Full wwPDB X-ray Structure Validation Report ⓘ

Apr 29, 2024 – 07:40 am BST

PDB ID	:	6FRN
Title	:	Structure of F420H2 oxidase (FprA) co-crystallized with 10mM Tb-Xo4 and calcium chloride
Authors	:	Engilberge, S.; Riobe, F.; Di Pietro, S.; Wagner, T.; Shima, S.; Girard, E.; Dumont, E.; Maury, O.
Deposited on	:	2018-02-16
Resolution	:	1.74 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:

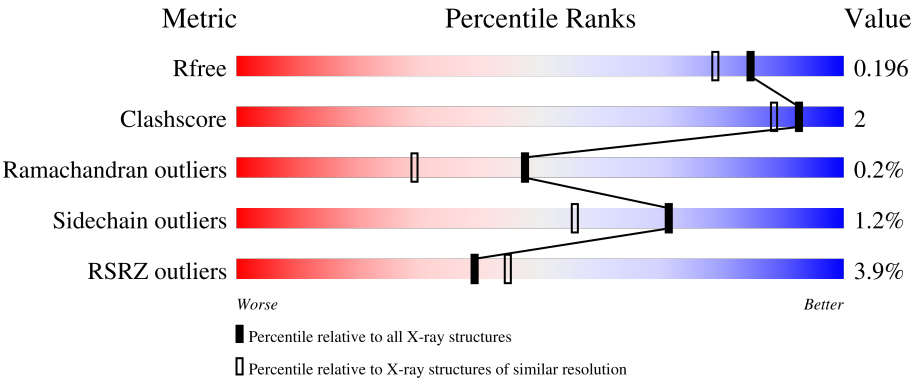
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 1.74 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	3764 (1.76-1.72)
Clashscore	141614	3923 (1.76-1.72)
Ramachandran outliers	138981	3878 (1.76-1.72)
Sidechain outliers	138945	3878 (1.76-1.72)
RSRZ outliers	127900	3705 (1.76-1.72)

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	410	4% 95%
1	B	410	4% 93% 5%
1	C	410	3% 96%
1	D	410	3% 95% 5%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GOL	D	513	-	-	X	-

2 Entry composition

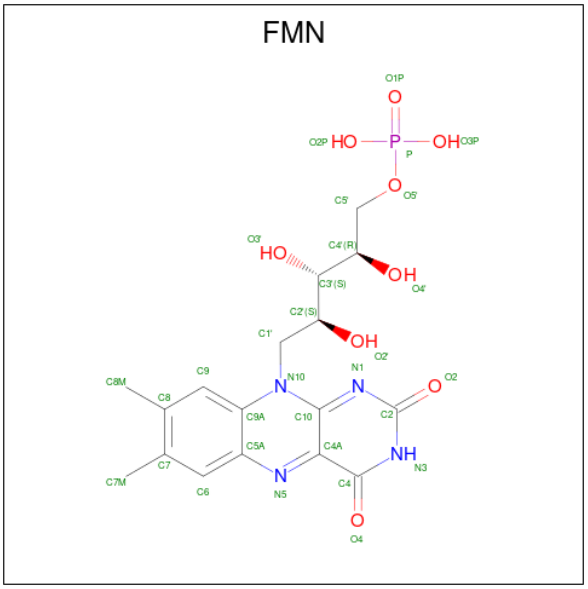
There are 9 unique types of molecules in this entry. The entry contains 27293 atoms, of which 13143 are hydrogens and 0 are deuteriums.

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 F420H2 oxidase (FprA).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	403	Total	C	H	N	O	S	0	1	0
			6389	2066	3196	513	594	20			
1	B	403	Total	C	H	N	O	S	0	0	0
			6371	2060	3184	513	594	20			
1	C	409	Total	C	H	N	O	S	0	1	0
			6489	2102	3243	523	601	20			
1	D	409	Total	C	H	N	O	S	0	1	0
			6490	2102	3244	523	601	20			

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			50	17	19	4	9	1		
2	B	1	Total	C	H	N	O	P	0	0
			50	17	19	4	9	1		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	C	1	Total	C	H	N	O	P	0	0
			50	17	19	4	9	1		
2	D	1	Total	C	H	N	O	P	0	0
			50	17	19	4	9	1		

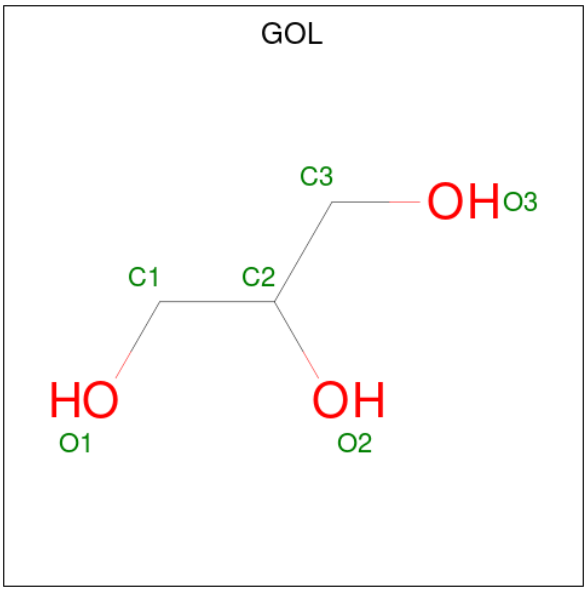
- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Ca	0	0
			3	3		
3	B	2	Total	Ca	0	0
			2	2		
3	C	5	Total	Ca	0	0
			5	5		
3	D	5	Total	Ca	0	0
			5	5		

- Molecule 4 is TERBIUM(III) ION (three-letter code: TB) (formula: Tb).

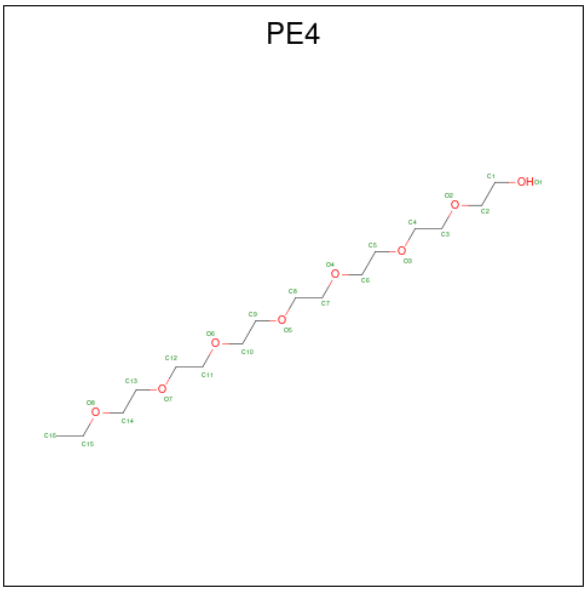
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Tb	0	0
			1	1		
4	B	1	Total	Tb	0	0
			1	1		
4	C	1	Total	Tb	0	0
			1	1		
4	D	1	Total	Tb	0	0
			1	1		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



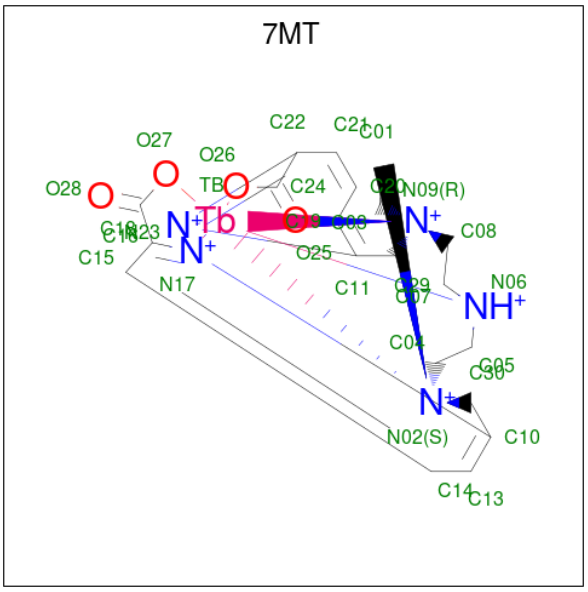
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			12	3	6	3		
5	B	1	Total	C	H	O	0	0
			12	3	6	3		
5	C	1	Total	C	H	O	0	0
			12	3	6	3		
5	C	1	Total	C	H	O	0	0
			11	3	5	3		
5	D	1	Total	C	H	O	0	0
			13	3	7	3		
5	D	1	Total	C	H	O	0	0
			12	3	6	3		

- Molecule 6 is 2-{2-[2-(2-{2-[2-(2-ETHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHOXY)-ETHOXY]-ETHOXY}-ETHANOL (three-letter code: PE4) (formula: $C_{16}H_{34}O_8$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	H	O	0	0
			24	8	12	4		
6	B	1	Total	C	H	O	0	0
			24	8	12	4		
6	C	1	Total	C	H	O	0	0
			24	8	12	4		
6	C	1	Total	C	H	O	0	0
			24	8	12	4		
6	D	1	Total	C	H	O	0	0
			24	8	12	4		
6	D	1	Total	C	H	O	0	0
			24	8	12	4		

- Molecule 7 is Tb-Xo4 (three-letter code: 7MT) (formula: $C_{20}H_{23}N_5O_4Tb$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
7	C	1	Total	C	H	N	O	Tb	0	0
			53	20	23	5	4	1		
7	C	1	Total	C	H	N	O	Tb	0	0
			53	20	23	5	4	1		
7	D	1	Total	C	H	N	O	Tb	0	0
			53	20	23	5	4	1		
7	D	1	Total	C	H	N	O	Tb	0	0
			53	20	23	5	4	1		

- Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	1	Total	Na	0	0
			1	1		

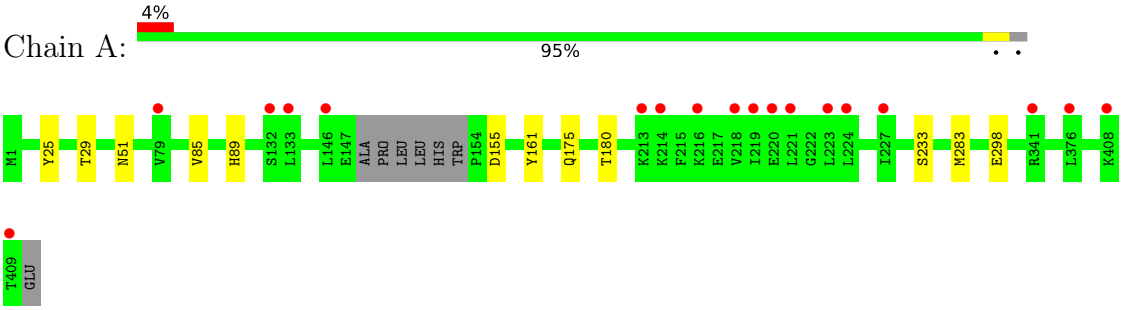
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	219	Total	O	0	0
			219	219		
9	B	216	Total	O	0	0
			216	216		
9	C	233	Total	O	0	0
			233	233		
9	D	238	Total	O	0	0
			238	238		

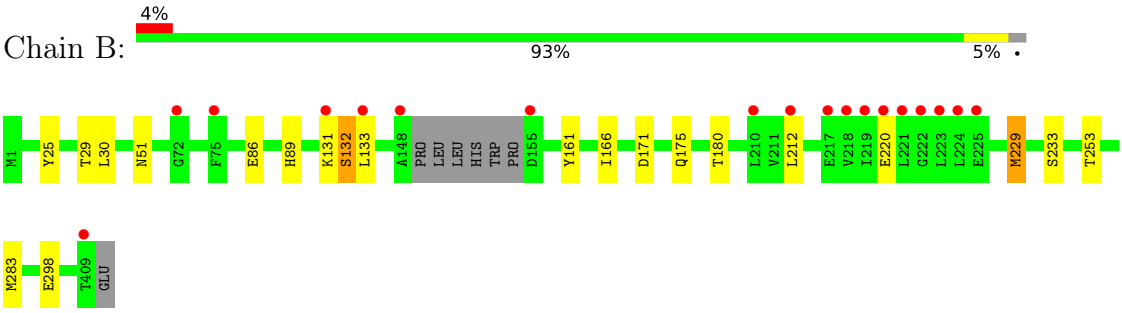
3 Residue-property plots (i)

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.

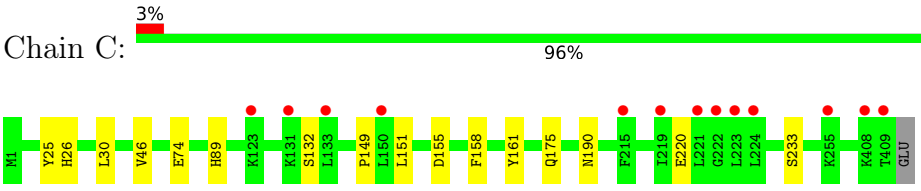
• Molecule 1: F420H2 oxidase (FprA)



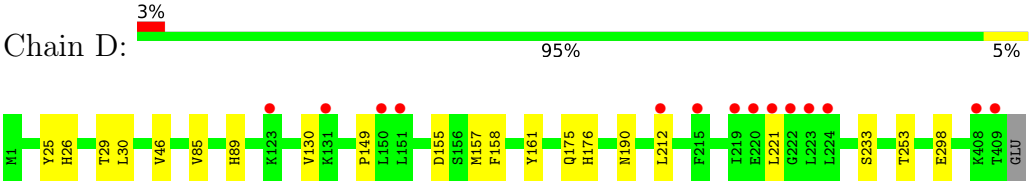
• Molecule 1: F420H2 oxidase (FprA)



• Molecule 1: F420H2 oxidase (FprA)



• Molecule 1: F420H2 oxidase (FprA)



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	73.66Å 144.97Å 74.21Å 90.00° 91.78° 90.00°	Depositor
Resolution (Å)	25.48 – 1.74 42.83 – 1.74	Depositor EDS
% Data completeness (in resolution range)	98.2 (25.48-1.74) 99.0 (42.83-1.74)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.99 (at 1.74Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.164 , 0.189 0.174 , 0.196	Depositor DCC
R_{free} test set	7783 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	27.3	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.44 , 62.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.010 for l,k,-h 0.049 for h,-k,-l 0.027 for l,-k,h	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	27293	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, CA, NA, TB, PE4, GOL, 7MT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.47	0/3268	0.63	0/4406
1	B	0.51	1/3258 (0.0%)	0.63	0/4392
1	C	0.50	0/3326	0.65	0/4490
1	D	0.50	0/3326	0.64	0/4490
All	All	0.49	1/13178 (0.0%)	0.64	0/17778

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	229	MET	SD-CE	-5.50	1.47	1.77

