Full wwPDB X-ray Structure Validation Report ⓘ

Nov 20, 2023 – 01:13 AM JST

PDB ID	:	7CC3
Title	:	Versatile cis-prenyltransferase MM_0014 from Methanosarcina mazei (crystal type: co-FG)
Authors	:	Unno, H.; Hemmi, H.
Deposited on	:	2020-06-16
Resolution	:	1.72 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:

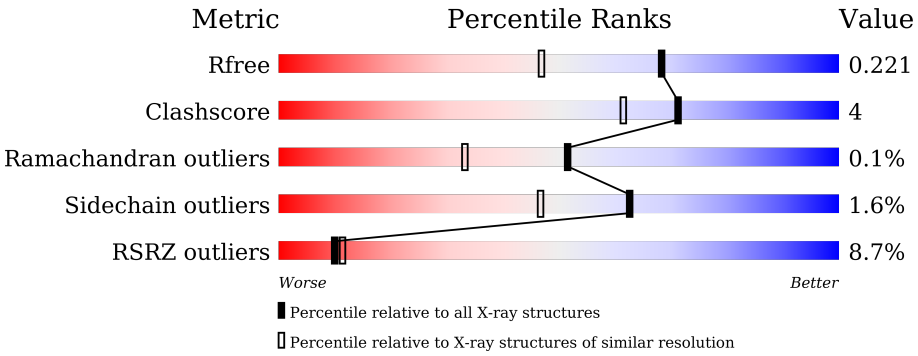
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 1.72 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	5722 (1.74-1.70)
Clashscore	141614	6152 (1.74-1.70)
Ramachandran outliers	138981	6051 (1.74-1.70)
Sidechain outliers	138945	6051 (1.74-1.70)
RSRZ outliers	127900	5629 (1.74-1.70)

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	224	6% 84% 9% 6%
1	B	224	8% 87% 12% .
1	C	224	12% 82% 14% .
1	D	224	10% 85% 7% 8%
1	E	224	9% 86% 10% .
1	F	224	8% 83% 8% 9%

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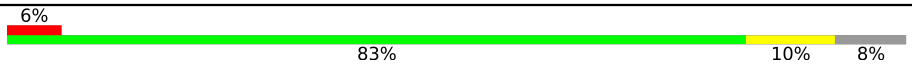
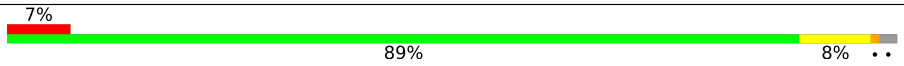
Mol	Chain	Length	Quality of chain
1	G	224	
1	H	224	

2 Entry composition (i)

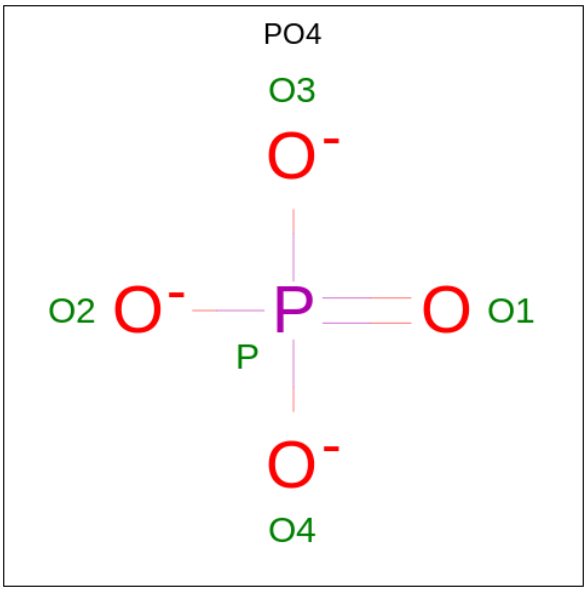
There are 7 unique types of molecules in this entry. The entry contains 15202 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 cis-prenyltransferase MM_0014.

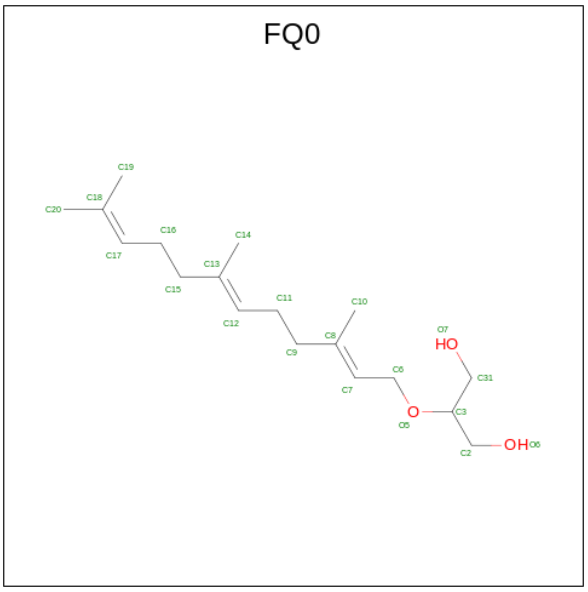
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	211	Total	C	N	O	S	0	0	0
			1726	1118	293	308	7			
1	B	221	Total	C	N	O	S	0	0	0
			1794	1156	305	326	7			
1	C	216	Total	C	N	O	S	0	0	0
			1755	1132	299	318	6			
1	D	206	Total	C	N	O	S	0	0	0
			1686	1092	287	301	6			
1	E	215	Total	C	N	O	S	0	0	0
			1747	1128	297	316	6			
1	F	204	Total	C	N	O	S	0	0	0
			1670	1084	285	295	6			
1	G	207	Total	C	N	O	S	0	1	0
			1700	1102	288	304	6			
1	H	220	Total	C	N	O	S	0	0	0
			1787	1154	303	323	7			

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P) (labeled as "Ligand of Interest" by depositor).



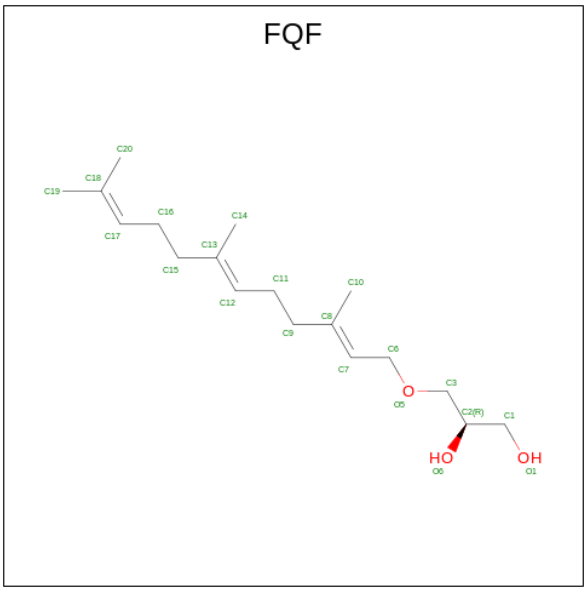
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0
2	F	1	Total O P 5 4 1	0	0
2	H	1	Total O P 5 4 1	0	0

- Molecule 3 is 2-[(2E,6E)-3,7,11-trimethyldodeca-2,6,10-trienoxy]propane-1,3-diol (three-letter code: FQ0) (formula: $C_{18}H_{32}O_3$) (labeled as "Ligand of Interest" by depositor).



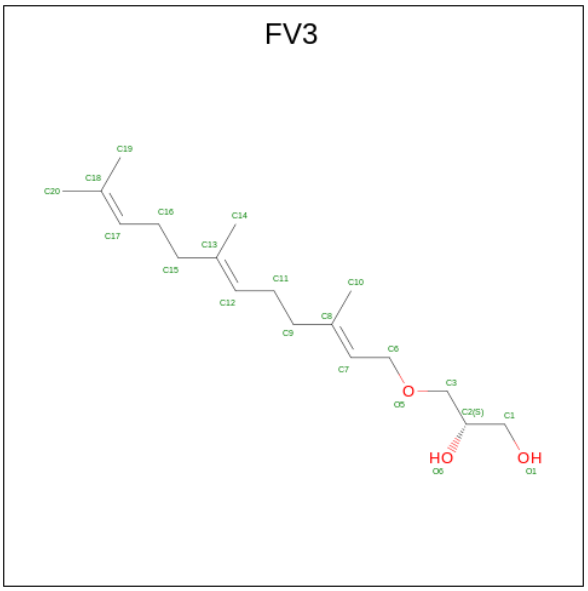
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 21 18 3	0	0
3	B	1	Total C O 21 18 3	0	0
3	C	1	Total C O 21 18 3	0	0
3	D	1	Total C O 21 18 3	0	0
3	E	1	Total C O 21 18 3	0	0
3	F	1	Total C O 21 18 3	0	0
3	G	1	Total C O 21 18 3	0	0
3	H	1	Total C O 21 18 3	0	0

- Molecule 4 is (2R)-3-[(2E,6E)-3,7,11-trimethyldodeca-2,6,10-trienoxy]propane-1,2-diol (three-letter code: FQF) (formula: $C_{18}H_{32}O_3$) (labeled as "Ligand of Interest" by depositor).



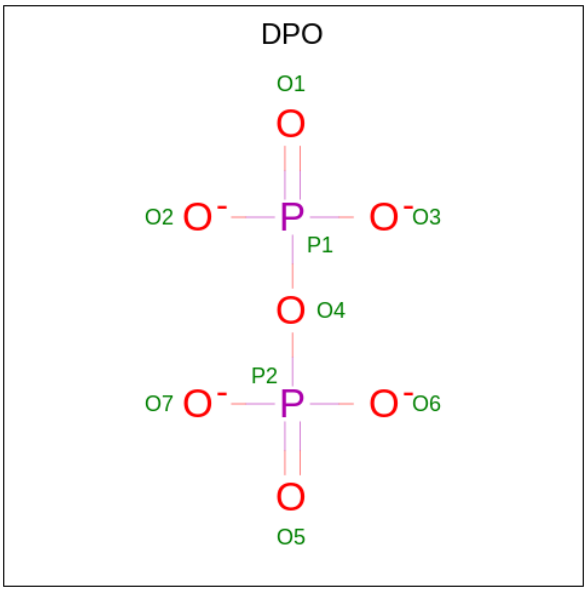
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 21 18 3	0	0
4	B	1	Total C O 21 18 3	0	0
4	C	1	Total C O 21 18 3	0	0
4	D	1	Total C O 21 18 3	0	0
4	E	1	Total C O 21 18 3	0	0
4	F	1	Total C O 21 18 3	0	0
4	G	1	Total C O 21 18 3	0	0
4	H	1	Total C O 21 18 3	0	0

- Molecule 5 is (2S)-3-[(2E,6E)-3,7,11-trimethyldodeca-2,6,10-trienoxy]propane-1,2-diol (three-letter code: FV3) (formula: $C_{18}H_{32}O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 21 18 3	0	0
5	B	1	Total C O 21 18 3	0	0
5	C	1	Total C O 21 18 3	0	0
5	D	1	Total C O 21 18 3	0	0
5	E	1	Total C O 21 18 3	0	0
5	F	1	Total C O 21 18 3	0	0
5	G	1	Total C O 21 18 3	0	0
5	H	1	Total C O 21 18 3	0	0

- Molecule 6 is DIPHOSPHATE (three-letter code: DPO) (formula: O_7P_2) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total O P 9 7 2	0	0
6	E	1	Total O P 9 7 2	0	0
6	G	1	Total O P 9 7 2	0	0

- Molecule 7 is water.

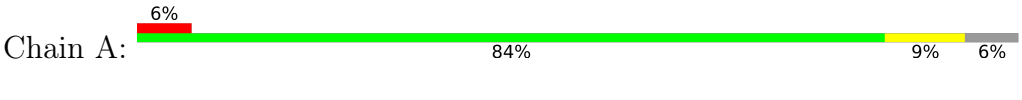
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	123	Total O 123 123	0	0
7	B	109	Total O 109 109	0	0
7	C	71	Total O 71 71	0	0
7	D	84	Total O 84 84	0	0
7	E	104	Total O 104 104	0	0
7	F	71	Total O 71 71	0	0
7	G	103	Total O 103 103	0	0
7	H	116	Total O 116 116	0	0

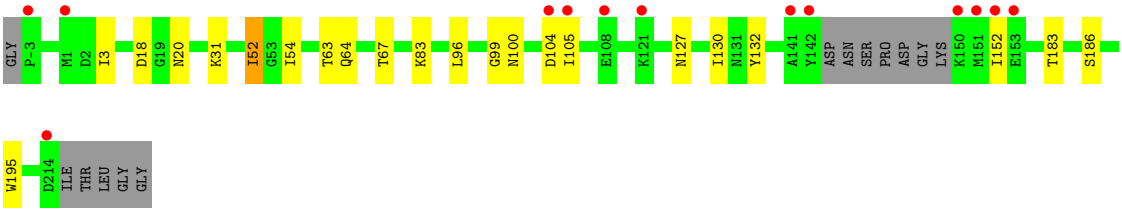
3 Residue-property plots (i)

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: cis-prenyltransferase MM_0014

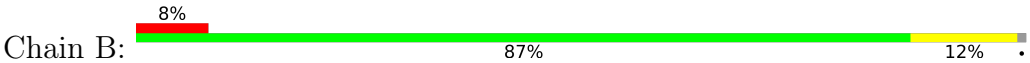
Chain A:

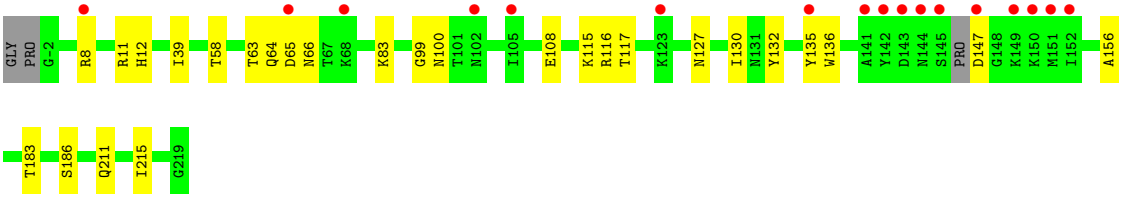




• Molecule 1: cis-prenyltransferase MM_0014

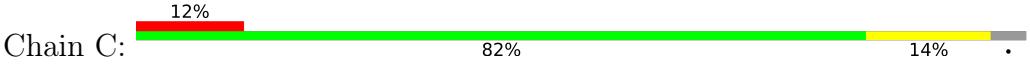
Chain B:

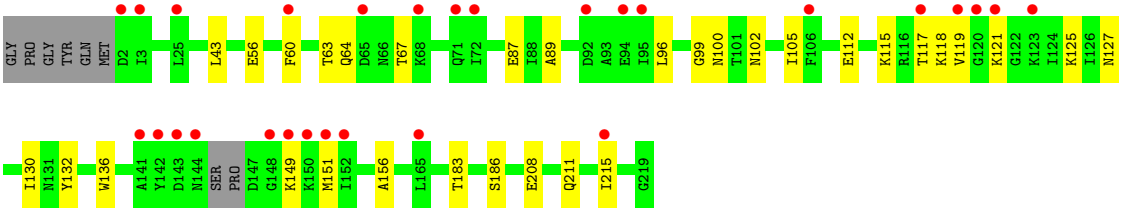




• Molecule 1: cis-prenyltransferase MM_0014

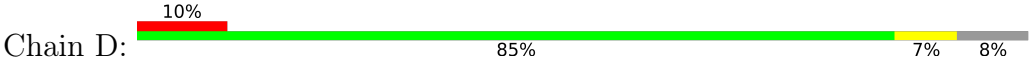
Chain C:

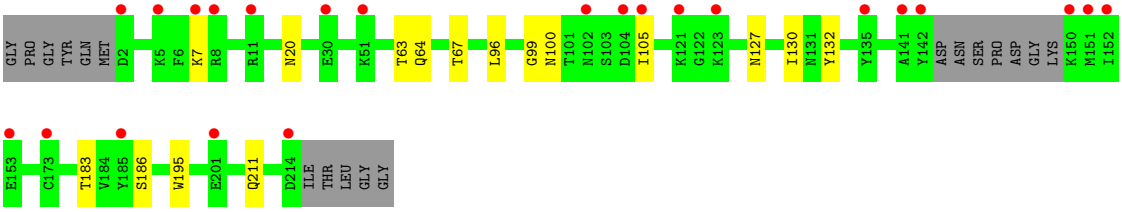




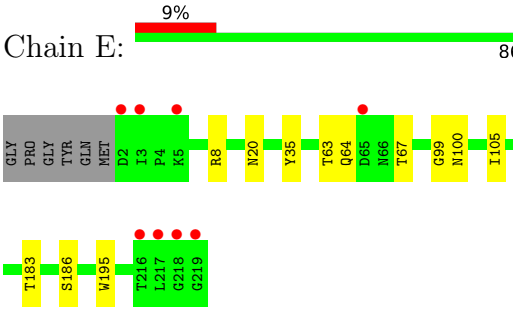
• Molecule 1: cis-prenyltransferase MM_0014

Chain D:

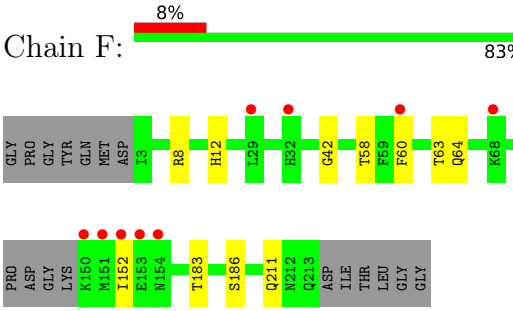




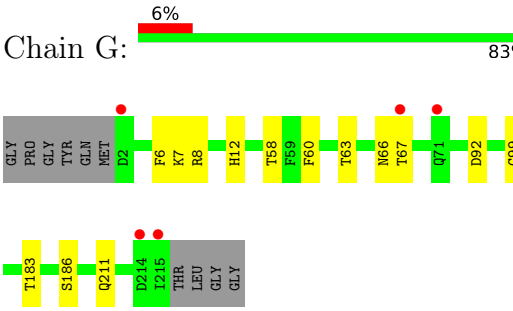
• Molecule 1: cis-prenyltransferase MM_0014



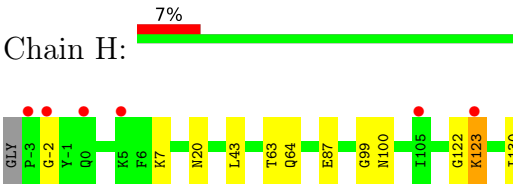
• Molecule 1: cis-prenyltransferase MM_0014



• Molecule 1: cis-prenyltransferase MM_0014



• Molecule 1: cis-prenyltransferase MM_0014



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	99.05Å 99.22Å 193.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.06 – 1.72 48.06 – 1.72	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.06-1.72) 99.6 (48.06-1.72)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	191.28 (at 1.72Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.196 , 0.213 0.206 , 0.221	Depositor DCC
R_{free} test set	9998 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	30.6	Xtriage
Anisotropy	0.009	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 40.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	15202	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.34% 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: FQF, FV3, DPO, PO4, FQ0

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	0.61	0/1769	0.71	0/2390
1	B	0.63	0/1836	0.71	0/2478
1	C	0.62	0/1796	0.68	0/2425
1	D	0.62	0/1727	0.69	0/2334
1	E	0.62	0/1788	0.69	0/2414
1	F	0.62	0/1711	0.66	0/2312
1	G	0.61	0/1744	0.66	0/2357
1	H	0.62	0/1830	0.69	0/2470
All	All	0.62	0/14201	0.69	0/19180

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1726	0	1730	13	0
1	B	1794	0	1793	14	0
1	C	1755	0	1756	18	0
1	D	1686	0	1691	9	0
1	E	1747	0	1750	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1670	0	1683	11	0
1	G	1700	0	1708	12	0
1	H	1787	0	1789	11	0
2	A	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	F	5	0	0	0	0
2	H	5	0	0	0	0
3	A	21	0	0	0	0
3	B	21	0	0	0	0
3	C	21	0	0	1	0
3	D	21	0	0	0	0
3	E	21	0	0	0	0
3	F	21	0	0	0	0
3	G	21	0	0	1	0
3	H	21	0	0	1	0
4	A	21	0	0	0	0
4	B	21	0	0	2	0
4	C	21	0	0	1	0
4	D	21	0	0	1	0
4	E	21	0	0	0	0
4	F	21	0	0	1	0
4	G	21	0	0	1	0
4	H	21	0	0	0	0
5	A	21	0	0	1	0
5	B	21	0	0	0	0
5	C	21	0	0	0	0
5	D	21	0	0	1	0
5	E	21	0	0	0	0
5	F	21	0	0	0	0
5	G	21	0	0	2	0
5	H	21	0	0	1	0
6	B	9	0	0	1	0
6	E	9	0	0	1	0
6	G	9	0	0	0	0
7	A	123	0	0	0	0
7	B	109	0	0	0	0
7	C	71	0	0	1	0
7	D	84	0	0	0	0
7	E	104	0	0	0	0
7	F	71	0	0	1	0
7	G	103	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	H	116	0	0	0	0
All	All	15202	0	13900	100	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 4.

All (100) 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:89:ALA:O	1:C:119:VAL:HG21	1.82	0.80
3:H:302:FQ0:C14	5:H:304:FV3:C9	2.51	0.77
3:G:302:FQ0:C12	5:G:304:FV3:C10	2.55	0.75
1:B:116:ARG:HH22	1:B:127:ASN:HD21	1.33	0.73
1:D:64:GLN:HE22	1:D:100:ASN:HD22	1.38	0.72
1:A:64:GLN:HE22	1:A:100:ASN:HD22	1.40	0.69
1:B:11:ARG:HD3	1:C:102:ASN:HA	1.75	0.68
1:A:52:ILE:HD11	1:A:54:ILE:HD11	1.75	0.68
1:E:64:GLN:HE22	1:E:100:ASN:HD22	1.42	0.68
1:B:115:LYS:O	1:B:117:THR:HG23	1.96	0.65
1:B:215:ILE:O	1:C:112:GLU:HA	1.98	0.64
1:C:215:ILE:O	1:E:112:GLU:HA	1.98	0.63
1:A:3:ILE:HG21	1:A:52:ILE:HG22	1.81	0.62
1:C:119:VAL:HG22	7:C:416:HOH:O	2.00	0.61
1:G:99:GLY:HA3	1:G:130:ILE:O	2.01	0.60
4:D:303:FQF:C10	5:D:304:FV3:C12	2.72	0.59
1:C:64:GLN:HE22	1:C:100:ASN:HD22	1.51	0.59
1:H:63:THR:HA	1:H:132:TYR:O	2.04	0.58
1:H:122:GLY:O	1:H:123:LYS:HG3	2.04	0.58
1:G:67:THR:HG21	1:G:105:ILE:HG21	1.85	0.58
1:A:152:ILE:HG21	1:B:135:TYR:CE2	2.40	0.57
1:F:64:GLN:HE22	1:F:100:ASN:HD22	1.54	0.56
1:A:67:THR:HG21	1:A:105:ILE:HG21	1.87	0.56
4:G:303:FQF:C12	5:G:304:FV3:C10	2.74	0.56
1:H:64:GLN:HE22	1:H:100:ASN:HD22	1.54	0.55
1:F:99:GLY:HA3	1:F:130:ILE:O	2.06	0.55
1:E:115:LYS:O	1:E:117:THR:HG23	2.07	0.55
1:B:99:GLY:HA3	1:B:130:ILE:O	2.08	0.54
1:D:99:GLY:HA3	1:D:130:ILE:O	2.07	0.54
1:G:6:PHE:HA	1:G:211:GLN:HE22	1.73	0.54
1:B:116:ARG:HH22	1:B:127:ASN:ND2	2.03	0.54
1:A:99:GLY:HA3	1:A:130:ILE:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:THR:HA	1:B:132:TYR:O	2.08	0.54
1:E:63:THR:HA	1:E:132:TYR:O	2.09	0.53
1:G:92:ASP:HB2	1:G:123:LYS:HE2	1.90	0.53
1:F:63:THR:HA	1:F:132:TYR:O	2.08	0.53
1:C:63:THR:HA	1:C:132:TYR:O	2.08	0.53
1:G:7:LYS:H	1:G:211:GLN:NE2	2.06	0.53
1:G:63:THR:HA	1:G:132:TYR:O	2.10	0.52
1:D:64:GLN:NE2	1:D:100:ASN:HD22	2.07	0.52
1:F:8:ARG:H	1:F:211:GLN:HE21	1.57	0.51
1:E:20:ASN:HD21	1:E:195:TRP:HD1	1.58	0.51
1:F:116:ARG:HH21	1:F:127:ASN:HD21	1.57	0.51
1:C:64:GLN:NE2	1:C:100:ASN:HD22	2.08	0.51
1:E:183:THR:HA	1:E:186:SER:OG	2.12	0.50
1:F:12:HIS:HE1	1:F:58:THR:OG1	1.95	0.50
1:A:31:LYS:NZ	1:C:118:LYS:O	2.41	0.50
1:H:20:ASN:HD21	1:H:195:TRP:HD1	1.59	0.50
1:E:99:GLY:HA3	1:E:130:ILE:O	2.13	0.49
1:E:64:GLN:NE2	1:E:100:ASN:HD22	2.07	0.49
1:B:64:GLN:HE22	1:B:100:ASN:HD22	1.59	0.48
1:A:64:GLN:NE2	1:A:100:ASN:HD22	2.10	0.48
1:B:12:HIS:HE1	1:B:58:THR:OG1	1.96	0.48
1:C:115:LYS:O	1:C:117:THR:HG23	2.14	0.48
1:D:67:THR:HG21	1:D:105:ILE:HG21	1.96	0.48
1:B:39:ILE:HD13	1:B:83:LYS:HG2	1.96	0.47
1:H:7:LYS:H	1:H:211:GLN:NE2	2.12	0.47
1:H:64:GLN:NE2	1:H:100:ASN:HD22	2.12	0.47
1:H:99:GLY:HA3	1:H:130:ILE:O	2.14	0.47
1:H:43:LEU:HD21	1:H:87:GLU:HB3	1.97	0.47
1:H:7:LYS:H	1:H:211:GLN:HE22	1.62	0.47
1:E:135:TYR:CE2	1:F:152:ILE:HG21	2.50	0.47
1:F:8:ARG:NH2	7:F:402:HOH:O	2.47	0.46
1:D:63:THR:HA	1:D:132:TYR:O	2.14	0.46
1:G:67:THR:CG2	1:G:105:ILE:HG21	2.45	0.46
1:C:67:THR:HG21	1:C:105:ILE:HG21	1.98	0.46
1:C:208:GLU:O	1:C:211:GLN:HG2	2.16	0.46
1:E:67:THR:HG21	1:E:105:ILE:HG21	1.98	0.46
1:A:18:ASP:OD1	5:A:304:FV3:O1	2.33	0.46
1:G:63:THR:H	1:G:66:ASN:ND2	2.13	0.46
1:A:183:THR:HA	1:A:186:SER:OG	2.16	0.45
1:A:20:ASN:HD21	1:A:195:TRP:HD1	1.65	0.44
1:H:214:ASP:HB3	1:H:217:LEU:HD22	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:THR:HA	1:A:132:TYR:O	2.16	0.44
1:C:99:GLY:HA3	1:C:130:ILE:O	2.18	0.44
1:B:183:THR:HA	1:B:186:SER:OG	2.18	0.44
1:G:183:THR:HA	1:G:186:SER:OG	2.19	0.43
1:B:136:TRP:CH2	1:B:156:ALA:HB1	2.53	0.43
3:C:302:FQ0:C10	4:C:303:FQF:C12	2.90	0.43
1:F:183:THR:HA	1:F:186:SER:OG	2.18	0.43
1:E:35:TYR:CZ	6:E:301:DPO:O2	2.72	0.43
1:D:7:LYS:H	1:D:211:GLN:HE22	1.67	0.43
1:A:96:LEU:O	1:A:127:ASN:HA	2.18	0.43
1:C:136:TRP:CH2	1:C:156:ALA:HB1	2.54	0.42
1:C:183:THR:HA	1:C:186:SER:OG	2.20	0.42
1:D:183:THR:HA	1:D:186:SER:OG	2.20	0.42
6:B:301:DPO:O1	4:B:303:FQF:O6	2.38	0.42
1:G:8:ARG:H	1:G:211:GLN:HE21	1.67	0.42
1:F:96:LEU:HB3	1:F:127:ASN:HD22	1.83	0.41
1:G:12:HIS:HE1	1:G:58:THR:OG1	2.03	0.41
1:D:96:LEU:O	1:D:127:ASN:HA	2.21	0.41
1:F:42:GLY:HA3	4:F:303:FQF:C17	2.49	0.41
1:H:136:TRP:CH2	1:H:156:ALA:HB1	2.56	0.41
1:E:162:ARG:NH1	1:E:164:ASP:OD1	2.48	0.41
1:C:96:LEU:HB3	1:C:127:ASN:HD22	1.86	0.41
1:B:66:ASN:ND2	4:B:303:FQF:C1	2.84	0.40
1:D:20:ASN:HD21	1:D:195:TRP:HD1	1.68	0.40
1:C:56:GLU:HA	1:C:125:LYS:O	2.22	0.40
1:G:115:LYS:O	1:G:117:THR:HG23	2.22	0.40
1:C:43:LEU:HD21	1:C:87:GLU:HB3	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	207/224 (92%)	205 (99%)	2 (1%)	0	100	100
1	B	217/224 (97%)	212 (98%)	5 (2%)	0	100	100
1	C	212/224 (95%)	209 (99%)	3 (1%)	0	100	100
1	D	202/224 (90%)	200 (99%)	2 (1%)	0	100	100
1	E	211/224 (94%)	208 (99%)	3 (1%)	0	100	100
1	F	200/224 (89%)	197 (98%)	3 (2%)	0	100	100
1	G	204/224 (91%)	202 (99%)	2 (1%)	0	100	100
1	H	216/224 (96%)	213 (99%)	2 (1%)	1 (0%)	29	13
All	All	1669/1792 (93%)	1646 (99%)	22 (1%)	1 (0%)	51	33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	-2	GLY

