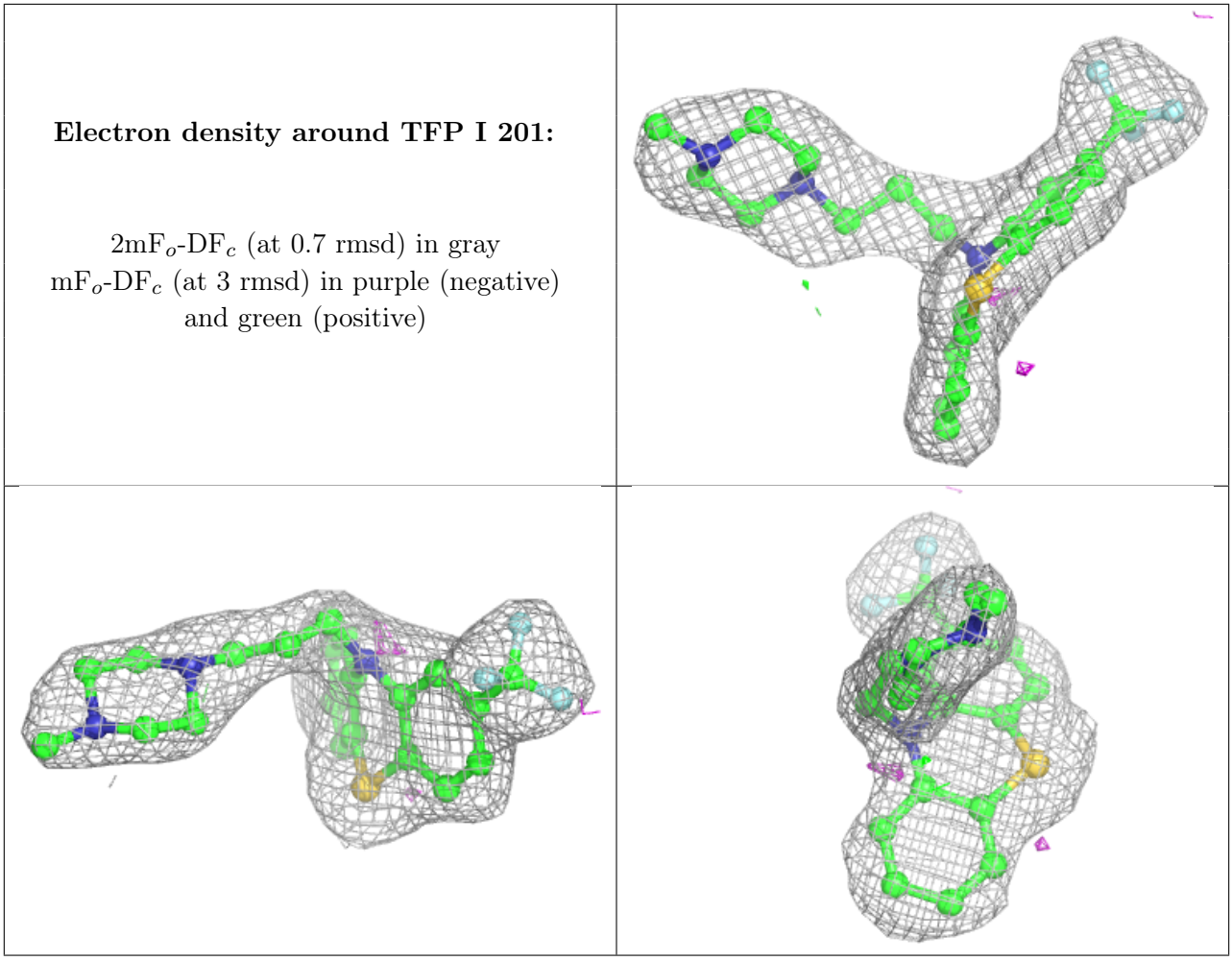
Electron density around TFP M 201:

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



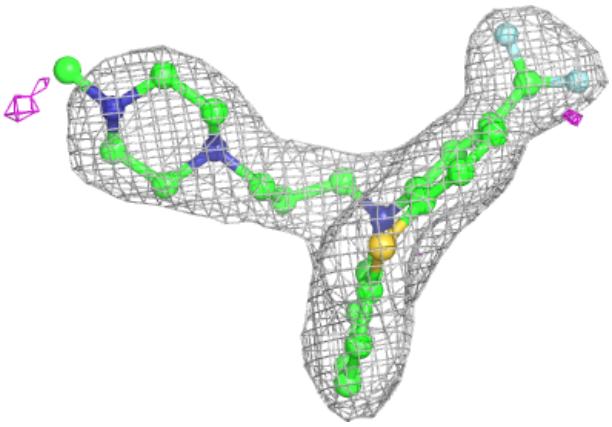
Electron density around TFP I 201:

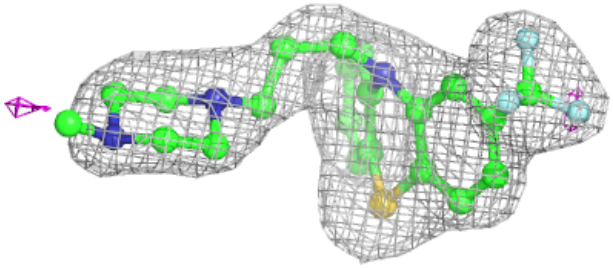
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

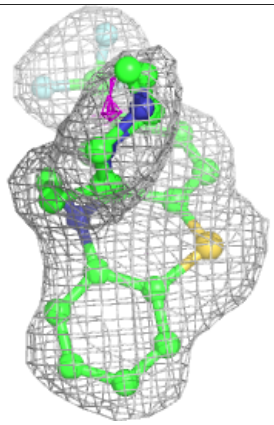


Electron density around TFP K 201:

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

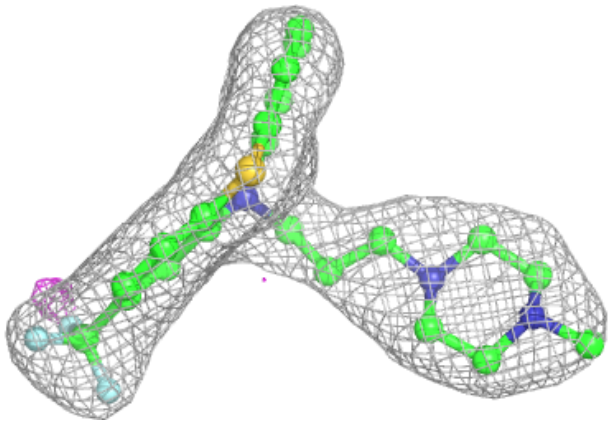


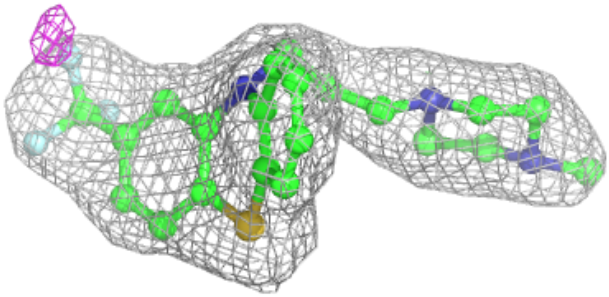


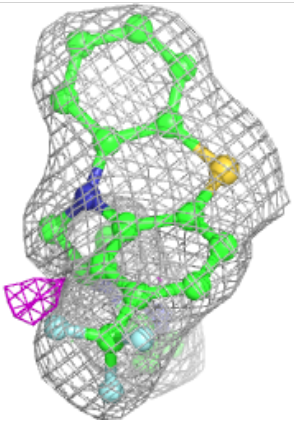


Electron density around TFP R 201:

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

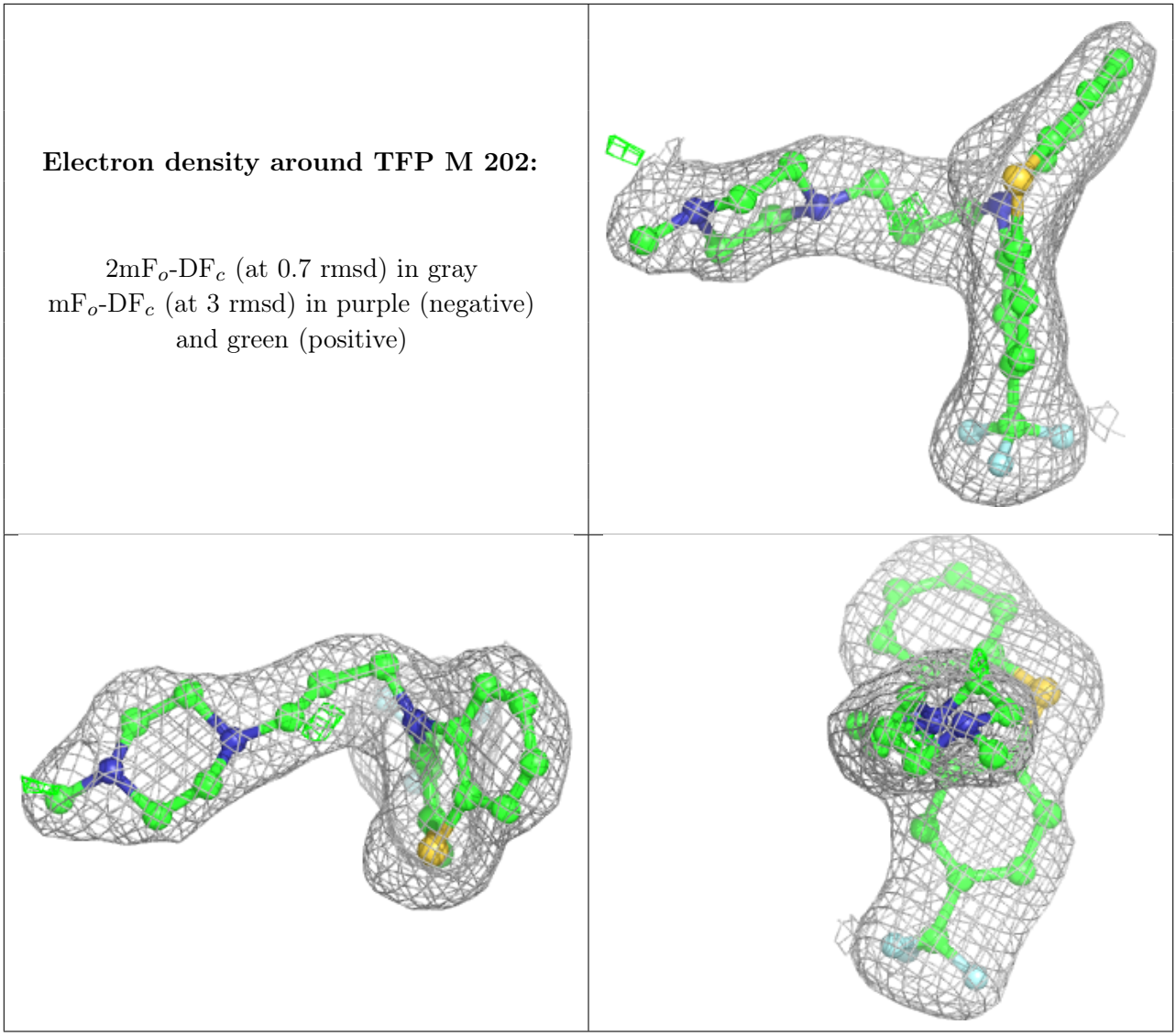






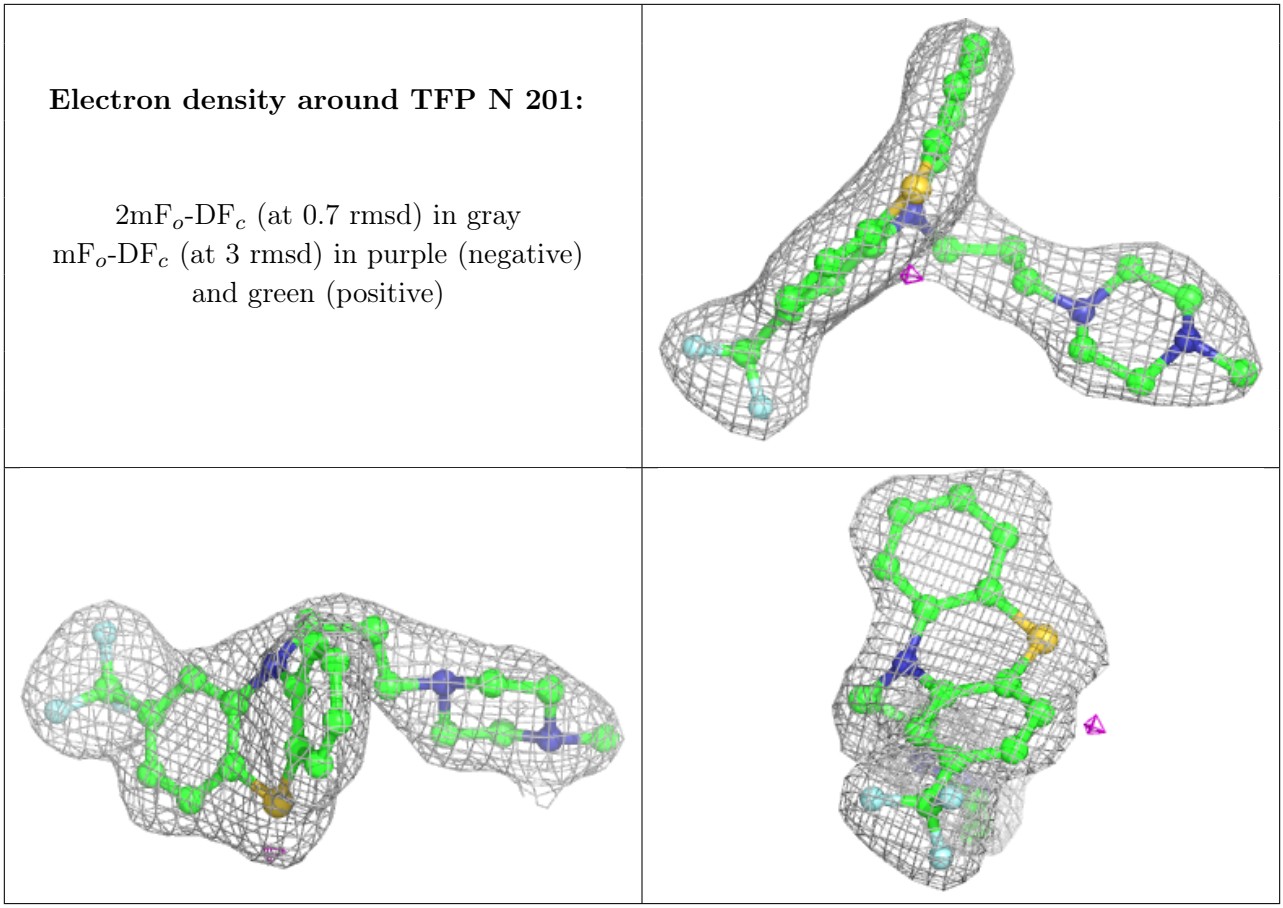
Electron density around TFP M 202:

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



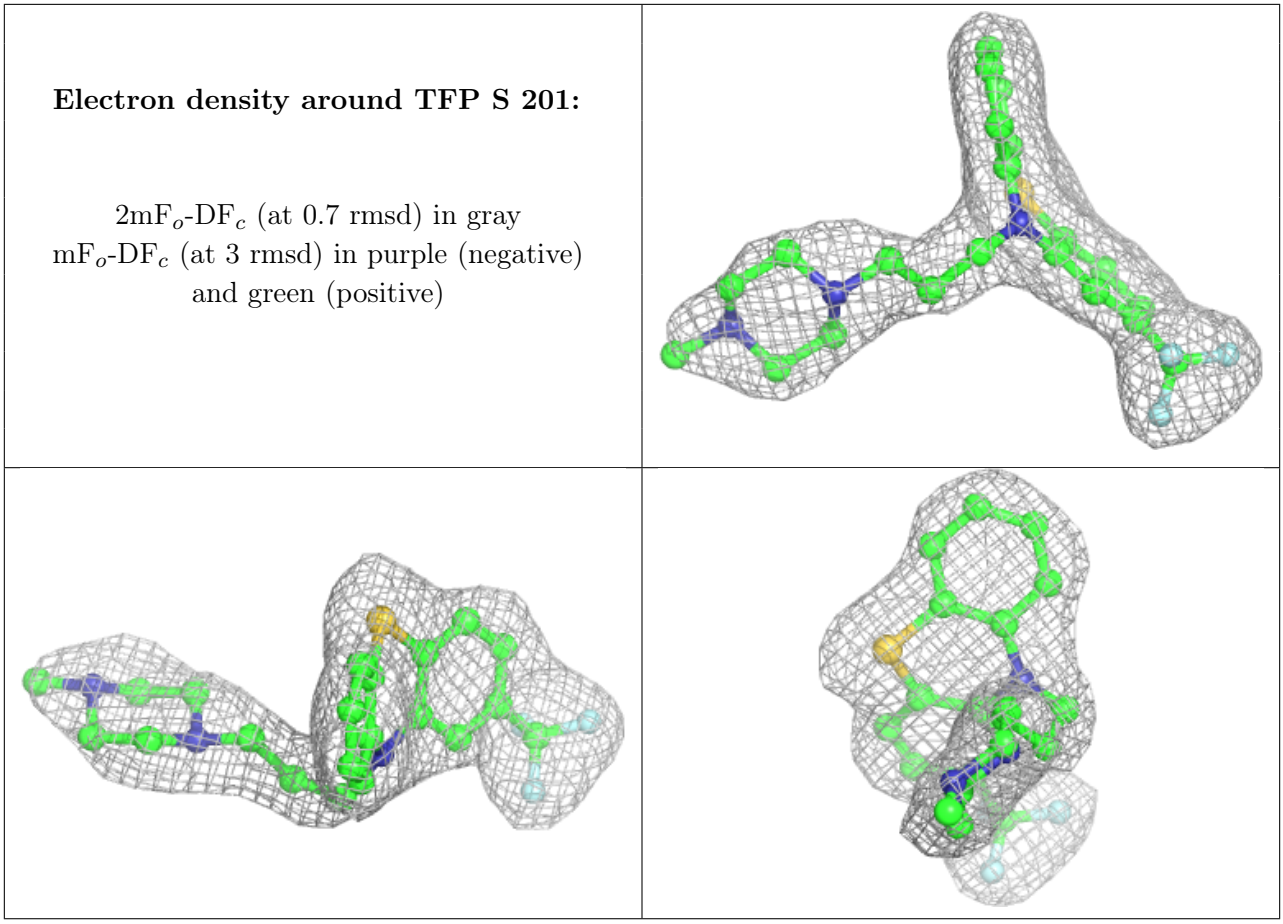
Electron density around TFP N 201:

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



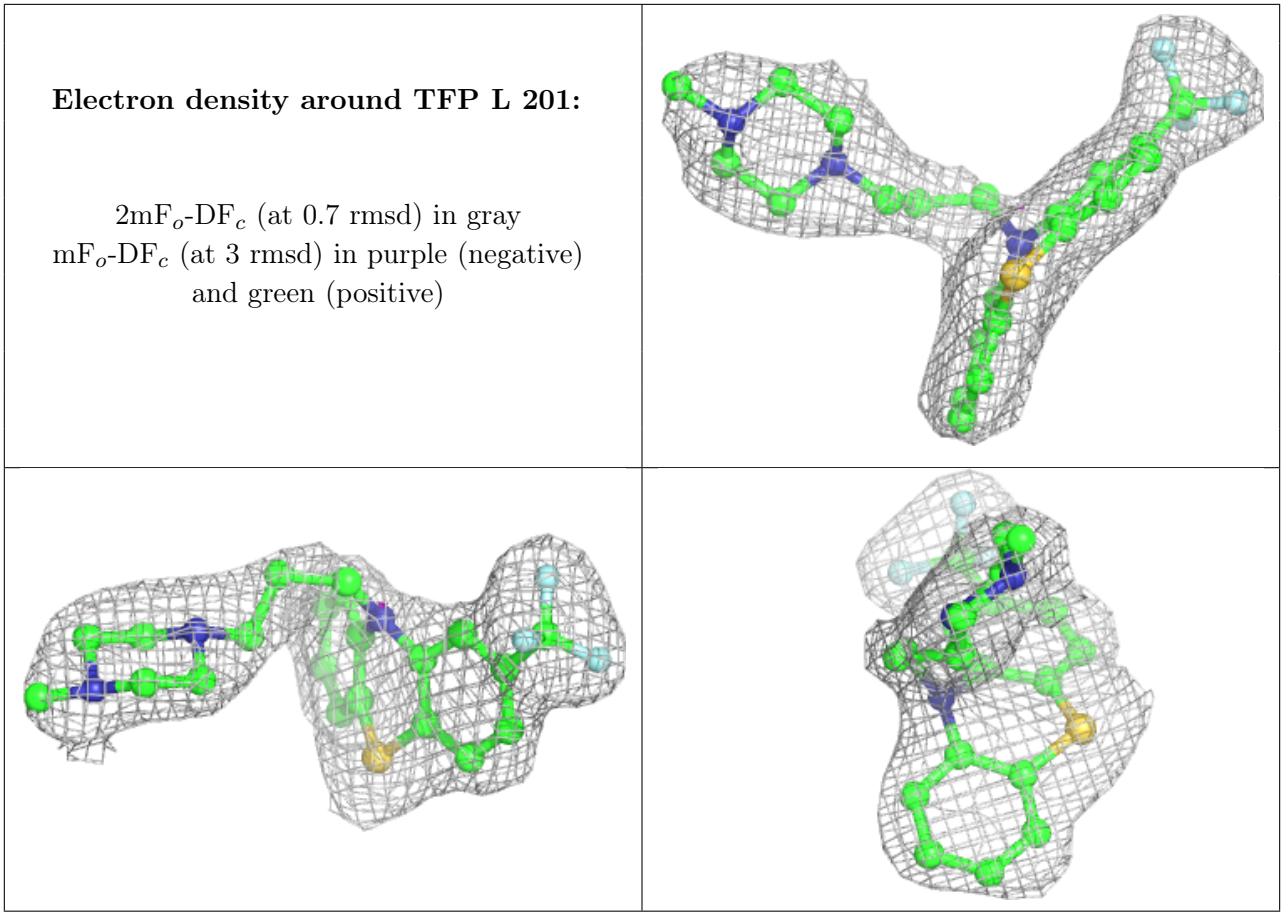
Electron density around TFP S 201:

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



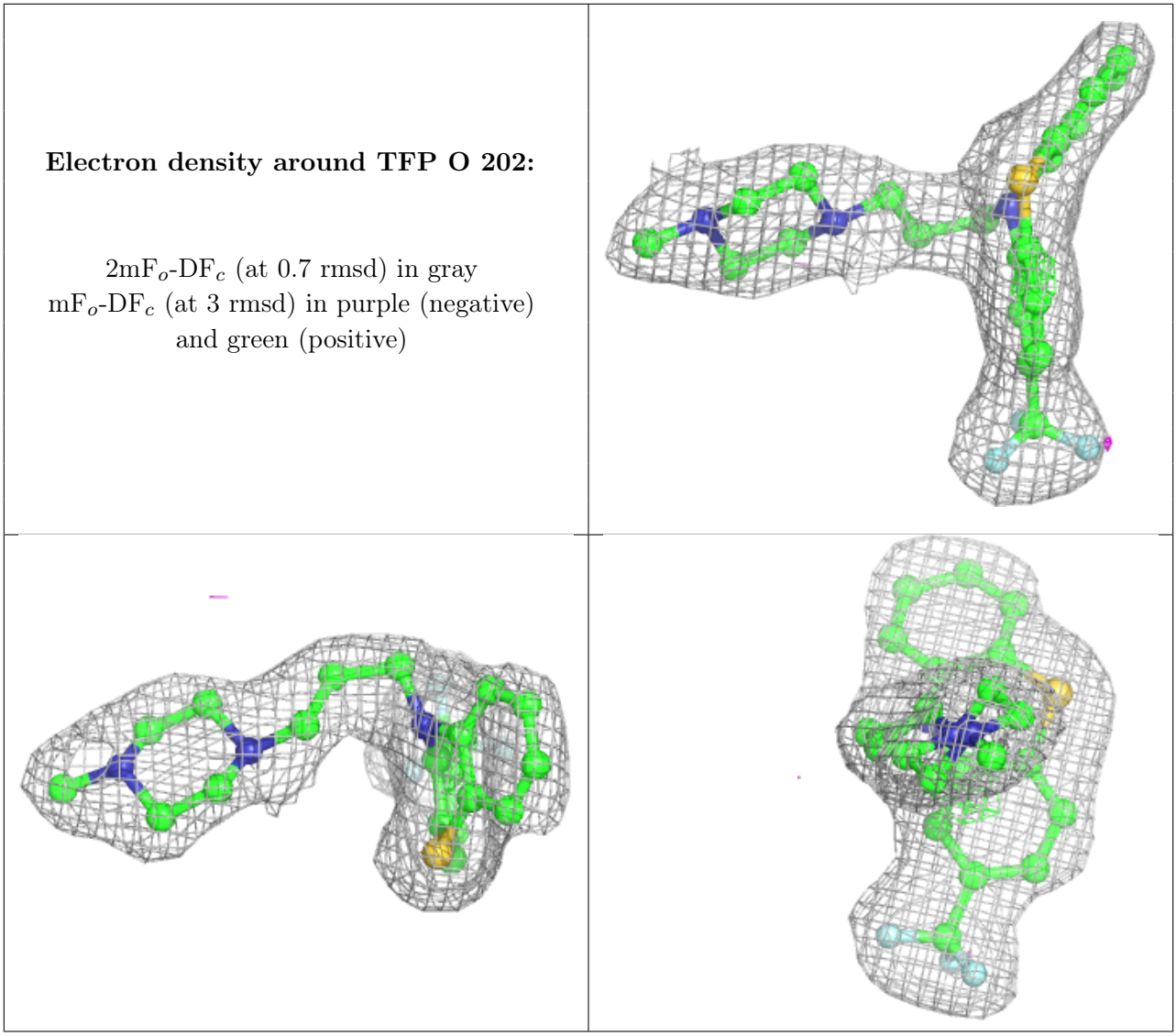
Electron density around TFP L 201:

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



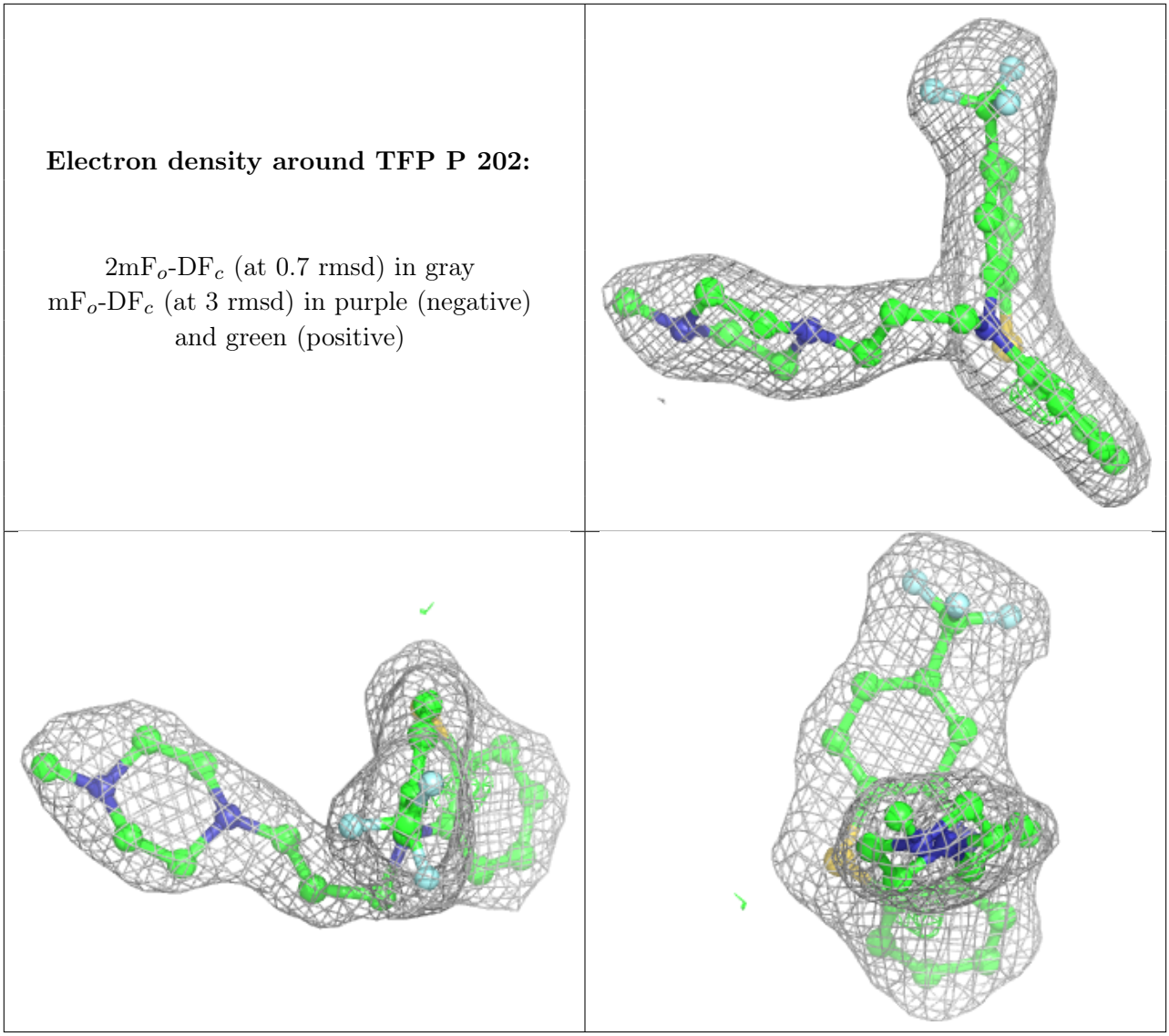
Electron density around TFP O 202:

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



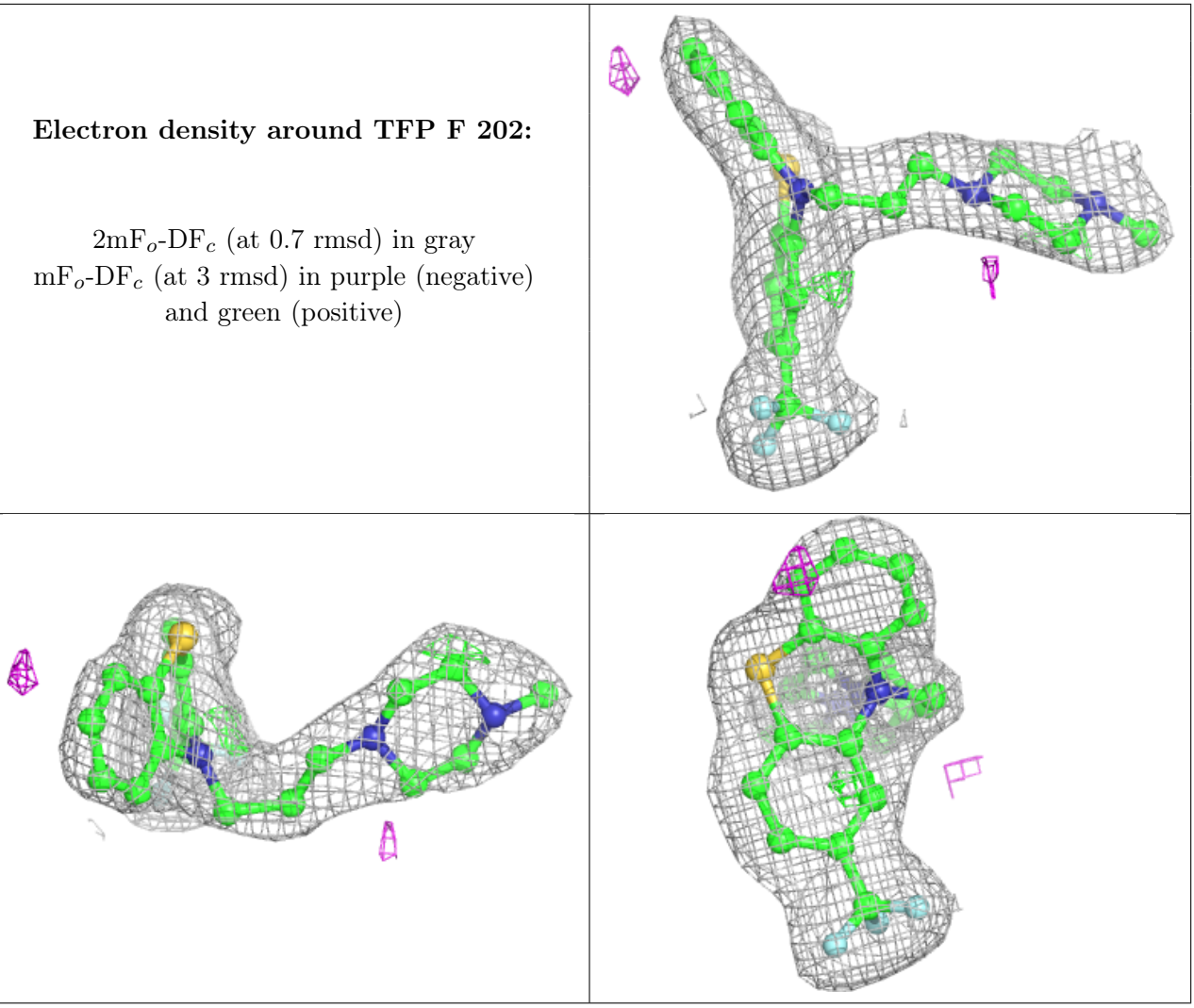
Electron density around TFP P 202:

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



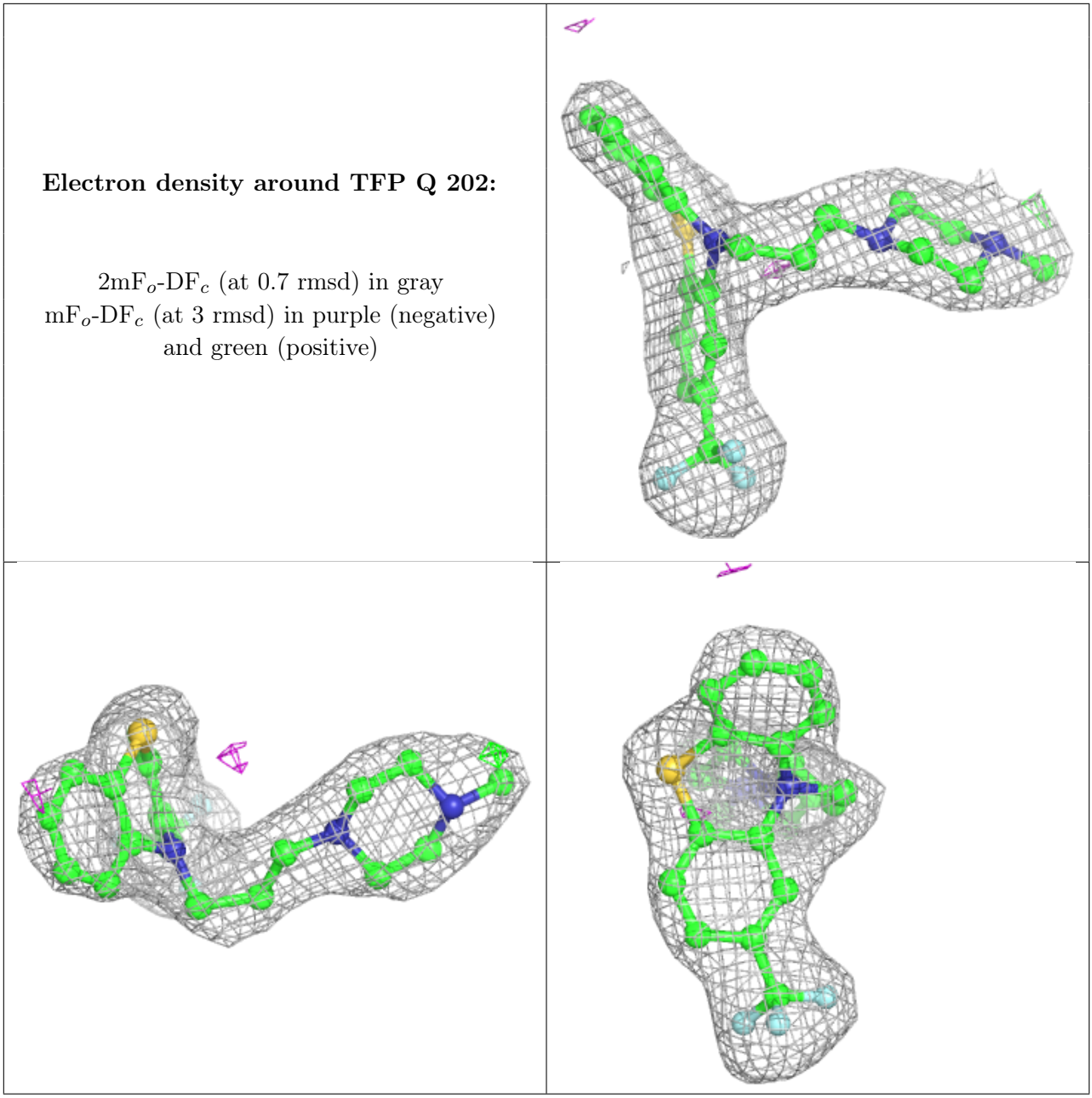
Electron density around TFP F 202:

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



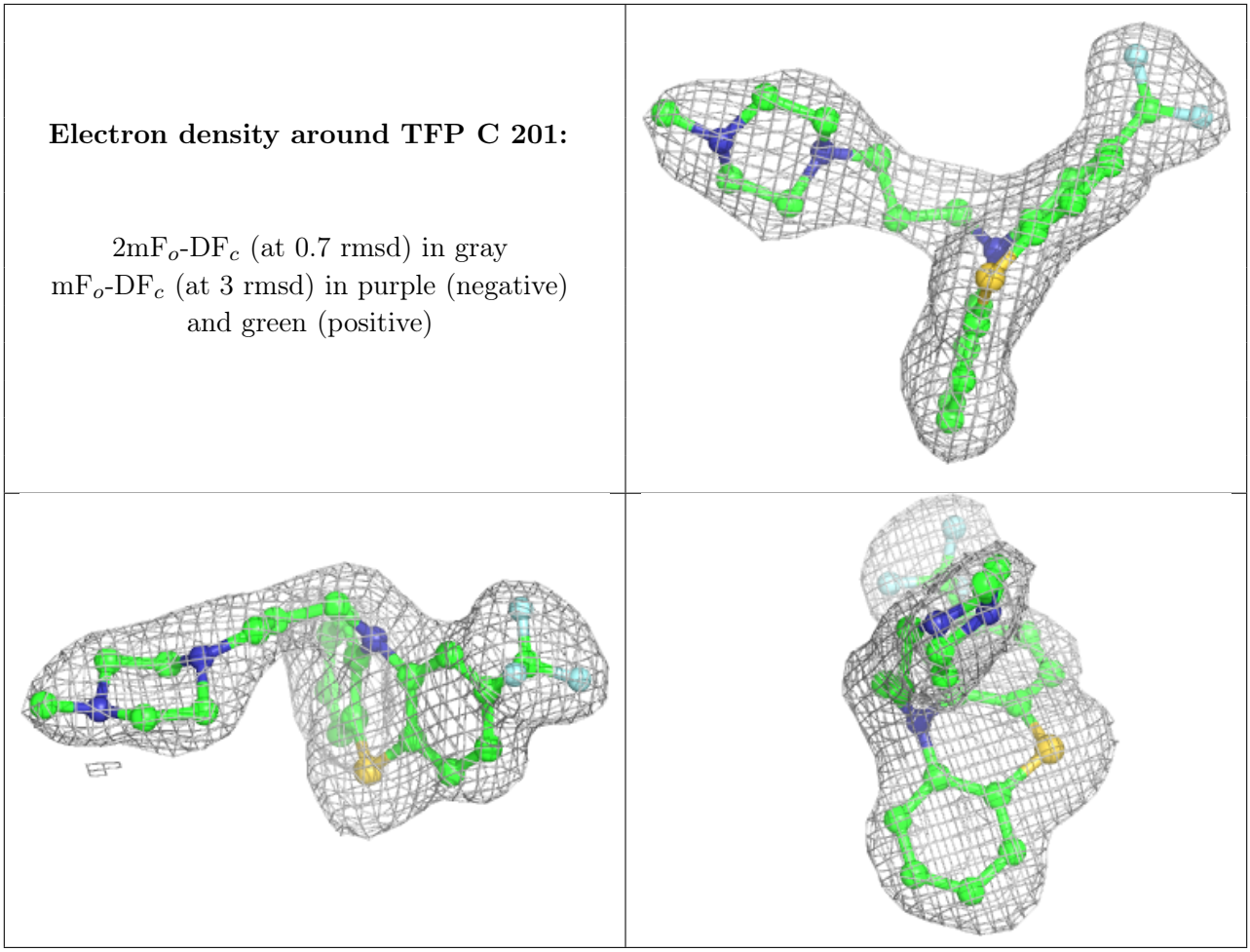
Electron density around TFP Q 202:

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



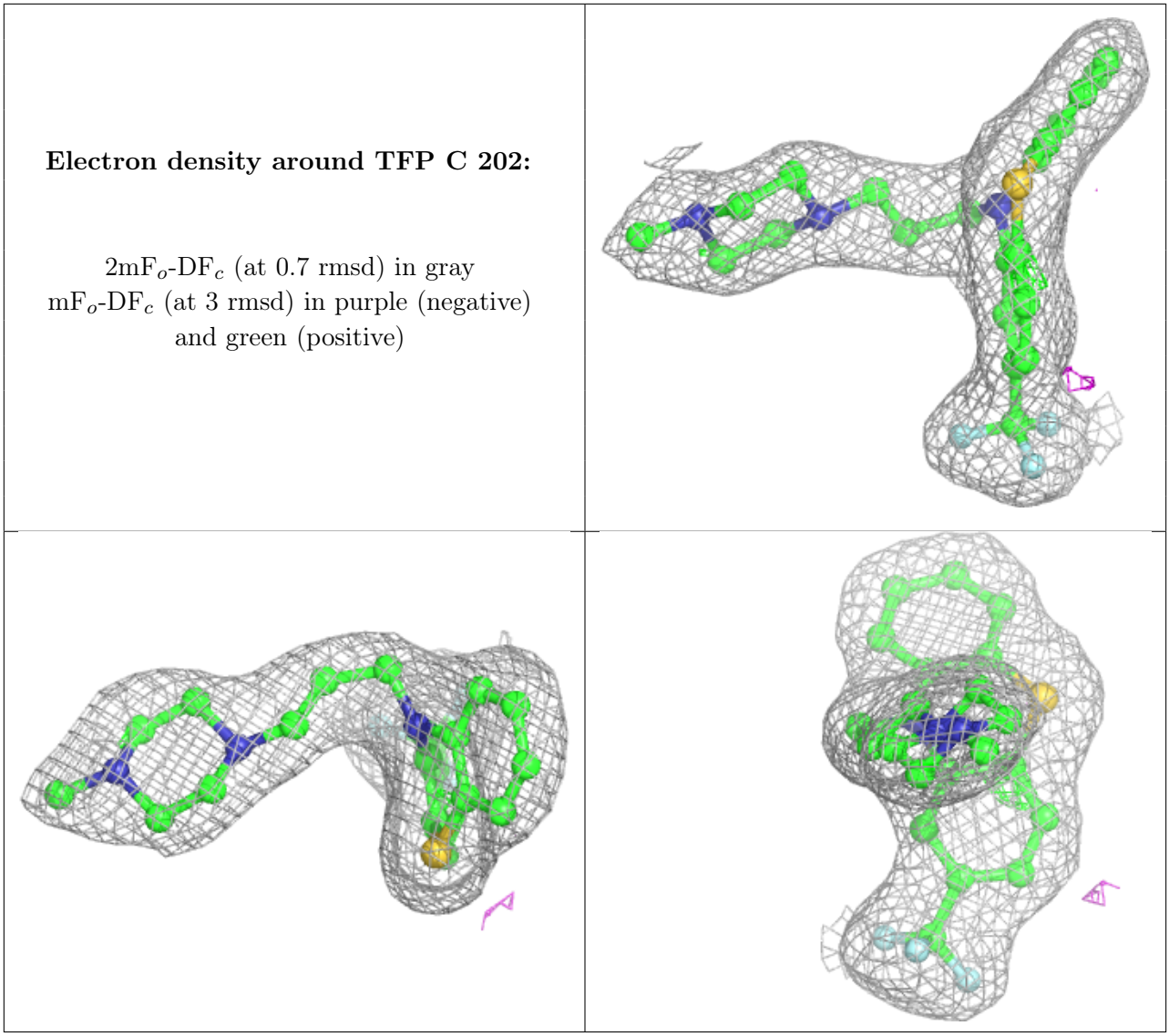
Electron density around TFP C 201:

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



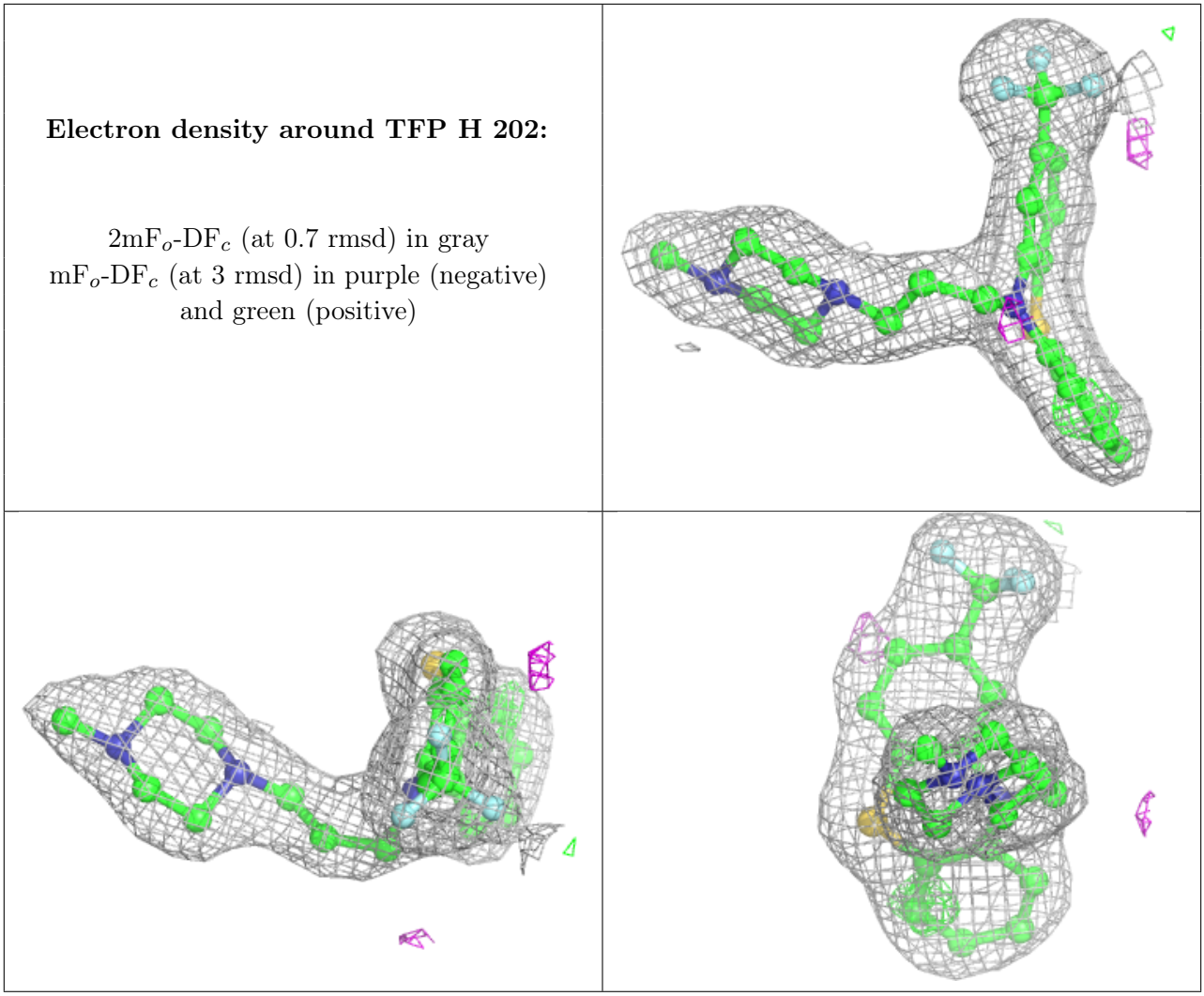
Electron density around TFP C 202:

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



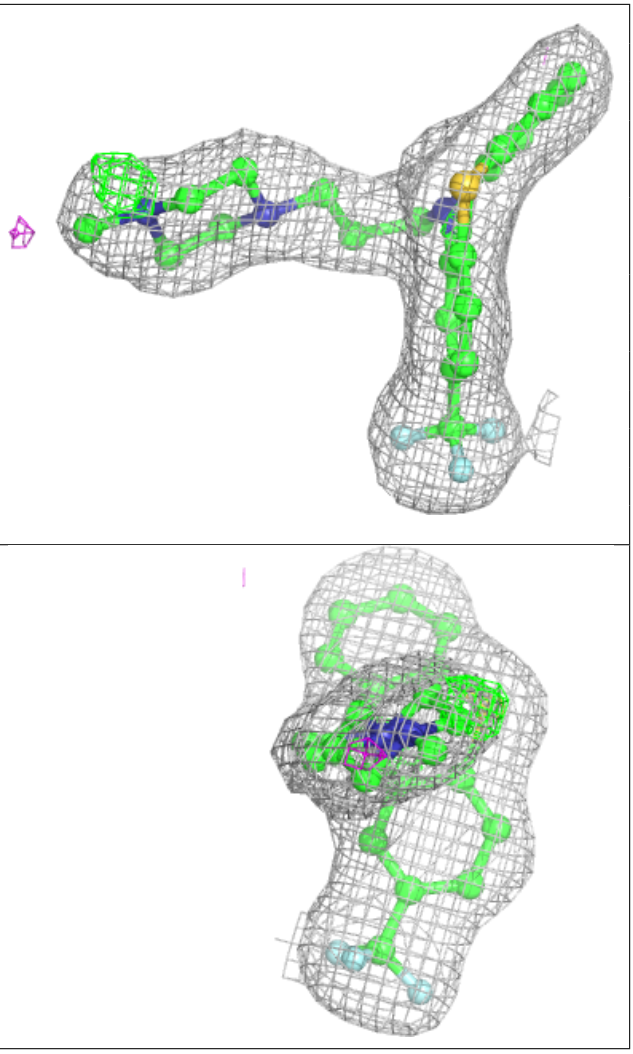
Electron density around TFP H 202:

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



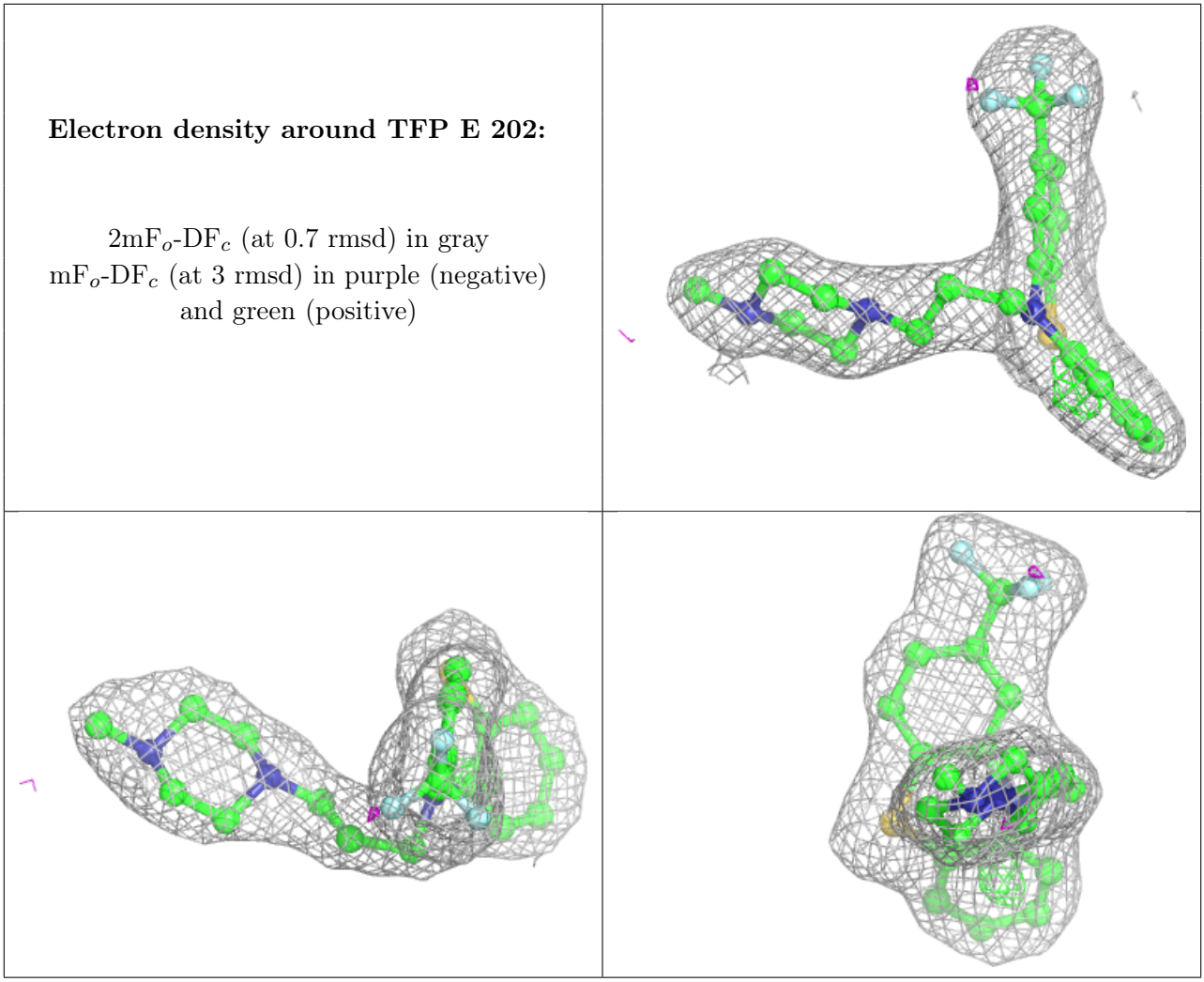
Electron density around TFP I 202:

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



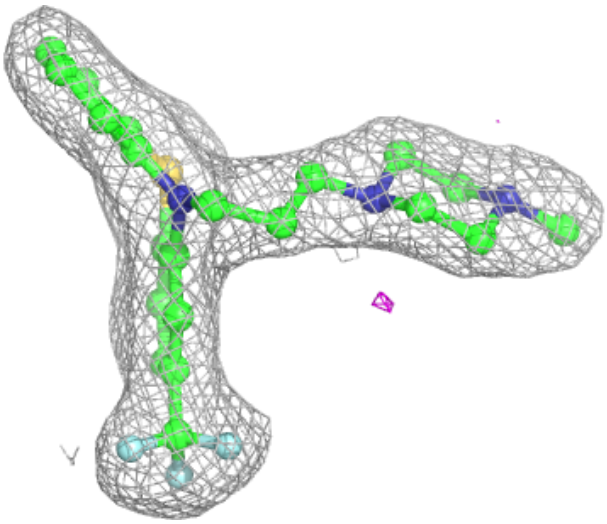
Electron density around TFP E 202:

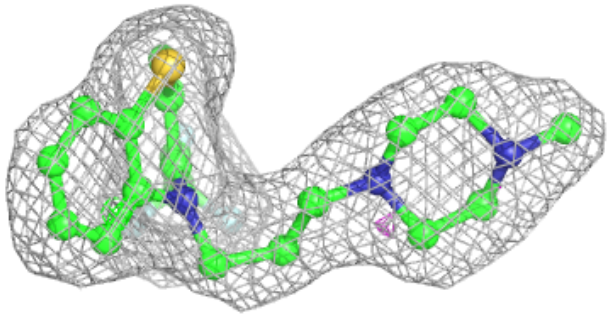
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

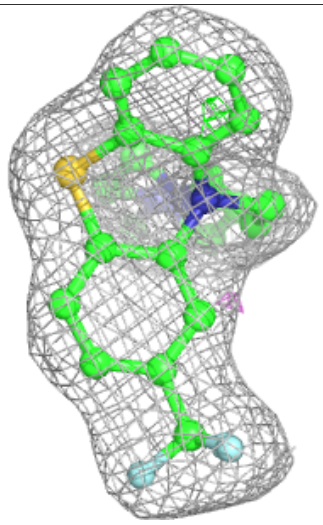


Electron density around TFP K 202:

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

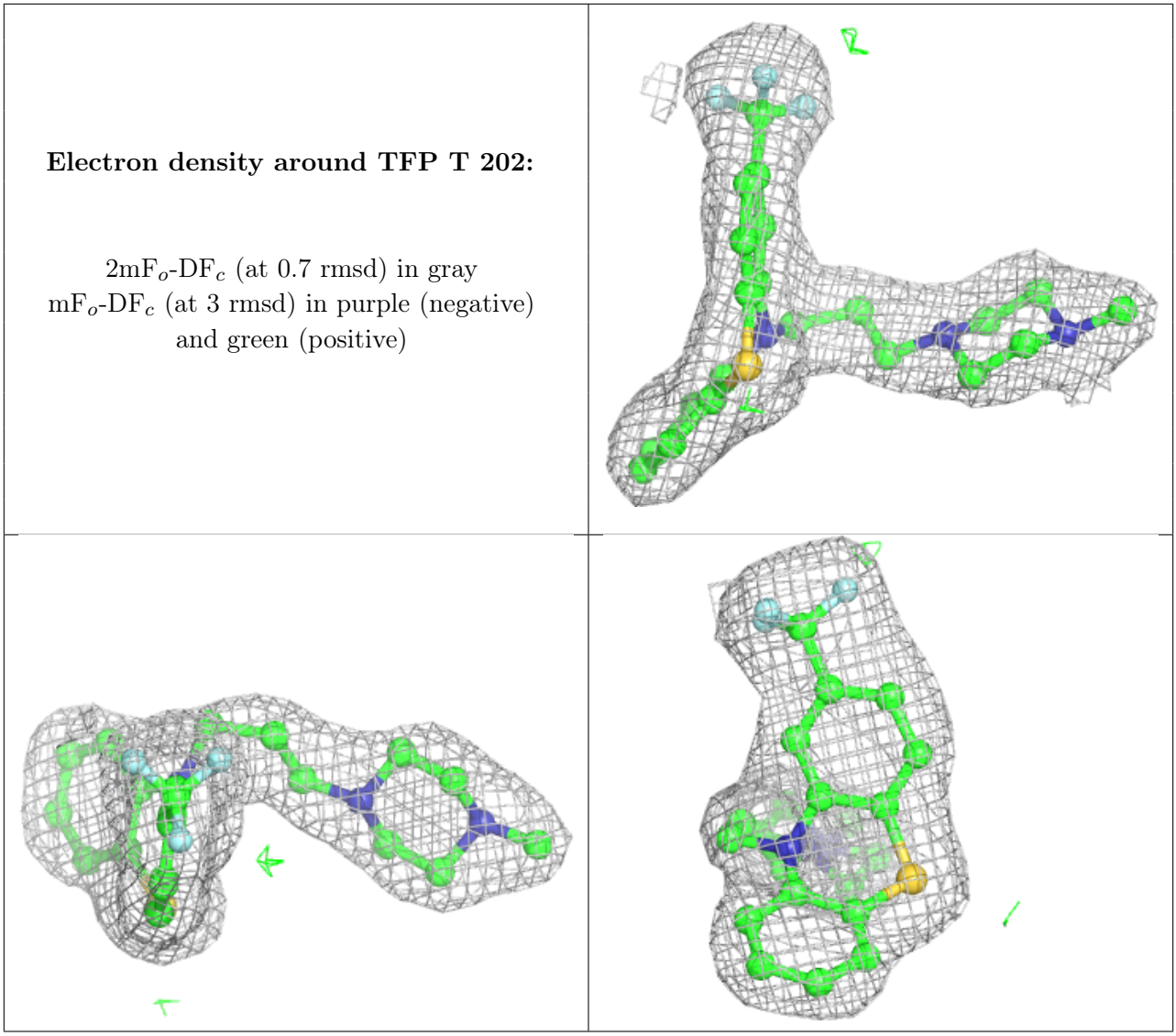






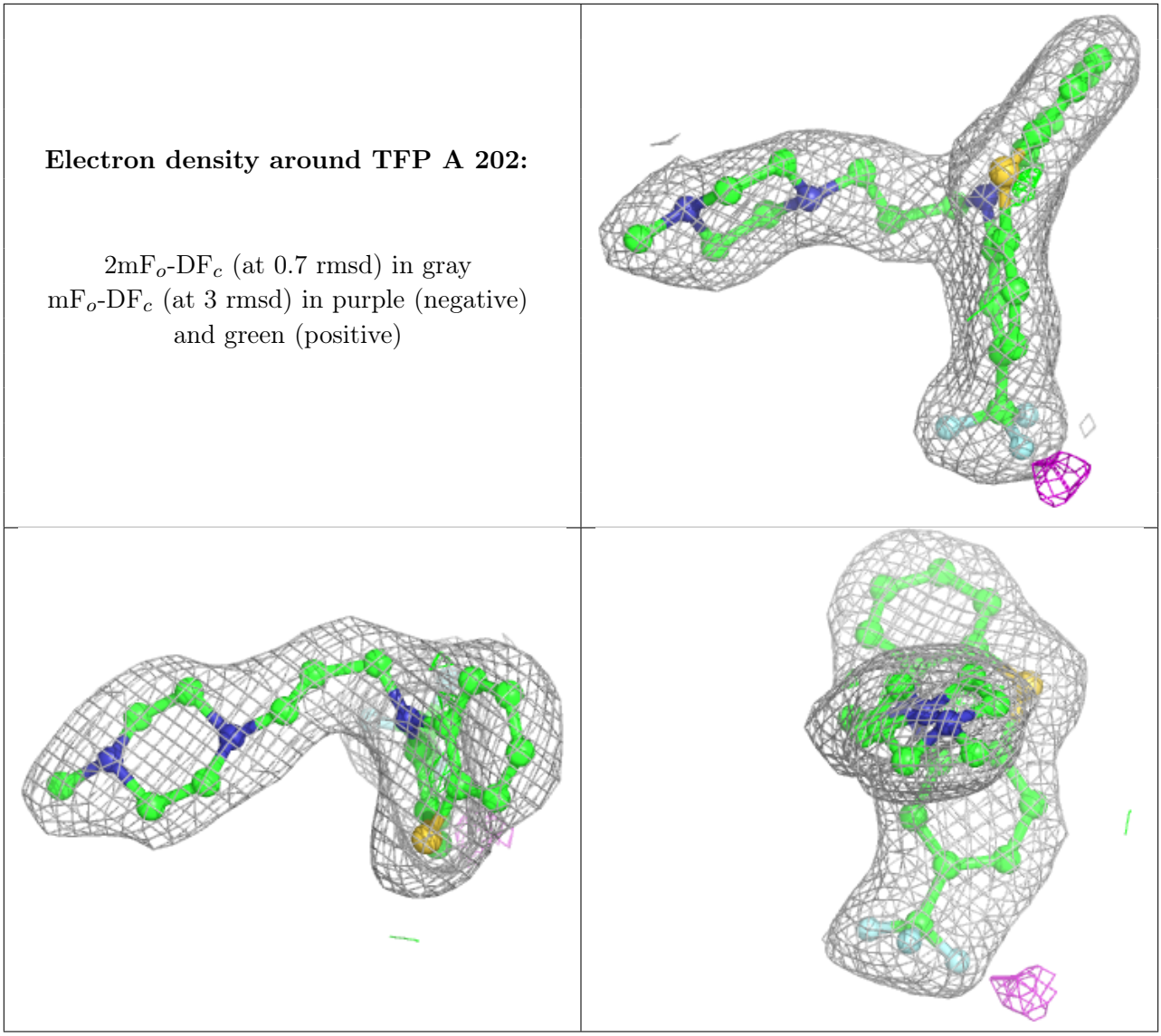
Electron density around TFP T 202:

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



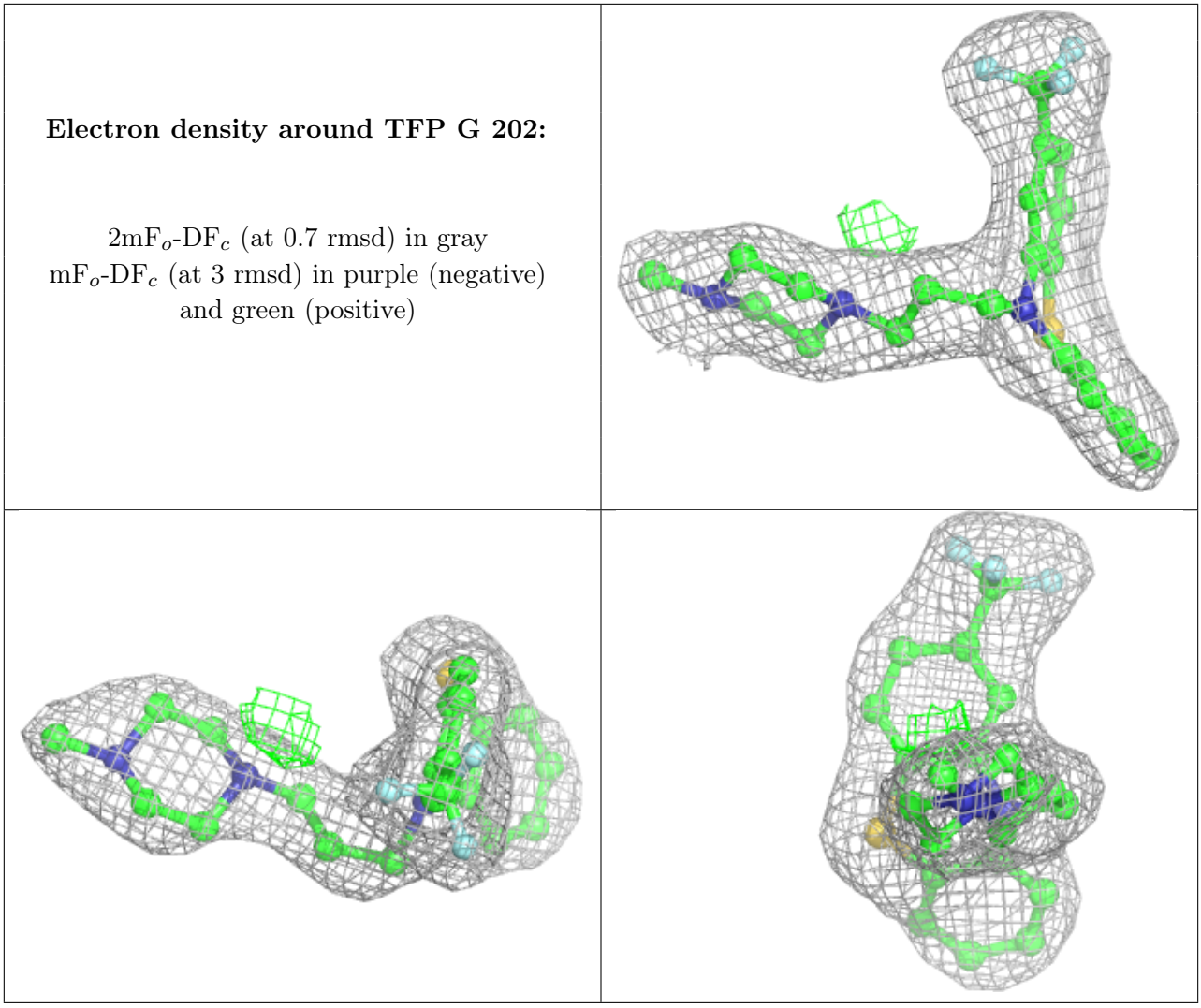
Electron density around TFP A 202:

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



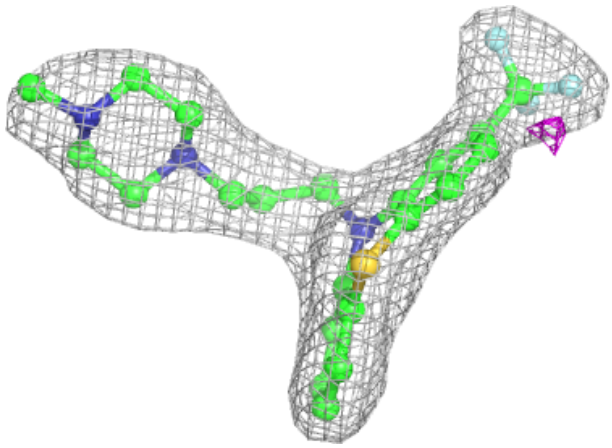
Electron density around TFP G 202:

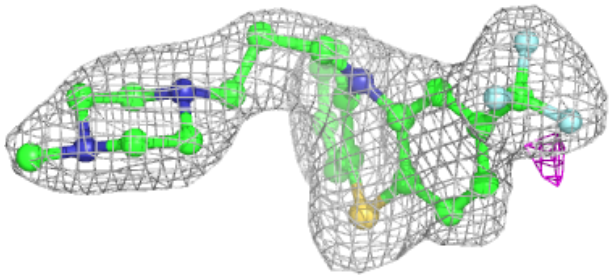
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

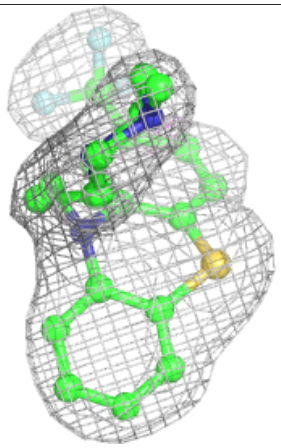


Electron density around TFP A 201:

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

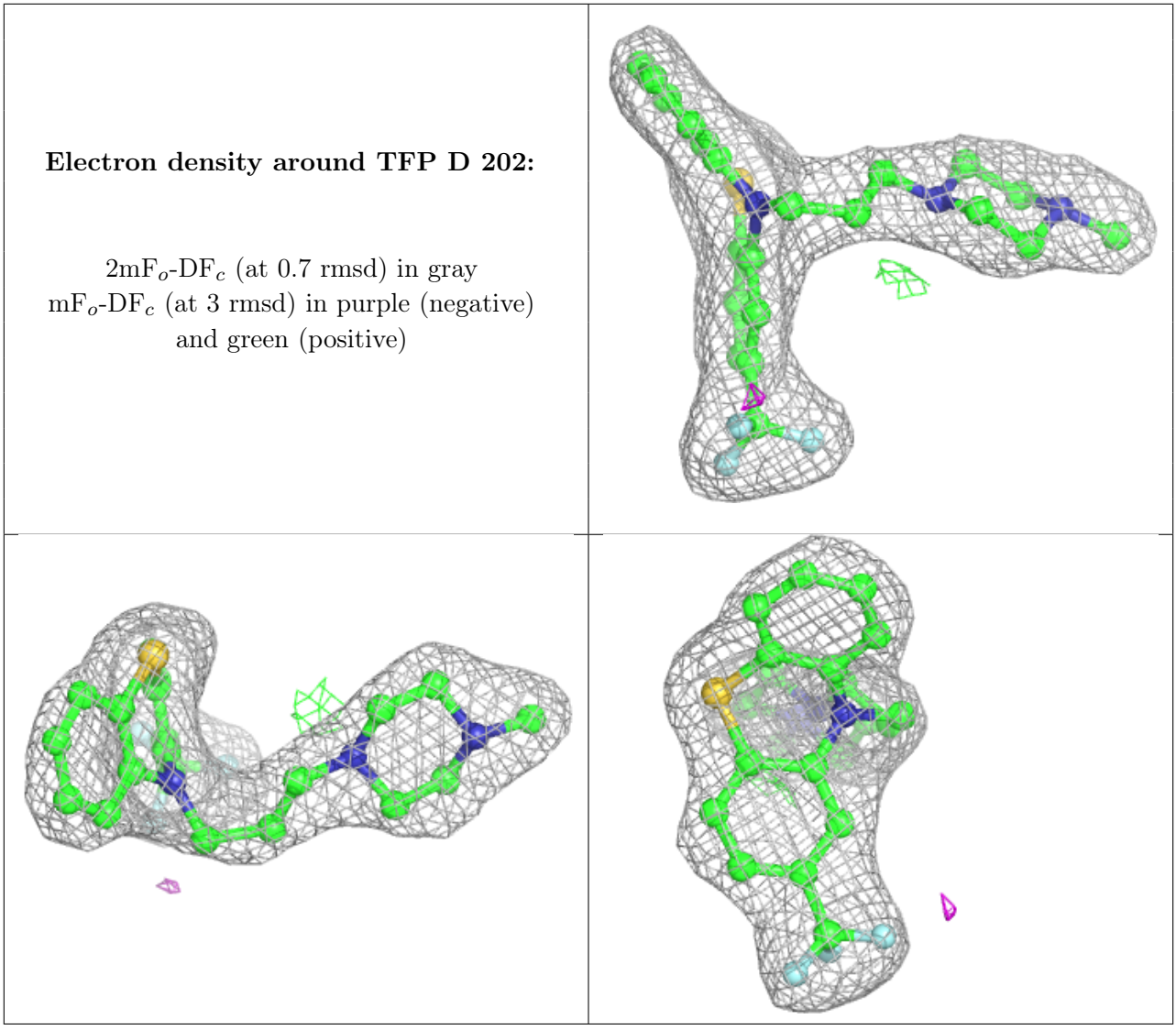






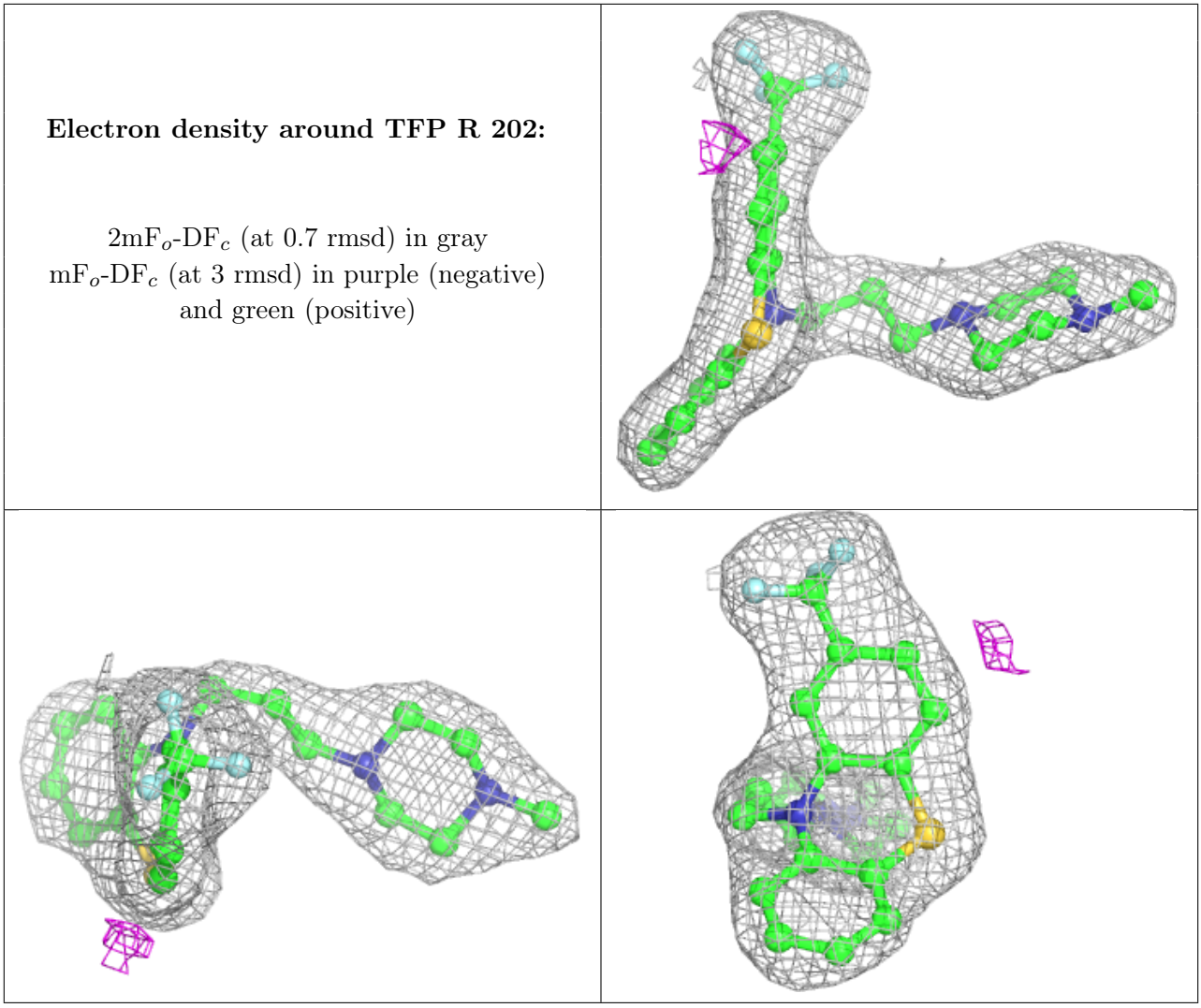
Electron density around TFP D 202:

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



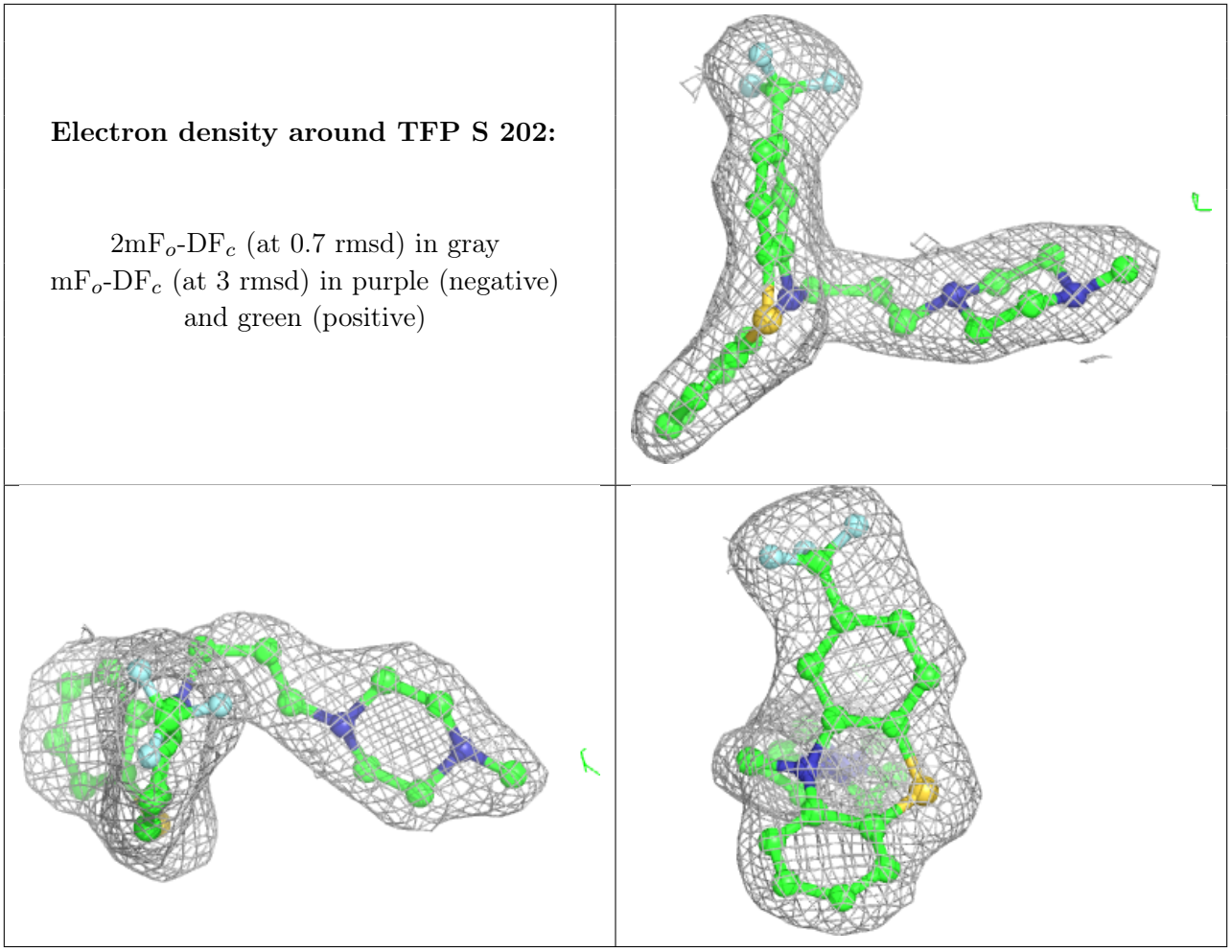
Electron density around TFP R 202:

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



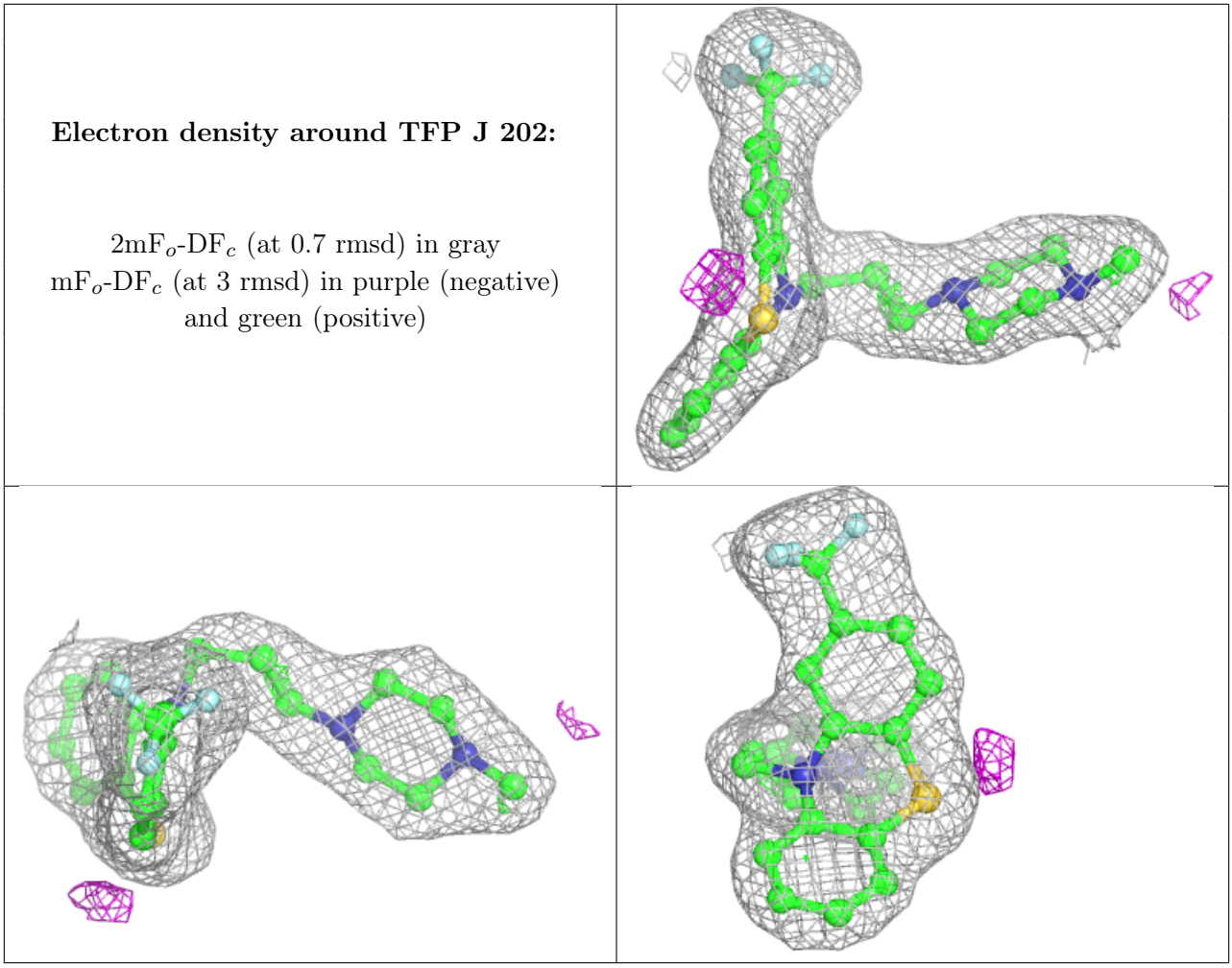
Electron density around TFP S 202:

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



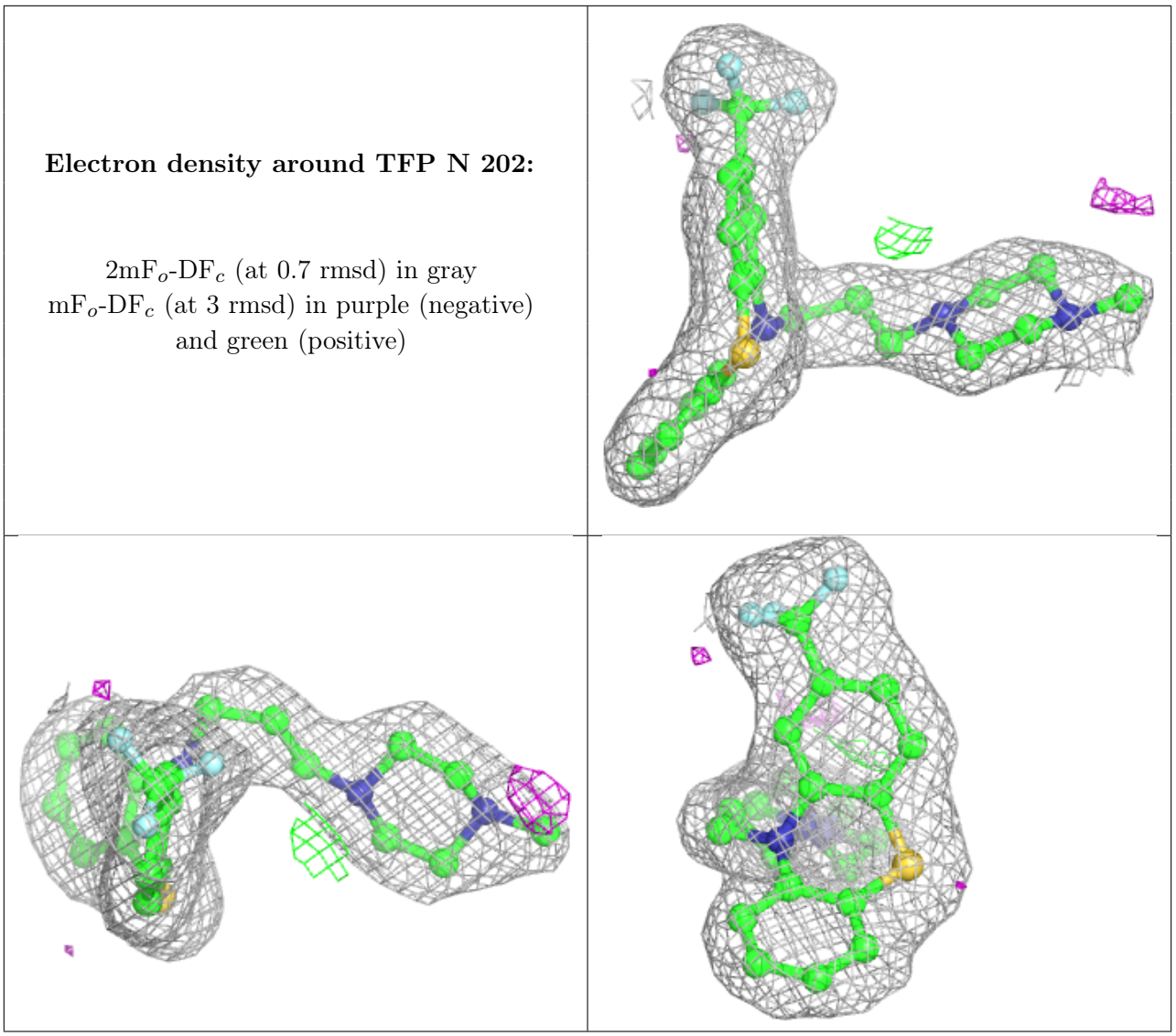
Electron density around TFP J 202:

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



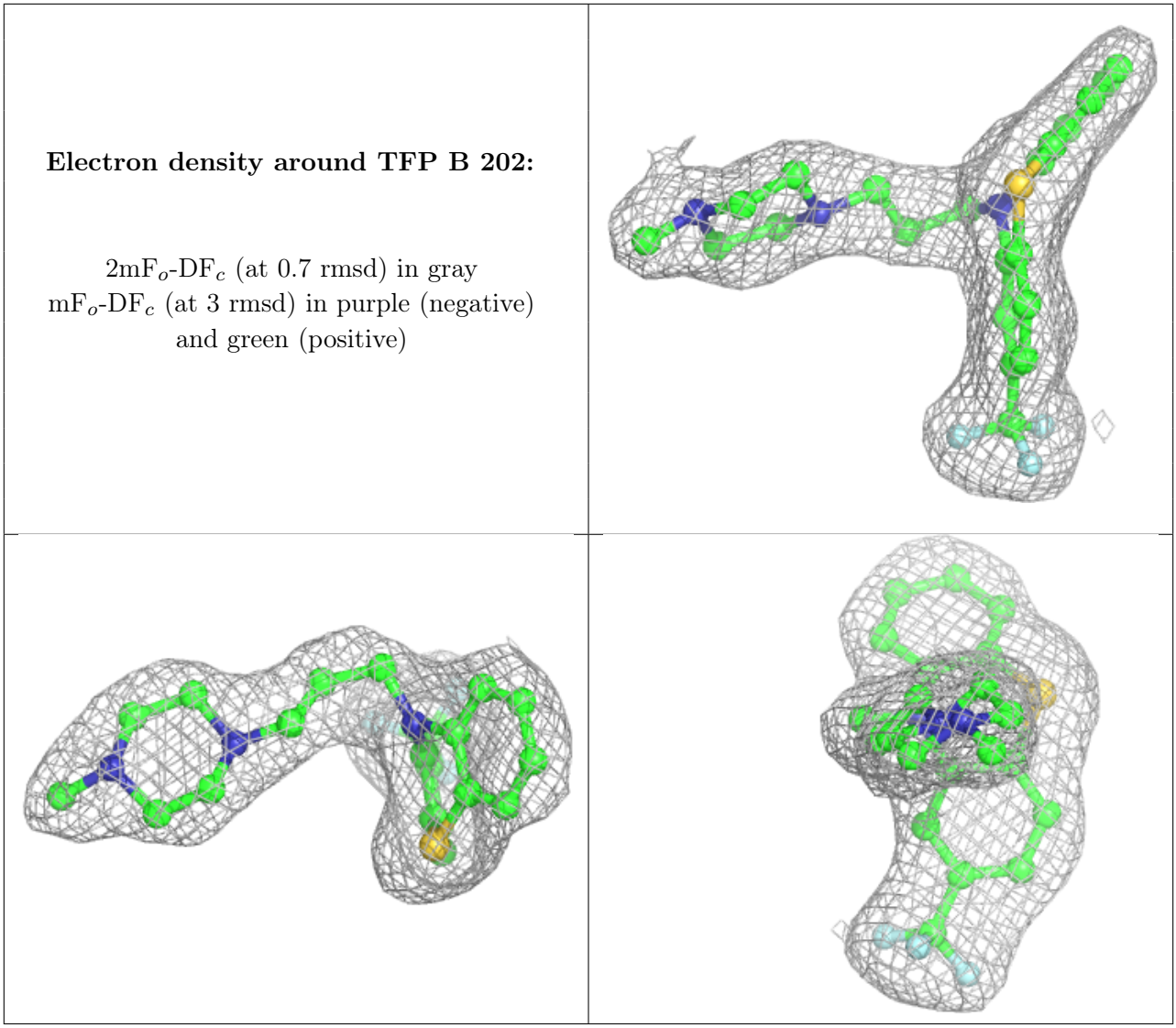
Electron density around TFP N 202:

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



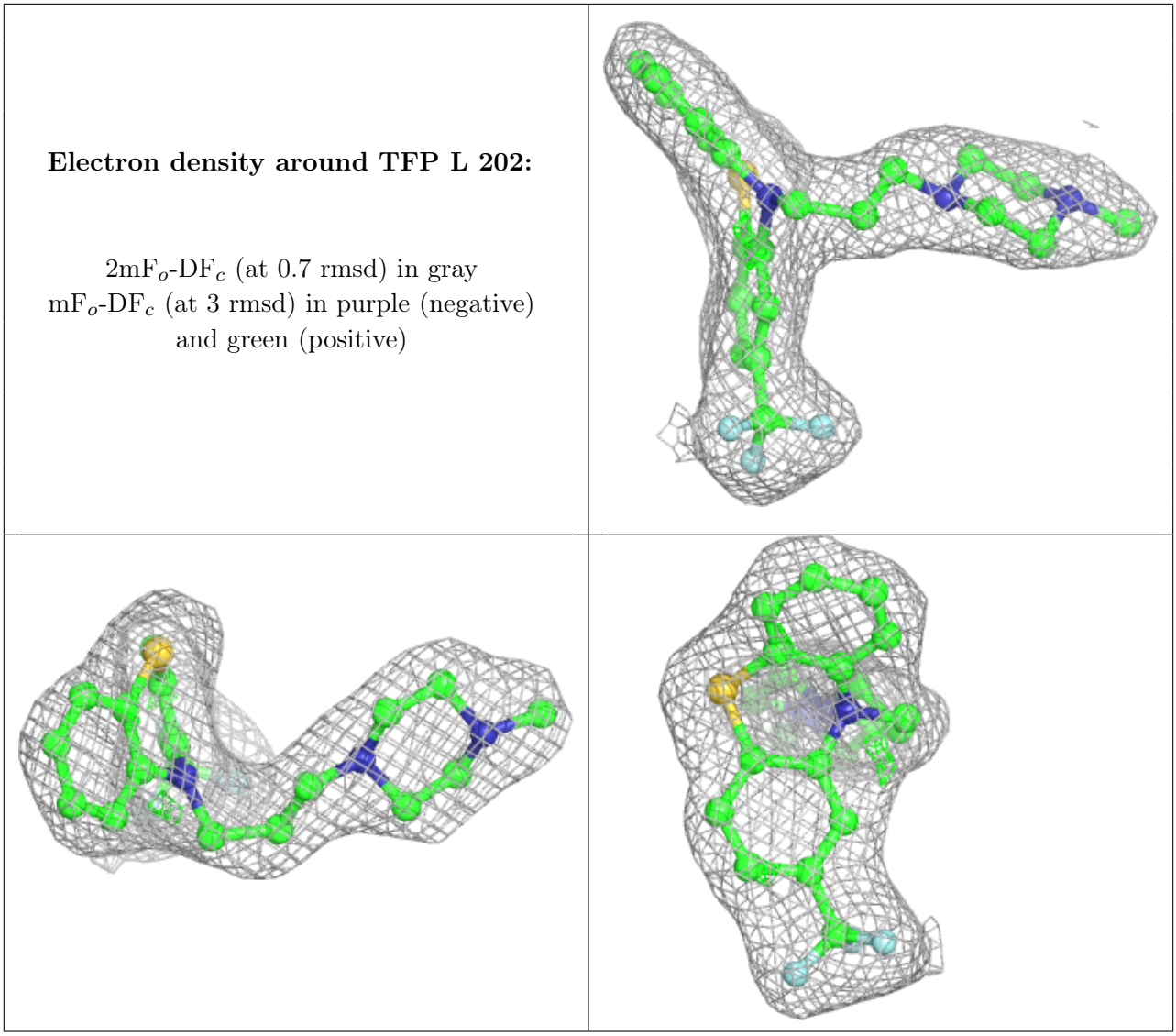
Electron density around TFP B 202:

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



Electron density around TFP L 202:

$2mF_o$-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.