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3193	3196	3196	7	0
1	B	3187	3184	3184	10	0
1	C	3246	3243	3244	9	0
1	D	3246	3244	3244	15	0
2	A	31	19	19	0	0
2	B	31	19	19	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	31	19	19	0	0
2	D	31	19	19	0	0
3	A	3	0	0	0	0
3	B	2	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	6	6	6	2	0
5	B	6	6	6	2	0
5	C	12	11	12	4	0
5	D	12	13	12	7	0
6	B	24	24	24	0	0
6	C	24	24	24	2	0
6	D	24	24	24	0	0
7	C	60	46	0	1	0
7	D	60	46	0	0	0
8	D	1	0	0	0	0
9	A	219	0	0	0	0
9	B	216	0	0	1	0
9	C	233	0	0	1	0
9	D	238	0	0	0	0
All	All	14150	13143	13052	40	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (40) 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:C:190[B]:ASN:OD1	1:D:190[B]:ASN:OD1	2.09	0.70
1:D:26:HIS:NE2	5:D:513:GOL:H31	2.19	0.58
6:C:510:PE4:H111	9:C:605:HOH:O	2.07	0.55
1:D:25:TYR:HE2	5:D:513:GOL:H2	1.71	0.55
1:D:85:VAL:HG13	1:D:155:ASP:HB2	1.90	0.54
1:C:25:TYR:CE2	5:C:513:GOL:H2	2.43	0.54
1:D:25:TYR:CE2	5:D:513:GOL:H2	2.45	0.52
1:D:176:HIS:NE2	5:D:513:GOL:H32	2.26	0.51
1:A:25:TYR:CE2	5:A:506:GOL:H2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:508:7MT:C05	7:C:508:7MT:C03	2.90	0.49
1:B:171:ASP:OD2	5:B:507:GOL:H32	2.11	0.49
1:D:130:VAL:HG21	1:D:157:MET:SD	2.52	0.49
1:D:212:LEU:HD21	1:D:253:THR:HG23	1.96	0.48
1:A:283:MET:SD	1:B:180:THR:HG22	2.54	0.48
1:A:180:THR:HG22	1:B:283:MET:SD	2.53	0.48
1:D:26:HIS:NE2	5:D:513:GOL:C3	2.78	0.47
1:B:166:ILE:HG23	1:B:229:MET:HE2	1.96	0.47
1:D:46:VAL:HG23	5:D:512:GOL:H11	1.96	0.46
1:B:25:TYR:CE2	5:B:507:GOL:H2	2.50	0.46
1:D:89:HIS:CE1	1:D:233:SER:HB2	2.51	0.46
1:A:89:HIS:CE1	1:A:233:SER:HB2	2.51	0.46
1:B:89:HIS:CE1	1:B:233:SER:HB2	2.52	0.45
1:A:85[B]:VAL:HG23	1:A:155:ASP:HB2	1.99	0.45
1:C:46:VAL:HG23	5:C:512:GOL:H32	1.99	0.45
1:C:46:VAL:HG23	5:C:512:GOL:C3	2.48	0.44
1:C:89:HIS:CE1	1:C:233:SER:HB2	2.52	0.44
1:A:25:TYR:HE2	5:A:506:GOL:H2	1.83	0.43
1:D:46:VAL:HG23	5:D:512:GOL:C1	2.49	0.43
1:D:149:PRO:HG3	1:D:158:PHE:CD1	2.54	0.43
1:B:212:LEU:HD21	1:B:253:THR:HG23	2.01	0.42
1:B:86:GLU:HG2	9:B:616:HOH:O	2.18	0.42
1:C:149:PRO:HG3	1:C:158:PHE:CG	2.54	0.42
1:A:29:THR:HG21	1:A:298:GLU:HG3	2.02	0.42
1:B:131:LYS:O	1:B:132:SER:HB2	2.20	0.42
1:C:26:HIS:HE2	5:C:513:GOL:C1	2.34	0.41
1:D:149:PRO:HG3	1:D:158:PHE:CG	2.55	0.41
1:C:74:GLU:OE1	6:C:511:PE4:C8	2.68	0.41
1:C:149:PRO:HG3	1:C:158:PHE:CD1	2.55	0.41
1:B:29:THR:HG21	1:B:298:GLU:HG3	2.02	0.40
1:D:29:THR:HG21	1:D:298:GLU:HG3	2.03	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	400/410 (98%)	389 (97%)	10 (2%)	1 (0%)	41	23
1	B	399/410 (97%)	390 (98%)	7 (2%)	2 (0%)	29	12
1	C	408/410 (100%)	397 (97%)	10 (2%)	1 (0%)	47	29
1	D	408/410 (100%)	398 (98%)	10 (2%)	0	100	100
All	All	1615/1640 (98%)	1574 (98%)	37 (2%)	4 (0%)	47	29

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	132	SER
1	C	132	SER
1	A	51	ASN
1	B	51	ASN

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	343/348 (99%)	341 (99%)	2 (1%)	86	79
1	B	341/348 (98%)	336 (98%)	5 (2%)	65	47
1	C	348/348 (100%)	342 (98%)	6 (2%)	60	41
1	D	348/348 (100%)	344 (99%)	4 (1%)	73	59
All	All	1380/1392 (99%)	1363 (99%)	17 (1%)	71	56

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	161	TYR
1	A	175	GLN
1	B	30	LEU
1	B	133	LEU

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Mol	Chain	Res	Type
1	B	161	TYR
1	B	175	GLN
1	B	220	GLU
1	C	30	LEU
1	C	151	LEU
1	C	155	ASP
1	C	161	TYR
1	C	175	GLN
1	C	220	GLU
1	D	30	LEU
1	D	161	TYR
1	D	175	GLN
1	D	221	LEU

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

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 40 ligands modelled in this entry, 20 are monoatomic - leaving 20 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	7MT	C	509	1,7	21,38,38	1.43	2 (9%)	20,76,76	1.64	4 (20%)
5	GOL	D	513	4	5,5,5	1.33	1 (20%)	5,5,5	1.07	0
6	PE4	C	510	-	11,11,23	0.41	0	10,10,22	0.37	0
6	PE4	D	511	-	11,11,23	0.49	0	10,10,22	0.48	0
7	7MT	D	508	1,3,7	21,38,38	1.11	1 (4%)	20,76,76	1.42	2 (10%)
6	PE4	B	506	-	11,11,23	0.52	0	10,10,22	0.68	0
7	7MT	C	508	1,3,7	21,38,38	1.12	1 (4%)	20,76,76	1.81	6 (30%)
7	7MT	D	509	1,7	21,38,38	1.43	2 (9%)	20,76,76	1.64	4 (20%)
2	FMN	B	501	-	33,33,33	1.42	4 (12%)	48,50,50	1.23	7 (14%)
6	PE4	D	510	-	11,11,23	0.47	0	10,10,22	0.47	0
5	GOL	C	512	3	5,5,5	0.45	0	5,5,5	0.71	0
2	FMN	C	501	-	33,33,33	1.84	9 (27%)	48,50,50	1.48	7 (14%)
6	PE4	B	505	-	11,11,23	0.50	0	10,10,22	0.54	0
2	FMN	D	501	-	33,33,33	1.76	8 (24%)	48,50,50	1.42	10 (20%)
5	GOL	B	507	4	5,5,5	1.16	0	5,5,5	1.85	1 (20%)
2	FMN	A	501	-	33,33,33	1.85	9 (27%)	48,50,50	1.49	10 (20%)
5	GOL	A	506	4	5,5,5	1.05	0	5,5,5	1.07	0
5	GOL	D	512	3	5,5,5	0.48	0	5,5,5	0.76	0
5	GOL	C	513	4	5,5,5	1.25	0	5,5,5	2.47	1 (20%)
6	PE4	C	511	-	11,11,23	0.55	0	10,10,22	0.66	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	506	4	-	2/4/4/4	-
5	GOL	C	512	3	-	1/4/4/4	-
5	GOL	B	507	4	-	0/4/4/4	-
5	GOL	D	512	3	-	1/4/4/4	-
5	GOL	C	513	4	-	0/4/4/4	-
2	FMN	C	501	-	-	2/18/18/18	0/3/3/3
2	FMN	B	501	-	-	0/18/18/18	0/3/3/3
5	GOL	D	513	4	-	2/4/4/4	-
6	PE4	B	505	-	-	3/9/9/21	-
6	PE4	C	510	-	-	4/9/9/21	-
6	PE4	D	511	-	-	5/9/9/21	-
6	PE4	D	510	-	-	2/9/9/21	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PE4	C	511	-	-	6/9/9/21	-
2	FMN	D	501	-	-	0/18/18/18	0/3/3/3
6	PE4	B	506	-	-	3/9/9/21	-
2	FMN	A	501	-	-	1/18/18/18	0/3/3/3

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	FMN	C9A-C5A	5.03	1.49	1.41
2	C	501	FMN	C9A-C5A	4.27	1.48	1.41
2	D	501	FMN	C9A-C5A	4.07	1.48	1.41
7	D	509	7MT	C30-C10	3.88	1.55	1.51
7	C	509	7MT	C30-C10	3.86	1.55	1.51
2	A	501	FMN	C4-N3	-3.85	1.31	1.38
2	A	501	FMN	C9A-C5A	3.73	1.47	1.41
7	C	509	7MT	C29-C11	3.56	1.55	1.51
7	D	509	7MT	C29-C11	3.54	1.55	1.51
7	C	508	7MT	C30-C10	3.51	1.55	1.51
2	D	501	FMN	C4-N3	-3.38	1.32	1.38
2	B	501	FMN	C8-C7	3.33	1.49	1.40
2	C	501	FMN	P-O3P	-3.31	1.42	1.54
2	C	501	FMN	P-O2P	-3.27	1.42	1.54
2	A	501	FMN	C5A-N5	-3.22	1.33	1.39
2	C	501	FMN	C4-N3	-3.18	1.32	1.38
2	A	501	FMN	P-O3P	-3.16	1.42	1.54
2	D	501	FMN	P-O3P	-2.91	1.43	1.54
2	D	501	FMN	C5A-N5	-2.86	1.33	1.39
2	D	501	FMN	P-O2P	-2.84	1.43	1.54
2	A	501	FMN	C2-N3	-2.80	1.32	1.39
2	C	501	FMN	C2-N3	-2.80	1.32	1.39
2	A	501	FMN	P-O2P	-2.76	1.44	1.54
7	D	508	7MT	C30-C10	2.72	1.54	1.51
5	D	513	GOL	O2-C2	-2.70	1.35	1.43
2	C	501	FMN	C5A-N5	-2.57	1.34	1.39
2	A	501	FMN	C8-C7	2.56	1.47	1.40
2	A	501	FMN	P-O1P	-2.53	1.42	1.50
2	D	501	FMN	C2-N3	-2.46	1.33	1.39
2	B	501	FMN	C4A-N5	2.46	1.35	1.30
2	C	501	FMN	O2'-C2'	-2.41	1.38	1.43
2	A	501	FMN	O2'-C2'	-2.39	1.38	1.43
2	B	501	FMN	C4-N3	-2.37	1.34	1.38
2	D	501	FMN	O2-C2	-2.35	1.19	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	FMN	C1'-C2'	-2.31	1.49	1.52
2	C	501	FMN	P-O1P	-2.20	1.43	1.50
2	D	501	FMN	P-O1P	-2.15	1.43	1.50

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	513	GOL	O1-C1-C2	-4.82	87.09	110.20
7	C	508	7MT	O27-C18-C16	4.55	122.41	115.78
2	A	501	FMN	C4-C4A-N5	3.98	123.89	118.23
2	C	501	FMN	O3P-P-O2P	3.49	120.99	107.64
7	D	508	7MT	O27-C18-C16	3.20	120.45	115.78
2	D	501	FMN	C4-C4A-N5	3.12	122.68	118.23
7	C	509	7MT	O26-C24-O25	-2.96	119.96	125.24
7	D	509	7MT	O27-C18-O28	-2.93	120.02	125.24
7	C	509	7MT	O27-C18-O28	-2.92	120.04	125.24
7	C	508	7MT	O26-C24-O25	-2.91	120.04	125.24
7	D	509	7MT	O26-C24-O25	-2.91	120.05	125.24
7	C	509	7MT	O26-C24-C22	2.91	120.02	115.78
7	D	509	7MT	O27-C18-C16	2.90	120.02	115.78
7	C	509	7MT	O27-C18-C16	2.89	120.00	115.78
2	C	501	FMN	O4-C4-C4A	-2.88	118.95	126.60
7	C	508	7MT	O26-C24-C22	2.88	119.98	115.78
7	D	509	7MT	O26-C24-C22	2.87	119.96	115.78
5	B	507	GOL	O1-C1-C2	-2.85	96.53	110.20
7	C	508	7MT	C19-C11-N23	2.82	123.71	121.75
2	A	501	FMN	C10-N1-C2	2.76	122.42	116.90
2	B	501	FMN	C4-C4A-N5	2.72	122.10	118.23
2	A	501	FMN	C4A-C10-N1	-2.70	118.46	124.73
2	C	501	FMN	C4A-C10-N1	-2.69	118.49	124.73
2	B	501	FMN	C4A-C10-N1	-2.68	118.51	124.73
2	C	501	FMN	O2'-C2'-C3'	2.65	115.54	109.10
2	D	501	FMN	O2-C2-N1	-2.61	117.50	121.83
2	D	501	FMN	C4A-C10-N1	-2.52	118.89	124.73
2	C	501	FMN	C4-C4A-N5	2.48	121.76	118.23
2	A	501	FMN	C4A-C10-N10	2.45	120.06	116.48
2	A	501	FMN	C4A-C4-N3	2.44	119.38	113.19
2	D	501	FMN	O3P-P-O2P	2.42	116.88	107.64
2	D	501	FMN	O4-C4-C4A	-2.37	120.30	126.60
2	D	501	FMN	C4A-C4-N3	2.37	119.21	113.19
7	C	508	7MT	C13-C10-N17	-2.36	120.11	121.75
2	A	501	FMN	O5'-C5'-C4'	2.30	115.50	109.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	D	508	7MT	C19-C11-N23	2.28	123.34	121.75
2	B	501	FMN	C10-N1-C2	2.26	121.42	116.90
2	D	501	FMN	C4-N3-C2	-2.25	121.49	125.64
2	B	501	FMN	O4-C4-C4A	-2.23	120.68	126.60
2	D	501	FMN	C10-N1-C2	2.22	121.34	116.90
2	A	501	FMN	O4-C4-C4A	-2.21	120.74	126.60
2	D	501	FMN	N3-C2-N1	2.21	123.71	119.38
2	C	501	FMN	C10-N1-C2	2.20	121.29	116.90
2	B	501	FMN	C4A-C4-N3	2.17	118.69	113.19
2	A	501	FMN	C4-N3-C2	-2.16	121.64	125.64
7	C	508	7MT	O28-C18-C16	-2.16	115.19	119.05
2	A	501	FMN	C9A-C5A-N5	-2.13	120.11	122.43
2	D	501	FMN	C9A-C5A-N5	-2.07	120.18	122.43
2	B	501	FMN	C4-N3-C2	-2.07	121.83	125.64
2	A	501	FMN	O2P-P-O5'	-2.05	101.27	106.73
2	B	501	FMN	C4A-C10-N10	2.05	119.47	116.48
2	C	501	FMN	C4A-C4-N3	2.05	118.38	113.19

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	506	GOL	O1-C1-C2-C3
6	B	505	PE4	O7-C13-C14-O8
6	C	511	PE4	O7-C13-C14-O8
6	C	511	PE4	O6-C10-C9-O5
6	D	510	PE4	O7-C13-C14-O8
5	D	513	GOL	C1-C2-C3-O3
6	C	510	PE4	O7-C13-C14-O8
5	A	506	GOL	O1-C1-C2-O2
5	D	513	GOL	O2-C2-C3-O3
6	D	511	PE4	O6-C10-C9-O5
2	C	501	FMN	C5'-O5'-P-O1P
6	B	506	PE4	O7-C13-C14-O8
6	C	510	PE4	C13-C14-O8-C15
6	B	505	PE4	O6-C10-C9-O5
6	B	505	PE4	C12-C11-O6-C10
6	D	510	PE4	C9-C10-O6-C11
6	C	511	PE4	C14-C13-O7-C12
6	C	510	PE4	C9-C10-O6-C11
6	C	511	PE4	C13-C14-O8-C15
2	A	501	FMN	C5'-O5'-P-O1P

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Mol	Chain	Res	Type	Atoms
5	D	512	GOL	O1-C1-C2-C3
6	D	511	PE4	C13-C14-O8-C15
6	C	511	PE4	C12-C11-O6-C10
6	D	511	PE4	O7-C13-C14-O8
6	C	511	PE4	C10-C9-O5-C8
6	D	511	PE4	C10-C9-O5-C8
6	B	506	PE4	C12-C11-O6-C10
2	C	501	FMN	C5'-O5'-P-O3P
6	B	506	PE4	C9-C10-O6-C11
6	D	511	PE4	C11-C12-O7-C13
5	C	512	GOL	C1-C2-C3-O3
6	C	510	PE4	O6-C11-C12-O7

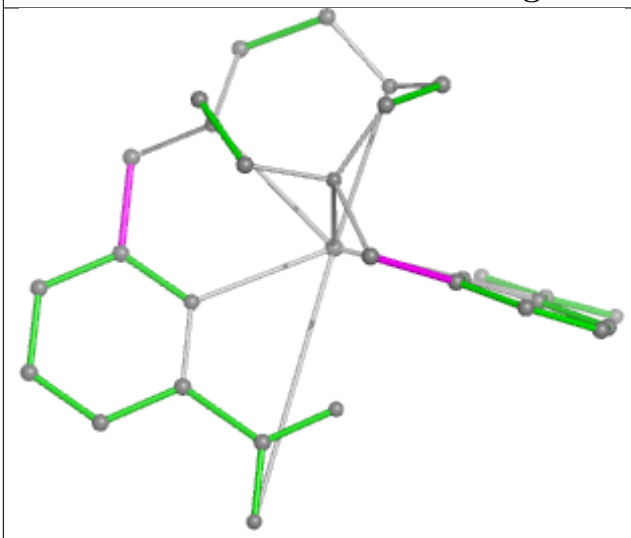
There are no ring outliers.

9 monomers are involved in 18 short contacts:

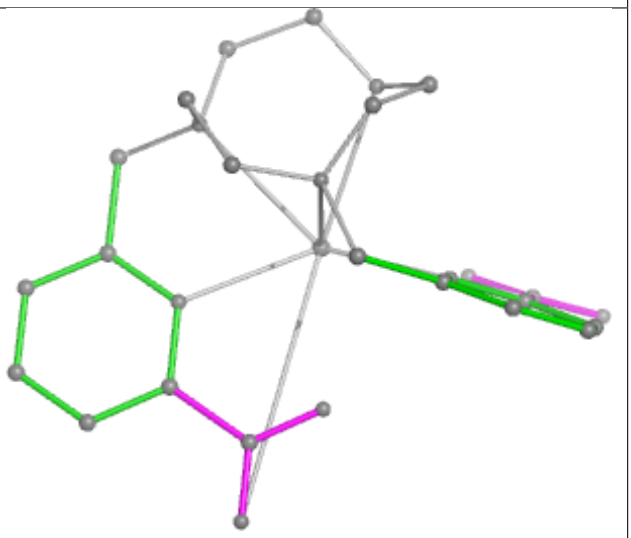
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	513	GOL	5	0
6	C	510	PE4	1	0
7	C	508	7MT	1	0
5	C	512	GOL	2	0
5	B	507	GOL	2	0
5	A	506	GOL	2	0
5	D	512	GOL	2	0
5	C	513	GOL	2	0
6	C	511	PE4	1	0

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.