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	184/193 (95%)	181 (98%)	3 (2%)	62	47
1	B	191/193 (99%)	186 (97%)	5 (3%)	46	26
1	C	187/193 (97%)	183 (98%)	4 (2%)	53	35
1	D	180/193 (93%)	180 (100%)	0	100	100
1	E	186/193 (96%)	183 (98%)	3 (2%)	62	47
1	F	178/193 (92%)	177 (99%)	1 (1%)	86	80
1	G	182/193 (94%)	179 (98%)	3 (2%)	62	47
1	H	190/193 (98%)	185 (97%)	5 (3%)	46	26
All	All	1478/1544 (96%)	1454 (98%)	24 (2%)	62	47

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	ILE
1	A	83	LYS
1	A	104	ASP
1	B	8	ARG
1	B	65	ASP
1	B	108	GLU
1	B	147	ASP
1	B	211	GLN
1	C	60	PHE
1	C	121	LYS
1	C	149	LYS
1	C	151	MET
1	E	8	ARG
1	E	149	LYS
1	E	151	MET
1	F	60	PHE
1	G	60	PHE
1	G	121	LYS
1	G	150	LYS
1	H	123	LYS
1	H	149	LYS
1	H	151	MET
1	H	211	GLN
1	H	217	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	64	GLN
1	A	66	ASN
1	A	131	ASN
1	A	211	GLN
1	A	213	GLN
1	B	12	HIS
1	B	64	GLN
1	B	66	ASN
1	B	127	ASN
1	B	131	ASN
1	B	211	GLN
1	B	213	GLN
1	C	12	HIS
1	C	64	GLN

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Mol	Chain	Res	Type
1	C	127	ASN
1	C	131	ASN
1	C	211	GLN
1	C	213	GLN
1	D	20	ASN
1	D	64	GLN
1	D	66	ASN
1	D	131	ASN
1	D	211	GLN
1	E	20	ASN
1	E	32	HIS
1	E	64	GLN
1	E	131	ASN
1	E	211	GLN
1	E	213	GLN
1	F	12	HIS
1	F	64	GLN
1	F	127	ASN
1	F	131	ASN
1	F	211	GLN
1	F	213	GLN
1	G	12	HIS
1	G	66	ASN
1	G	127	ASN
1	G	131	ASN
1	G	211	GLN
1	G	213	GLN
1	H	20	ASN
1	H	64	GLN
1	H	66	ASN
1	H	71	GLN
1	H	131	ASN
1	H	211	GLN
1	H	213	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

32 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	FQF	B	303	-	20,20,20	0.38	0	23,23,23	1.38	5 (21%)
2	PO4	H	301	-	4,4,4	0.58	0	6,6,6	0.42	0
3	FQ0	E	302	-	20,20,20	0.52	0	23,23,23	1.36	4 (17%)
5	FV3	F	304	-	20,20,20	0.37	0	23,23,23	1.61	6 (26%)
5	FV3	A	304	-	20,20,20	0.36	0	23,23,23	1.55	5 (21%)
2	PO4	A	301	-	4,4,4	1.03	0	6,6,6	0.39	0
2	PO4	C	301	-	4,4,4	0.61	0	6,6,6	0.42	0
3	FQ0	F	302	-	20,20,20	0.49	0	23,23,23	1.58	6 (26%)
5	FV3	G	304	-	20,20,20	0.36	0	23,23,23	1.52	6 (26%)
5	FV3	B	304	-	20,20,20	0.37	0	23,23,23	1.56	5 (21%)
6	DPO	G	301	-	6,8,8	0.76	0	13,13,13	0.75	0
2	PO4	F	301	-	4,4,4	0.65	0	6,6,6	0.43	0
4	FQF	H	303	-	20,20,20	0.43	0	23,23,23	1.46	5 (21%)
6	DPO	B	301	-	6,8,8	0.94	0	13,13,13	0.93	0
3	FQ0	B	302	-	20,20,20	0.51	0	23,23,23	1.77	4 (17%)
3	FQ0	A	302	-	20,20,20	0.47	0	23,23,23	1.77	6 (26%)
4	FQF	G	303	-	20,20,20	0.34	0	23,23,23	1.69	6 (26%)
4	FQF	C	303	-	20,20,20	0.37	0	23,23,23	1.58	6 (26%)
4	FQF	E	303	-	20,20,20	0.41	0	23,23,23	1.44	5 (21%)
4	FQF	D	303	-	20,20,20	0.34	0	23,23,23	1.65	6 (26%)
3	FQ0	G	302	-	20,20,20	0.43	0	23,23,23	1.69	6 (26%)
3	FQ0	H	302	-	20,20,20	0.52	0	23,23,23	1.42	5 (21%)
5	FV3	H	304	-	20,20,20	0.38	0	23,23,23	1.48	6 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	FQ0	D	302	-	20,20,20	0.45	0	23,23,23	1.81	5 (21%)
5	FV3	C	304	-	20,20,20	0.39	0	23,23,23	1.55	6 (26%)
5	FV3	E	304	-	20,20,20	0.38	0	23,23,23	1.52	5 (21%)
2	PO4	D	301	-	4,4,4	0.79	0	6,6,6	0.41	0
4	FQF	F	303	-	20,20,20	0.35	0	23,23,23	1.65	6 (26%)
6	DPO	E	301	-	6,8,8	0.88	0	13,13,13	0.75	0
3	FQ0	C	302	-	20,20,20	0.51	0	23,23,23	1.50	5 (21%)
4	FQF	A	303	-	20,20,20	0.38	0	23,23,23	1.81	6 (26%)
5	FV3	D	304	-	20,20,20	0.38	0	23,23,23	1.66	6 (26%)

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
4	FQF	B	303	-	-	6/21/21/21	-
3	FQ0	E	302	-	-	0/22/22/22	-
5	FV3	F	304	-	-	5/21/21/21	-
5	FV3	A	304	-	-	4/21/21/21	-
3	FQ0	F	302	-	-	6/22/22/22	-
5	FV3	G	304	-	-	2/21/21/21	-
5	FV3	B	304	-	-	4/21/21/21	-
6	DPO	G	301	-	-	3/6/6/6	-
4	FQF	H	303	-	-	8/21/21/21	-
6	DPO	B	301	-	-	0/6/6/6	-
3	FQ0	B	302	-	-	1/22/22/22	-
3	FQ0	A	302	-	-	2/22/22/22	-
4	FQF	G	303	-	-	2/21/21/21	-
4	FQF	C	303	-	-	5/21/21/21	-
4	FQF	E	303	-	-	4/21/21/21	-
4	FQF	D	303	-	-	6/21/21/21	-
3	FQ0	G	302	-	-	4/22/22/22	-
3	FQ0	H	302	-	-	0/22/22/22	-
5	FV3	H	304	-	-	7/21/21/21	-
3	FQ0	D	302	-	-	1/22/22/22	-
5	FV3	C	304	-	-	4/21/21/21	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	FV3	E	304	-	-	2/21/21/21	-
4	FQF	F	303	-	-	7/21/21/21	-
6	DPO	E	301	-	-	0/6/6/6	-
3	FQ0	C	302	-	-	4/22/22/22	-
4	FQF	A	303	-	-	7/21/21/21	-
5	FV3	D	304	-	-	4/21/21/21	-

There are no bond length outliers.

All (131) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	302	FQ0	C6-C7-C8	-5.22	117.02	126.04
3	D	302	FQ0	C6-C7-C8	-4.89	117.58	126.04
4	A	303	FQF	C6-C7-C8	-4.61	118.08	126.04
5	D	304	FV3	C6-C7-C8	-4.36	118.50	126.04
4	G	303	FQF	C6-C7-C8	-4.28	118.64	126.04
4	C	303	FQF	C6-C7-C8	-4.12	118.92	126.04
3	A	302	FQ0	C11-C12-C13	-4.12	117.75	127.66
5	F	304	FV3	C6-C7-C8	-4.01	119.11	126.04
5	B	304	FV3	C6-C7-C8	-3.96	119.19	126.04
5	C	304	FV3	C6-C7-C8	-3.82	119.43	126.04
4	F	303	FQF	C6-C7-C8	-3.80	119.48	126.04
4	A	303	FQF	C10-C8-C9	3.79	121.64	115.27
5	E	304	FV3	C6-C7-C8	-3.75	119.55	126.04
3	G	302	FQ0	C6-C7-C8	-3.58	119.84	126.04
3	F	302	FQ0	C6-C7-C8	-3.49	120.00	126.04
5	D	304	FV3	C14-C13-C15	3.42	121.03	115.27
4	D	303	FQF	C14-C13-C15	3.42	121.03	115.27
4	F	303	FQF	C14-C13-C15	3.38	120.95	115.27
4	C	303	FQF	C14-C13-C15	3.20	120.65	115.27
4	D	303	FQF	C6-C7-C8	-3.20	120.51	126.04
4	E	303	FQF	C14-C13-C15	3.19	120.64	115.27
4	G	303	FQF	C14-C13-C15	3.19	120.63	115.27
3	A	302	FQ0	C14-C13-C15	3.18	120.62	115.27
3	D	302	FQ0	C14-C13-C15	3.17	120.60	115.27
3	D	302	FQ0	C10-C8-C9	3.15	120.58	115.27
5	F	304	FV3	C11-C12-C13	-3.15	120.07	127.66
4	G	303	FQF	C10-C8-C9	3.13	120.54	115.27
3	C	302	FQ0	C11-C12-C13	-3.13	120.12	127.66
5	A	304	FV3	C6-C7-C8	-3.09	120.70	126.04
5	B	304	FV3	C14-C13-C15	3.09	120.46	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	303	FQF	C10-C8-C9	3.05	120.41	115.27
5	H	304	FV3	C14-C13-C15	3.03	120.37	115.27
5	E	304	FV3	C14-C13-C15	3.01	120.33	115.27
3	A	302	FQ0	C6-C7-C8	-2.99	120.87	126.04
3	G	302	FQ0	C14-C13-C15	2.99	120.30	115.27
5	C	304	FV3	C14-C13-C15	2.99	120.30	115.27
3	F	302	FQ0	C11-C12-C13	-2.97	120.51	127.66
4	H	303	FQF	C14-C13-C15	2.97	120.26	115.27
5	F	304	FV3	C10-C8-C9	2.96	120.25	115.27
3	C	302	FQ0	C6-C7-C8	-2.96	120.93	126.04
4	E	303	FQF	C6-C7-C8	-2.96	120.93	126.04
5	A	304	FV3	C11-C12-C13	-2.95	120.56	127.66
3	D	302	FQ0	C11-C12-C13	-2.94	120.58	127.66
5	H	304	FV3	C6-C7-C8	-2.94	120.97	126.04
5	G	304	FV3	C14-C13-C15	2.93	120.20	115.27
5	G	304	FV3	C6-C7-C8	-2.92	120.99	126.04
5	G	304	FV3	C10-C8-C9	2.91	120.17	115.27
4	H	303	FQF	C10-C8-C9	2.90	120.16	115.27
4	D	303	FQF	C10-C8-C9	2.90	120.14	115.27
5	A	304	FV3	C10-C8-C9	2.89	120.14	115.27
4	B	303	FQF	C14-C13-C15	2.89	120.13	115.27
4	A	303	FQF	C14-C13-C15	2.88	120.12	115.27
5	A	304	FV3	C14-C13-C15	2.88	120.12	115.27
3	G	302	FQ0	C2-C3-C31	-2.85	107.59	112.80
5	B	304	FV3	C10-C8-C9	2.85	120.06	115.27
3	E	302	FQ0	C10-C8-C9	2.83	120.03	115.27
4	F	303	FQF	C11-C12-C13	-2.82	120.87	127.66
3	F	302	FQ0	C14-C13-C15	2.82	120.01	115.27
5	H	304	FV3	C11-C12-C13	-2.80	120.92	127.66
3	H	302	FQ0	C14-C13-C15	2.80	119.98	115.27
4	H	303	FQF	C6-C7-C8	-2.78	121.23	126.04
5	F	304	FV3	C14-C13-C15	2.74	119.88	115.27
3	A	302	FQ0	C10-C8-C9	2.72	119.84	115.27
3	H	302	FQ0	C11-C12-C13	-2.70	121.15	127.66
3	G	302	FQ0	C10-C8-C9	2.70	119.82	115.27
5	G	304	FV3	C11-C12-C13	-2.69	121.18	127.66
3	A	302	FQ0	C19-C18-C20	2.68	120.53	114.60
3	E	302	FQ0	C14-C13-C15	2.67	119.77	115.27
4	H	303	FQF	C11-C12-C13	-2.64	121.31	127.66
3	H	302	FQ0	C10-C8-C9	2.64	119.70	115.27
5	H	304	FV3	C10-C8-C9	2.61	119.66	115.27
5	C	304	FV3	C11-C12-C13	-2.57	121.46	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	303	FQF	C10-C8-C9	2.57	119.59	115.27
3	C	302	FQ0	C14-C13-C15	2.57	119.59	115.27
3	G	302	FQ0	C11-C12-C13	-2.56	121.50	127.66
3	B	302	FQ0	C10-C8-C9	2.54	119.55	115.27
3	B	302	FQ0	C14-C13-C15	2.54	119.54	115.27
5	E	304	FV3	C11-C12-C13	-2.54	121.54	127.66
4	A	303	FQF	C11-C9-C8	-2.52	104.70	112.98
4	B	303	FQF	C6-C7-C8	-2.50	121.72	126.04
4	D	303	FQF	C16-C17-C18	-2.50	119.21	127.75
4	D	303	FQF	C20-C18-C19	2.45	120.01	114.60
3	E	302	FQ0	C11-C12-C13	-2.44	121.78	127.66
5	A	304	FV3	C19-C18-C20	2.44	119.99	114.60
4	F	303	FQF	C16-C17-C18	-2.44	119.42	127.75
3	F	302	FQ0	C10-C8-C9	2.42	119.34	115.27
4	A	303	FQF	C20-C18-C19	2.42	119.94	114.60
4	E	303	FQF	C10-C8-C9	2.40	119.30	115.27
4	E	303	FQF	C11-C12-C13	-2.40	121.89	127.66
4	G	303	FQF	C20-C18-C19	2.38	119.86	114.60
3	G	302	FQ0	C19-C18-C20	2.36	119.81	114.60
5	C	304	FV3	C10-C8-C9	2.34	119.21	115.27
4	G	303	FQF	C11-C12-C13	-2.34	122.02	127.66
4	B	303	FQF	C11-C12-C13	-2.34	122.03	127.66
5	G	304	FV3	C19-C18-C20	2.33	119.74	114.60
5	D	304	FV3	C10-C8-C9	2.30	119.15	115.27
4	C	303	FQF	C11-C12-C13	-2.30	122.13	127.66
5	H	304	FV3	C19-C18-C20	2.29	119.67	114.60
5	C	304	FV3	C19-C18-C20	2.29	119.67	114.60
3	H	302	FQ0	C6-C7-C8	-2.28	122.10	126.04
4	E	303	FQF	C20-C18-C19	2.28	119.64	114.60
5	D	304	FV3	C19-C18-C20	2.27	119.62	114.60
3	C	302	FQ0	C19-C18-C20	2.26	119.59	114.60
5	E	304	FV3	C19-C18-C20	2.25	119.58	114.60
3	H	302	FQ0	C19-C18-C20	2.25	119.57	114.60
5	D	304	FV3	C11-C12-C13	-2.25	122.25	127.66
5	E	304	FV3	C10-C8-C9	2.21	118.99	115.27
5	F	304	FV3	C19-C18-C20	2.21	119.48	114.60
3	B	302	FQ0	O7-C31-C3	-2.19	105.97	111.78
3	F	302	FQ0	C19-C18-C20	2.19	119.43	114.60
4	C	303	FQF	C16-C17-C18	-2.18	120.28	127.75
5	B	304	FV3	C11-C12-C13	-2.17	122.43	127.66
4	H	303	FQF	C20-C18-C19	2.16	119.38	114.60
3	A	302	FQ0	C14-C13-C12	-2.16	118.14	123.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	G	304	FV3	C10-C8-C7	-2.14	118.18	123.68
3	E	302	FQ0	C6-C7-C8	-2.14	122.35	126.04
4	C	303	FQF	C10-C8-C9	2.14	118.86	115.27
5	C	304	FV3	C16-C17-C18	-2.13	120.46	127.75
3	C	302	FQ0	C16-C17-C18	-2.12	120.49	127.75
4	B	303	FQF	C16-C17-C18	-2.12	120.51	127.75
5	D	304	FV3	C16-C17-C18	-2.11	120.53	127.75
3	D	302	FQ0	C19-C18-C20	2.11	119.26	114.60
4	G	303	FQF	C16-C17-C18	-2.10	120.59	127.75
5	B	304	FV3	C16-C17-C18	-2.10	120.59	127.75
5	F	304	FV3	C16-C17-C18	-2.08	120.65	127.75
5	H	304	FV3	C16-C17-C18	-2.07	120.69	127.75
3	F	302	FQ0	C16-C17-C18	-2.04	120.76	127.75
4	A	303	FQF	C11-C12-C13	-2.04	122.74	127.66
4	D	303	FQF	C11-C12-C13	-2.03	122.78	127.66
4	F	303	FQF	C20-C18-C19	2.02	119.07	114.60
4	C	303	FQF	C20-C18-C19	2.02	119.06	114.60

There are no chirality outliers.

All (98) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	302	FQ0	O6-C2-C3-O5
3	F	302	FQ0	O6-C2-C3-O5
3	G	302	FQ0	O5-C3-C31-O7
3	G	302	FQ0	O6-C2-C3-O5
4	B	303	FQF	O1-C1-C2-C3
4	B	303	FQF	C1-C2-C3-O5
4	E	303	FQF	C2-C3-O5-C6
4	E	303	FQF	O5-C6-C7-C8
4	F	303	FQF	O1-C1-C2-C3
4	H	303	FQF	O1-C1-C2-C3
4	H	303	FQF	O5-C6-C7-C8
5	A	304	FV3	O1-C1-C2-C3
5	C	304	FV3	O1-C1-C2-C3
5	D	304	FV3	C1-C2-C3-O5
5	F	304	FV3	O1-C1-C2-C3
5	H	304	FV3	C7-C8-C9-C11
5	H	304	FV3	C10-C8-C9-C11
4	B	303	FQF	O6-C2-C3-O5
5	F	304	FV3	O6-C2-C3-O5
4	B	303	FQF	C2-C3-O5-C6

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Mol	Chain	Res	Type	Atoms
4	A	303	FQF	C1-C2-C3-O5
4	D	303	FQF	C1-C2-C3-O5
4	H	303	FQF	C1-C2-C3-O5
5	B	304	FV3	C1-C2-C3-O5
5	F	304	FV3	C1-C2-C3-O5
4	A	303	FQF	O6-C2-C3-O5
4	D	303	FQF	O6-C2-C3-O5
4	H	303	FQF	O6-C2-C3-O5
5	B	304	FV3	O6-C2-C3-O5
4	B	303	FQF	O1-C1-C2-O6
4	E	303	FQF	C12-C11-C9-C8
4	F	303	FQF	O6-C2-C3-O5
4	F	303	FQF	C1-C2-C3-O5
4	A	303	FQF	O1-C1-C2-C3
4	C	303	FQF	O1-C1-C2-C3
4	D	303	FQF	O1-C1-C2-C3
4	G	303	FQF	O1-C1-C2-C3
5	B	304	FV3	O1-C1-C2-C3
5	H	304	FV3	O1-C1-C2-C3
5	D	304	FV3	O6-C2-C3-O5
5	H	304	FV3	O6-C2-C3-O5
5	F	304	FV3	C12-C11-C9-C8
4	D	303	FQF	O1-C1-C2-O6
4	F	303	FQF	O1-C1-C2-O6
4	G	303	FQF	O1-C1-C2-O6
5	A	304	FV3	O1-C1-C2-O6
5	B	304	FV3	O1-C1-C2-O6
5	C	304	FV3	O1-C1-C2-O6
5	F	304	FV3	O1-C1-C2-O6
4	C	303	FQF	C7-C6-O5-C3
5	H	304	FV3	C1-C2-C3-O5
5	E	304	FV3	C12-C11-C9-C8
4	A	303	FQF	O1-C1-C2-O6
4	H	303	FQF	O1-C1-C2-O6
5	H	304	FV3	O1-C1-C2-O6
5	C	304	FV3	C2-C3-O5-C6
4	F	303	FQF	C7-C6-O5-C3
5	D	304	FV3	C7-C6-O5-C3
4	E	303	FQF	O1-C1-C2-C3
3	B	302	FQ0	C12-C11-C9-C8
3	F	302	FQ0	C13-C15-C16-C17
5	G	304	FV3	C12-C11-C9-C8

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Mol	Chain	Res	Type	Atoms
3	F	302	FQ0	C31-C3-O5-C6
4	A	303	FQF	C2-C3-O5-C6
5	A	304	FV3	C2-C3-O5-C6
3	A	302	FQ0	C2-C3-C31-O7
3	C	302	FQ0	O6-C2-C3-C31
3	F	302	FQ0	O6-C2-C3-C31
3	G	302	FQ0	C2-C3-C31-O7
3	G	302	FQ0	O6-C2-C3-C31
4	D	303	FQF	C7-C6-O5-C3
5	A	304	FV3	C7-C6-O5-C3
5	G	304	FV3	C7-C6-O5-C3
5	H	304	FV3	C7-C6-O5-C3
3	C	302	FQ0	C7-C6-O5-C3
3	D	302	FQ0	C7-C6-O5-C3
3	F	302	FQ0	C7-C6-O5-C3
6	G	301	DPO	P1-O4-P2-O5
4	D	303	FQF	C2-C3-O5-C6
5	C	304	FV3	C12-C11-C9-C8
5	D	304	FV3	C12-C11-C9-C8
4	H	303	FQF	C12-C11-C9-C8
5	E	304	FV3	C2-C3-O5-C6
4	C	303	FQF	C12-C11-C9-C8
4	C	303	FQF	C2-C3-O5-C6
4	H	303	FQF	C7-C6-O5-C3
4	F	303	FQF	C2-C3-O5-C6
4	A	303	FQF	C10-C8-C9-C11
4	B	303	FQF	C12-C11-C9-C8
4	A	303	FQF	C7-C8-C9-C11
4	C	303	FQF	O1-C1-C2-O6
3	A	302	FQ0	O5-C3-C31-O7
3	C	302	FQ0	C10-C8-C9-C11
4	F	303	FQF	C10-C8-C9-C11
6	G	301	DPO	P1-O4-P2-O6
6	G	301	DPO	P1-O4-P2-O7
3	F	302	FQ0	C10-C8-C9-C11
4	H	303	FQF	C2-C3-O5-C6

There are no ring outliers.

14 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	303	FQF	2	0

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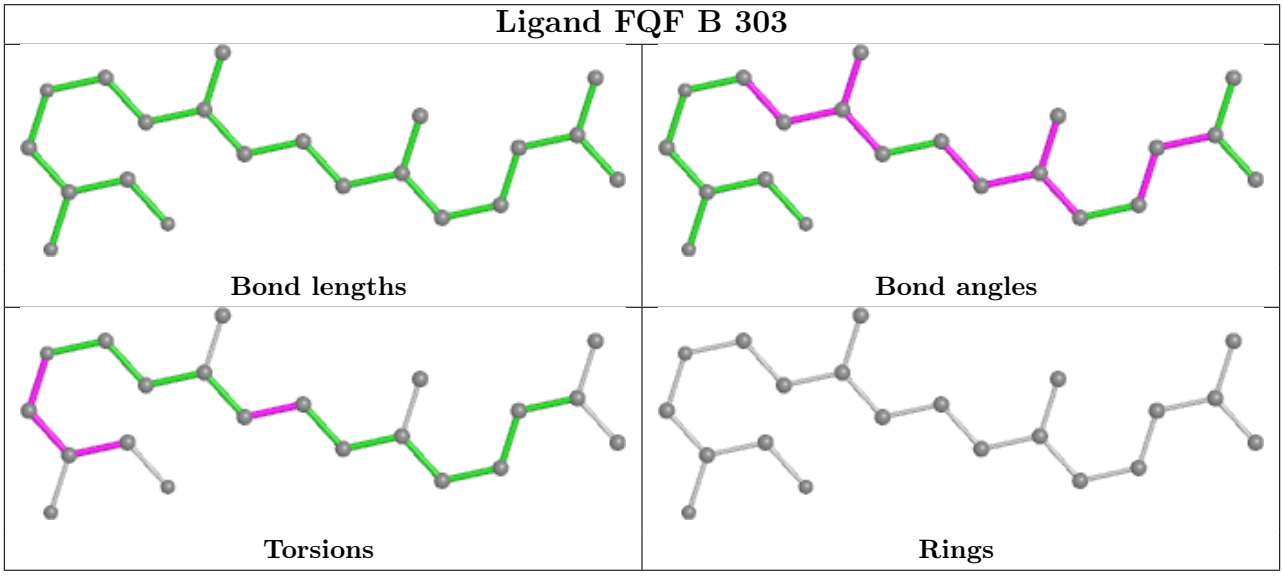
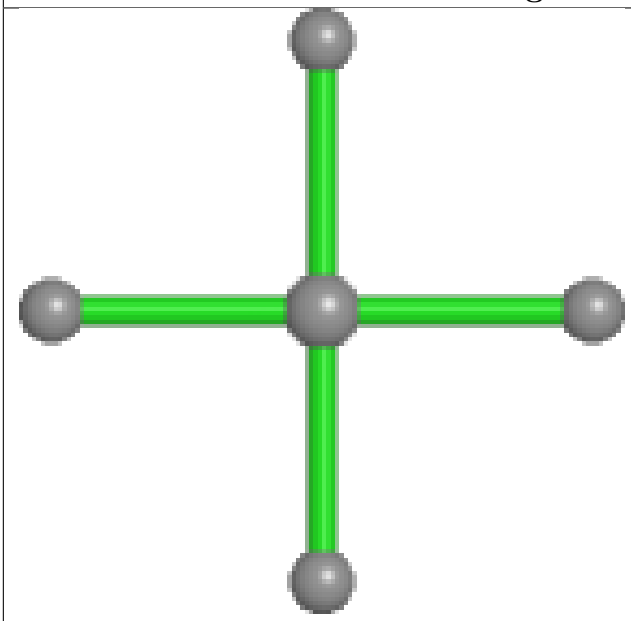
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	304	FV3	1	0
5	G	304	FV3	2	0
6	B	301	DPO	1	0
4	G	303	FQF	1	0
4	C	303	FQF	1	0
4	D	303	FQF	1	0
3	G	302	FQ0	1	0
3	H	302	FQ0	1	0
5	H	304	FV3	1	0
4	F	303	FQF	1	0
6	E	301	DPO	1	0
3	C	302	FQ0	1	0
5	D	304	FV3	1	0

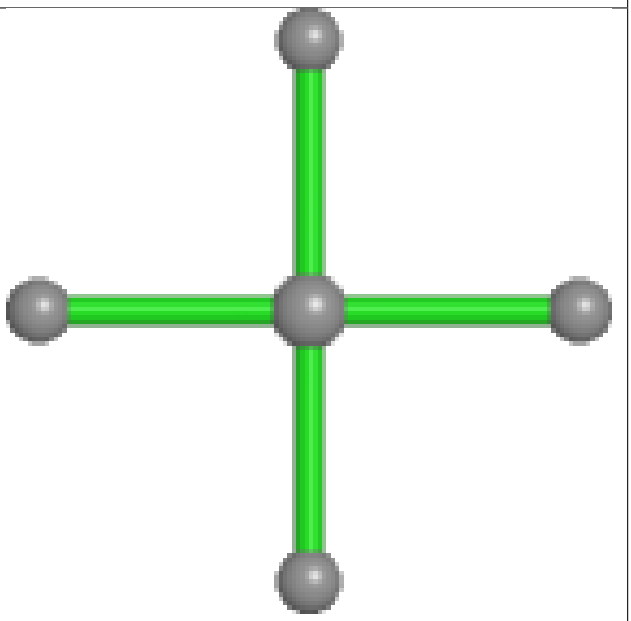
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