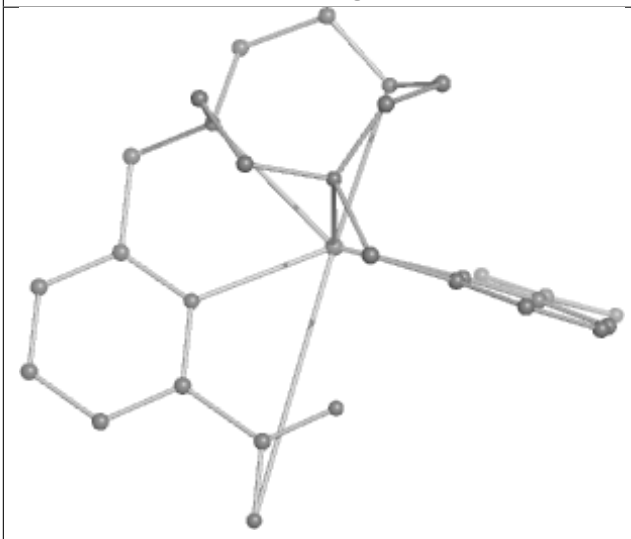
Ligand 7MT C 509



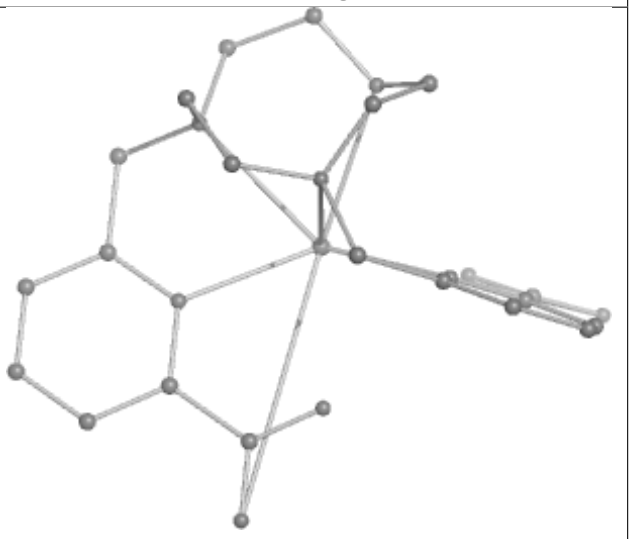
Bond lengths



Bond angles

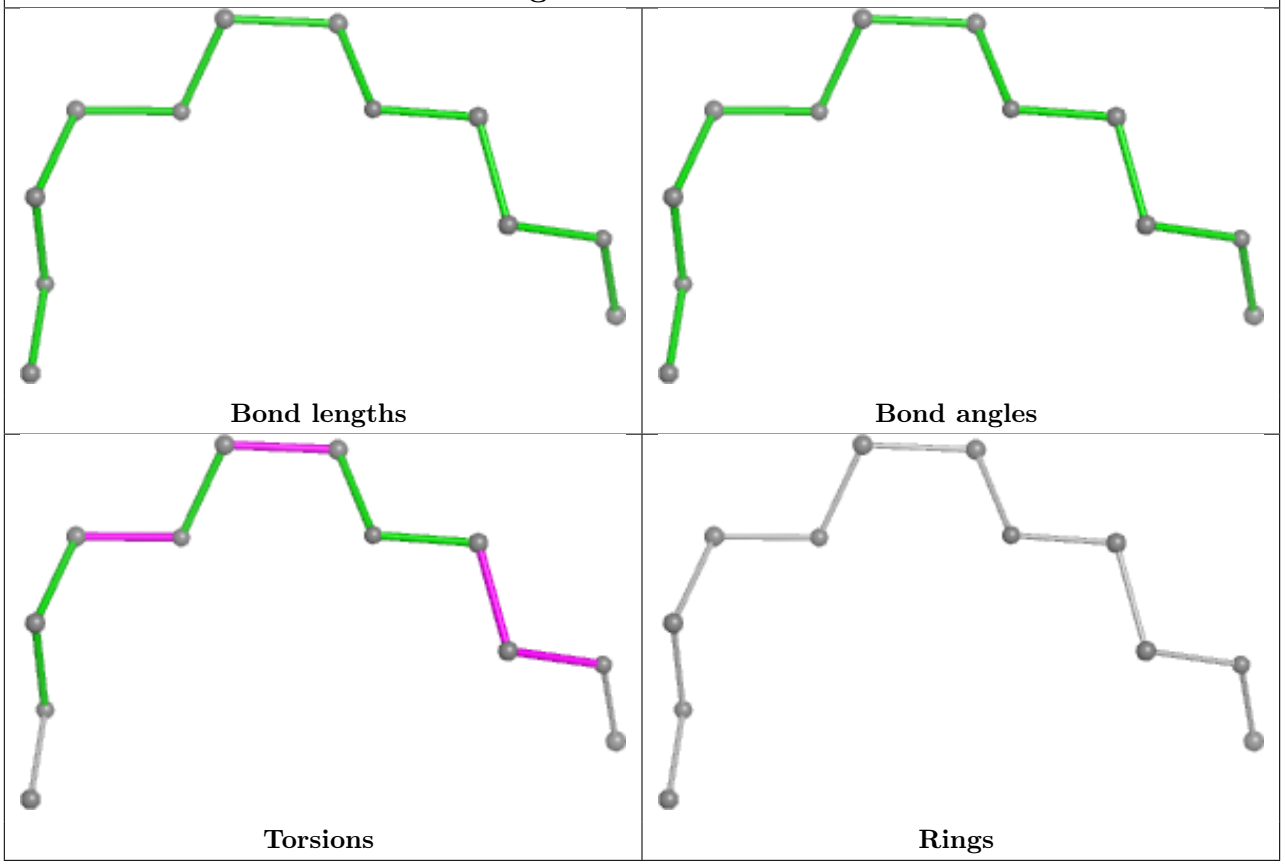


Torsions

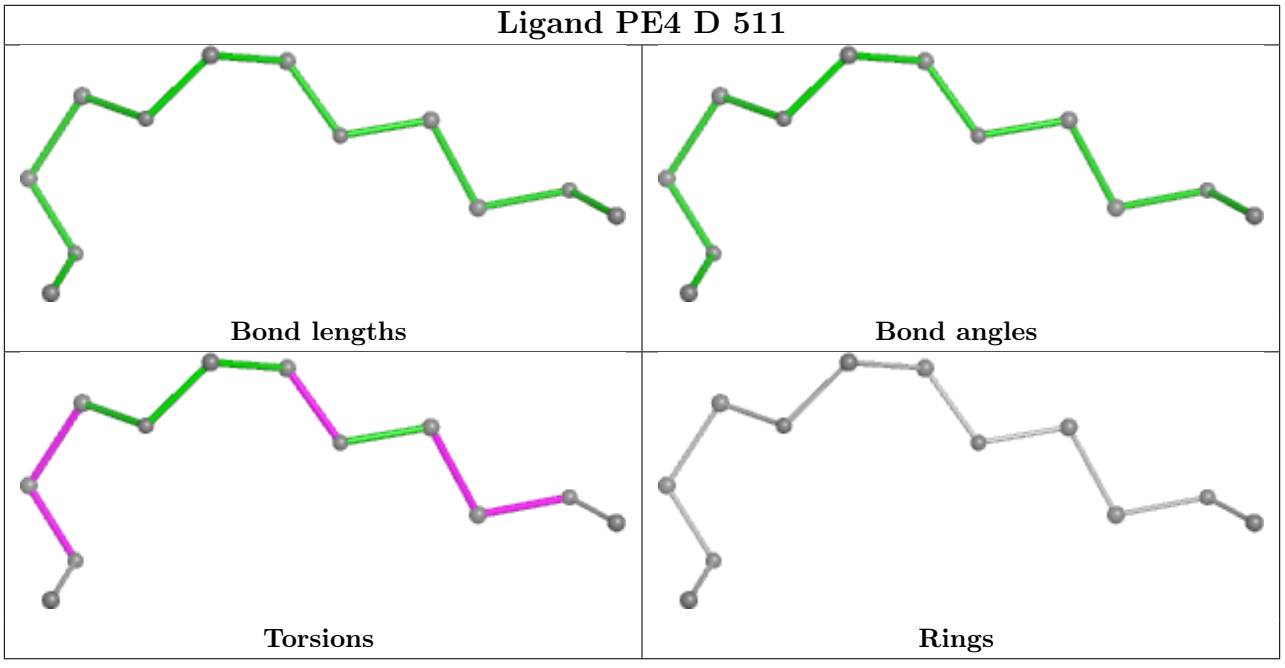


Rings

Ligand PE4 C 510



Ligand PE4 D 511



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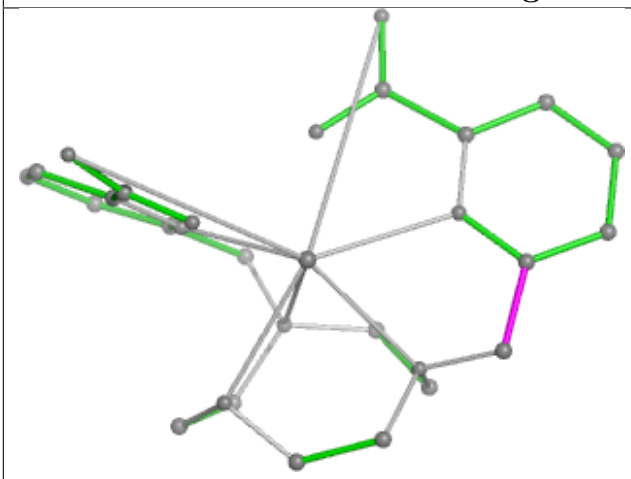
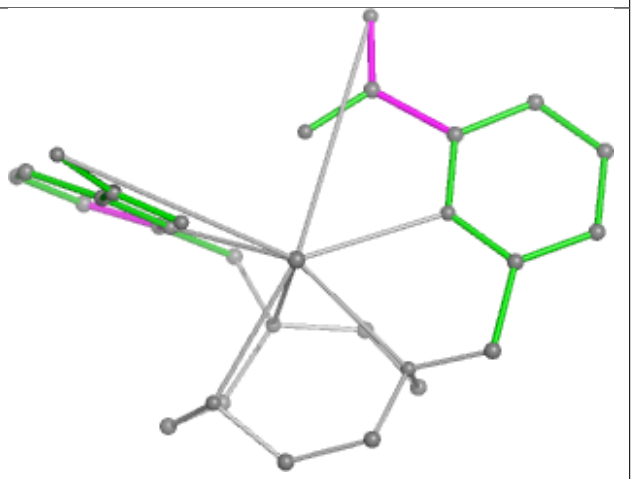
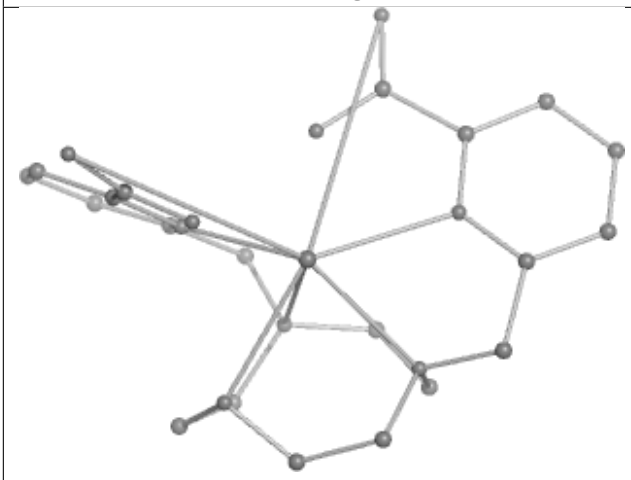


Bond lengths



Bond angles



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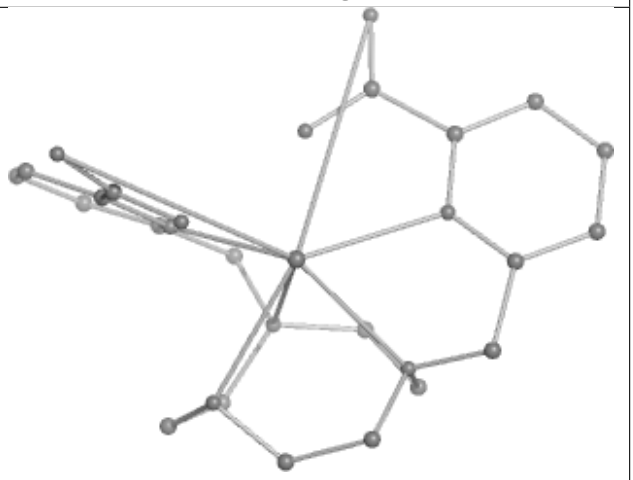
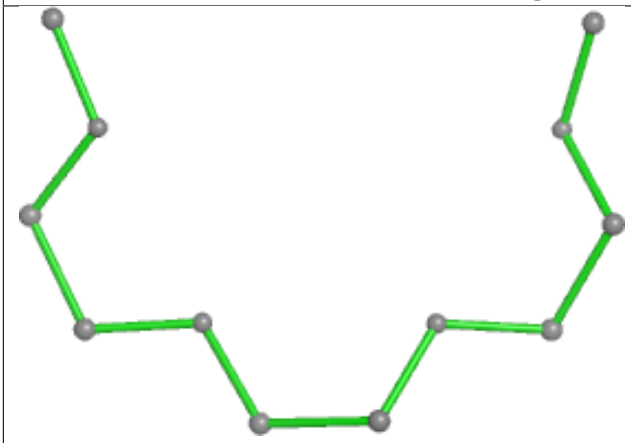
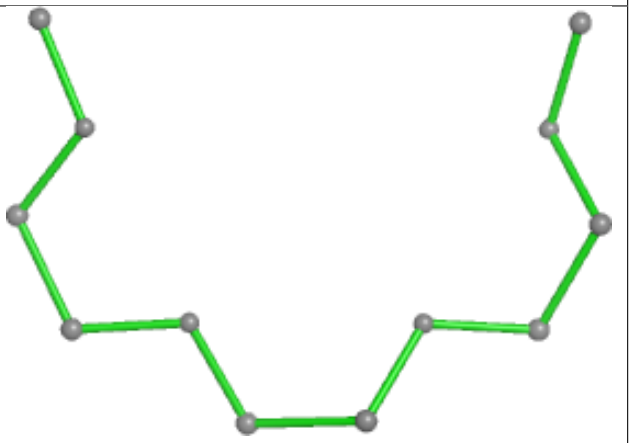