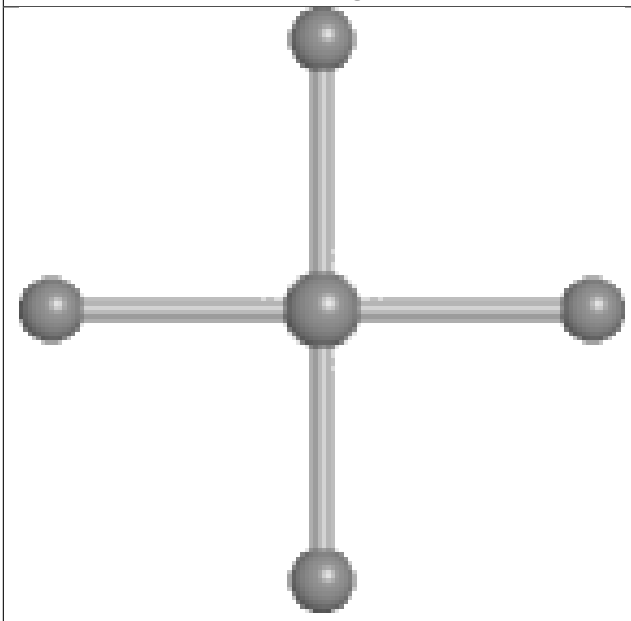
Ligand PO4 H 301



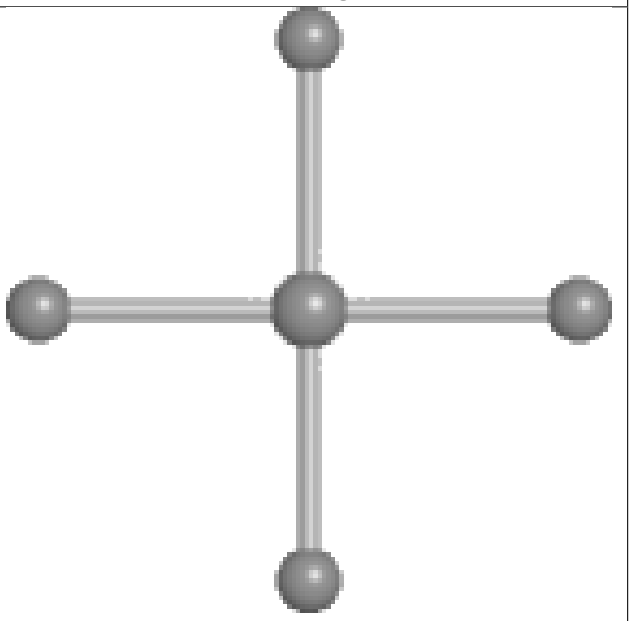
Bond lengths



Bond angles

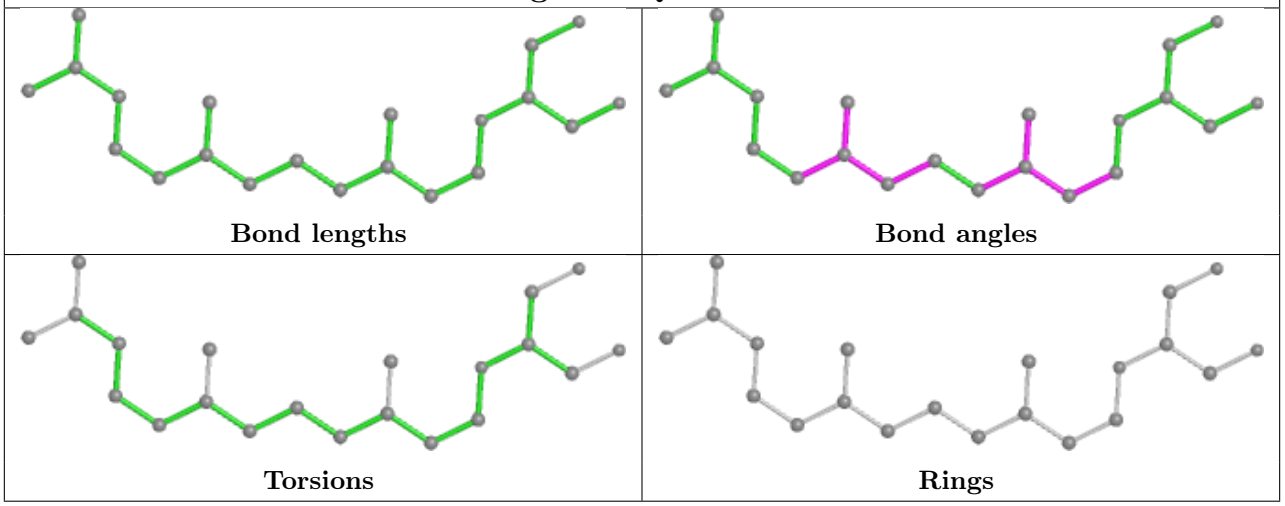


Torsions

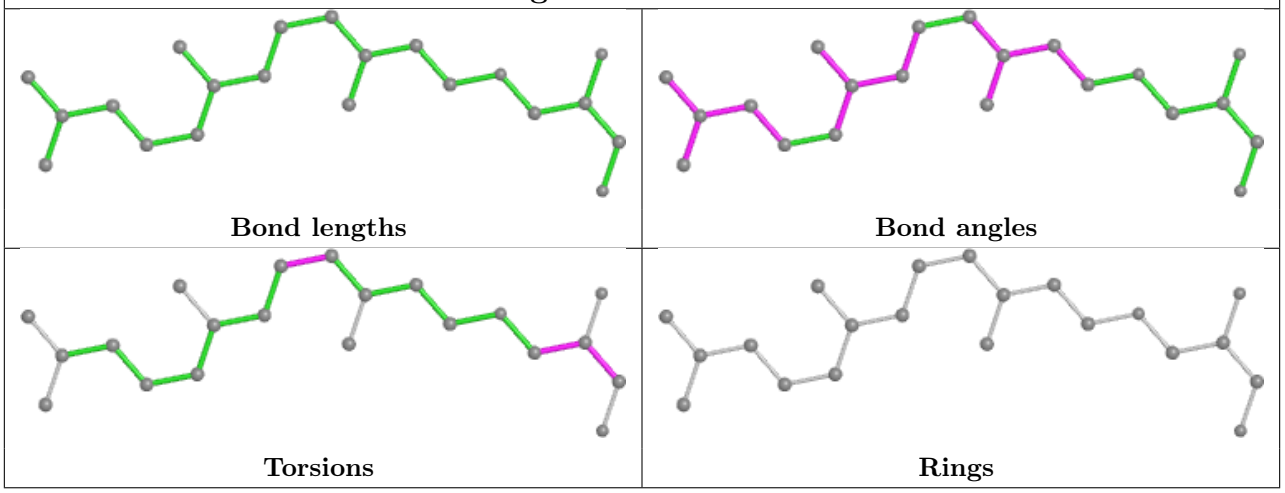


Rings

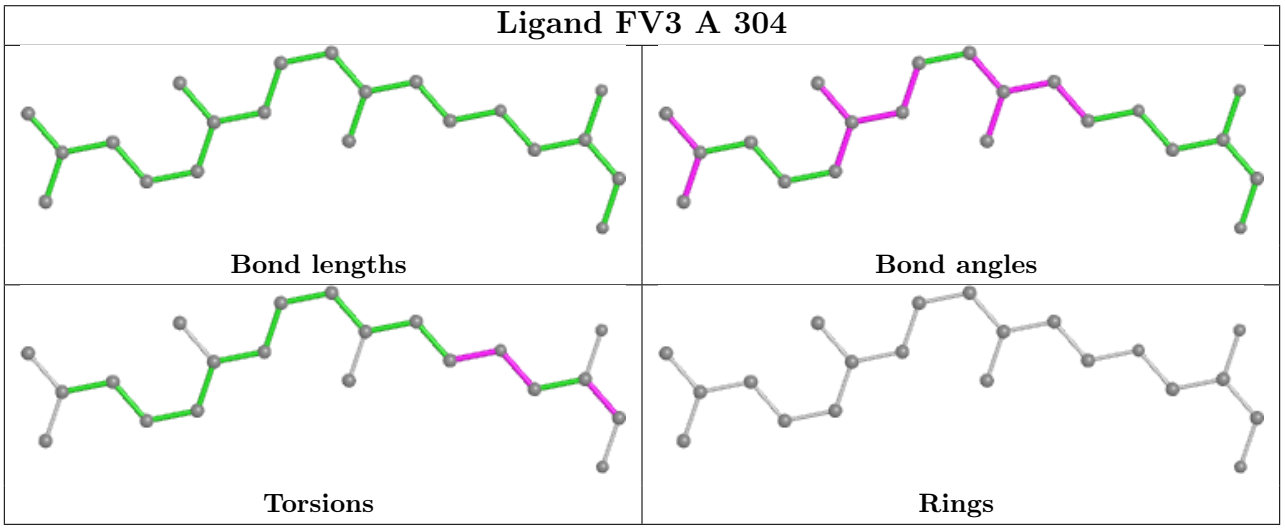
Ligand FQ0 E 302



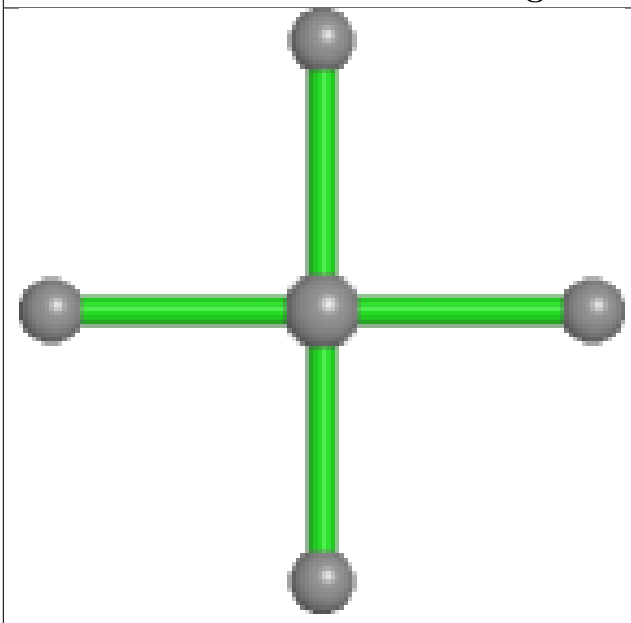
Ligand FV3 F 304



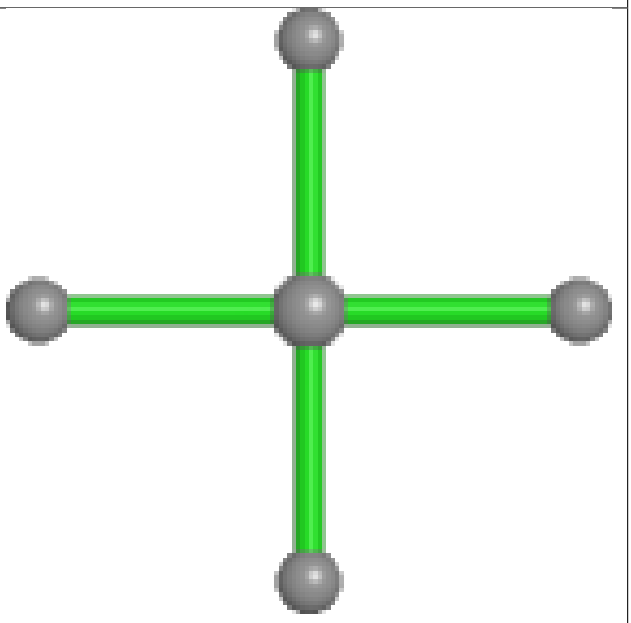
Ligand FV3 A 304



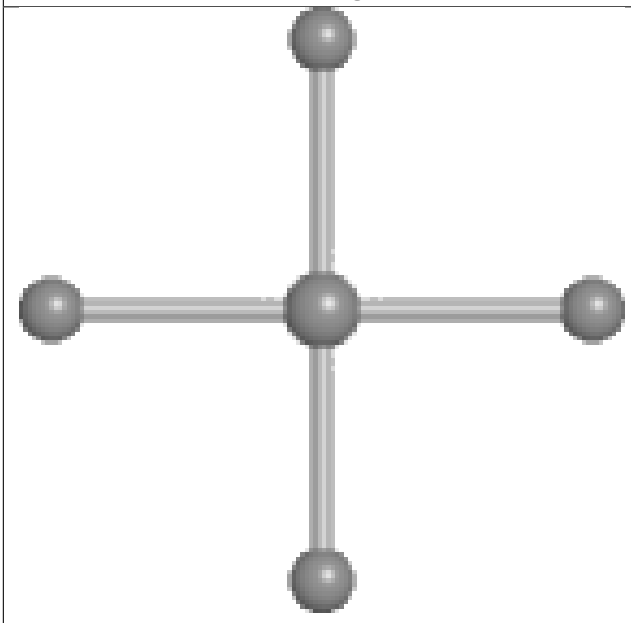
Ligand PO4 A 301



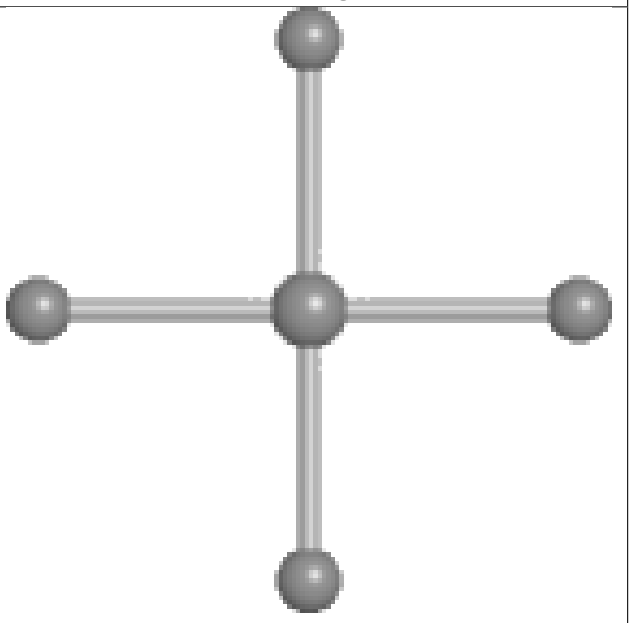
Bond lengths



Bond angles

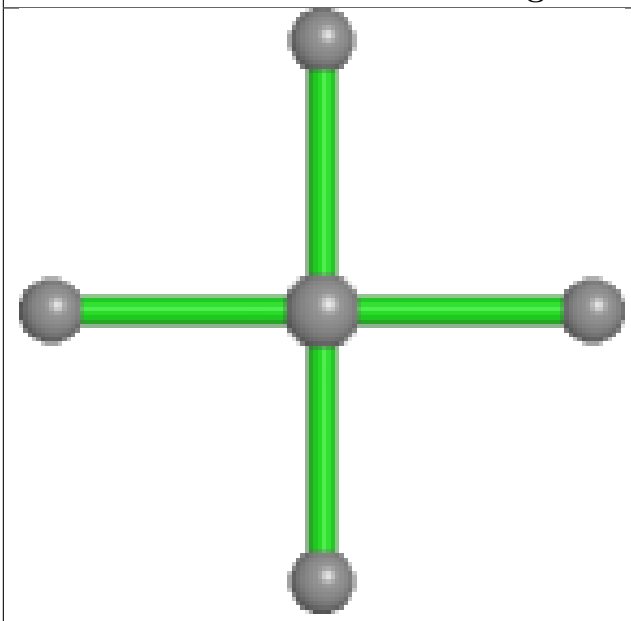


Torsions

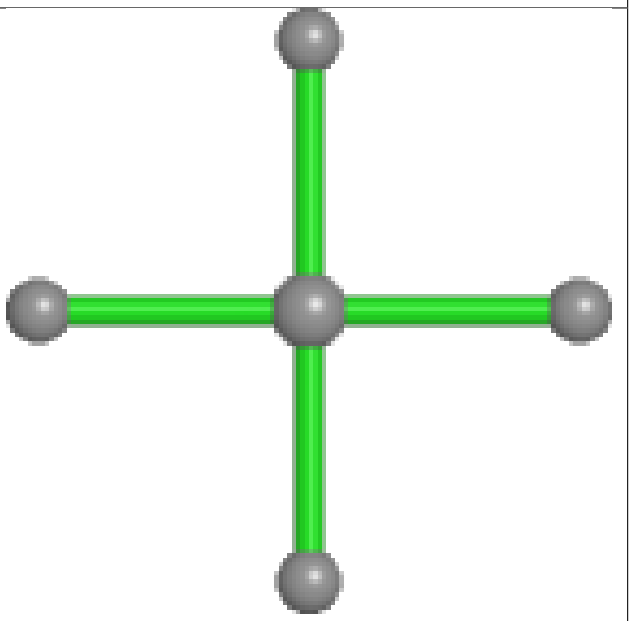


Rings

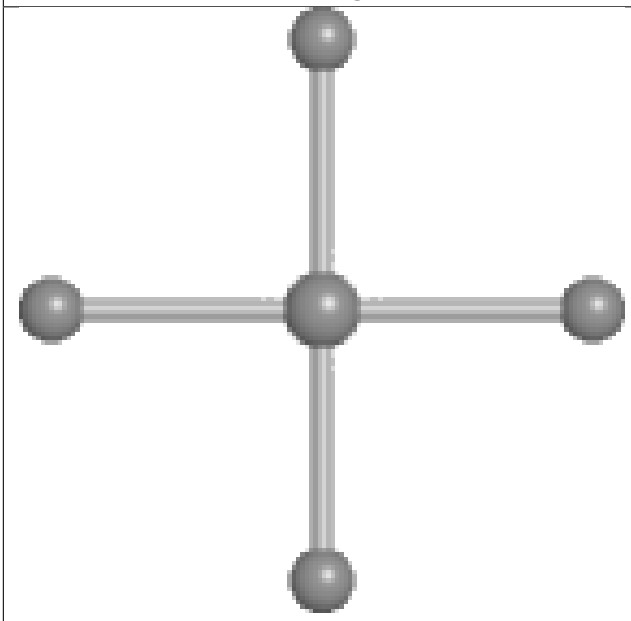
Ligand PO4 C 301



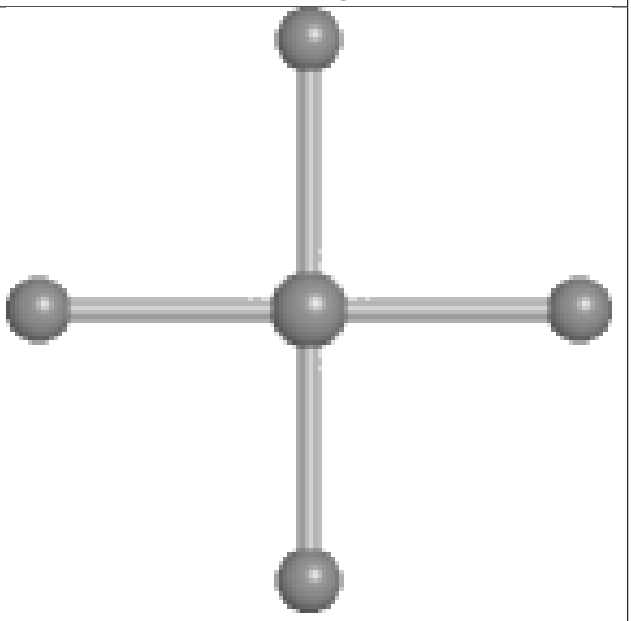
Bond lengths



Bond angles

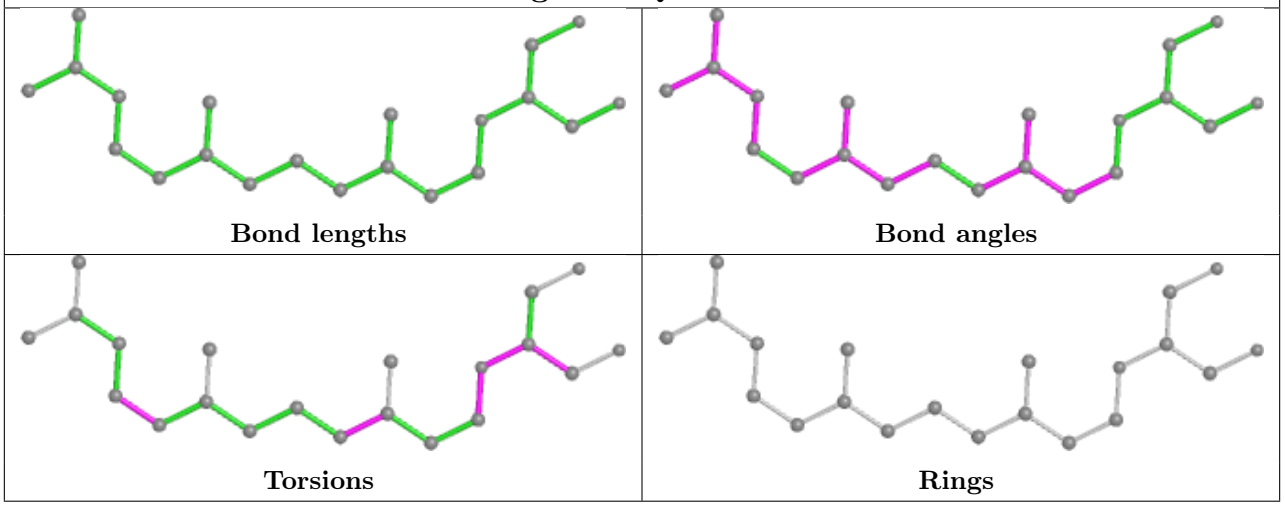


Torsions

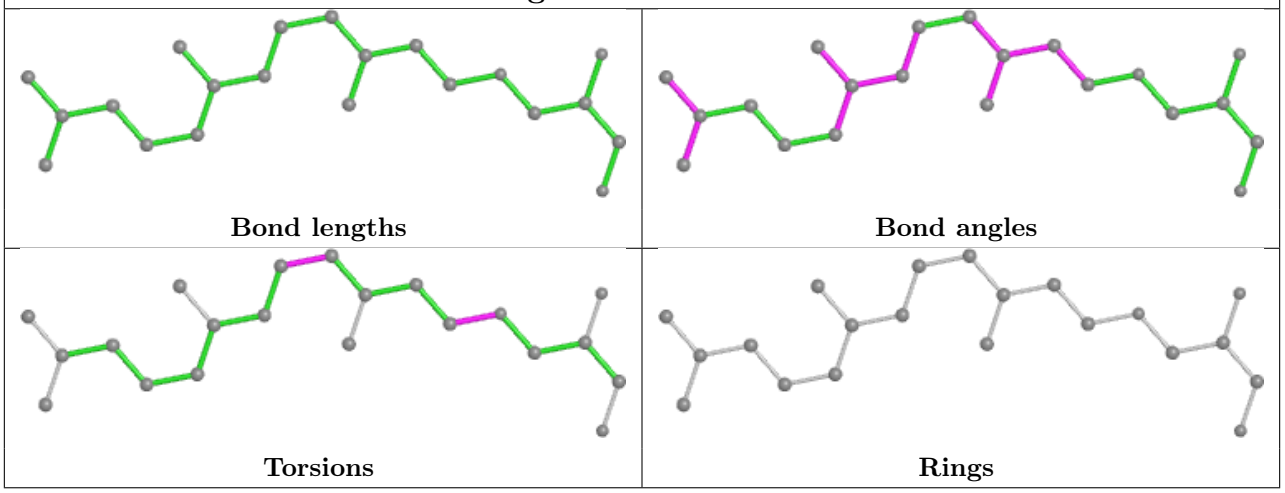


Rings

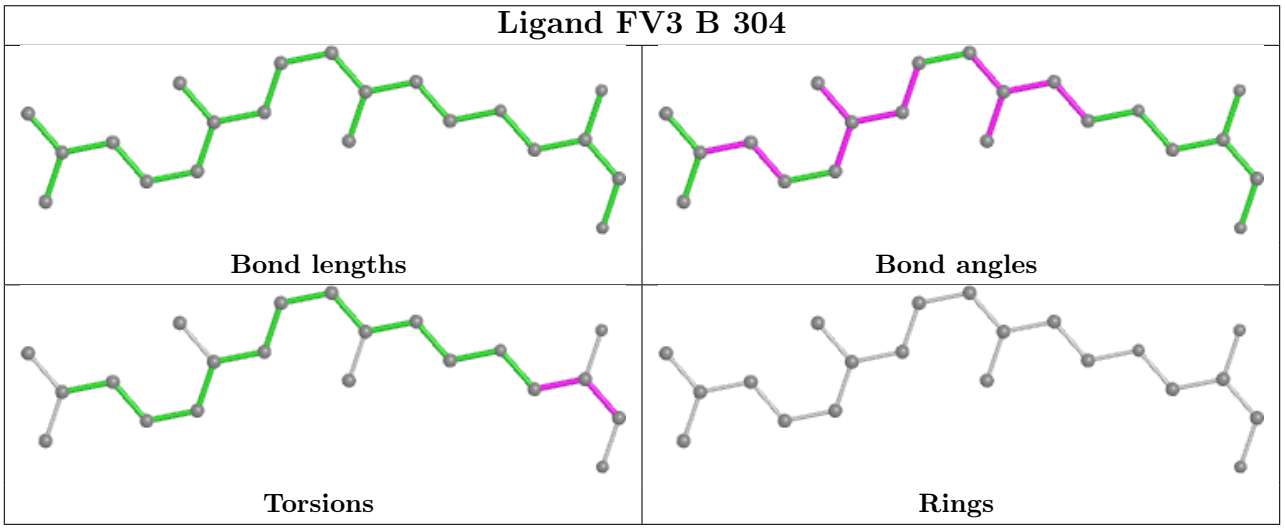
Ligand FQ0 F 302



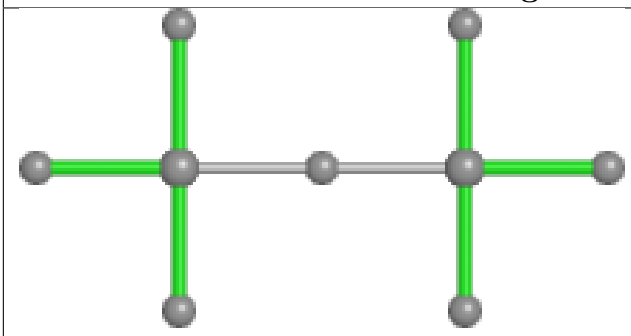
Ligand FV3 G 304



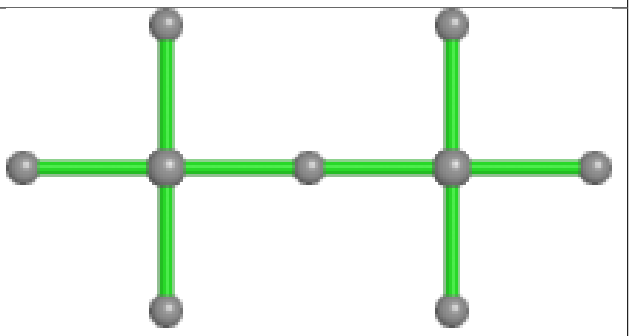
Ligand FV3 B 304



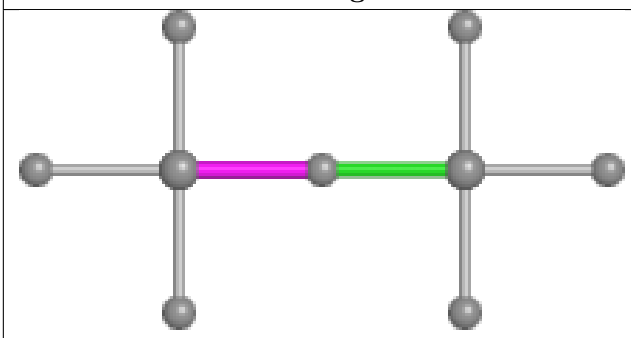
Ligand DPO G 301



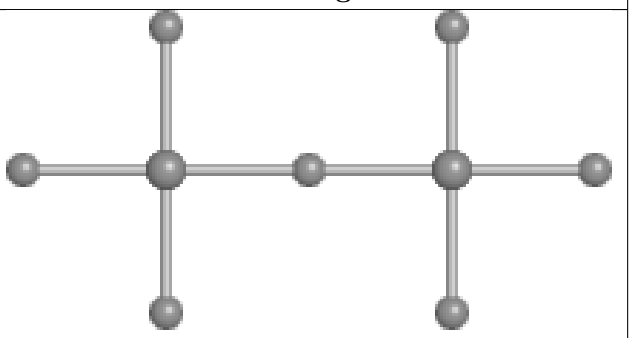
Bond lengths



Bond angles

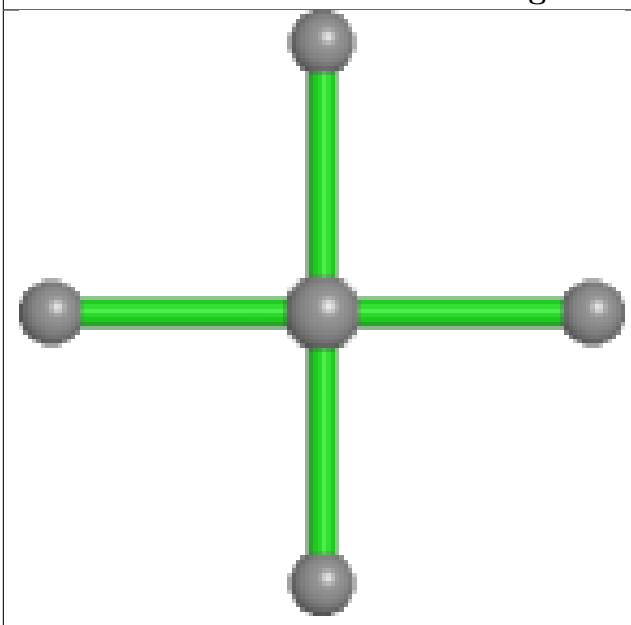


Torsions

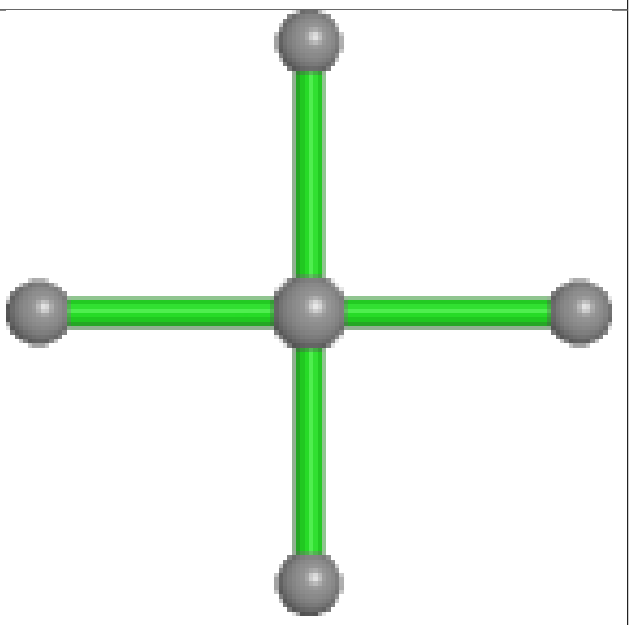


Rings

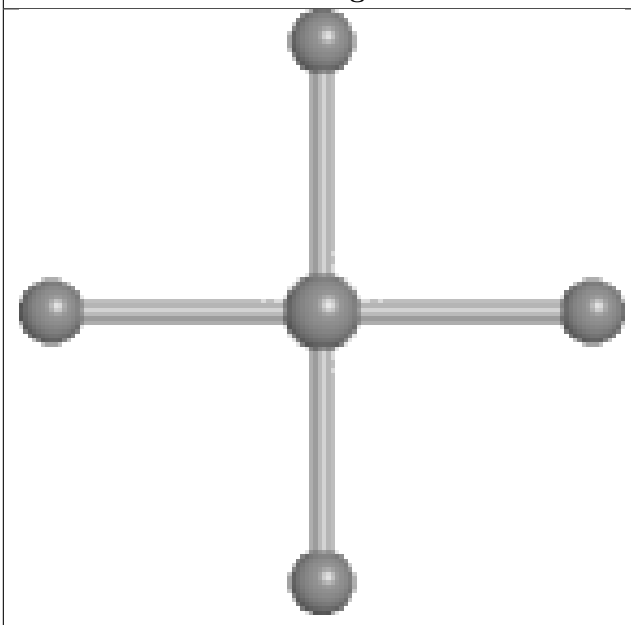
Ligand PO4 F 301



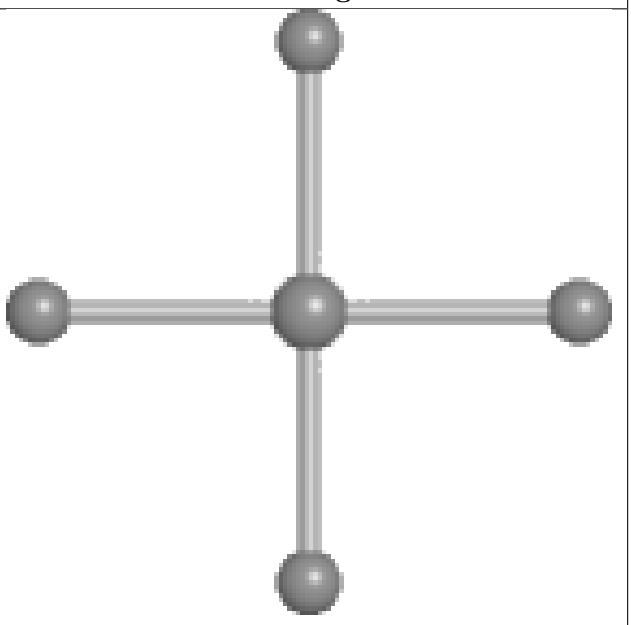
Bond lengths



Bond angles

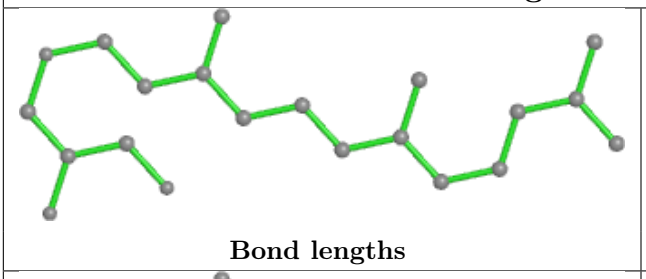


Torsions

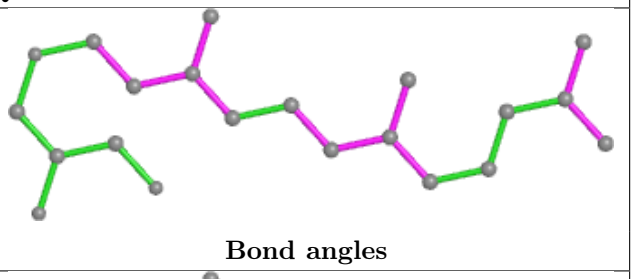


Rings

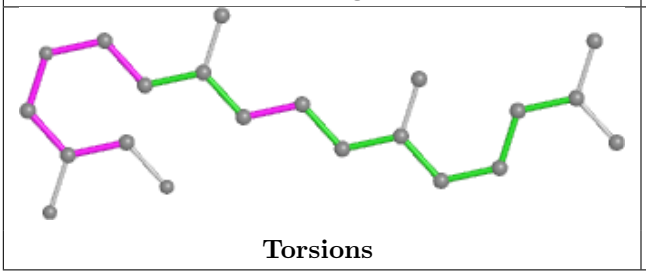
Ligand FQF H 303



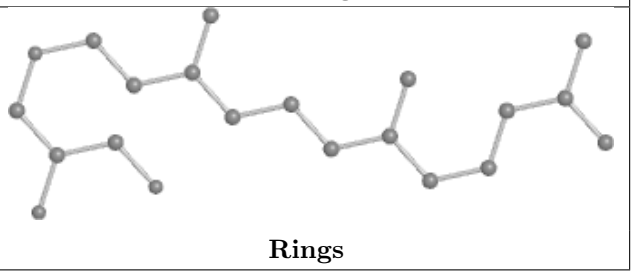
Bond lengths



Bond angles

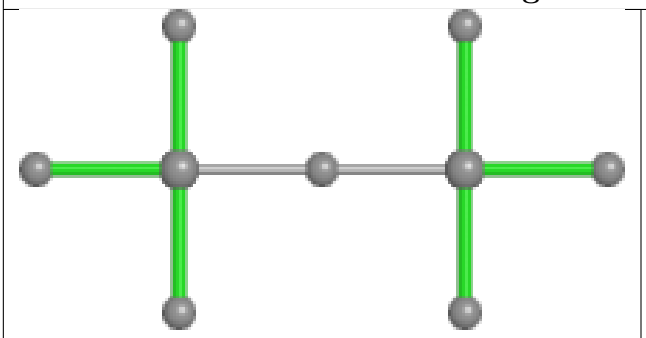


Torsions

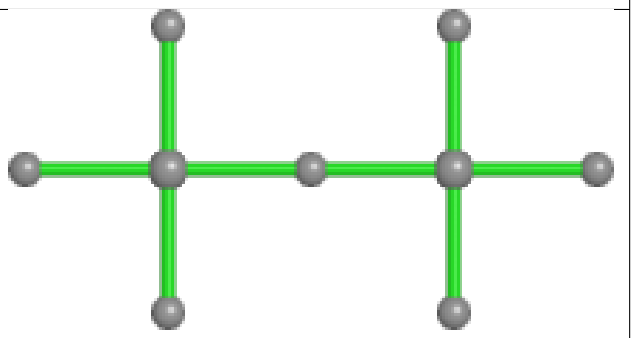


Rings

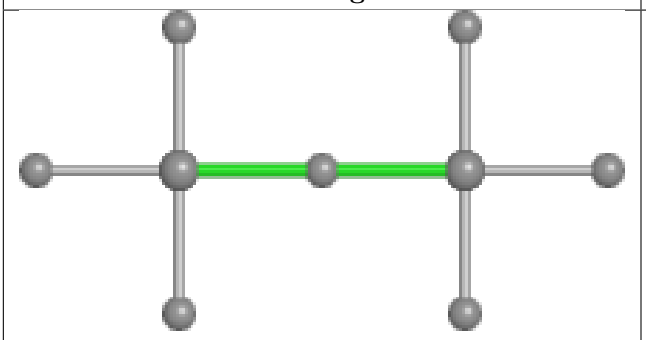
Ligand DPO B 301



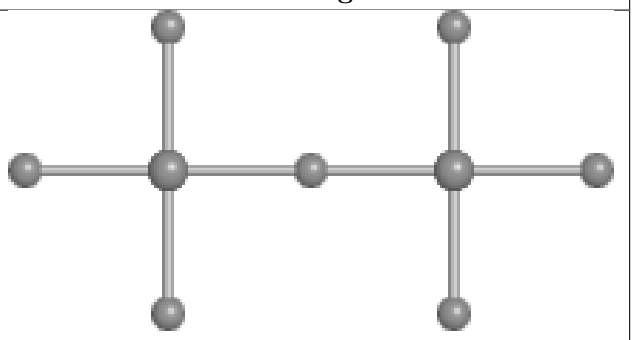
Bond lengths



Bond angles

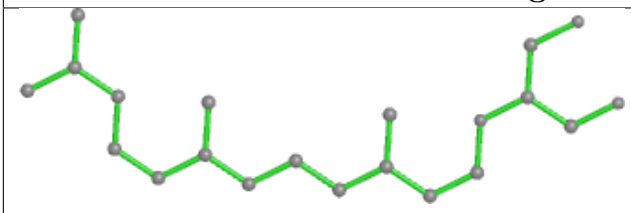


Torsions

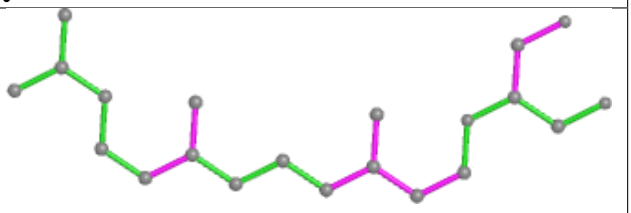


Rings

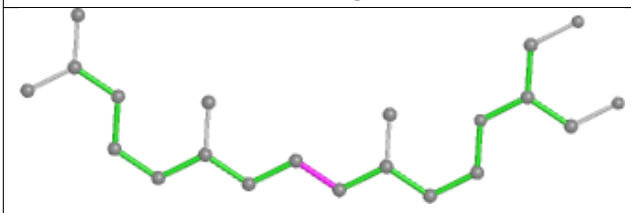
Ligand FQ0 B 302



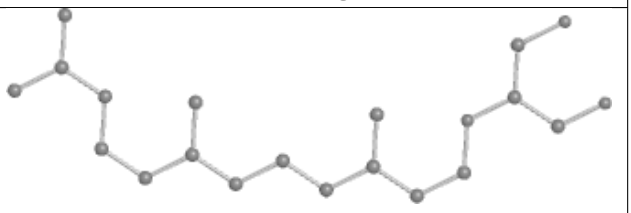
Bond lengths



Bond angles

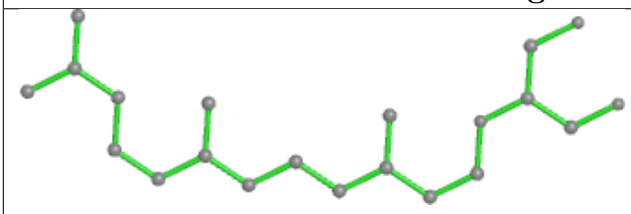


Torsions

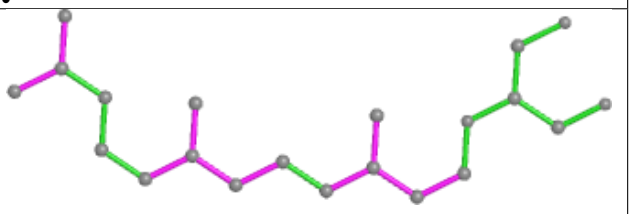


Rings

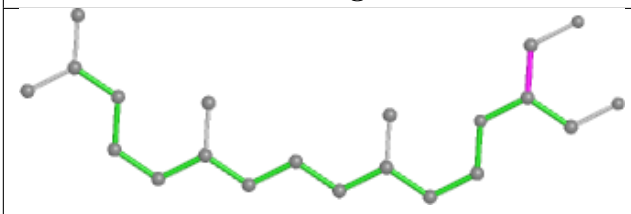
Ligand FQ0 A 302



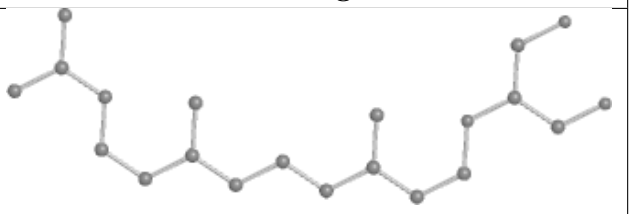
Bond lengths



Bond angles

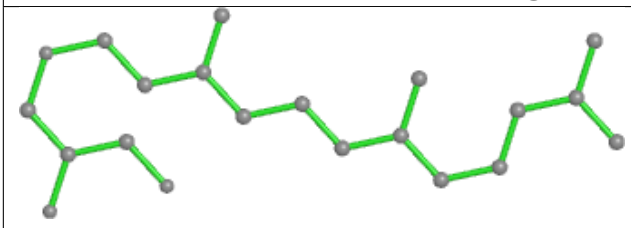


Torsions

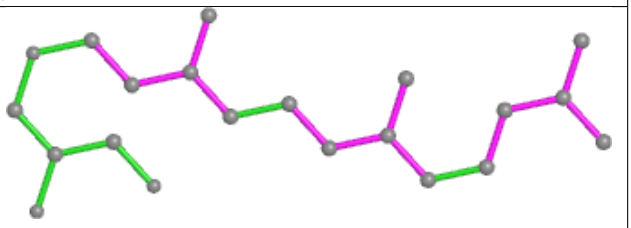


Rings

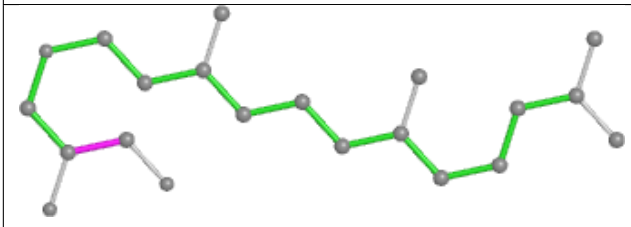
Ligand FQF G 303



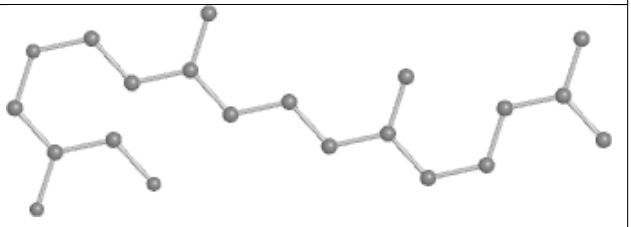
Bond lengths



Bond angles

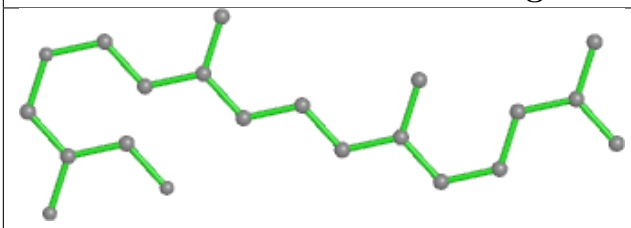


Torsions

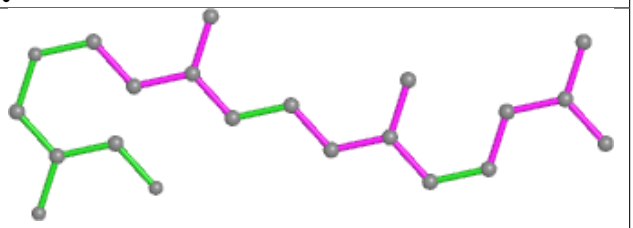


Rings

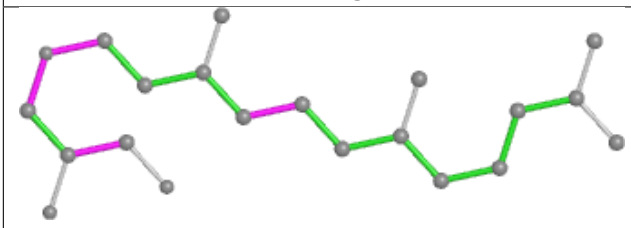
Ligand FQF C 303



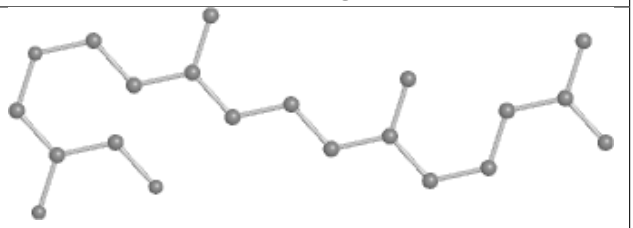