Rings

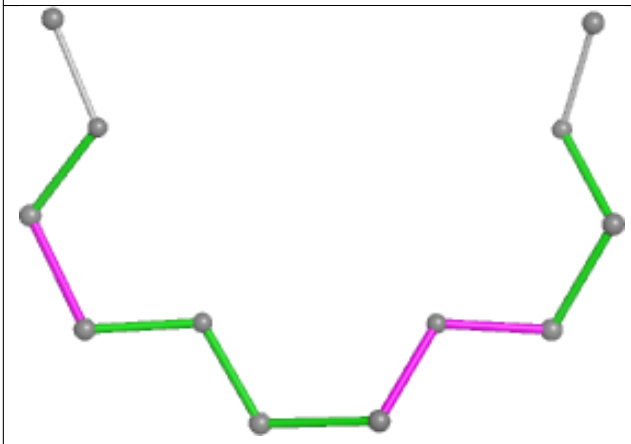
Ligand PE4 B 506



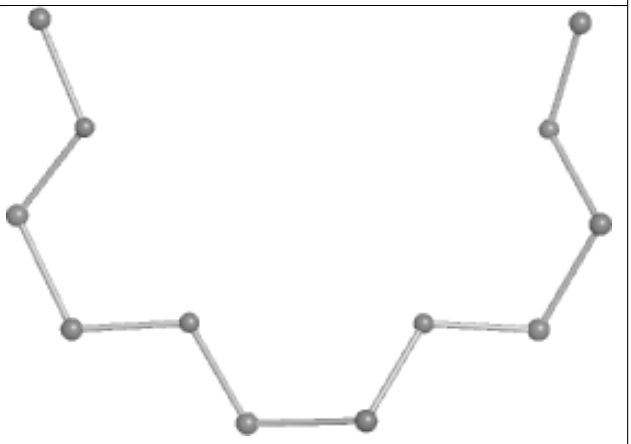
Bond lengths



Bond angles

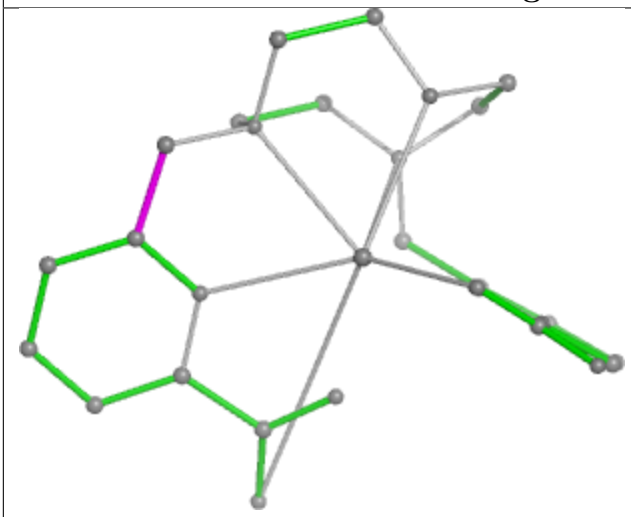


Torsions

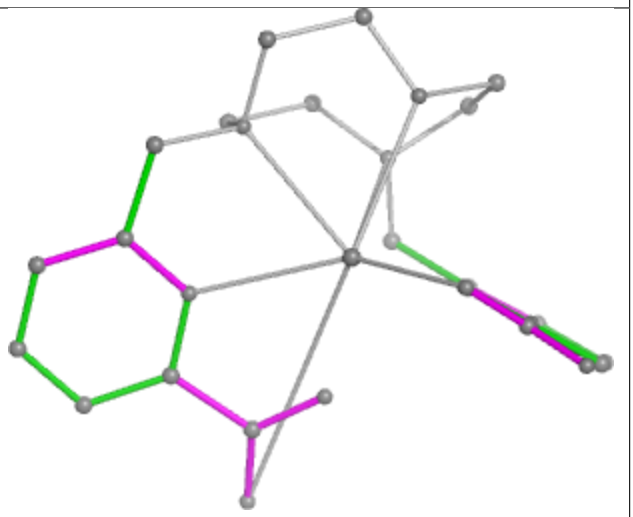


Rings

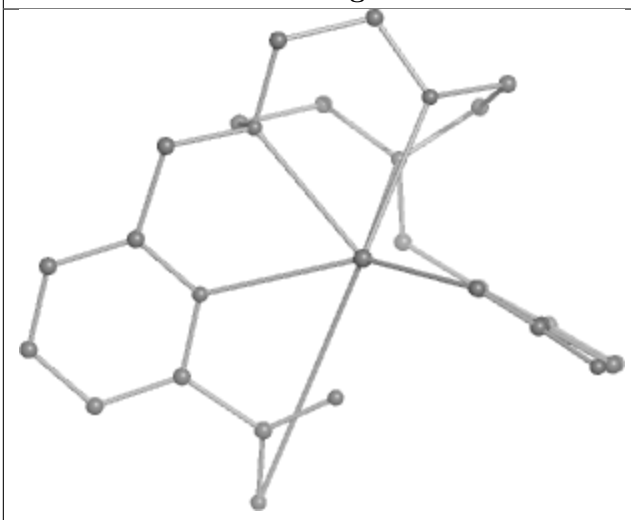
Ligand 7MT C 508



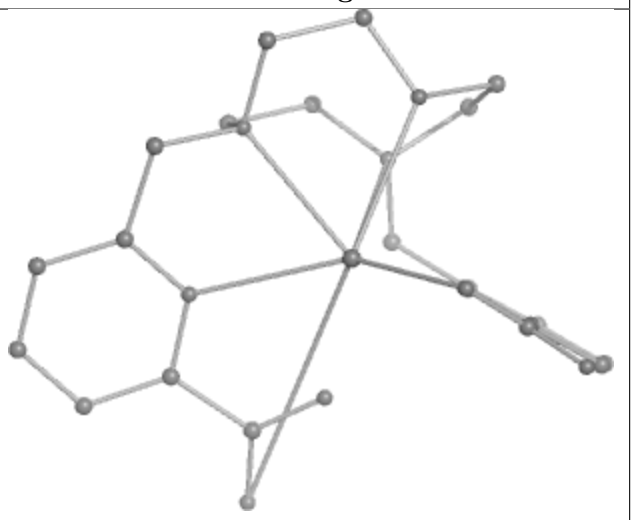
Bond lengths



Bond angles

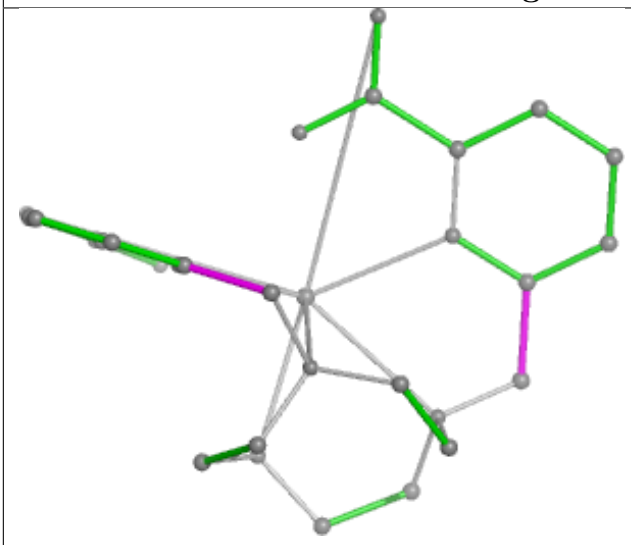


Torsions

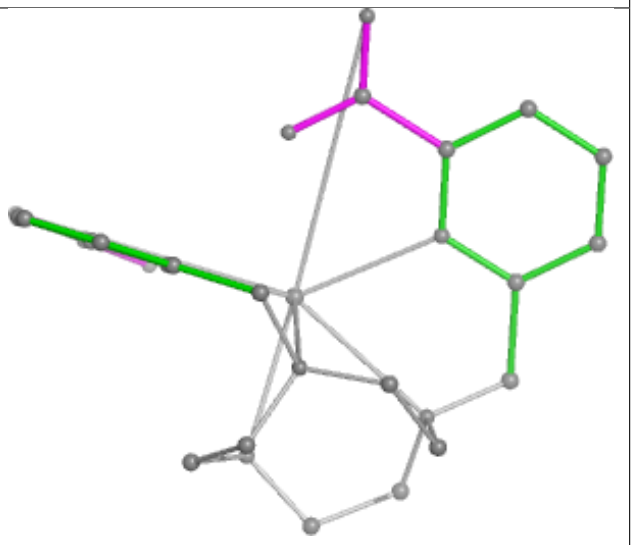


Rings

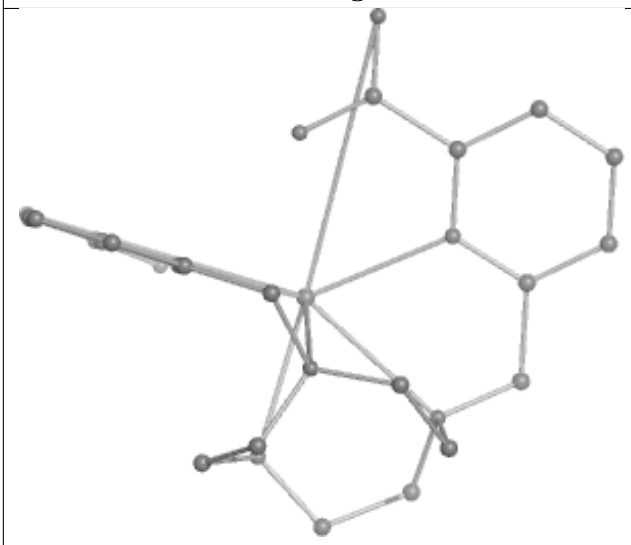
Ligand 7MT D 509



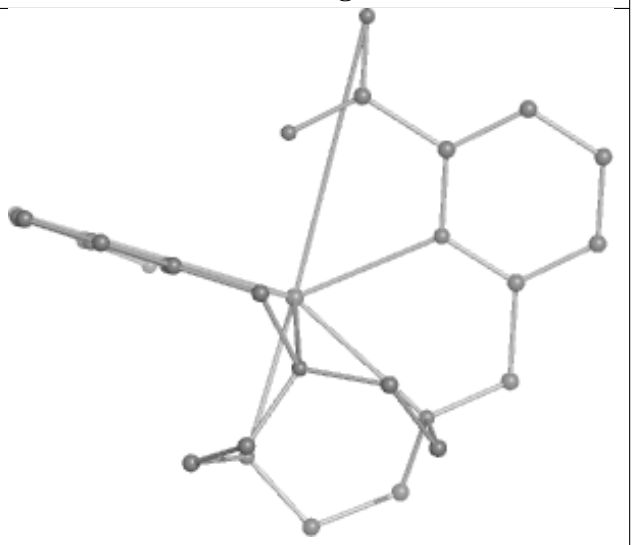
Bond lengths



Bond angles

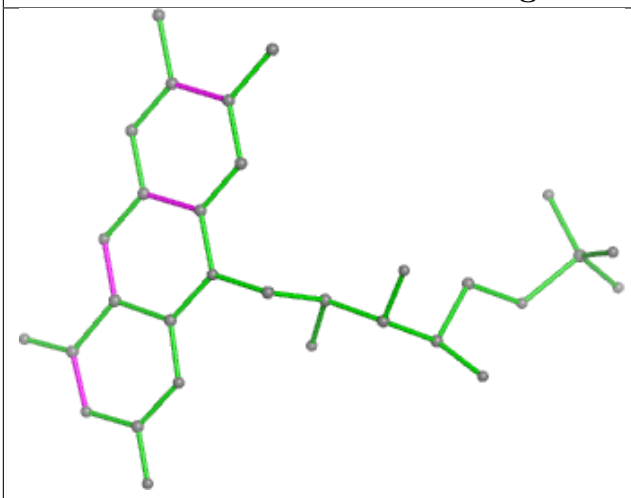


Torsions

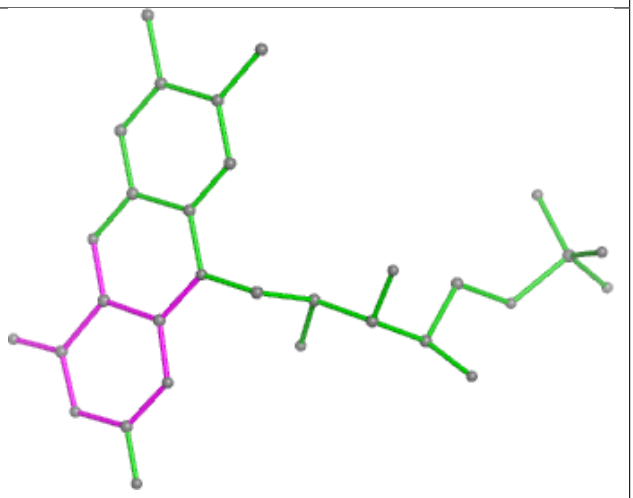


Rings

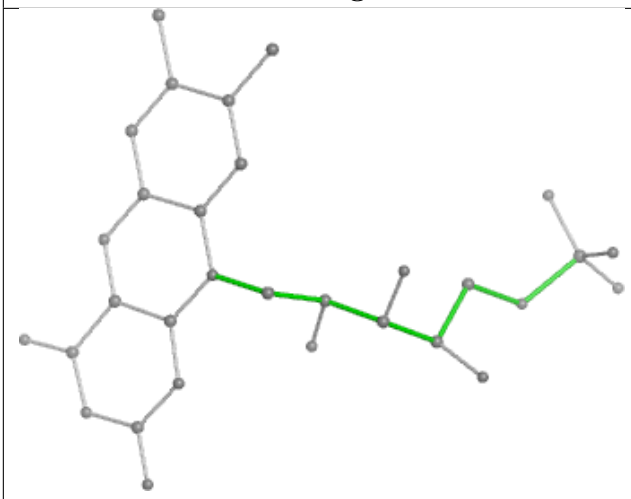
Ligand FMN B 501



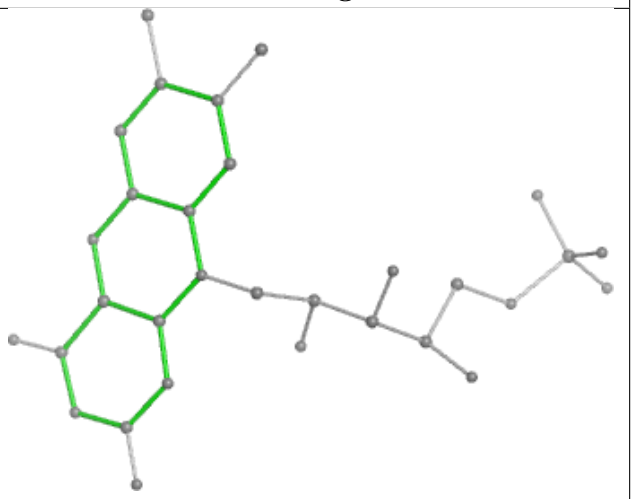
Bond lengths



Bond angles

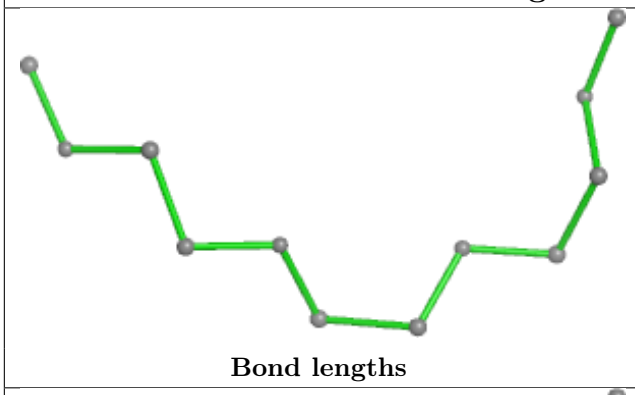


Torsions

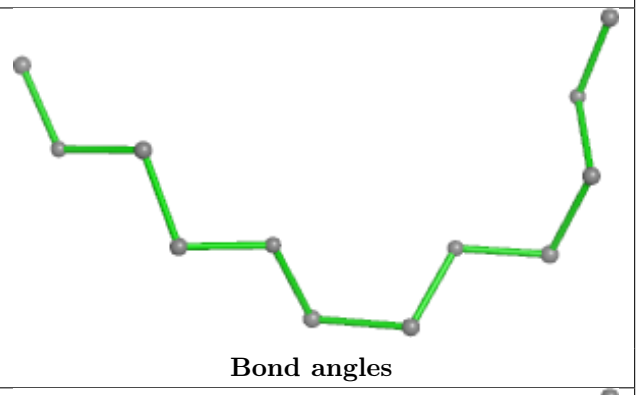


Rings

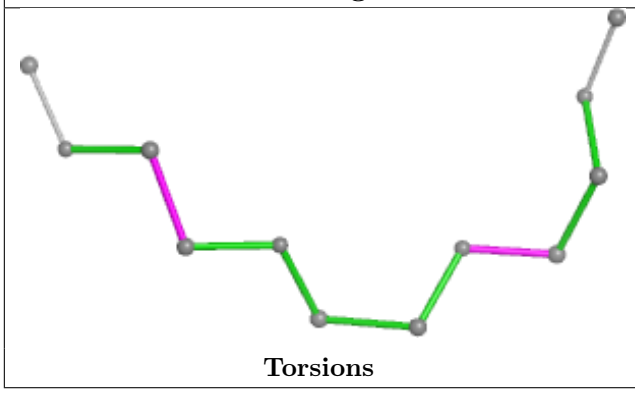
Ligand PE4 D 510



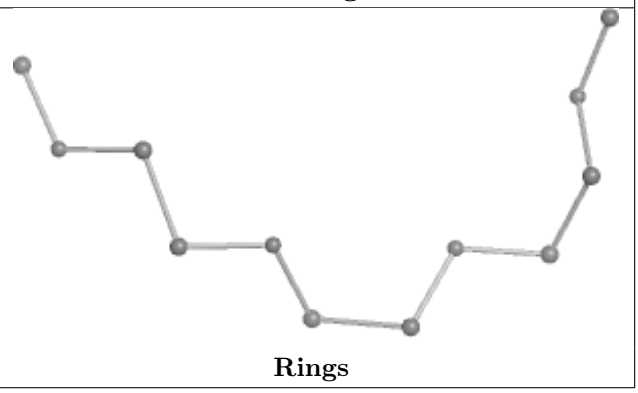
Bond lengths



Bond angles

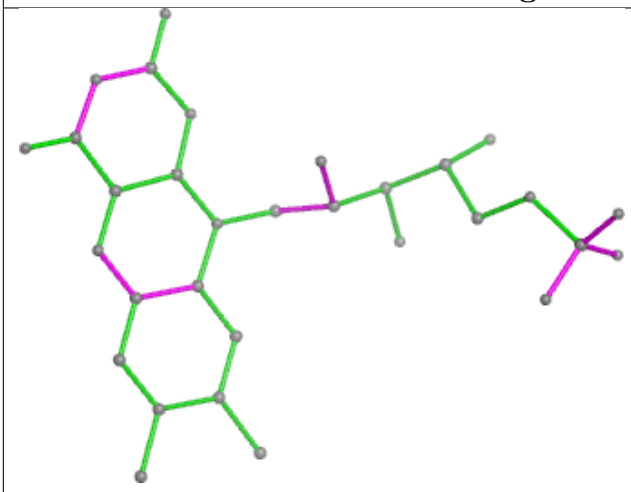


Torsions

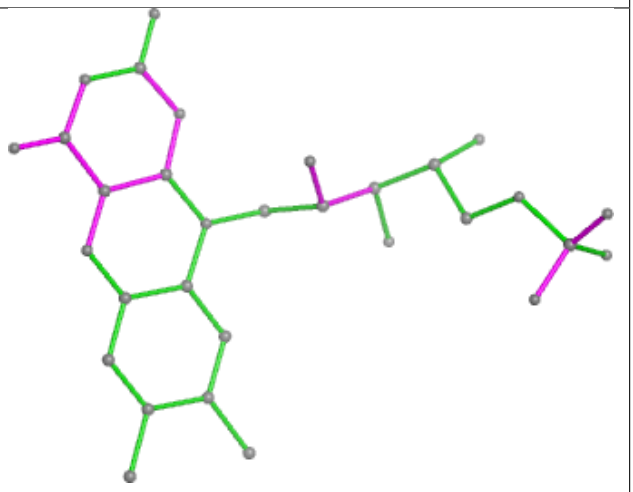


Rings

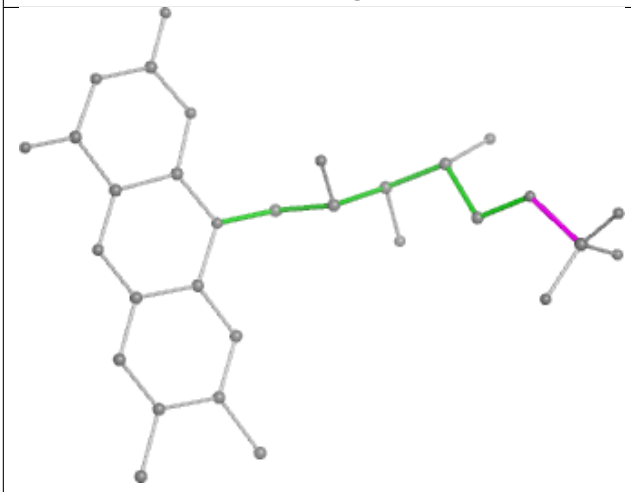
Ligand FMN C 501



Bond lengths



Bond angles



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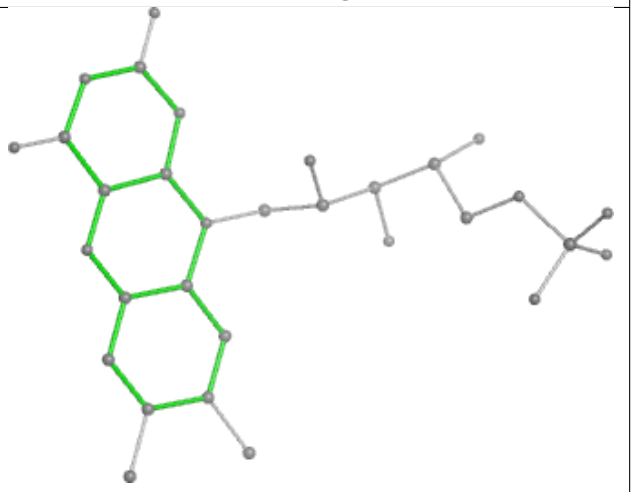
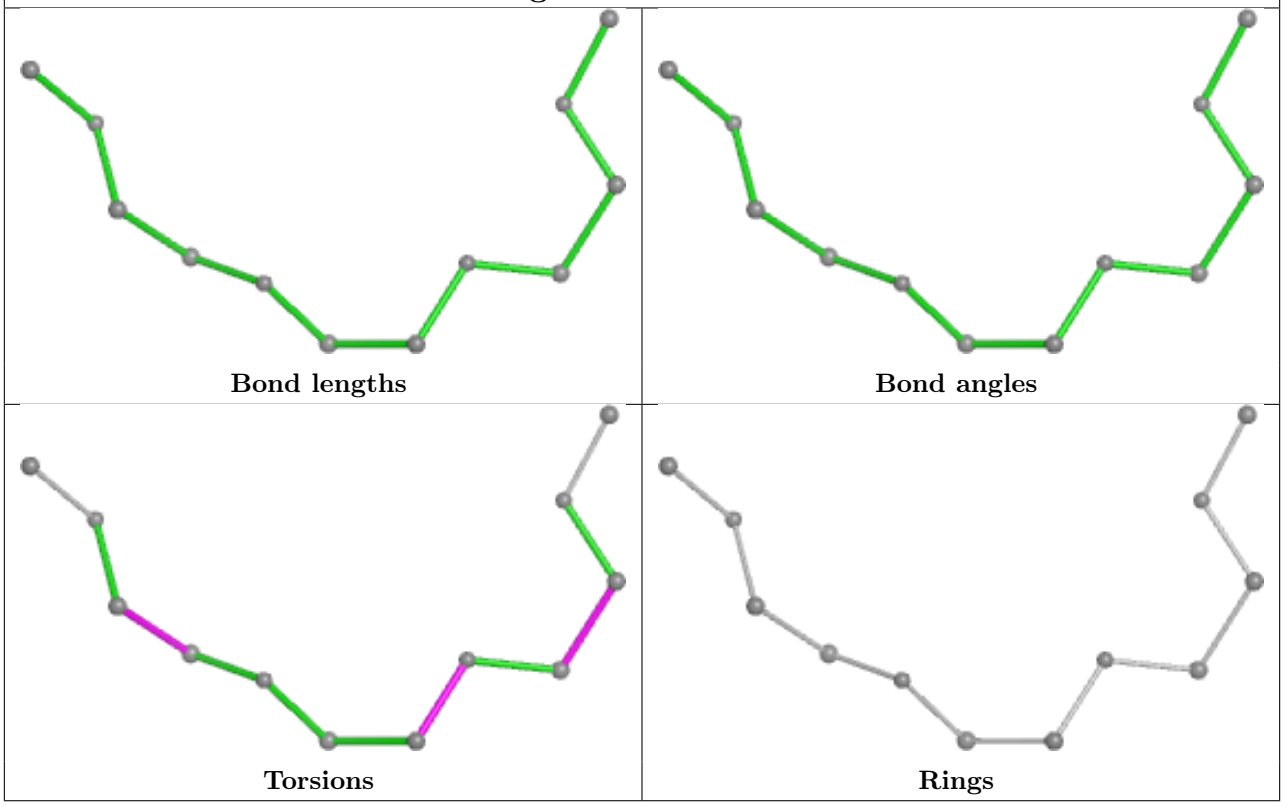
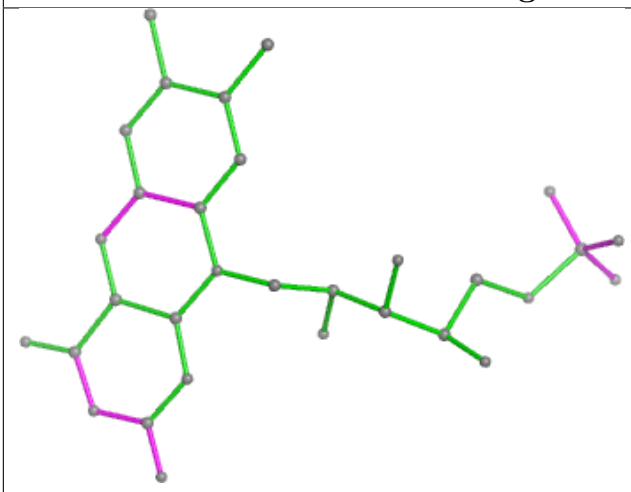