Bond lengths



Bond angles

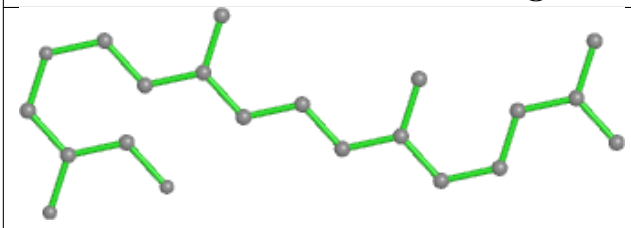


Torsions

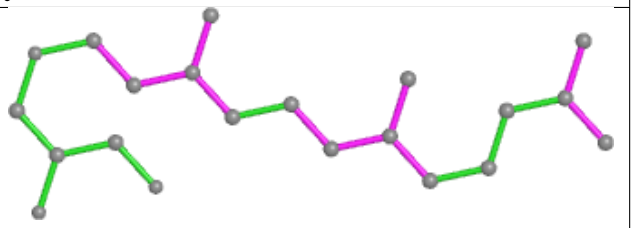


Rings

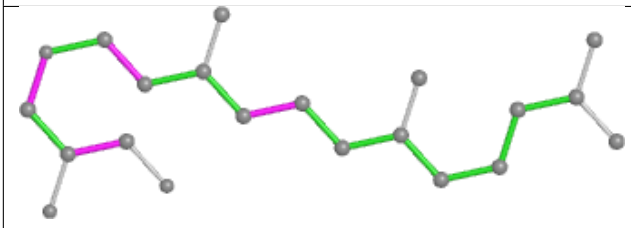
Ligand FQF E 303



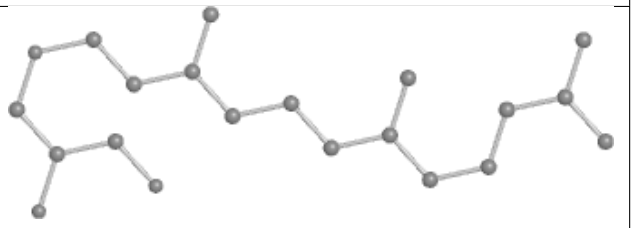
Bond lengths



Bond angles

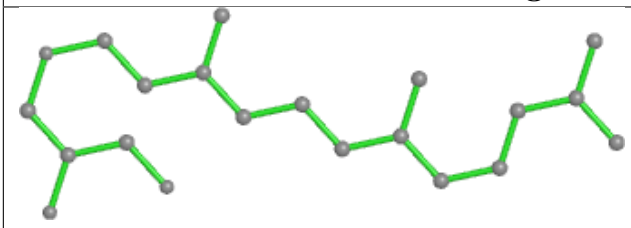


Torsions

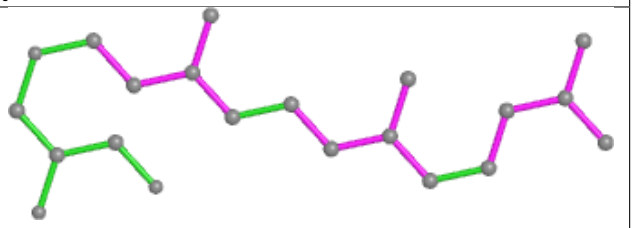


Rings

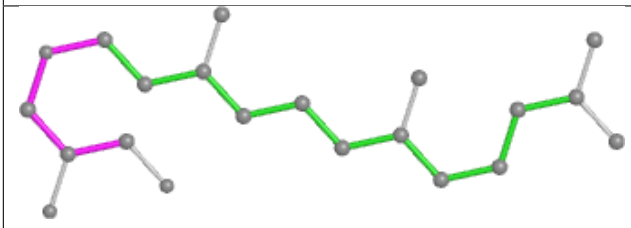
Ligand FQF D 303



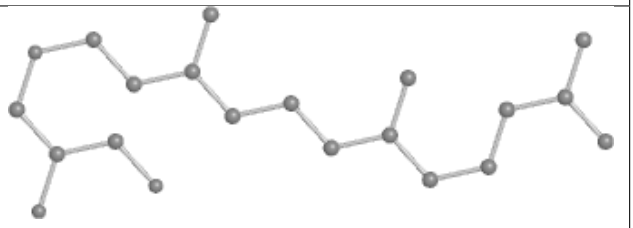
Bond lengths



Bond angles

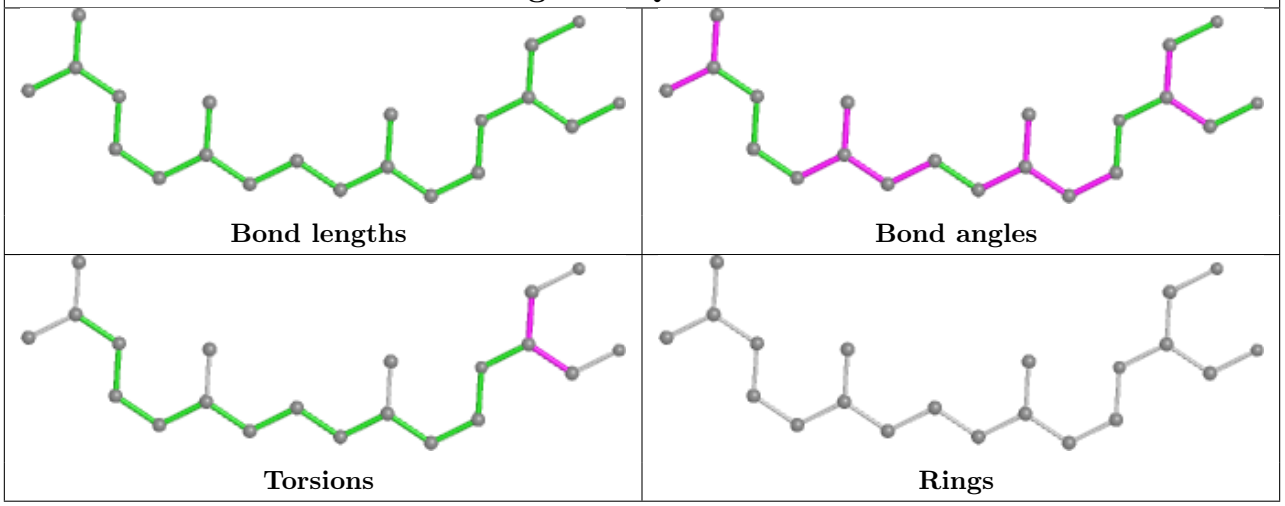


Torsions

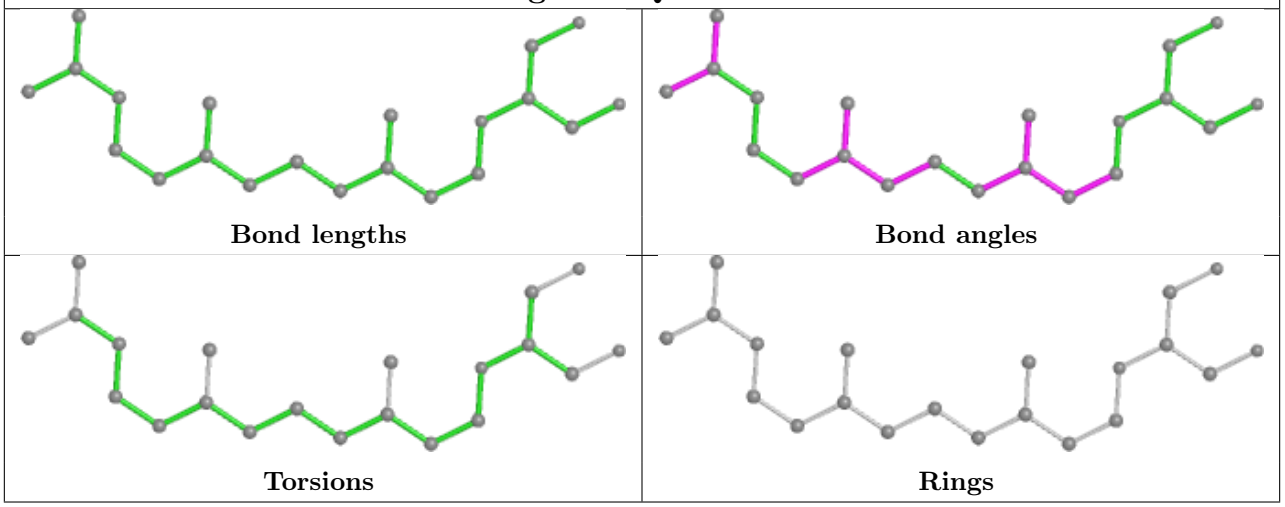


Rings

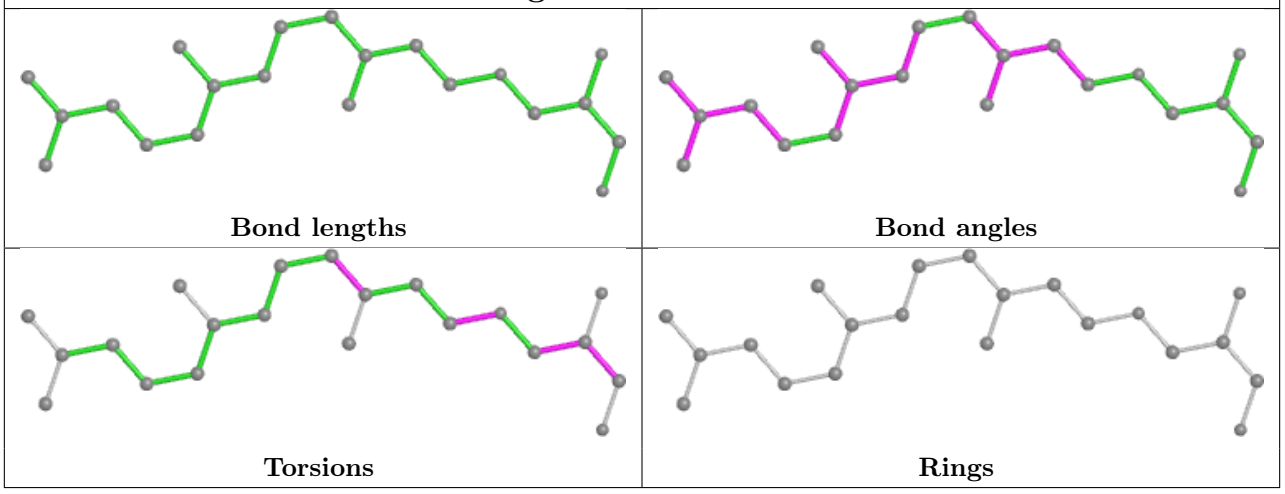
Ligand FQ0 G 302



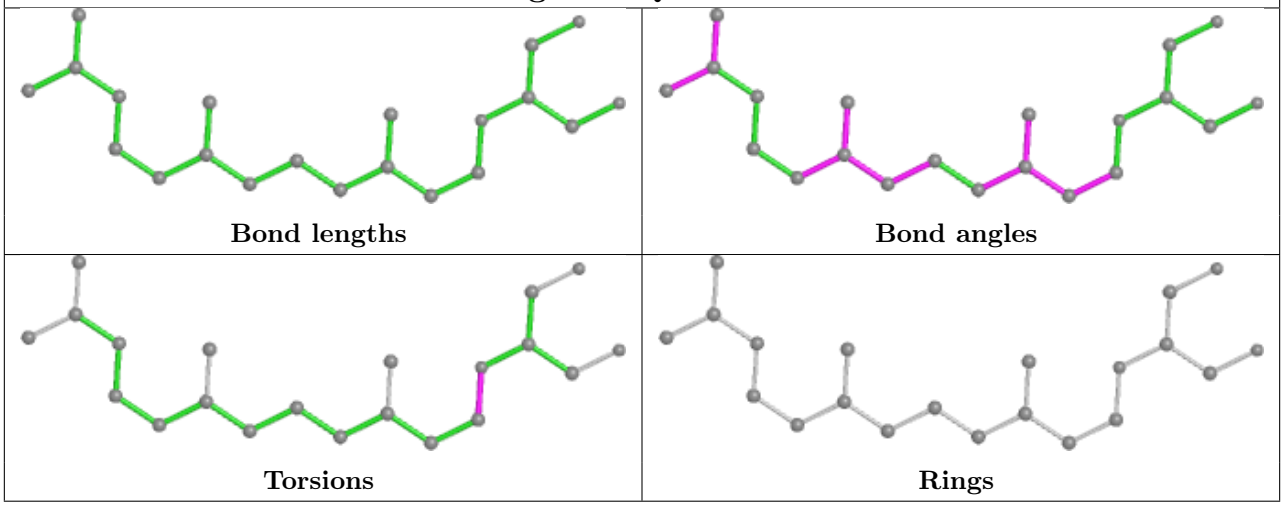
Ligand FQ0 H 302



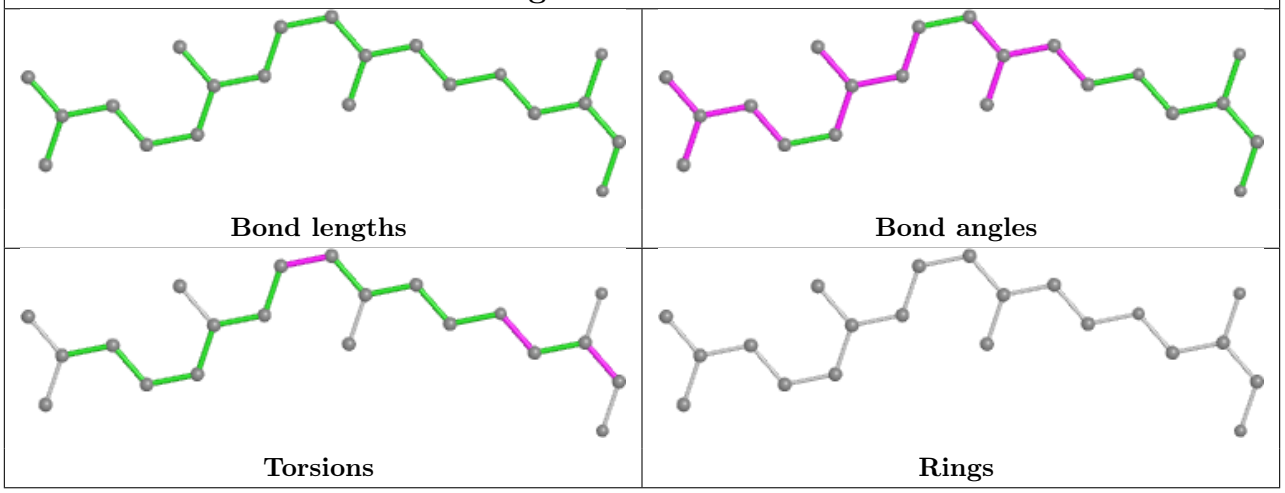
Ligand FV3 H 304



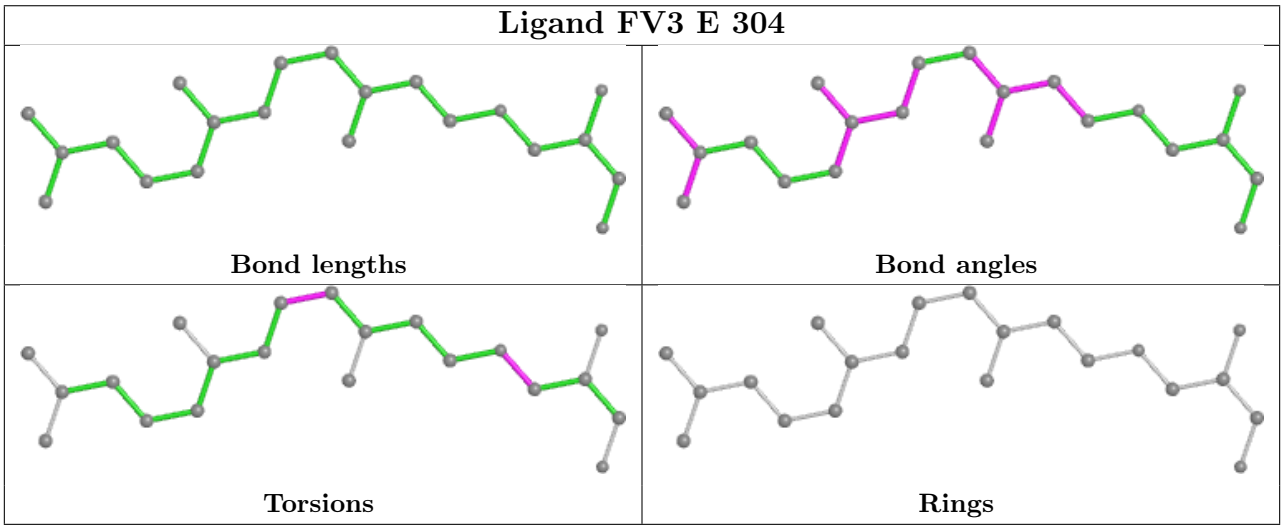
Ligand FQ0 D 302



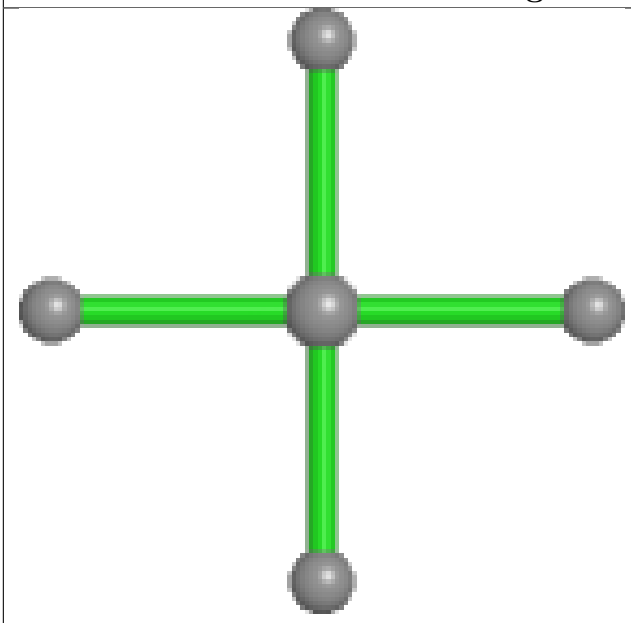
Ligand FV3 C 304



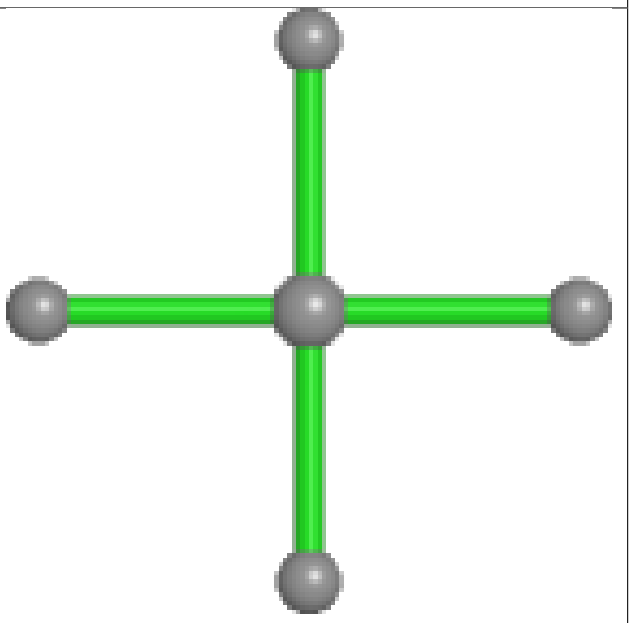
Ligand FV3 E 304



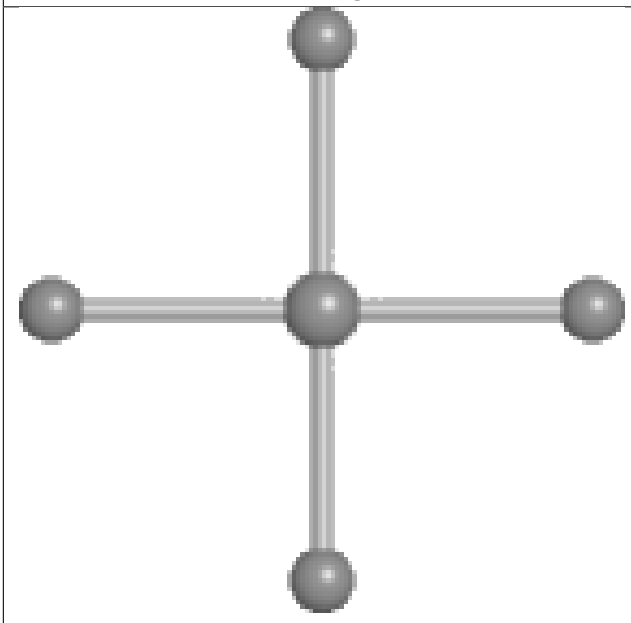
Ligand PO4 D 301



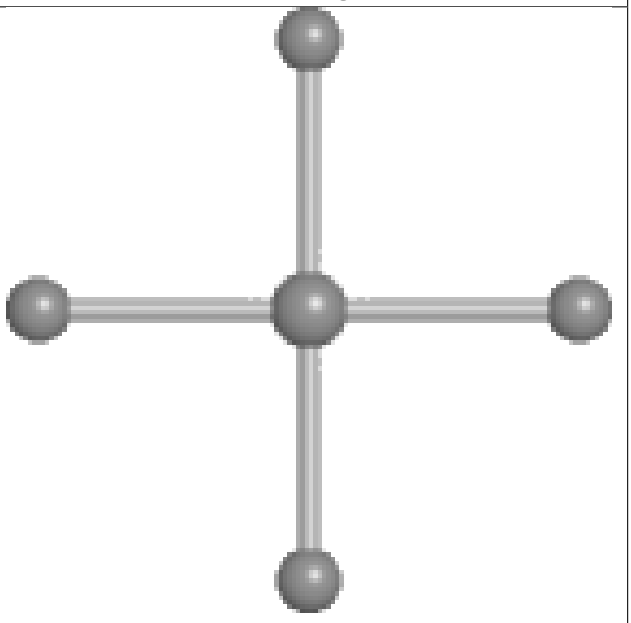
Bond lengths



Bond angles

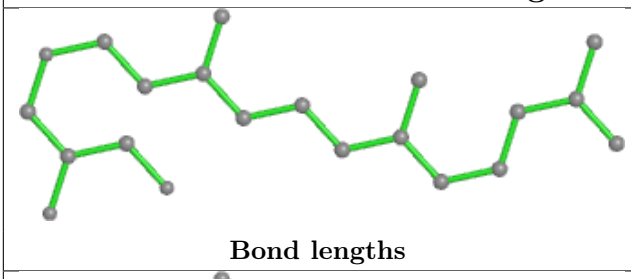


Torsions

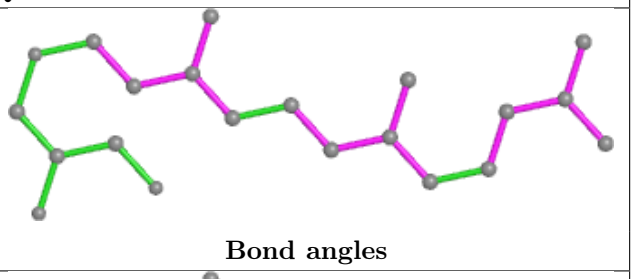


Rings

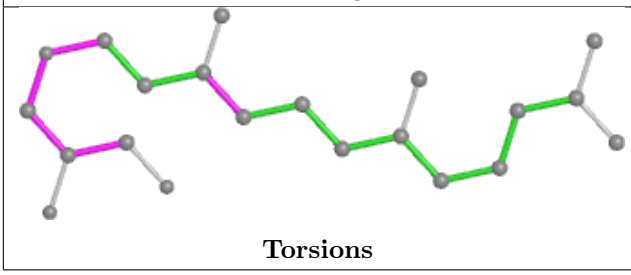
Ligand FQF F 303



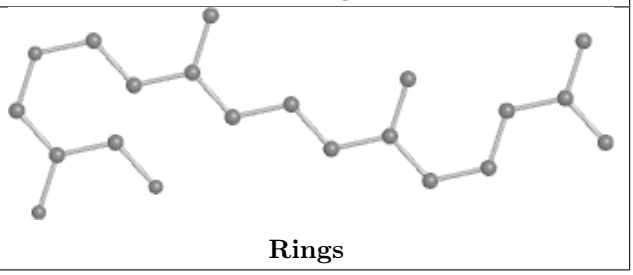
Bond lengths



Bond angles

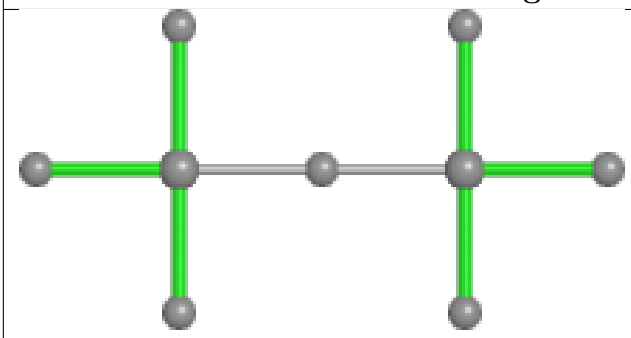


Torsions

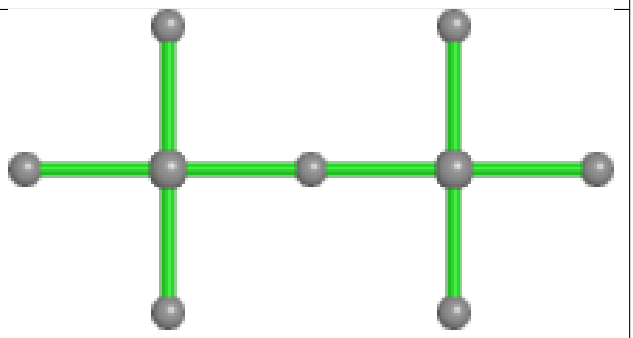


Rings

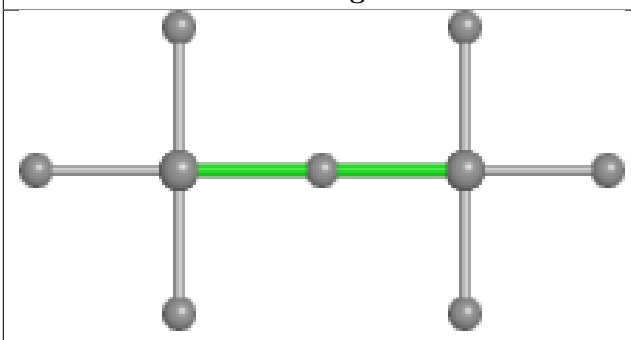
Ligand DPO E 301



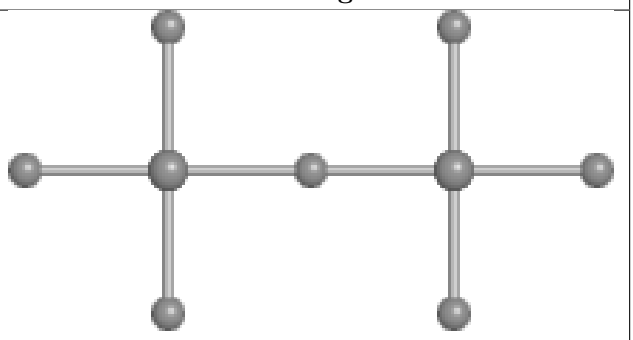
Bond lengths



Bond angles

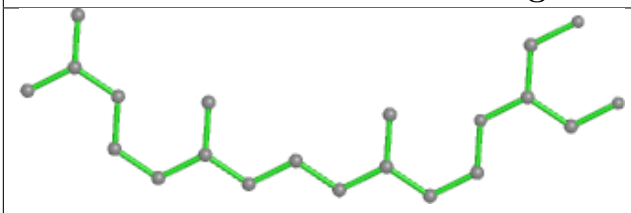


Torsions

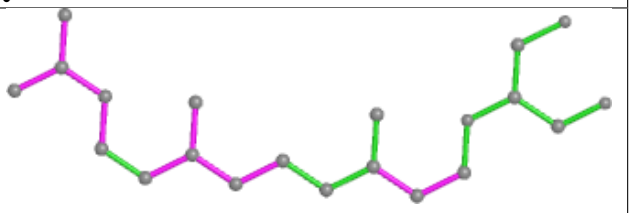


Rings

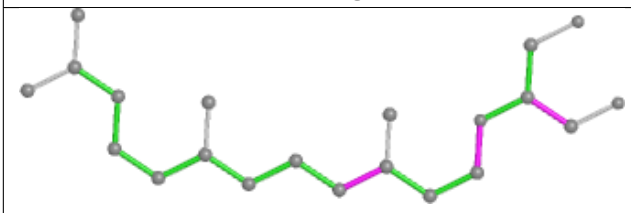
Ligand FQ0 C 302



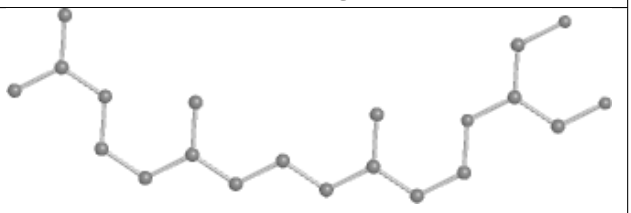
Bond lengths



Bond angles

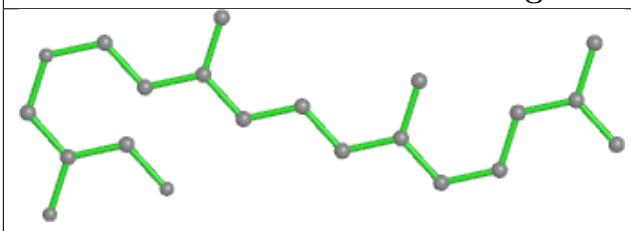


Torsions

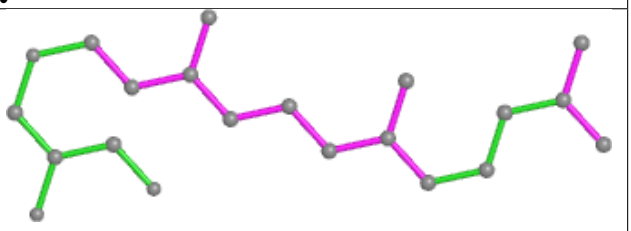


Rings

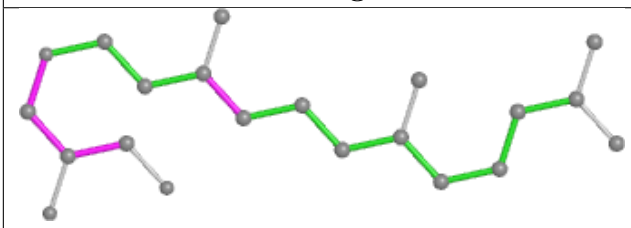
Ligand FQF A 303



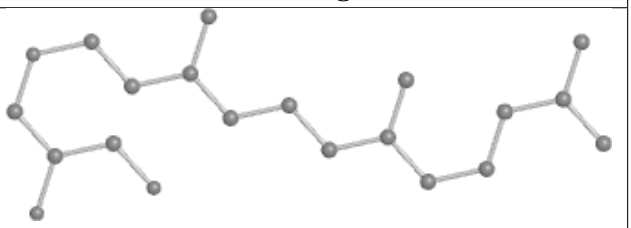
Bond lengths



Bond angles

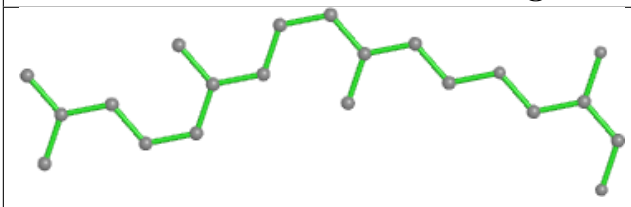


Torsions

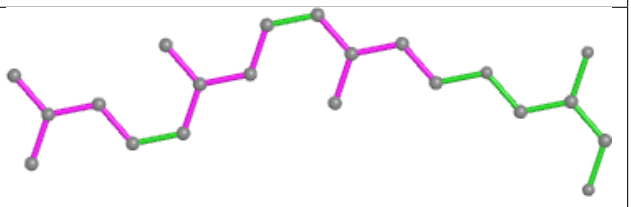


Rings

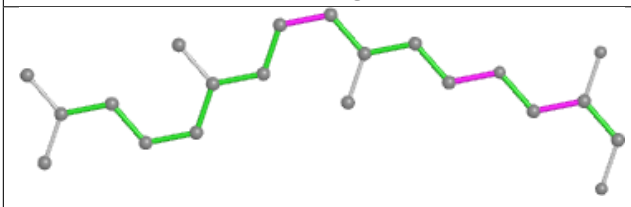
Ligand FV3 D 304



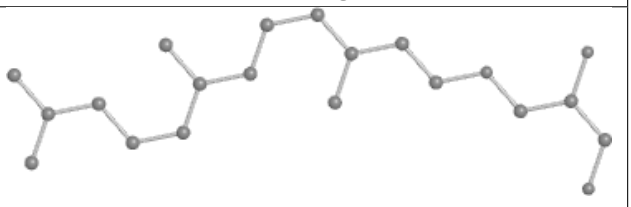
Bond lengths



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	211/224 (94%)	0.39	13 (6%)	20	23	20, 28, 52, 72	0
1	B	221/224 (98%)	0.50	17 (7%)	13	16	20, 27, 49, 83	0
1	C	216/224 (96%)	0.88	28 (12%)	3	3	23, 35, 60, 80	0
1	D	206/224 (91%)	0.54	23 (11%)	5	6	22, 32, 59, 73	0
1	E	215/224 (95%)	0.55	20 (9%)	8	9	22, 31, 56, 79	0
1	F	204/224 (91%)	0.48	19 (9%)	8	9	24, 34, 60, 79	0
1	G	207/224 (92%)	0.37	13 (6%)	20	22	21, 30, 53, 70	0
1	H	220/224 (98%)	0.55	15 (6%)	17	19	22, 32, 57, 87	0
All	All	1700/1792 (94%)	0.54	148 (8%)	10	11	20, 31, 57, 87	0