Rings

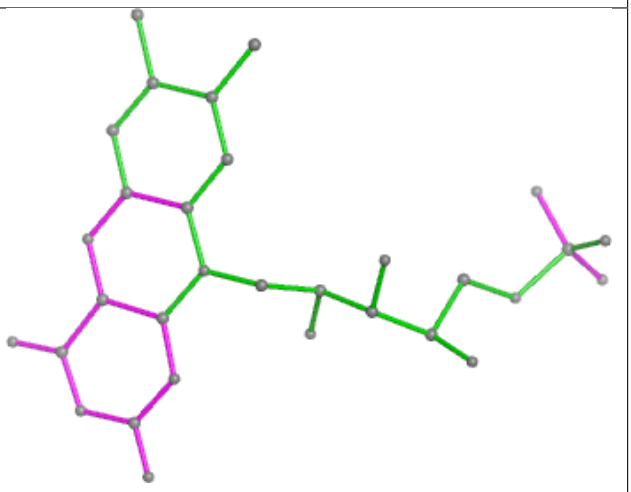
Ligand PE4 B 505



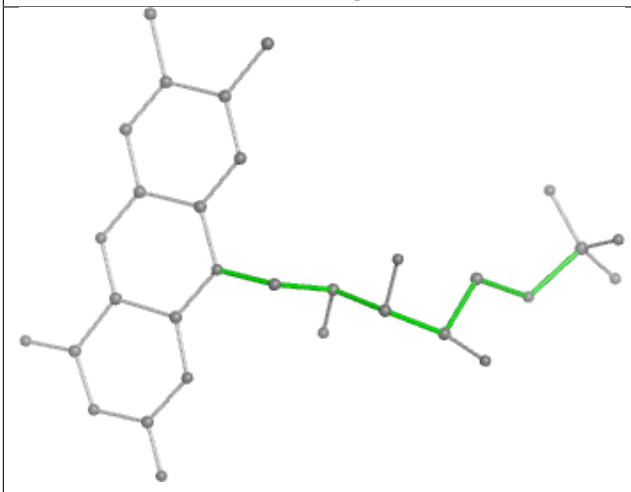
Ligand FMN D 501



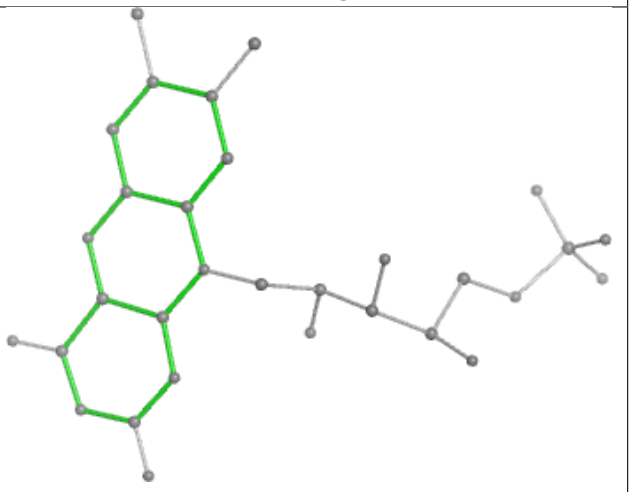
Bond lengths



Bond angles

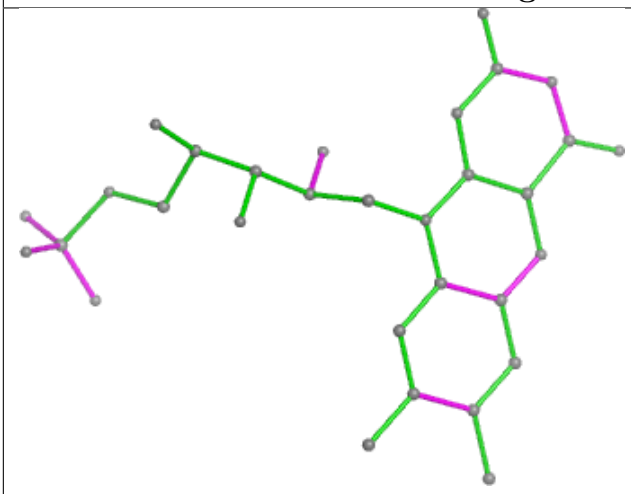


Torsions

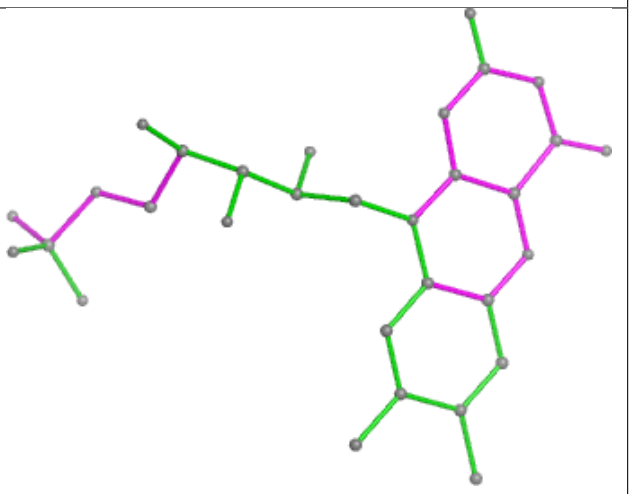


Rings

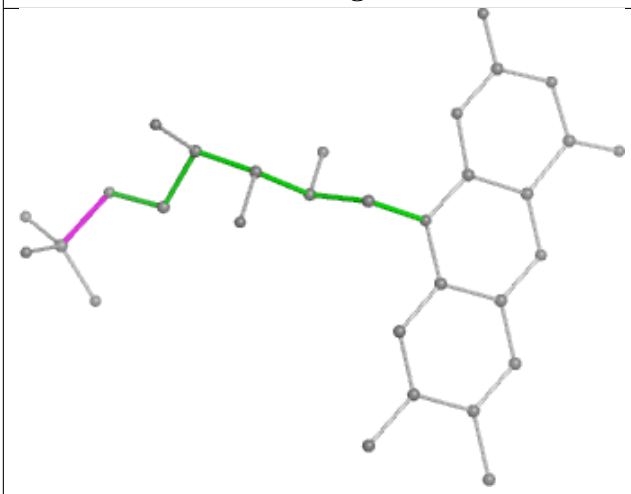
Ligand FMN A 501



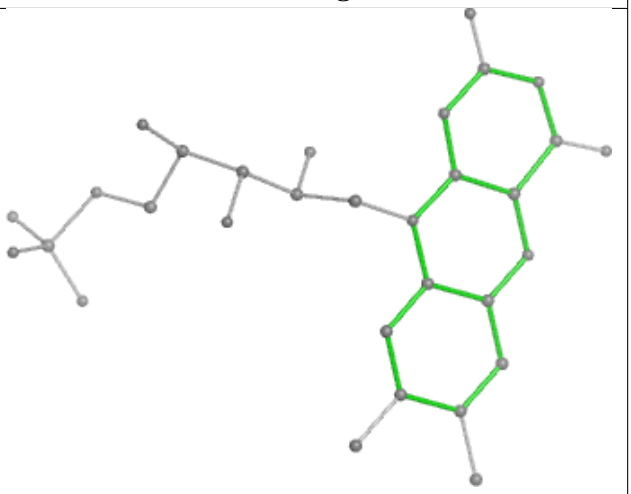
Bond lengths



Bond angles

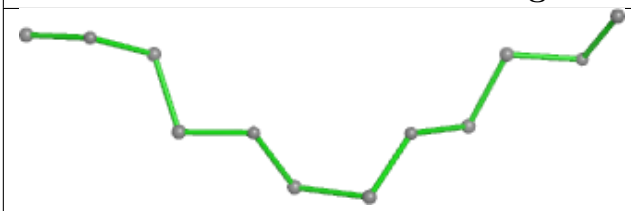


Torsions

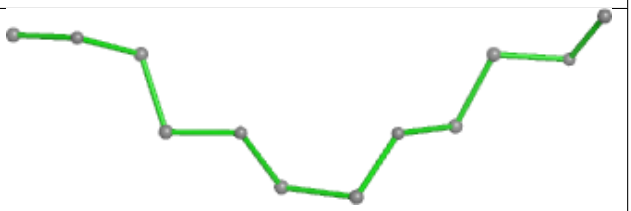


Rings

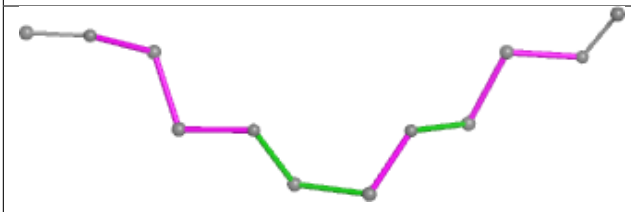
Ligand PE4 C 511



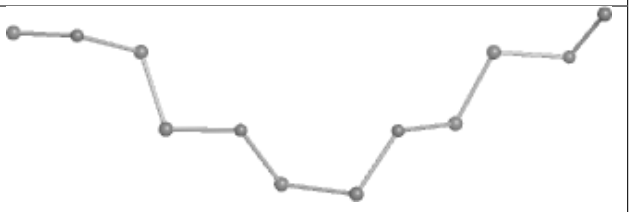
Bond lengths



Bond angles



Torsions



Rings

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	403/410 (98%)	0.25	18 (4%)	33	38	23, 33, 63, 92	0
1	B	403/410 (98%)	0.17	18 (4%)	33	38	23, 31, 64, 101	0
1	C	409/410 (99%)	0.15	13 (3%)	47	53	22, 31, 55, 82	0
1	D	409/410 (99%)	0.10	14 (3%)	45	51	21, 30, 53, 95	0
All	All	1624/1640 (99%)	0.17	63 (3%)	39	45	21, 31, 59, 101	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	133	LEU	9.4
1	B	409	THR	9.1
1	C	133	LEU	8.9
1	A	224	LEU	8.5
1	D	219	ILE	8.1
1	A	223	LEU	7.8
1	C	223	LEU	7.6
1	D	409	THR	6.7
1	B	221	LEU	6.6
1	B	222	GLY	6.1
1	B	133	LEU	6.0
1	D	223	LEU	6.0
1	B	219	ILE	5.9
1	B	223	LEU	5.4
1	C	221	LEU	5.4
1	C	408	LYS	5.0
1	C	219	ILE	4.9
1	A	221	LEU	4.8
1	D	150	LEU	4.8
1	A	409	THR	4.4
1	C	409	THR	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	220	GLU	4.2
1	D	224	LEU	4.2
1	D	151	LEU	3.9
1	B	225	GLU	3.8
1	B	148	ALA	3.8
1	C	215	PHE	3.7
1	A	220	GLU	3.5
1	B	218	VAL	3.5
1	C	150	LEU	3.4
1	C	224	LEU	3.3
1	D	212	LEU	3.3
1	D	221	LEU	3.3
1	A	218	VAL	3.2
1	A	219	ILE	3.2
1	B	224	LEU	3.1
1	D	220	GLU	3.0
1	A	376	LEU	2.9
1	D	408	LYS	2.9
1	C	131	LYS	2.8
1	B	155	ASP	2.8
1	B	72	GLY	2.8
1	C	123	LYS	2.7
1	A	146	LEU	2.6
1	B	75	PHE	2.5
1	A	216	LYS	2.5
1	C	255	LYS	2.4
1	D	215	PHE	2.4
1	A	214	LYS	2.4
1	A	227	ILE	2.3
1	B	212	LEU	2.3
1	D	123	LYS	2.3
1	C	222	GLY	2.3
1	A	213	LYS	2.3
1	B	210	LEU	2.2
1	D	131	LYS	2.2
1	A	408	LYS	2.2
1	B	131	LYS	2.2
1	A	132	SER	2.1
1	A	341	ARG	2.1
1	B	217	GLU	2.1
1	D	222	GLY	2.1
1	A	79	VAL	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
6	PE4	B	505	12/24	0.66	0.15	61,71,73,73	0
6	PE4	D	511	12/24	0.69	0.31	43,53,54,55	24
6	PE4	C	511	12/24	0.77	0.21	64,69,71,71	0
6	PE4	B	506	12/24	0.82	0.17	61,64,66,67	0
5	GOL	A	506	6/6	0.86	0.17	34,35,41,41	0
6	PE4	C	510	12/24	0.88	0.12	32,40,54,58	0
5	GOL	D	513	6/6	0.89	0.16	19,21,47,47	0
3	CA	C	506	1/1	0.89	0.05	53,53,53,53	0
3	CA	A	504	1/1	0.89	0.15	41,41,41,41	0
3	CA	B	503	1/1	0.90	0.18	39,39,39,39	0
5	GOL	B	507	6/6	0.90	0.12	29,35,38,44	0
6	PE4	D	510	12/24	0.91	0.13	38,40,58,65	0
3	CA	D	504	1/1	0.93	0.15	36,36,36,36	0
5	GOL	D	512	6/6	0.93	0.09	29,38,43,43	0
2	FMN	B	501	31/31	0.93	0.12	16,24,29,29	0
3	CA	A	503	1/1	0.94	0.06	65,65,65,65	0
5	GOL	C	513	6/6	0.94	0.11	23,33,40,41	0
5	GOL	C	512	6/6	0.95	0.07	32,35,40,40	0
2	FMN	D	501	31/31	0.96	0.08	20,29,34,36	0
3	CA	C	503	1/1	0.96	0.05	37,37,37,37	0
3	CA	C	504	1/1	0.97	0.17	35,35,35,35	0
2	FMN	C	501	31/31	0.97	0.08	22,29,38,40	0
2	FMN	A	501	31/31	0.97	0.09	20,25,28,30	0
3	CA	D	506	1/1	0.97	0.05	48,48,48,48	0
3	CA	C	505	1/1	0.98	0.11	26,26,26,26	0
3	CA	C	502	1/1	0.98	0.05	35,35,35,35	0
7	7MT	C	508	30/30	0.98	0.13	15,32,40,46	0

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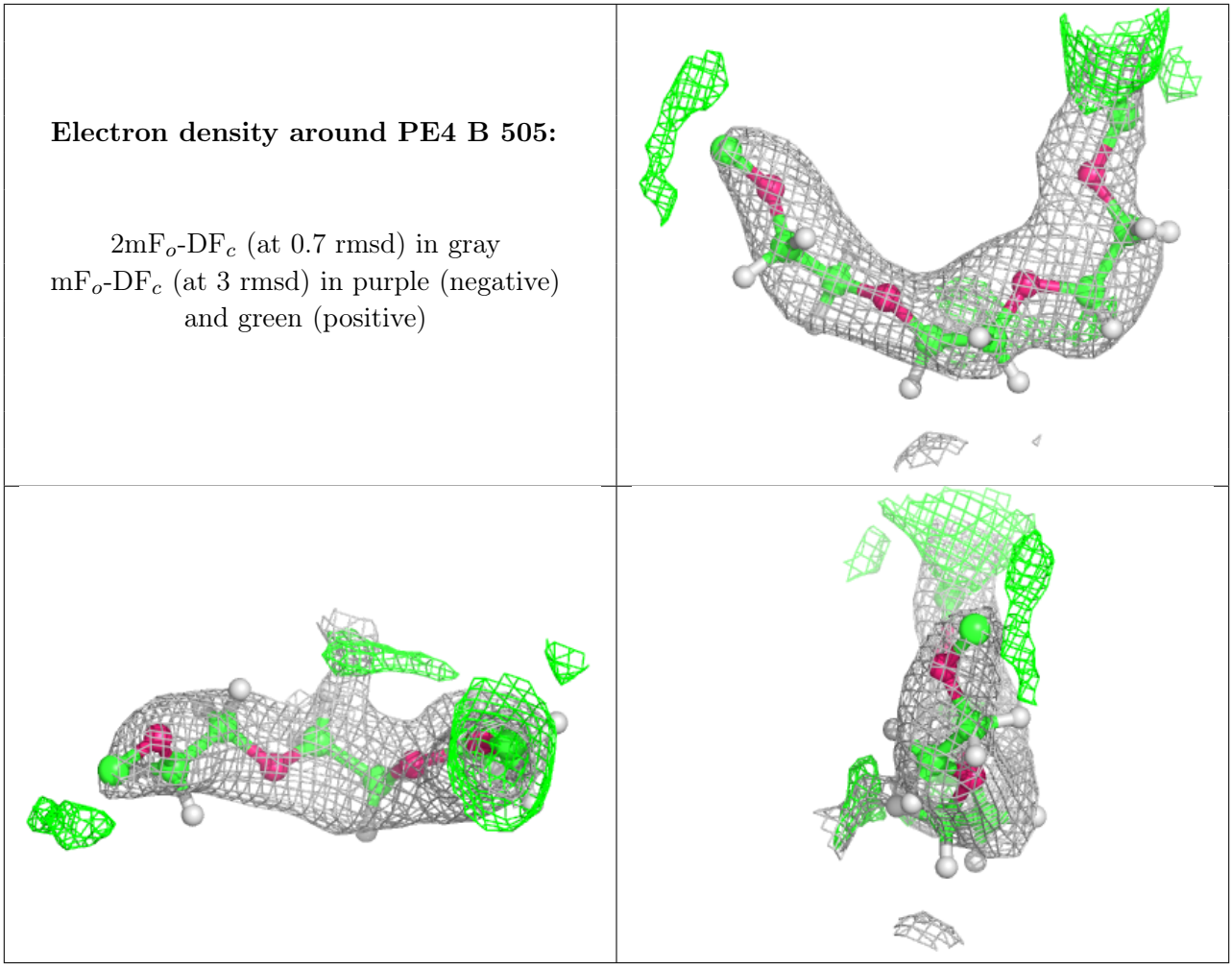
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	NA	D	514	1/1	0.98	0.18	35,35,35,35	0
3	CA	B	502	1/1	0.99	0.08	36,36,36,36	0
3	CA	D	502	1/1	0.99	0.08	32,32,32,32	0
3	CA	D	503	1/1	0.99	0.06	31,31,31,31	0
3	CA	A	502	1/1	0.99	0.04	35,35,35,35	0
7	7MT	C	509	30/30	0.99	0.11	25,32,38,41	0
7	7MT	D	508	30/30	0.99	0.10	23,35,39,40	0
7	7MT	D	509	30/30	0.99	0.10	24,33,39,42	0
3	CA	D	505	1/1	0.99	0.11	25,25,25,25	0
4	TB	B	504	1/1	1.00	0.06	29,29,29,29	0
4	TB	C	507	1/1	1.00	0.08	25,25,25,25	0
4	TB	D	507	1/1	1.00	0.08	25,25,25,25	0
4	TB	A	505	1/1	1.00	0.07	30,30,30,30	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.

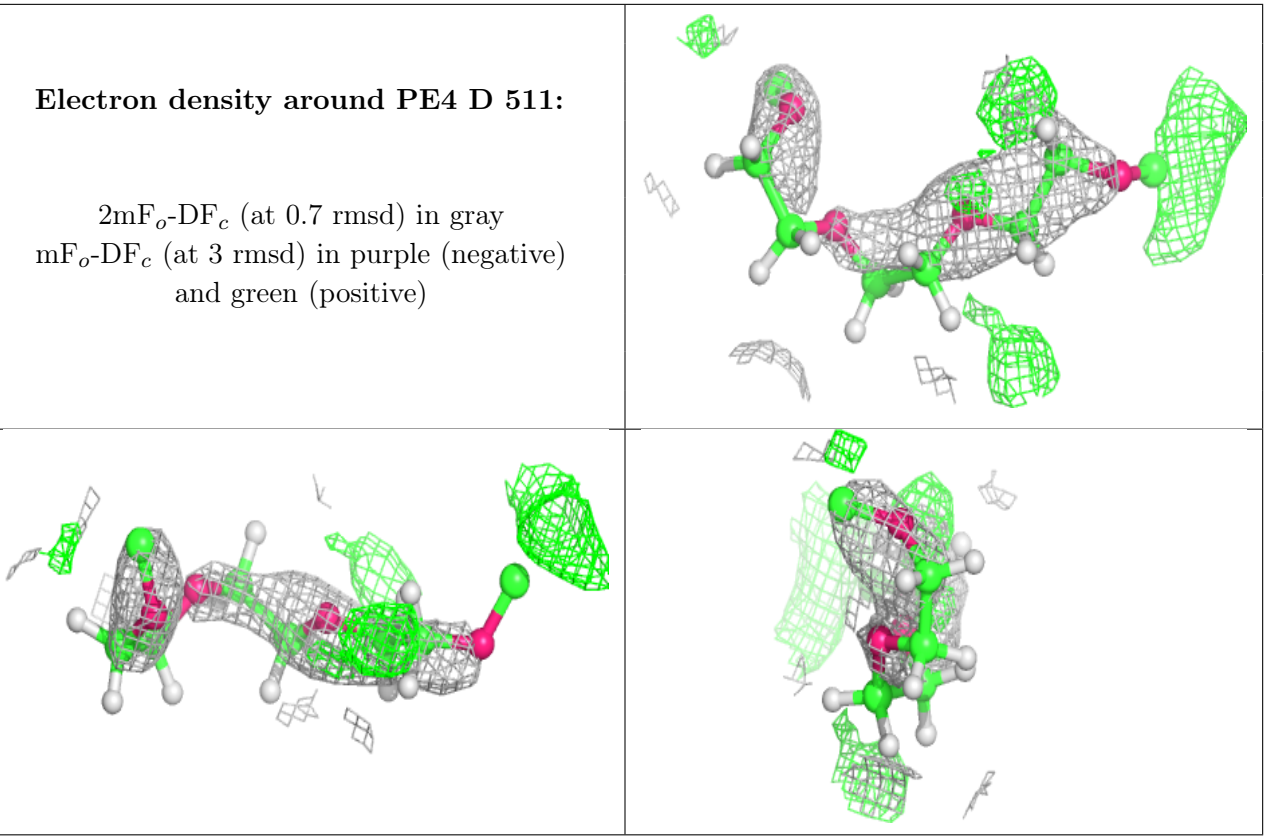
Electron density around PE4 B 505:

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



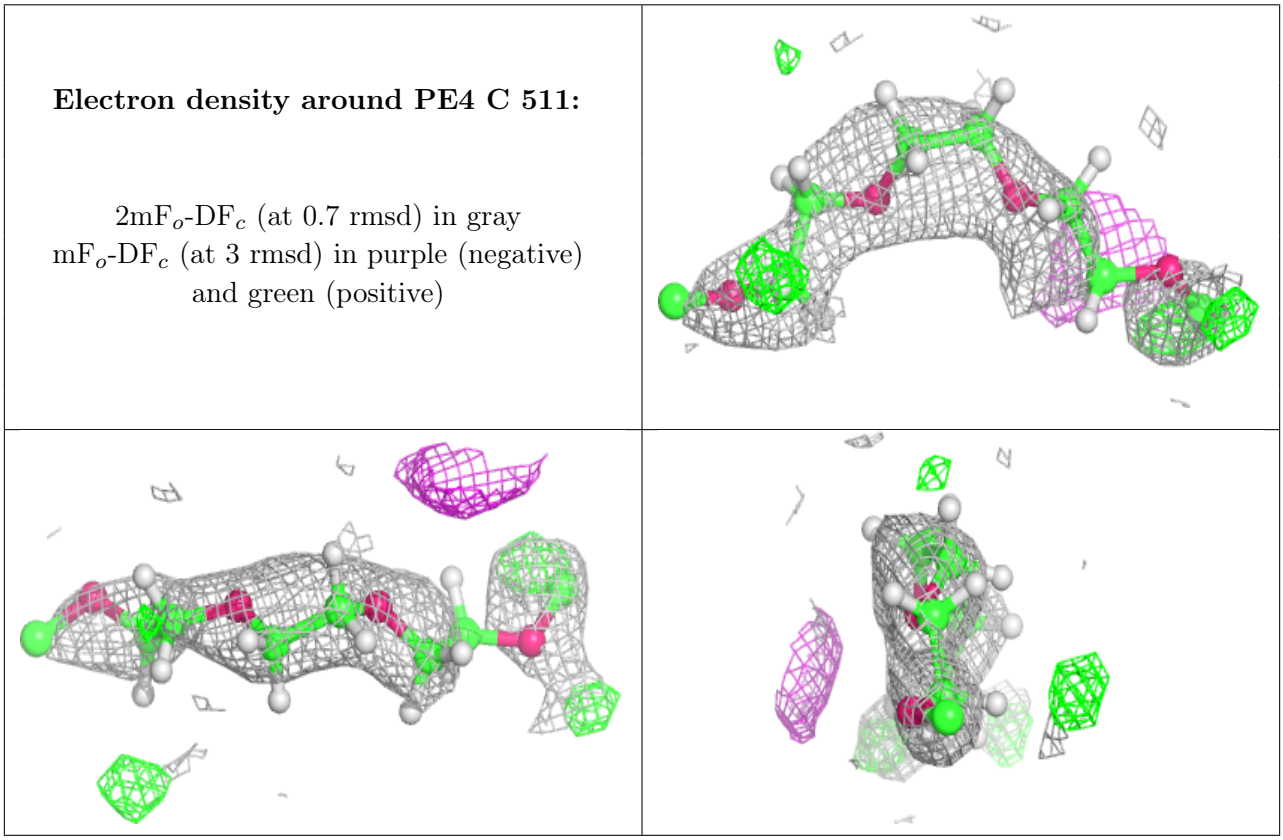
Electron density around PE4 D 511:

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



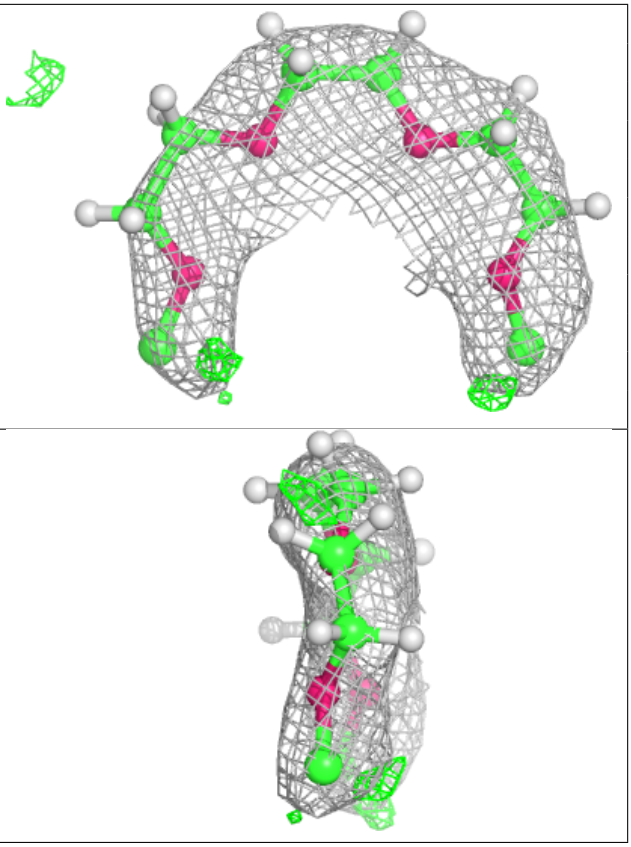
Electron density around PE4 C 511:

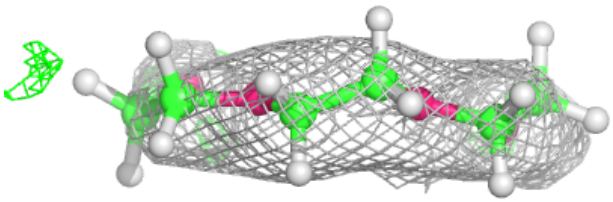
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around PE4 B 506:

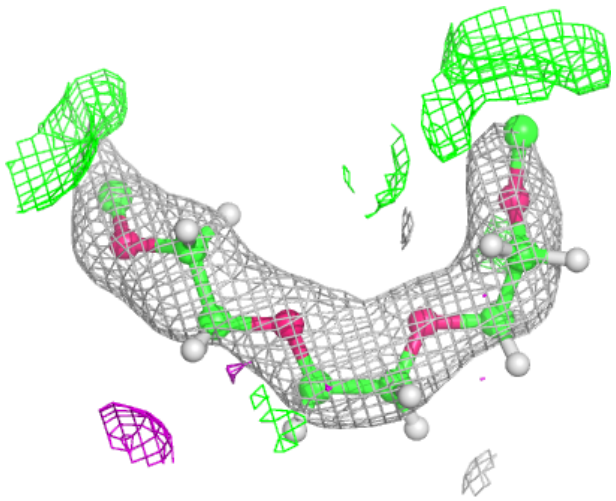
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

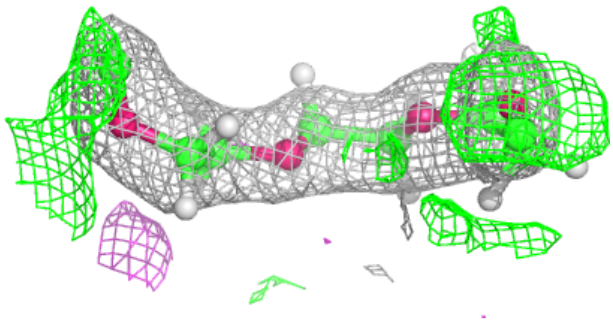


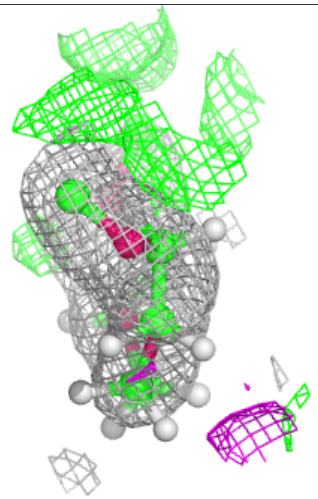


Electron density around PE4 C 510:

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

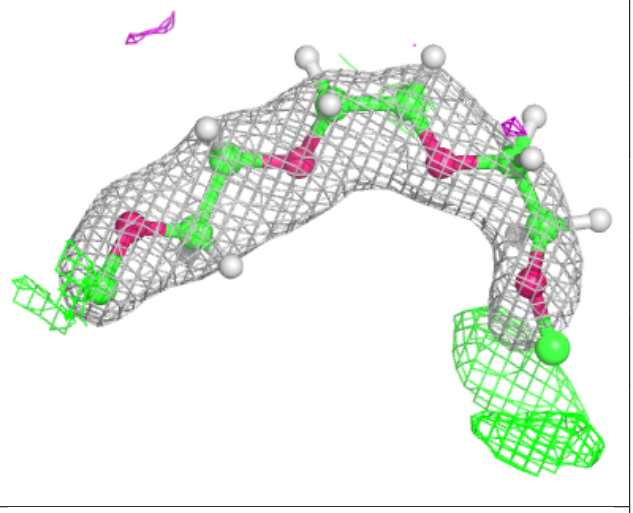


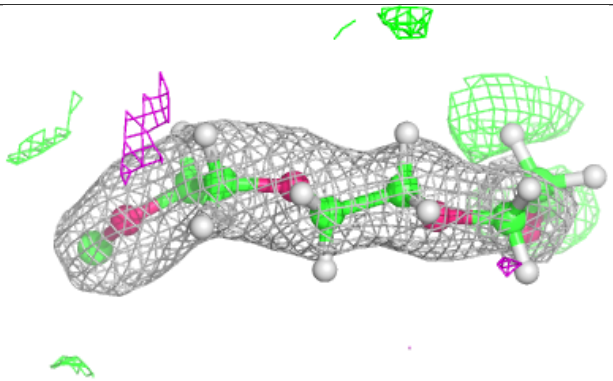


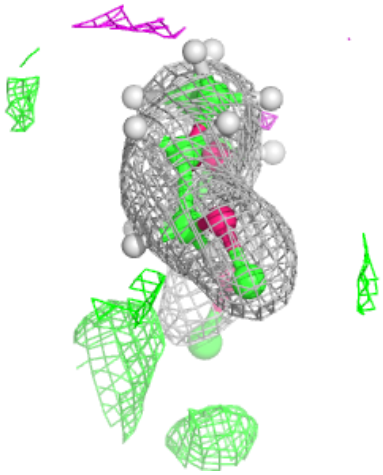


Electron density around PE4 D 510:

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

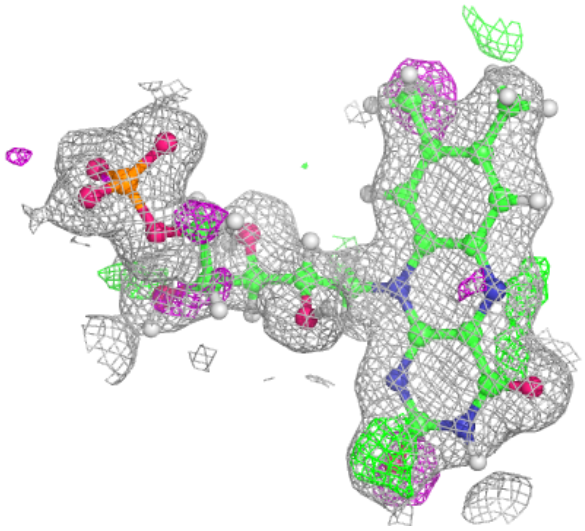


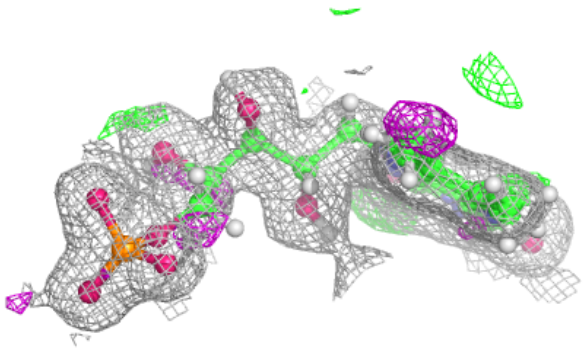


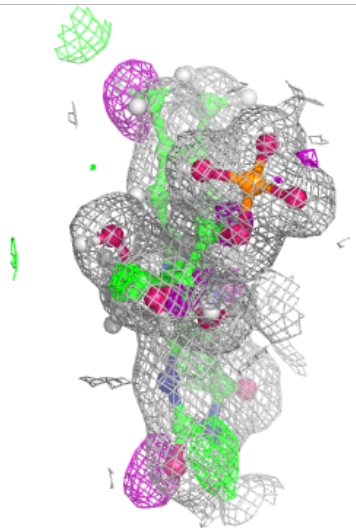


Electron density around FMN B 501:

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

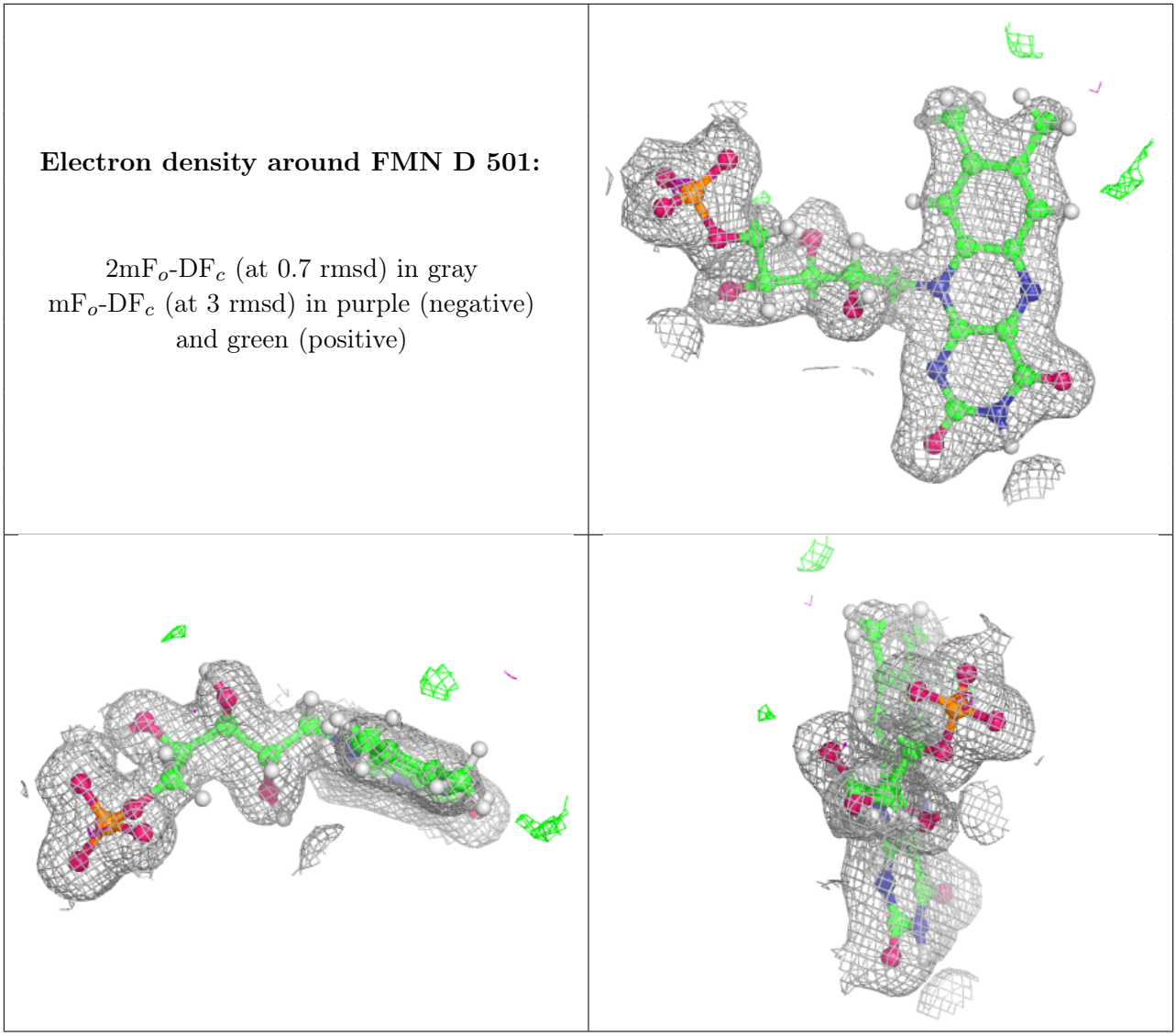






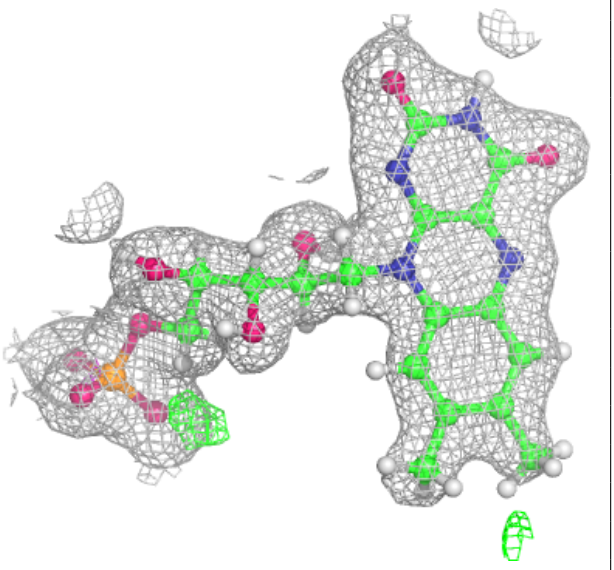
Electron density around FMN D 501:

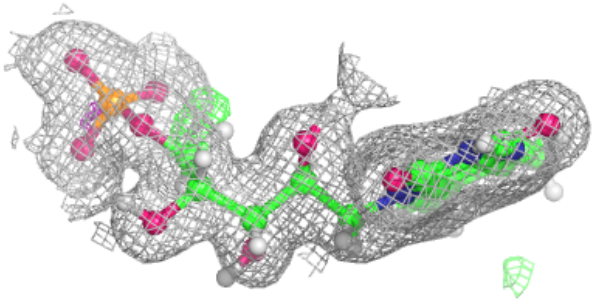
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

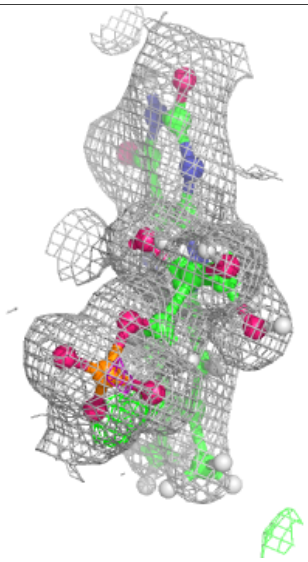


Electron density around FMN C 501:

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

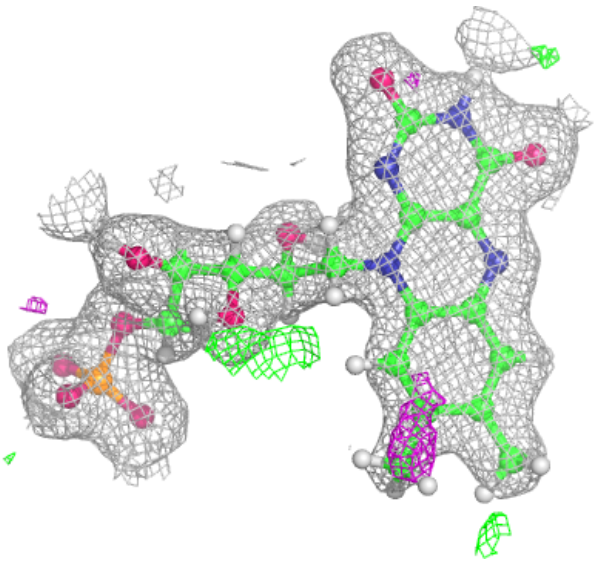


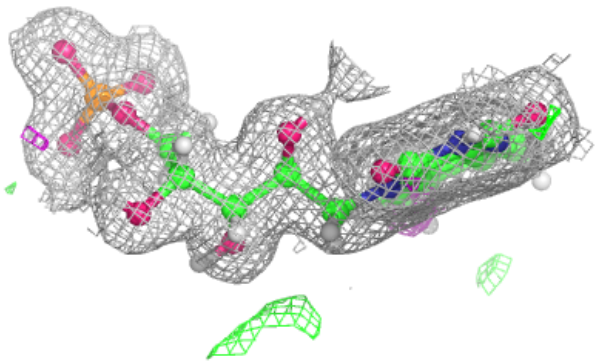


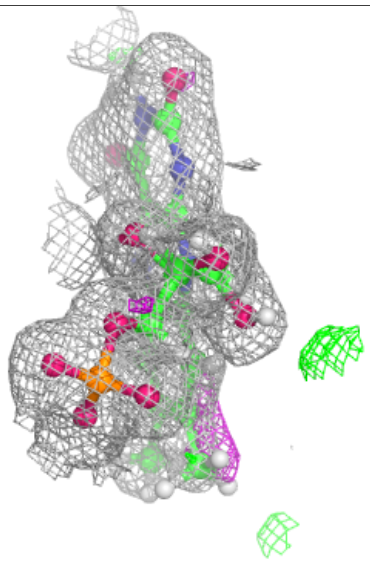


Electron density around FMN A 501:

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

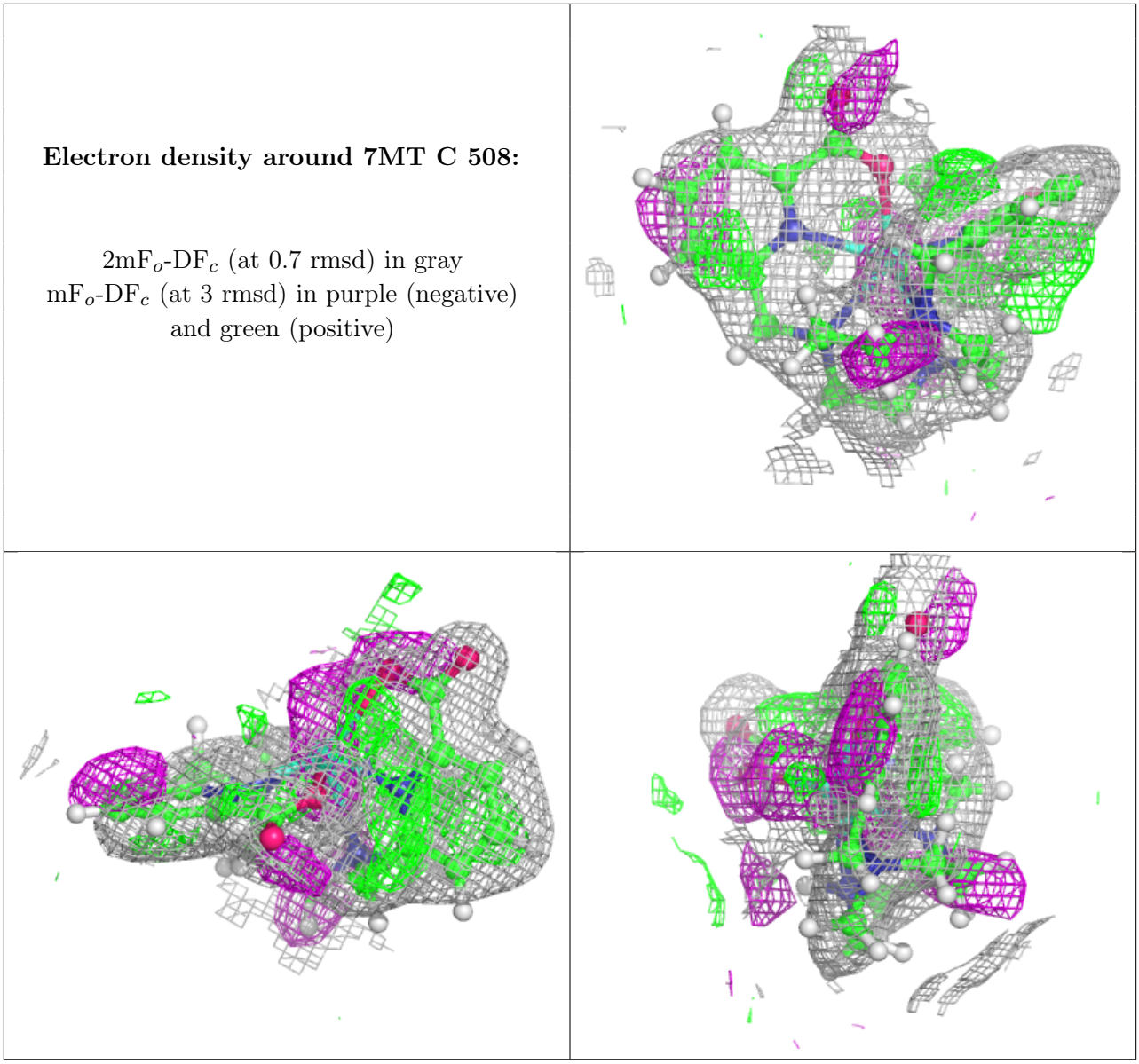






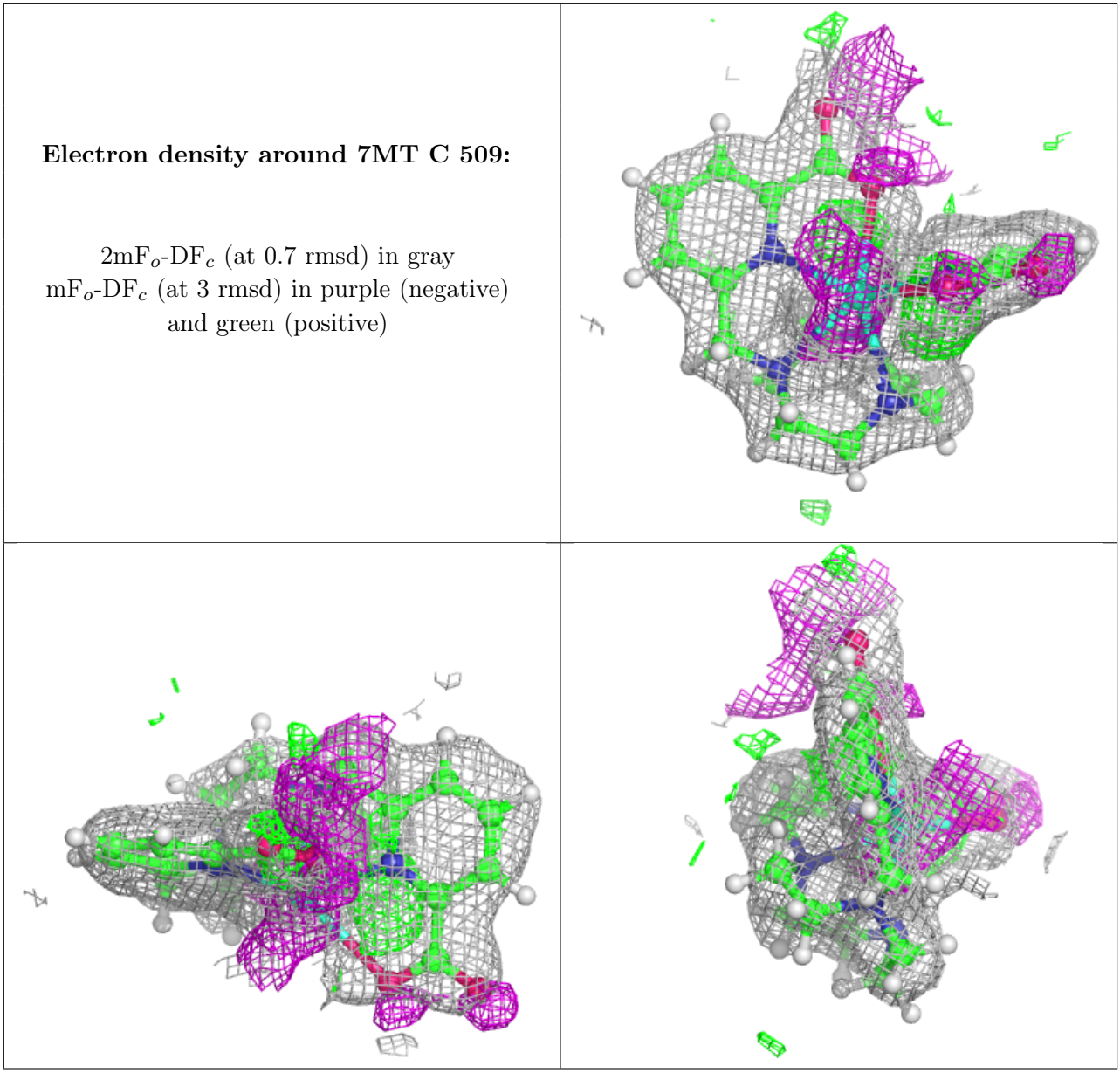
Electron density around 7MT C 508:

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



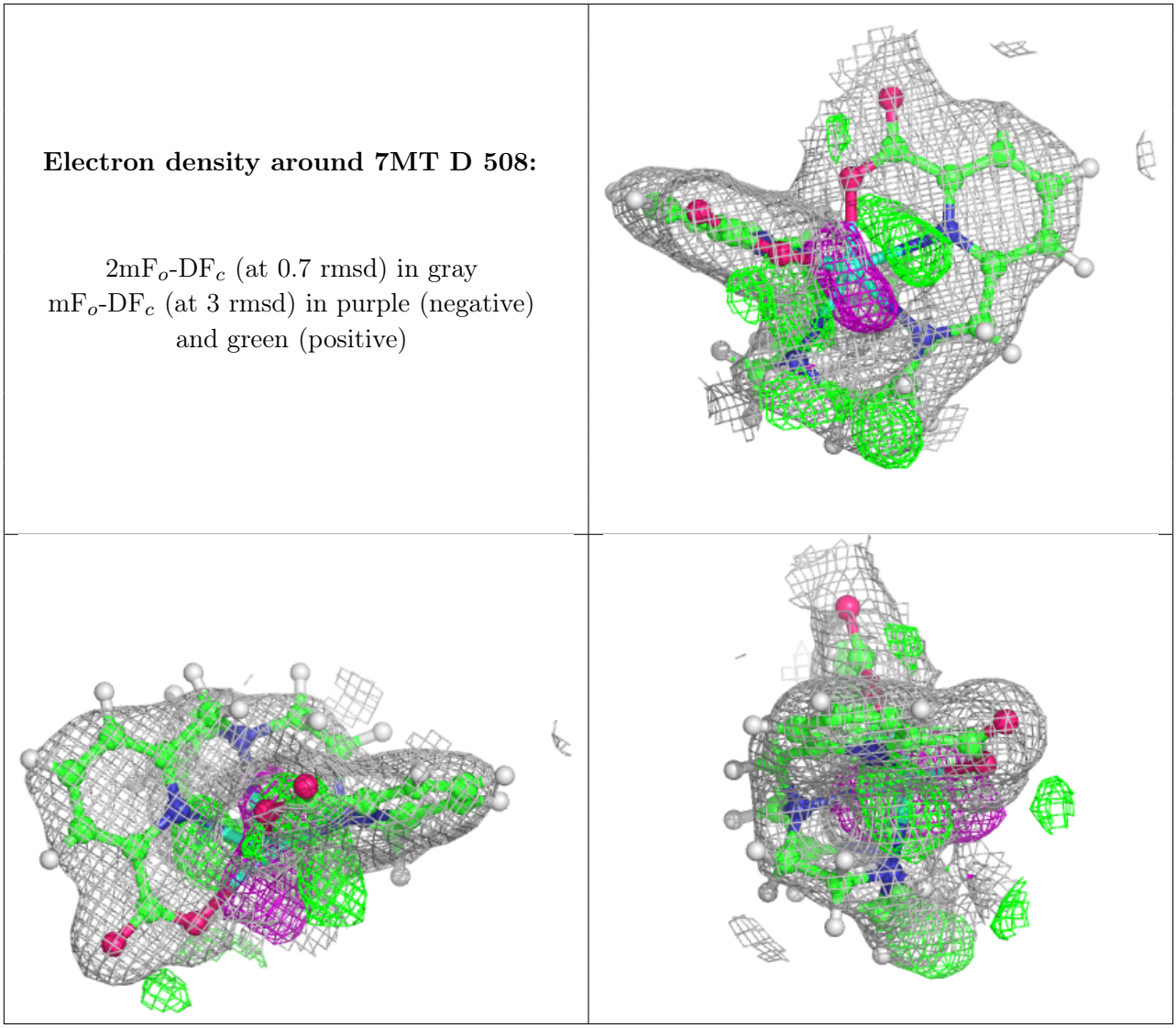
Electron density around 7MT C 509:

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



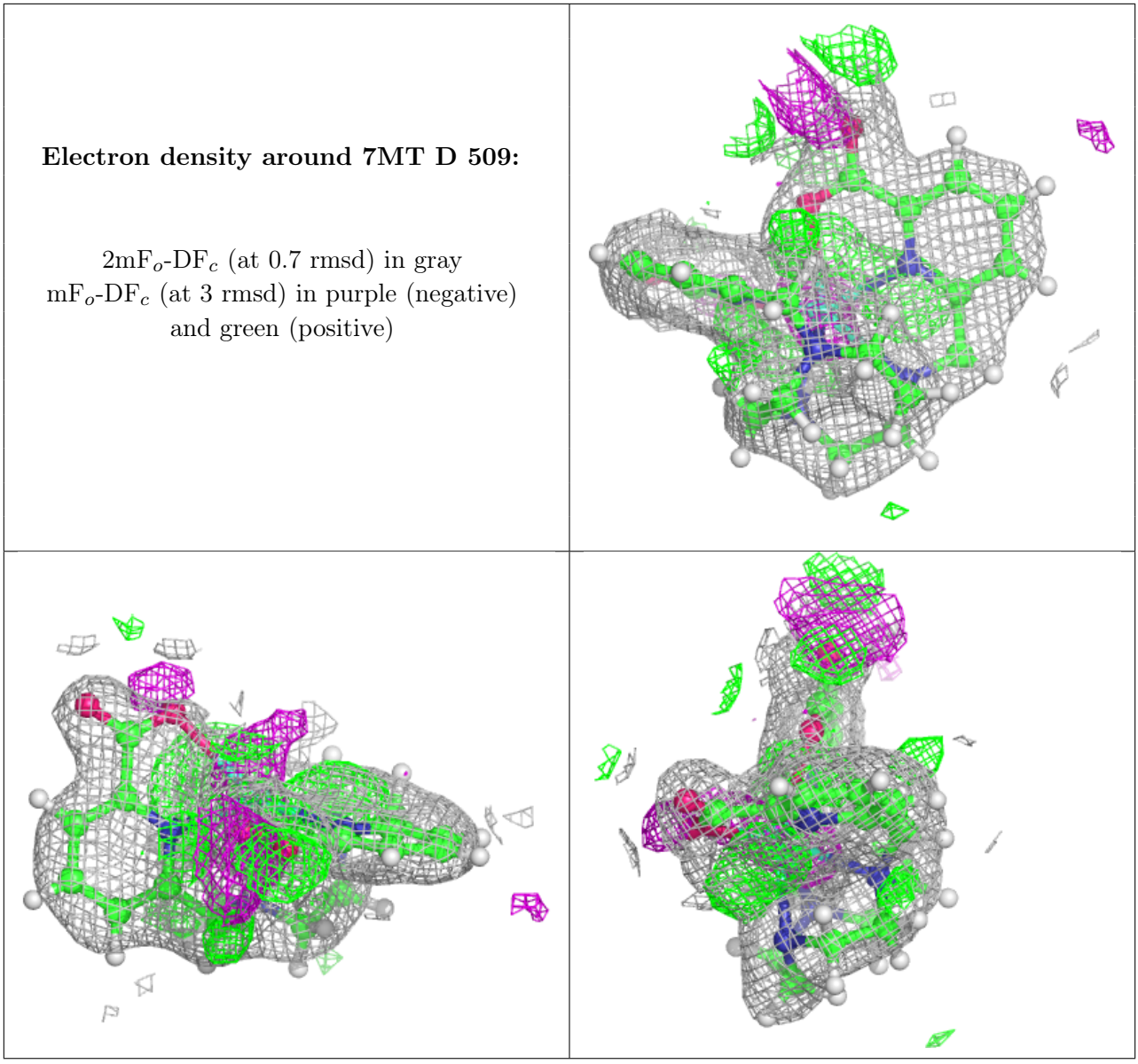
Electron density around 7MT D 508:

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



Electron density around 7MT D 509:

$2mF_o$-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.