All (148) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	150	LYS	7.8
1	C	148	GLY	7.5
1	H	142	TYR	7.4
1	H	152	ILE	6.5
1	D	150	LYS	6.5
1	C	141	ALA	6.4
1	G	141	ALA	6.4
1	B	142	TYR	6.3
1	G	151	MET	6.2
1	C	149	LYS	6.1
1	F	151	MET	5.9
1	E	3	ILE	5.8
1	H	151	MET	5.8
1	H	148	GLY	5.7
1	E	142	TYR	5.6
1	G	142	TYR	5.6

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Mol	Chain	Res	Type	RSRZ
1	D	104	ASP	5.5
1	C	152	ILE	5.5
1	E	219	GLY	5.5
1	C	142	TYR	5.4
1	H	-3	PRO	5.4
1	C	151	MET	5.3
1	C	123	LYS	5.2
1	H	150	LYS	5.2
1	F	68	LYS	5.1
1	B	151	MET	4.8
1	A	152	ILE	4.8
1	F	142	TYR	4.7
1	A	214	ASP	4.6
1	C	119	VAL	4.5
1	D	142	TYR	4.4
1	F	141	ALA	4.3
1	A	151	MET	4.3
1	H	5	LYS	4.3
1	B	105	ILE	4.2
1	C	121	LYS	4.2
1	D	2	ASP	4.2
1	H	-2	GLY	4.1
1	H	149	LYS	4.0
1	H	141	ALA	4.0
1	A	141	ALA	3.9
1	E	141	ALA	3.9
1	D	151	MET	3.8
1	A	105	ILE	3.8
1	A	150	LYS	3.7
1	D	5	LYS	3.7
1	F	153	GLU	3.6
1	D	123	LYS	3.6
1	B	141	ALA	3.6
1	G	71	GLN	3.6
1	C	215	ILE	3.5
1	H	123	LYS	3.5
1	A	142	TYR	3.4
1	E	149	LYS	3.4
1	F	72	ILE	3.4
1	D	214	ASP	3.4
1	E	147	ASP	3.4
1	B	152	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	G	150	LYS	3.3
1	A	-3	PRO	3.2
1	C	120	GLY	3.2
1	D	8	ARG	3.2
1	F	74	ARG	3.2
1	E	150	LYS	3.2
1	B	145	SER	3.2
1	D	153	GLU	3.1
1	C	60	PHE	3.1
1	G	102	ASN	3.1
1	E	123	LYS	3.1
1	D	121	LYS	3.1
1	F	152	ILE	3.1
1	C	117	THR	3.0
1	E	218	GLY	3.0
1	E	2	ASP	2.9
1	C	95	ILE	2.9
1	D	152	ILE	2.9
1	B	123	LYS	2.8
1	C	143	ASP	2.8
1	E	143	ASP	2.8
1	F	105	ILE	2.8
1	F	60	PHE	2.8
1	B	135	TYR	2.8
1	A	108	GLU	2.7
1	G	105	ILE	2.7
1	D	185	TYR	2.7
1	D	141	ALA	2.7
1	E	217	LEU	2.7
1	C	3	ILE	2.7
1	D	105	ILE	2.7
1	G	214	ASP	2.7
1	B	149	LYS	2.7
1	E	135	TYR	2.7
1	H	0	GLN	2.6
1	F	154	ASN	2.6
1	C	144	ASN	2.6
1	A	153	GLU	2.6
1	G	2	ASP	2.6
1	B	144	ASN	2.6
1	E	151	MET	2.6
1	G	215	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	68	LYS	2.5
1	A	104	ASP	2.5
1	A	121	LYS	2.5
1	G	67	THR	2.4
1	F	29	LEU	2.4
1	E	121	LYS	2.4
1	F	108	GLU	2.4
1	H	105	ILE	2.4
1	B	68	LYS	2.4
1	D	11	ARG	2.4
1	D	51	LYS	2.3
1	E	5	LYS	2.3
1	H	135	TYR	2.3
1	F	71	GLN	2.3
1	C	2	ASP	2.3
1	D	102	ASN	2.3
1	C	71	GLN	2.2
1	C	92	ASP	2.2
1	D	7	LYS	2.2
1	D	135	TYR	2.2
1	E	216	THR	2.2
1	A	1	MET	2.2
1	C	165	LEU	2.2
1	D	201	GLU	2.2
1	C	72	ILE	2.2
1	F	115	LYS	2.2
1	E	148	GLY	2.2
1	C	106	PHE	2.2
1	B	147	ASP	2.2
1	B	143	ASP	2.2
1	G	154	ASN	2.1
1	C	150	LYS	2.1
1	F	102	ASN	2.1
1	E	65	ASP	2.1
1	C	94	GLU	2.1
1	H	140	TYR	2.1
1	F	32	HIS	2.1
1	B	65	ASP	2.1
1	F	135	TYR	2.1
1	G	135	TYR	2.1
1	C	65	ASP	2.1
1	D	173	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	152	ILE	2.1
1	B	8	ARG	2.0
1	B	150	LYS	2.0
1	D	30	GLU	2.0
1	C	25	LEU	2.0
1	B	102	ASN	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	DPO	G	301	9/9	0.78	0.28	37,44,58,58	0
3	FQ0	F	302	21/21	0.80	0.19	29,30,30,31	21
4	FQF	F	303	21/21	0.83	0.16	26,30,35,36	21
5	FV3	F	304	21/21	0.84	0.18	40,46,50,51	21
3	FQ0	D	302	21/21	0.84	0.15	25,26,27,27	21
4	FQF	B	303	21/21	0.85	0.14	27,31,33,33	21
3	FQ0	B	302	21/21	0.85	0.13	17,22,25,26	21
4	FQF	C	303	21/21	0.86	0.17	28,31,39,41	21
5	FV3	D	304	21/21	0.86	0.16	30,33,40,42	21
5	FV3	E	304	21/21	0.87	0.14	26,31,36,37	21
5	FV3	C	304	21/21	0.87	0.17	31,34,42,43	21
5	FV3	G	304	21/21	0.87	0.18	32,36,47,48	21
5	FV3	H	304	21/21	0.87	0.18	35,38,42,42	21
3	FQ0	G	302	21/21	0.87	0.19	26,28,31,33	21
4	FQF	G	303	21/21	0.88	0.17	29,31,37,39	21
4	FQF	H	303	21/21	0.88	0.17	27,28,35,36	21
5	FV3	B	304	21/21	0.88	0.14	26,30,35,35	21

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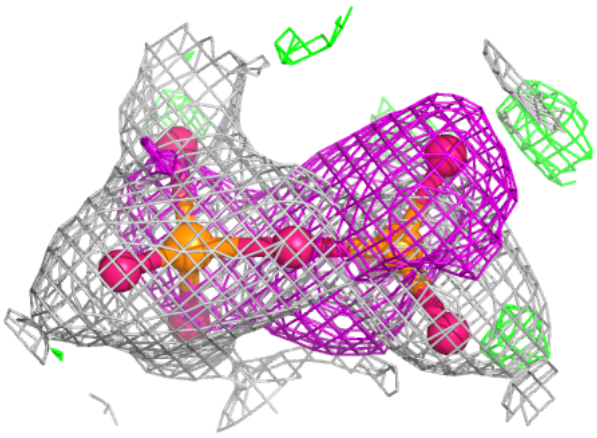
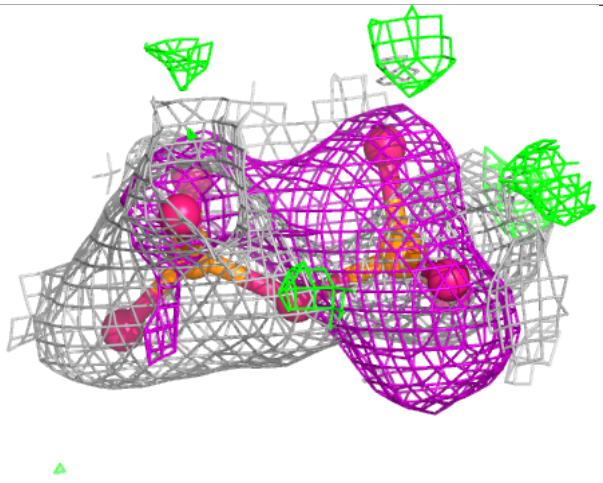
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	FQF	D	303	21/21	0.88	0.17	23,27,31,32	21
6	DPO	B	301	9/9	0.88	0.34	38,45,59,60	0
6	DPO	E	301	9/9	0.88	0.39	44,48,59,63	0
3	FQ0	H	302	21/21	0.88	0.14	20,22,25,26	21
3	FQ0	C	302	21/21	0.89	0.17	24,25,31,31	21
3	FQ0	A	302	21/21	0.90	0.13	19,21,25,25	21
5	FV3	A	304	21/21	0.90	0.13	27,29,41,43	21
3	FQ0	E	302	21/21	0.90	0.14	23,23,26,27	21
4	FQF	A	303	21/21	0.91	0.14	20,24,28,29	21
4	FQF	E	303	21/21	0.91	0.16	21,26,34,36	21
2	PO4	F	301	5/5	0.96	0.10	47,48,48,52	0
2	PO4	H	301	5/5	0.97	0.12	40,43,45,46	0
2	PO4	C	301	5/5	0.98	0.11	49,49,50,53	0
2	PO4	D	301	5/5	0.99	0.13	34,36,37,38	0
2	PO4	A	301	5/5	0.99	0.10	30,30,33,33	0

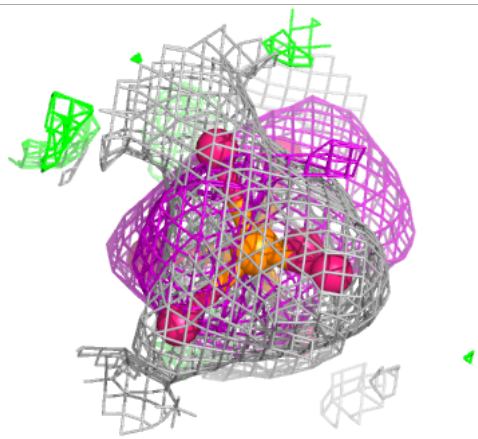
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DPO G 301:

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

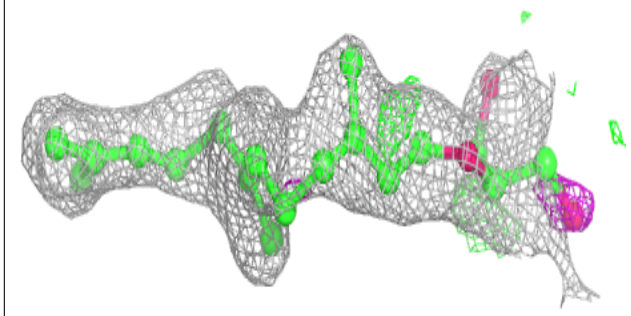


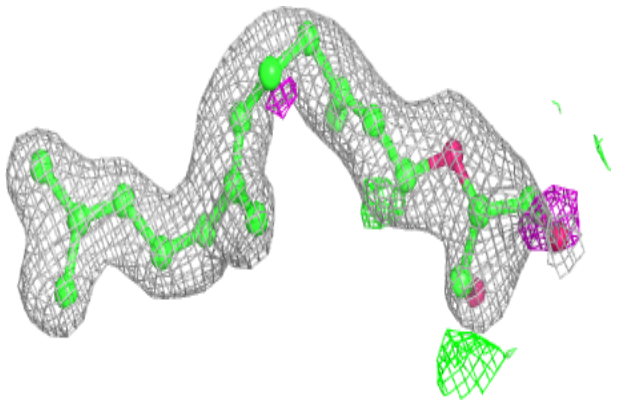


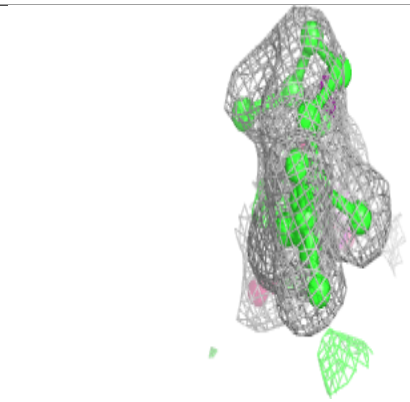


Electron density around FQ0 F 302:

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

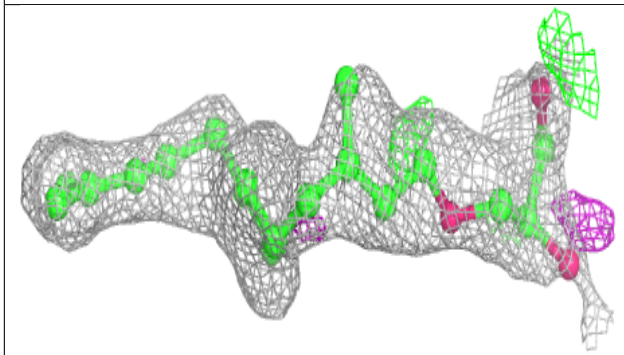


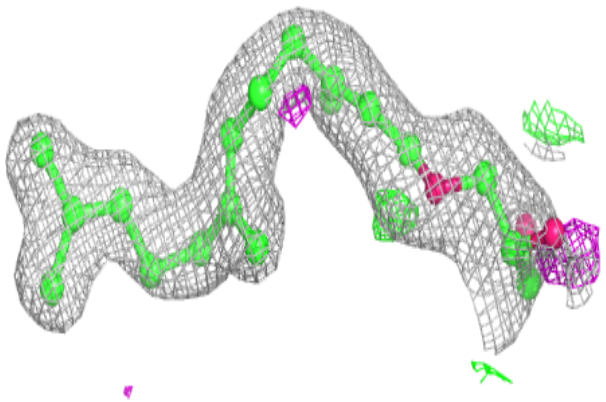


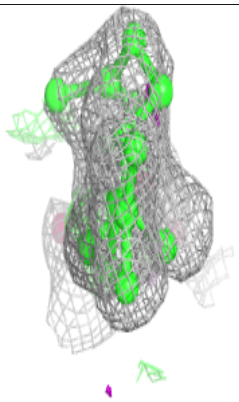


Electron density around FQF F 303:

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

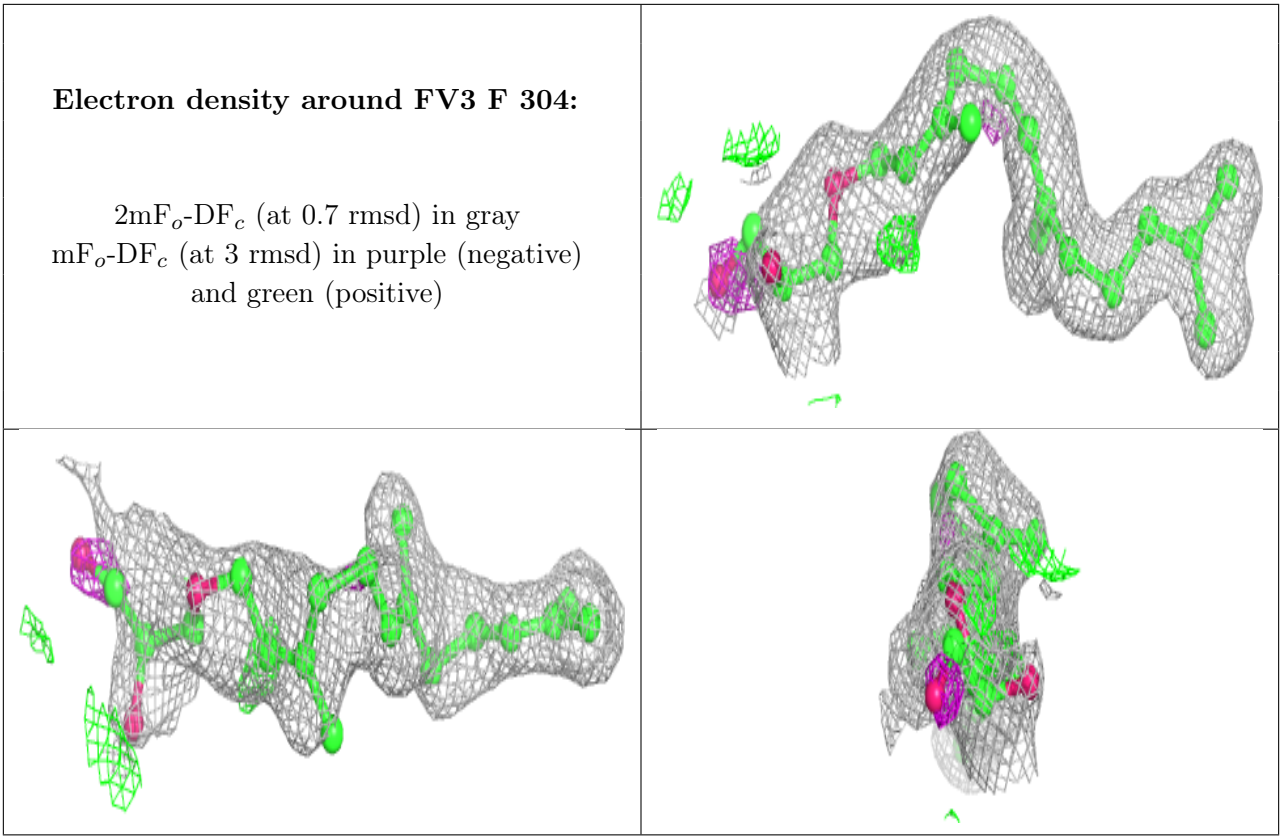






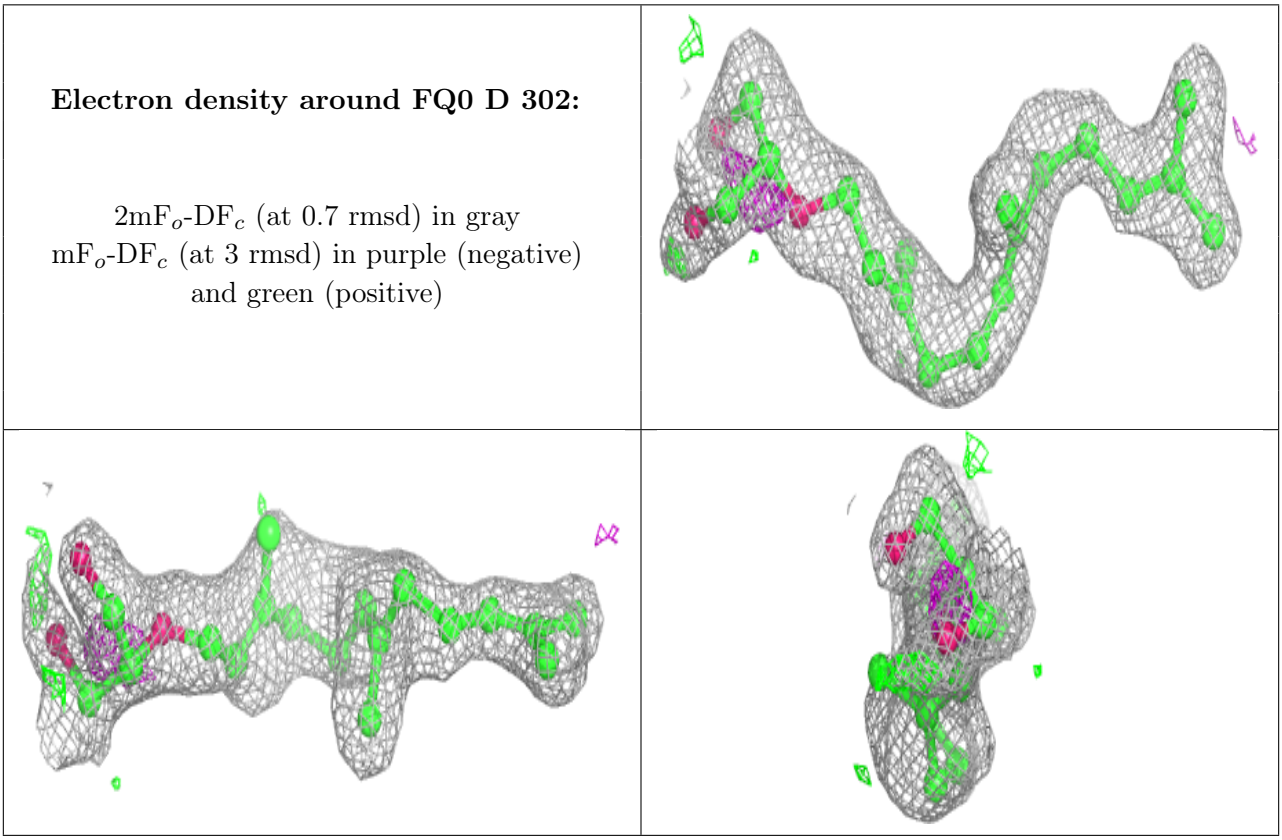
Electron density around FV3 F 304:

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



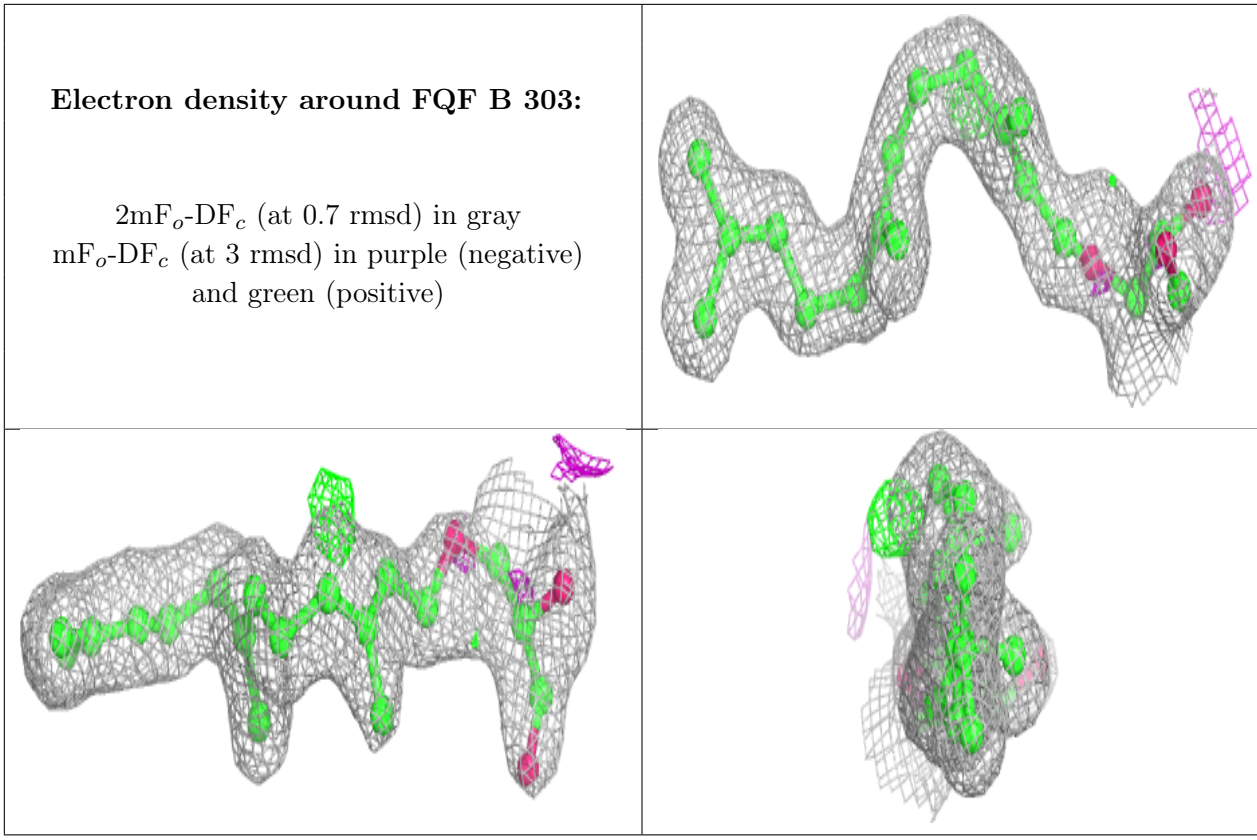
Electron density around FQ0 D 302:

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



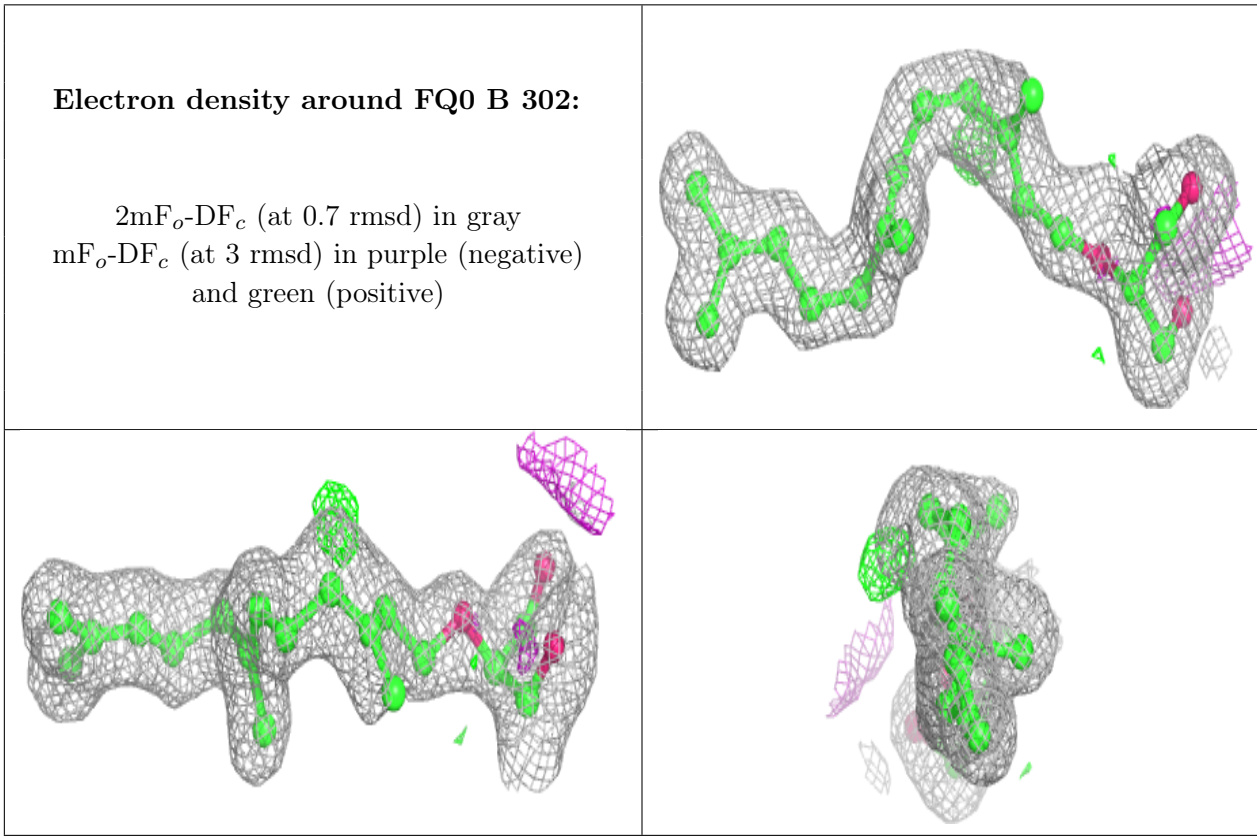
Electron density around FQF B 303:

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



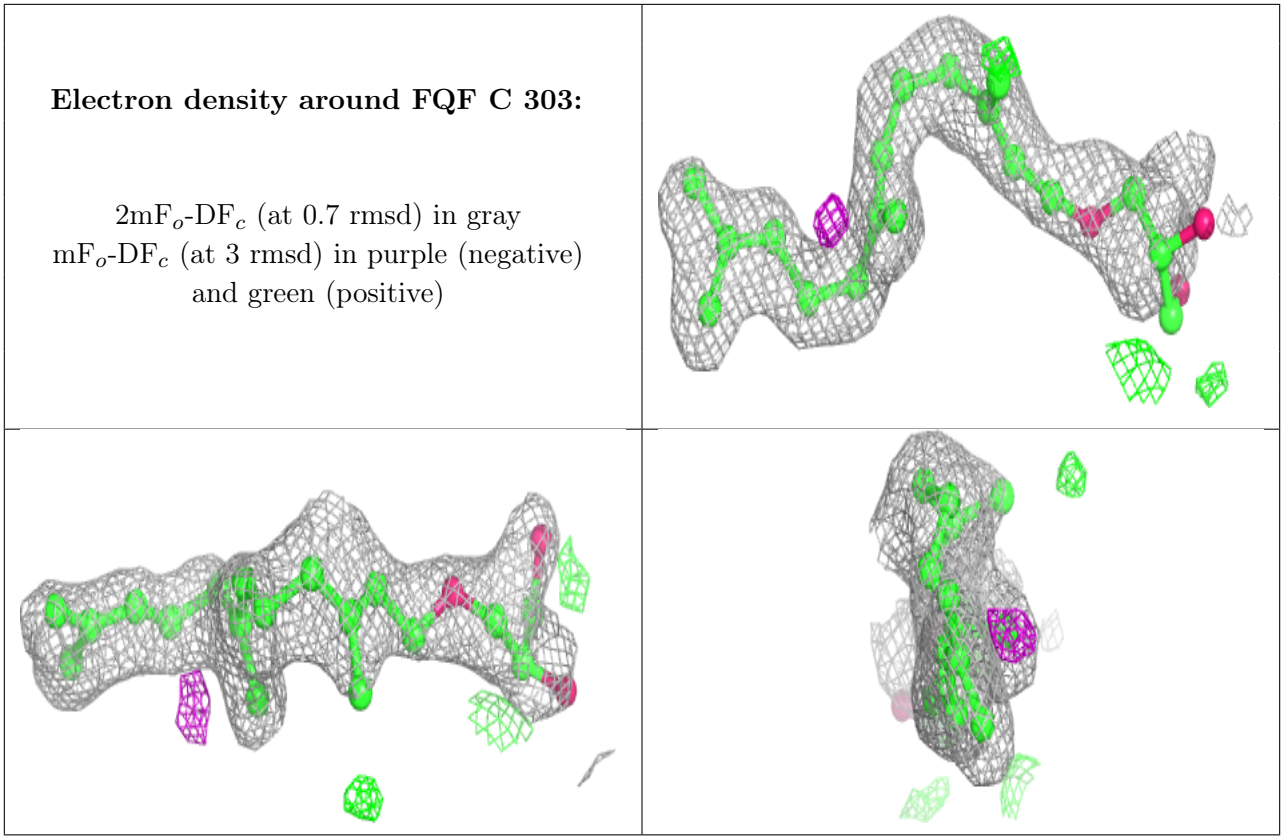
Electron density around FQ0 B 302:

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



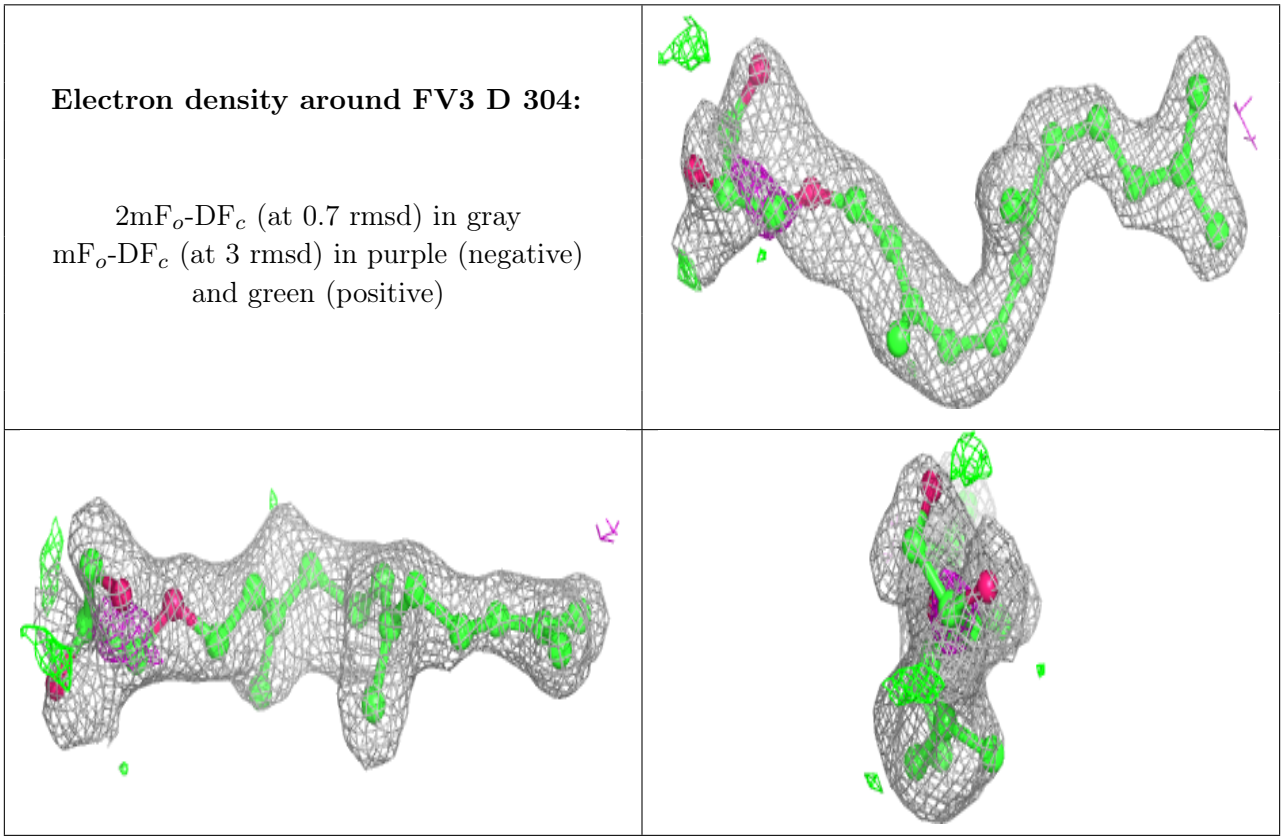
Electron density around FQF C 303:

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



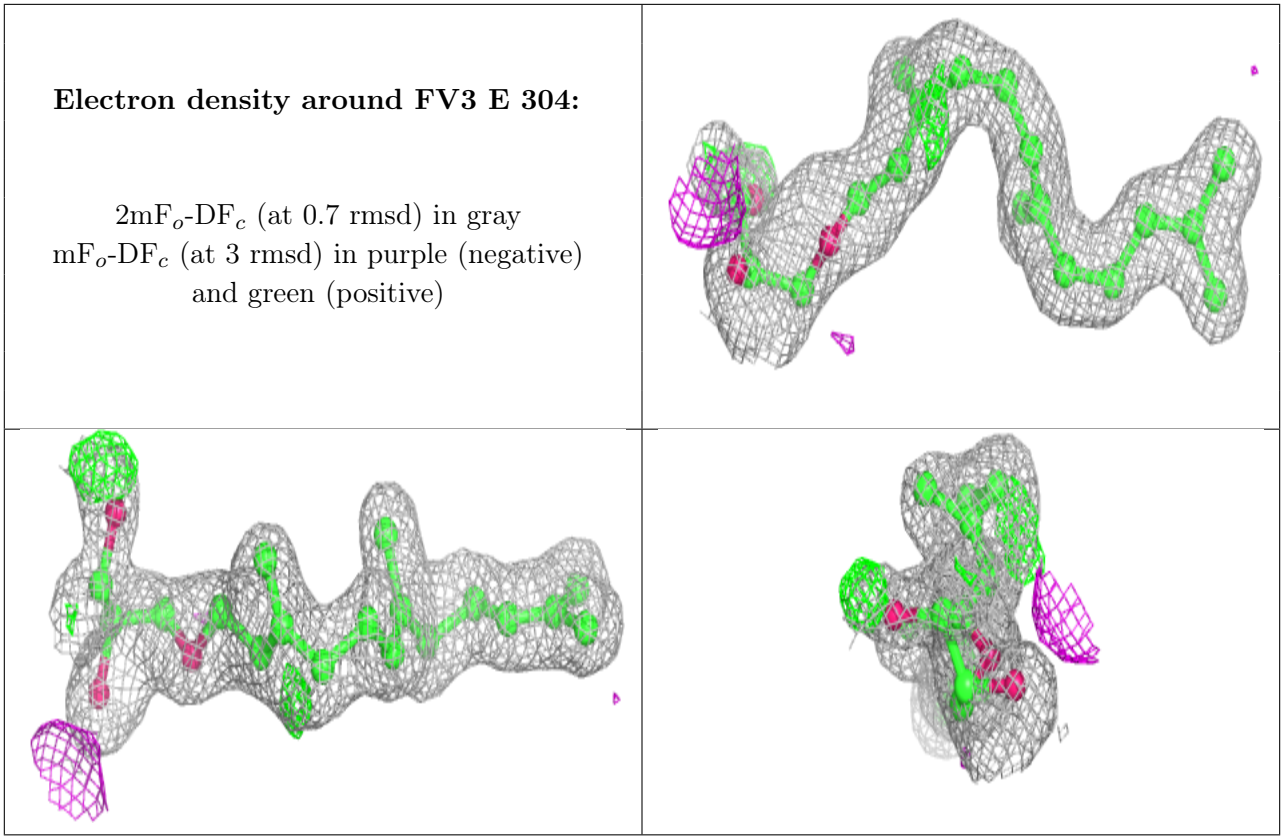
Electron density around FV3 D 304:

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



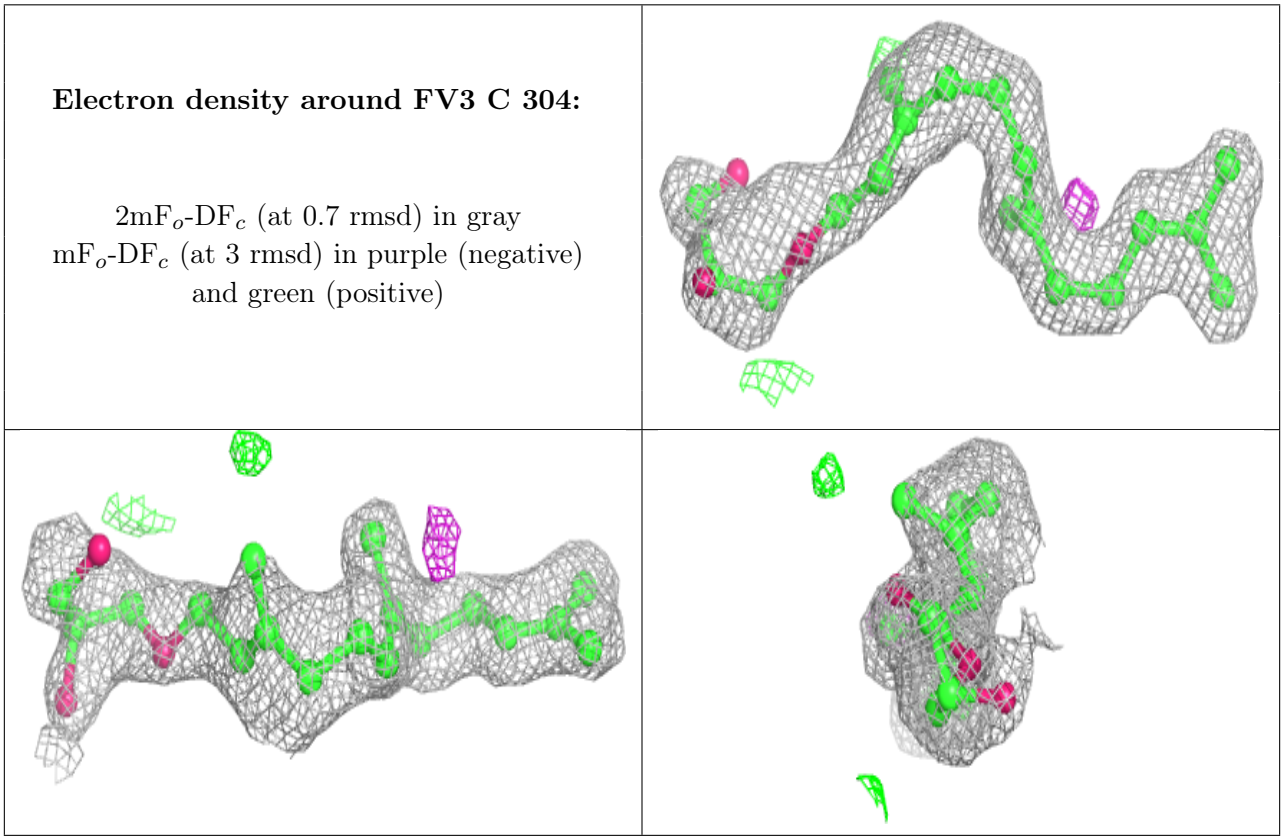
Electron density around FV3 E 304:

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



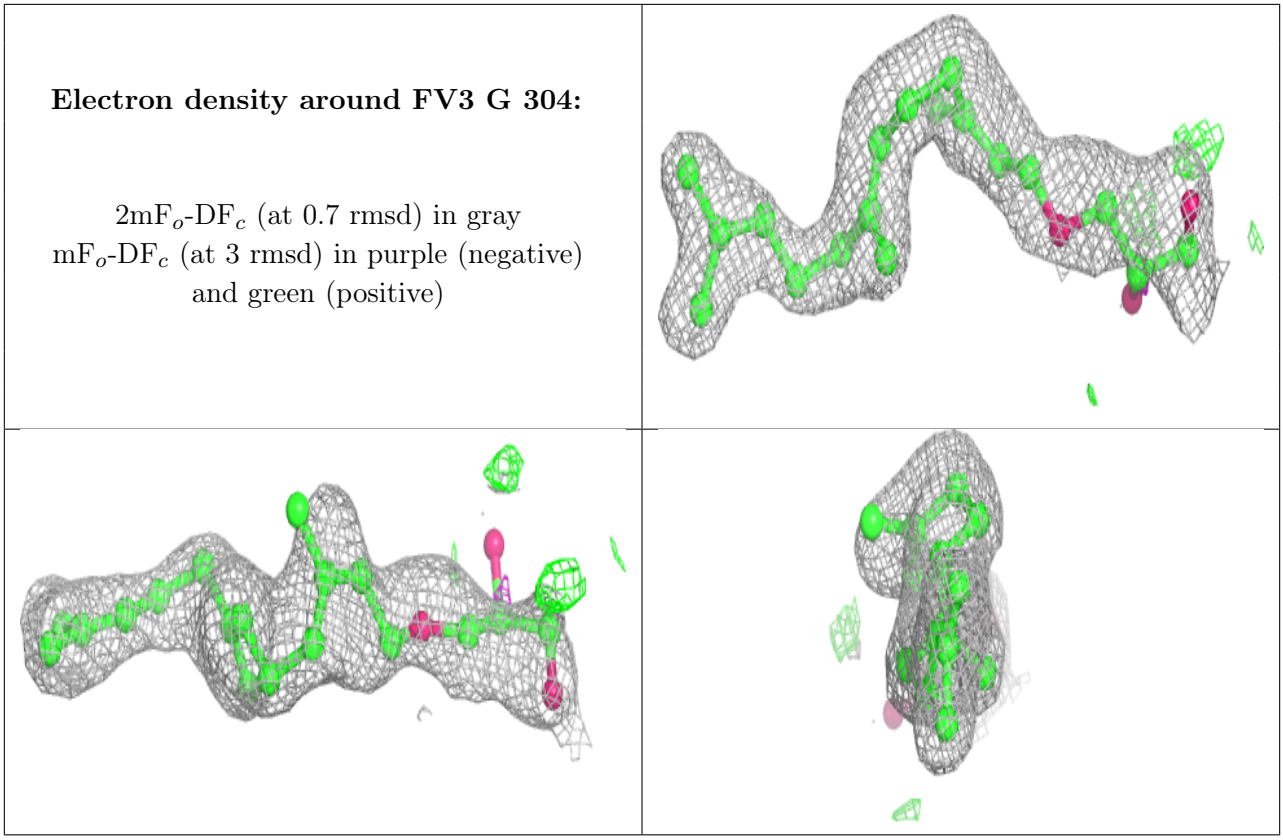
Electron density around FV3 C 304:

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



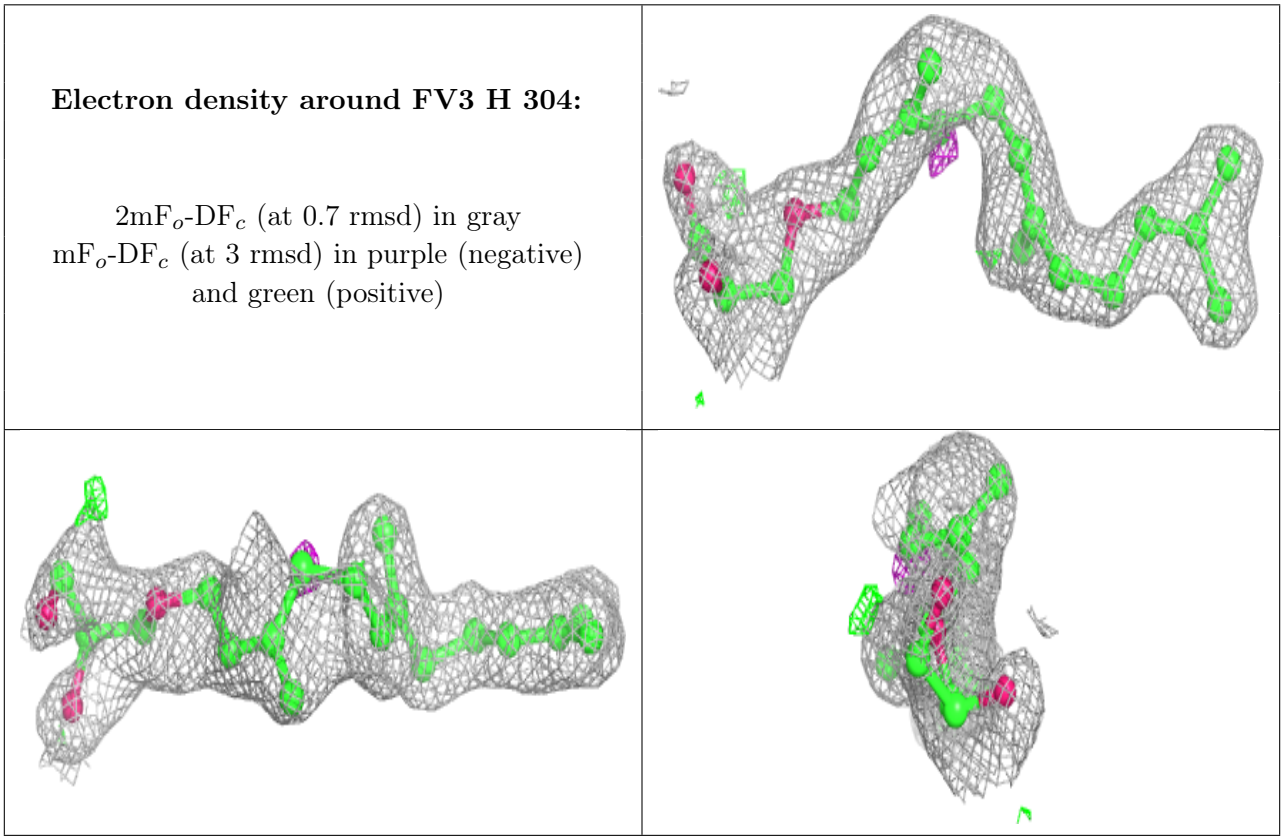
Electron density around FV3 G 304:

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



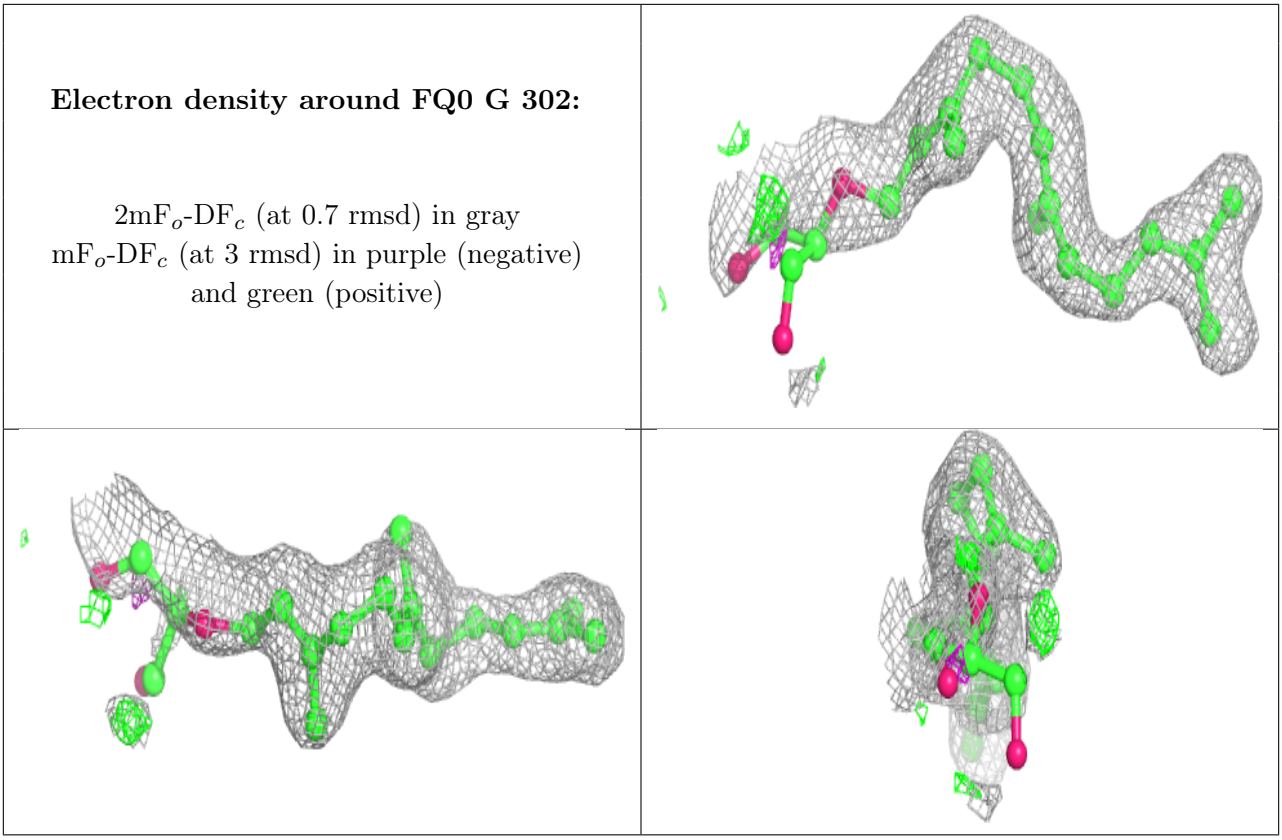
Electron density around FV3 H 304:

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



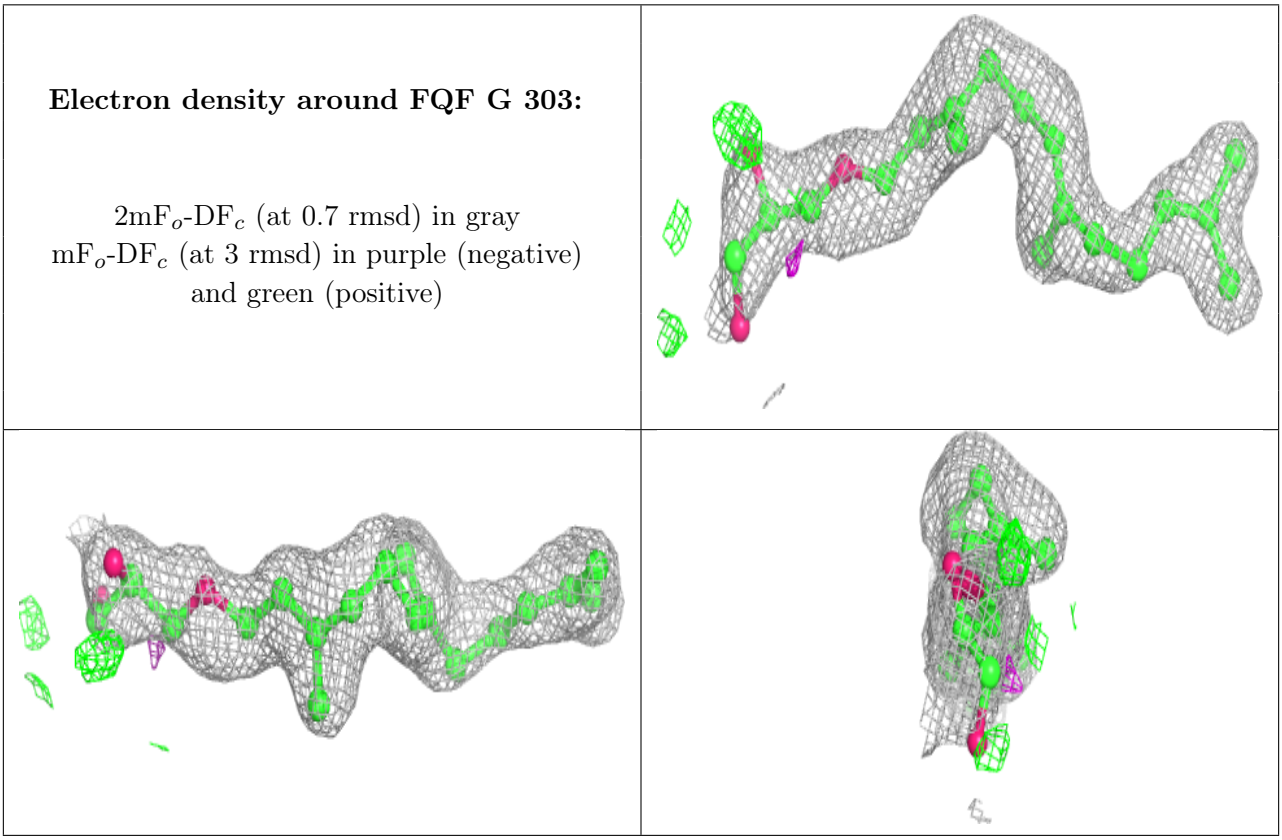
Electron density around FQ0 G 302:

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



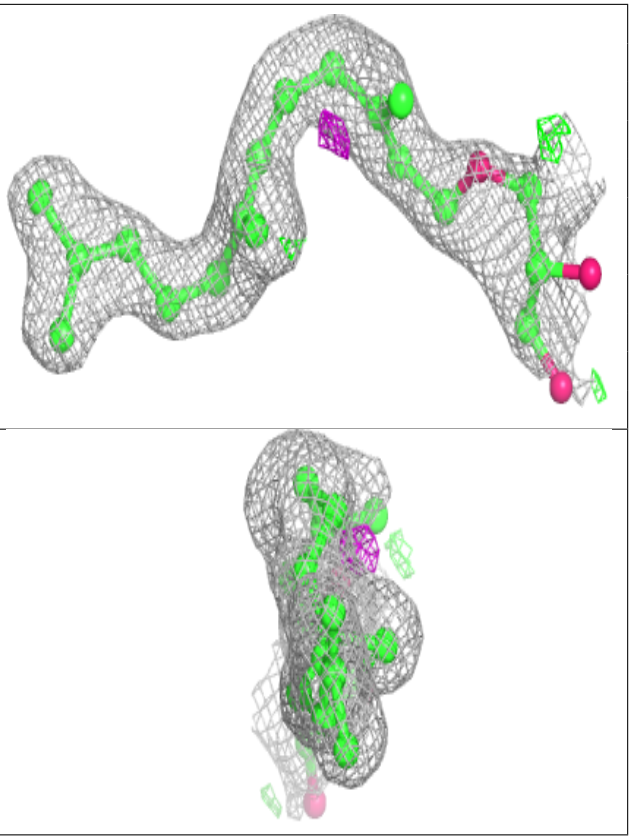
Electron density around FQF G 303:

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



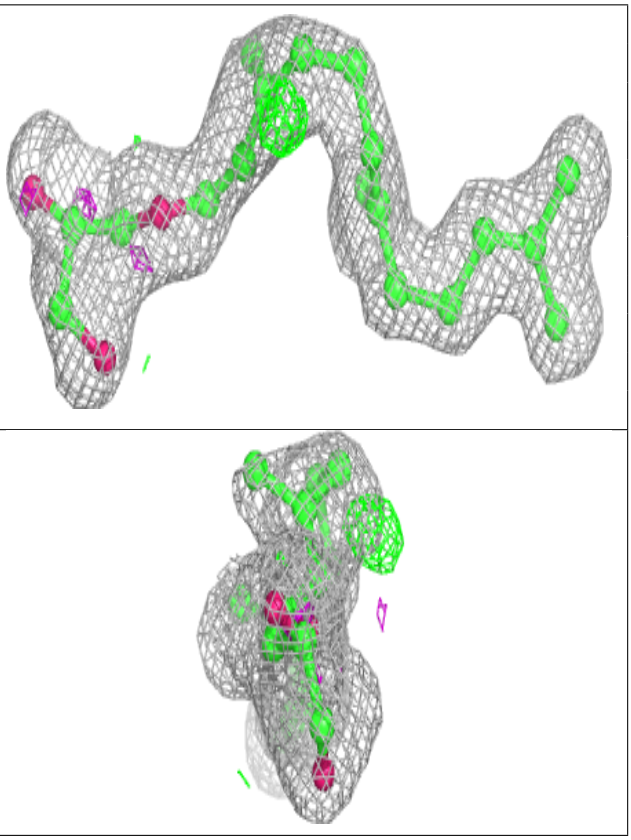
Electron density around FQF H 303:

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



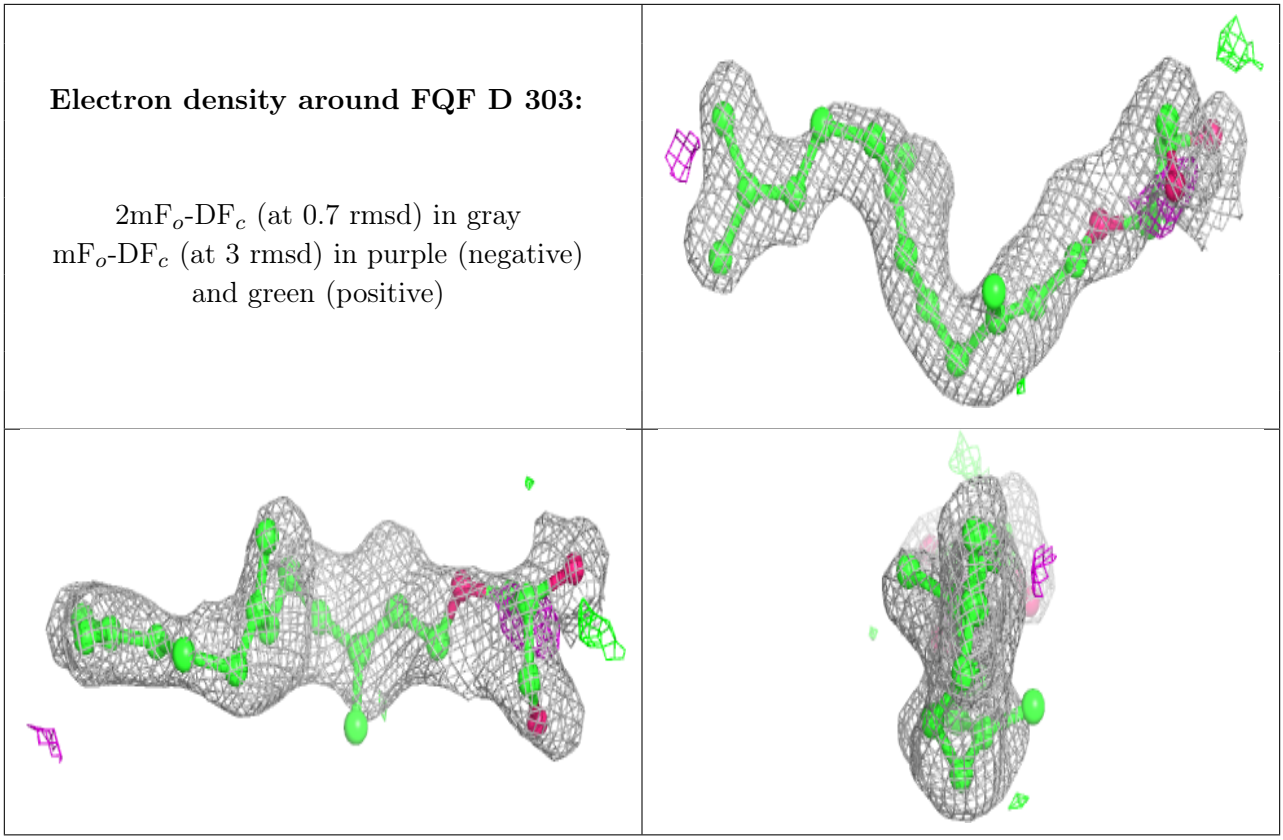
Electron density around FV3 B 304:

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



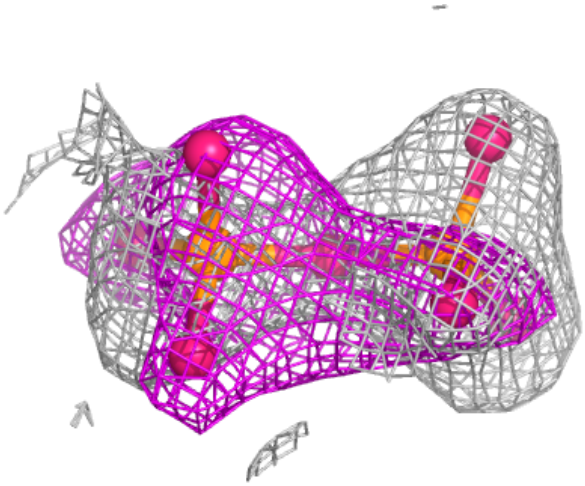
Electron density around FQF D 303:

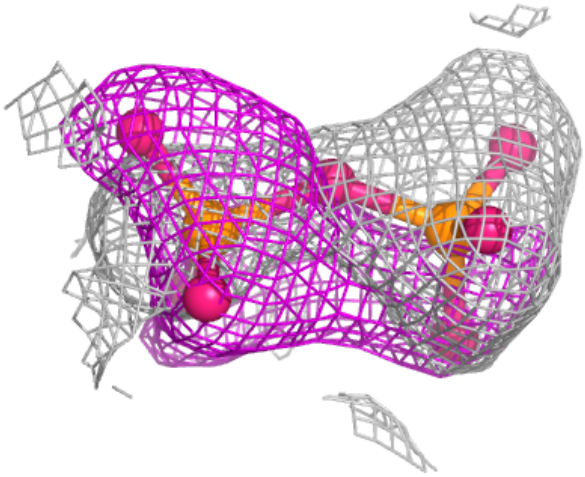
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

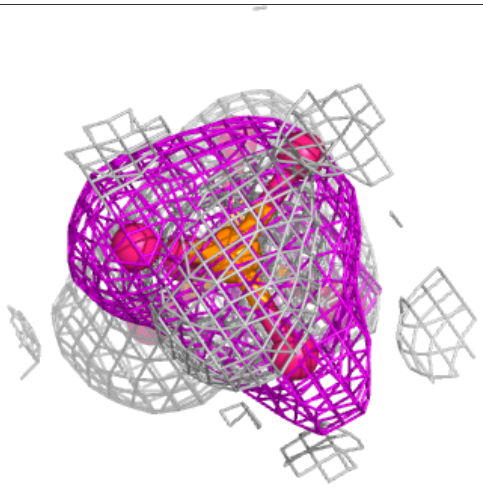


Electron density around DPO B 301:

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

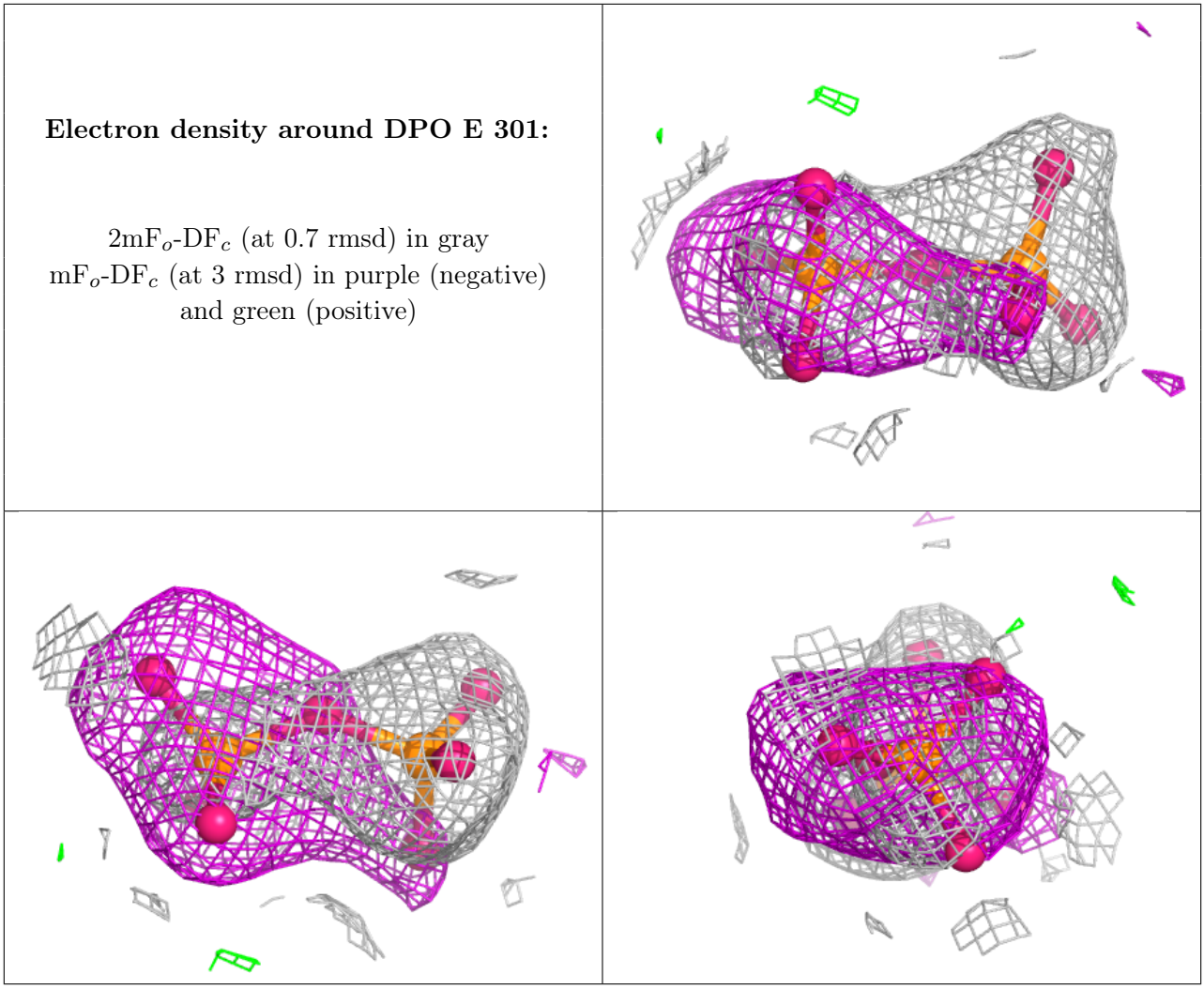






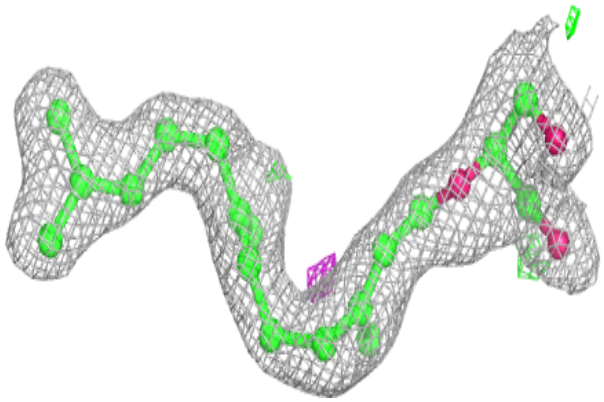
Electron density around DPO E 301:

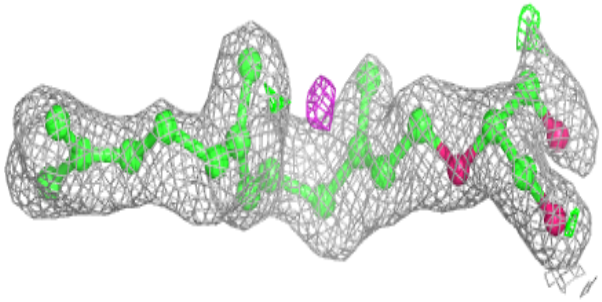
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

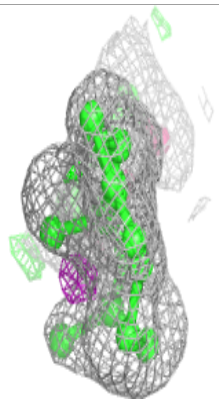


Electron density around FQ0 H 302:

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

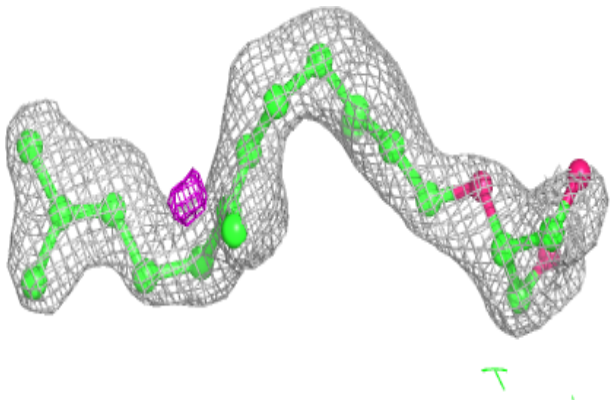


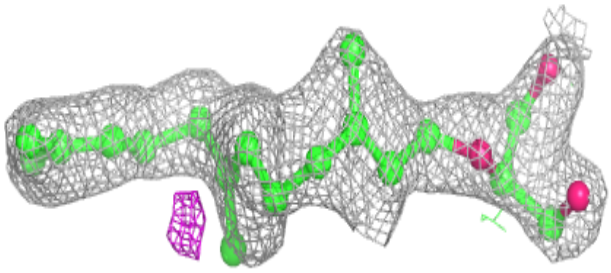


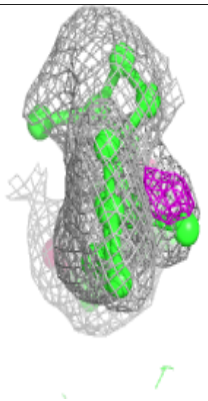


Electron density around FQ0 C 302:

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

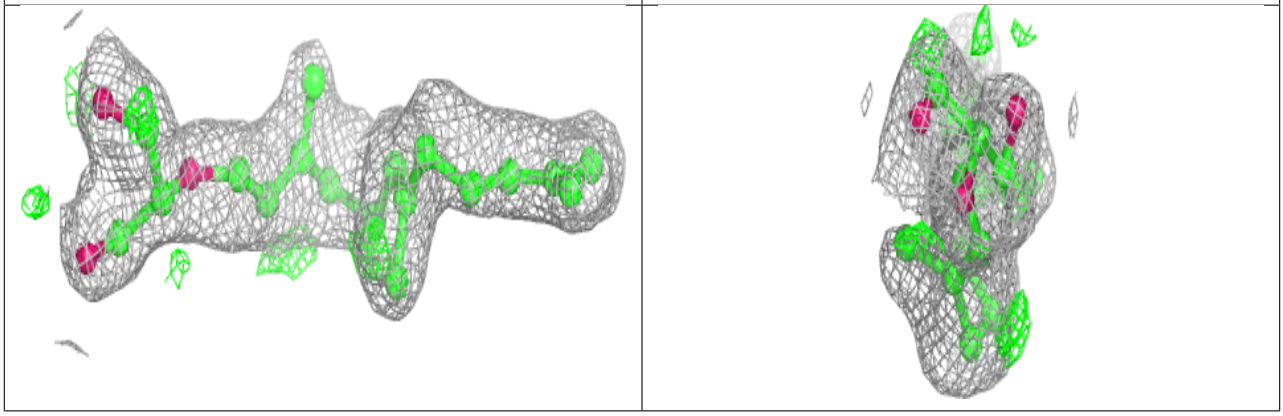






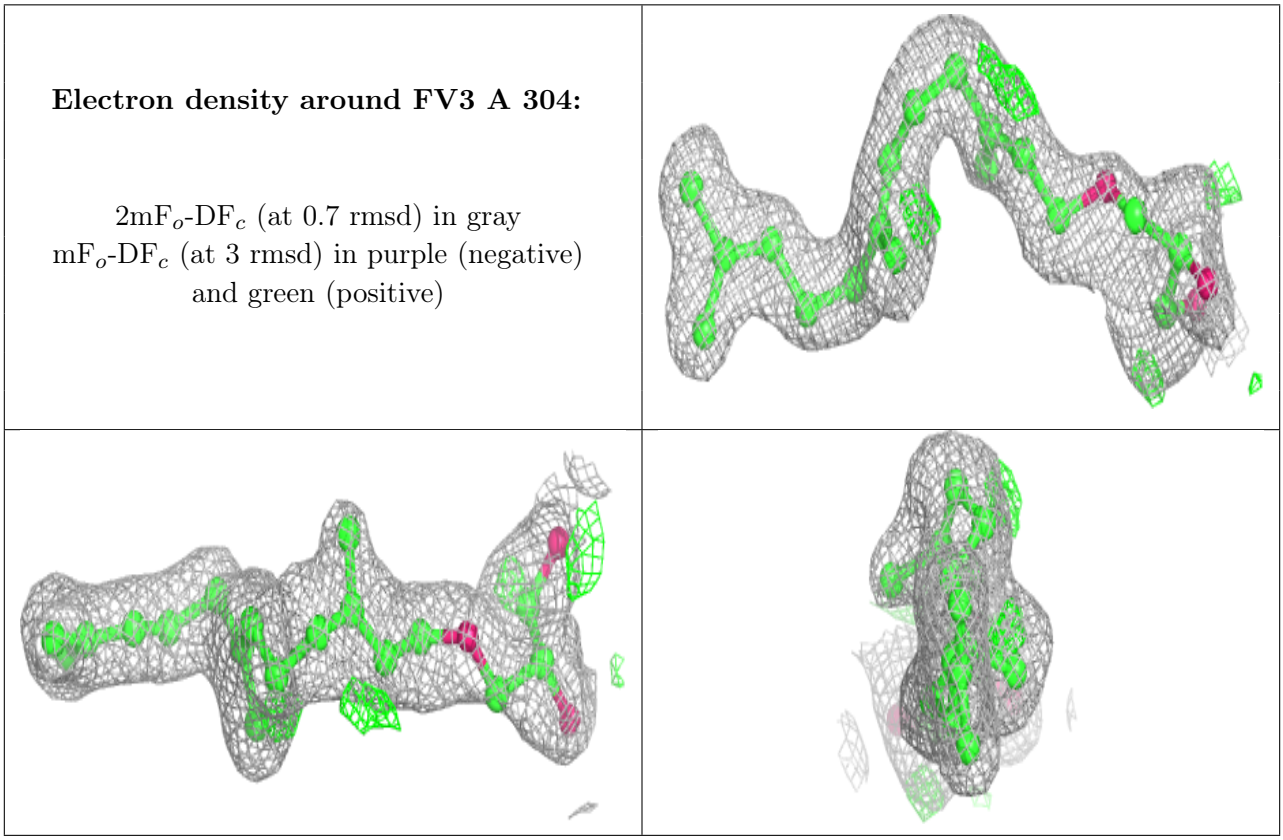
Electron density around FQ0 A 302:

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



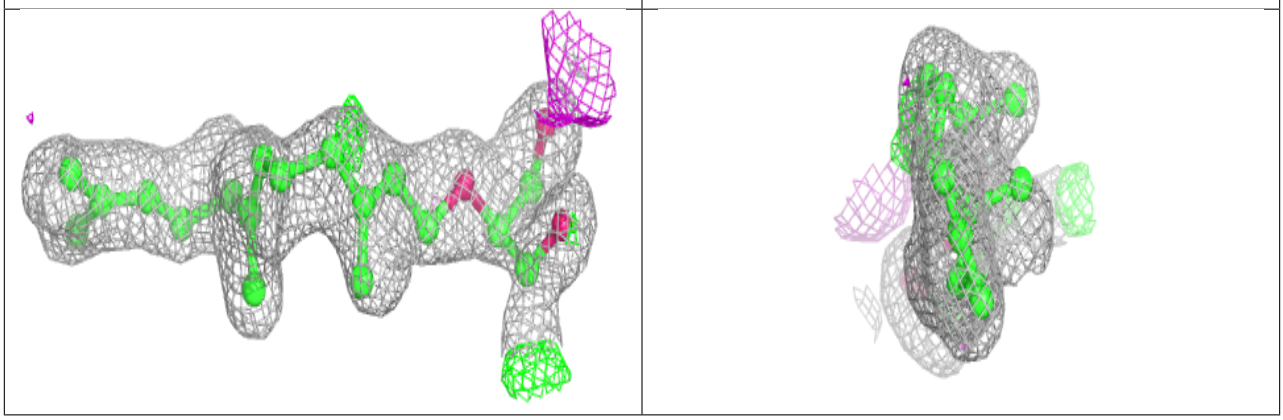
Electron density around FV3 A 304:

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



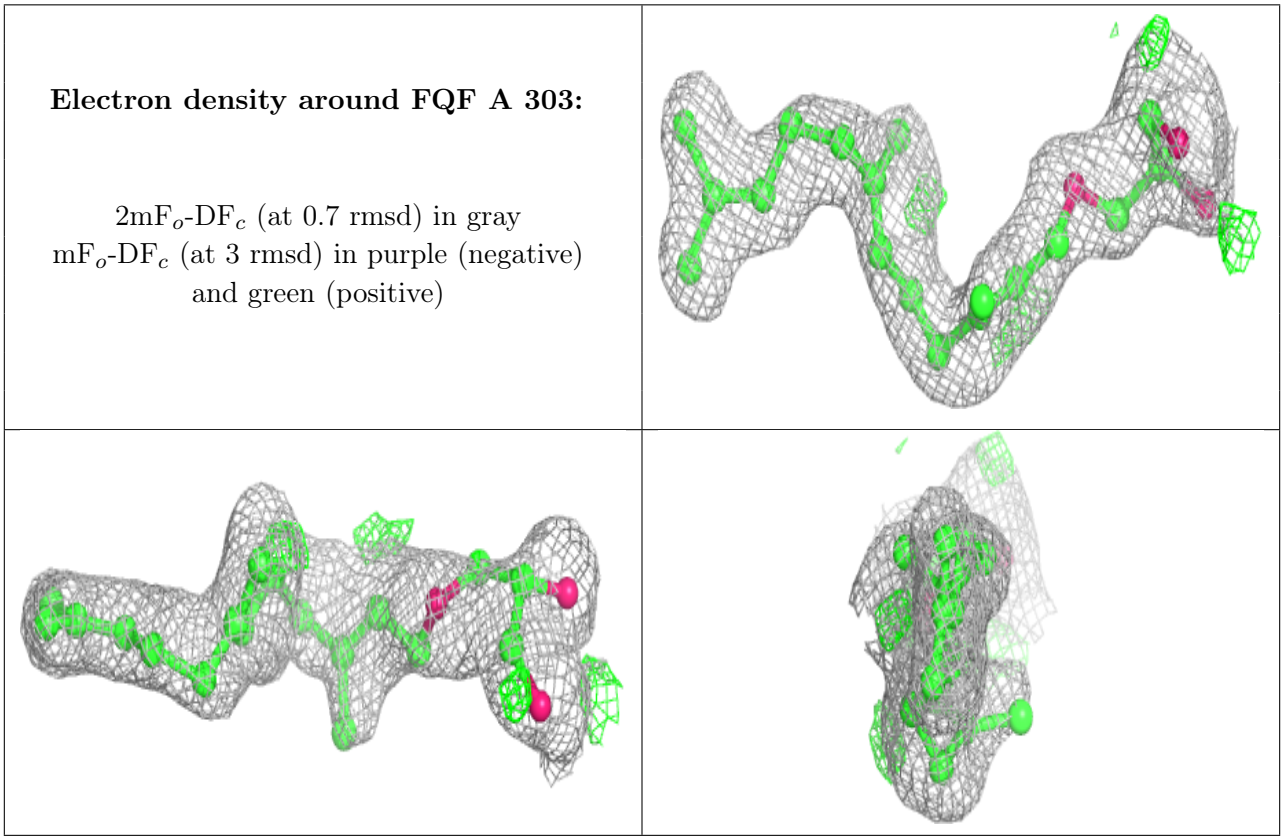
Electron density around FQ0 E 302:

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



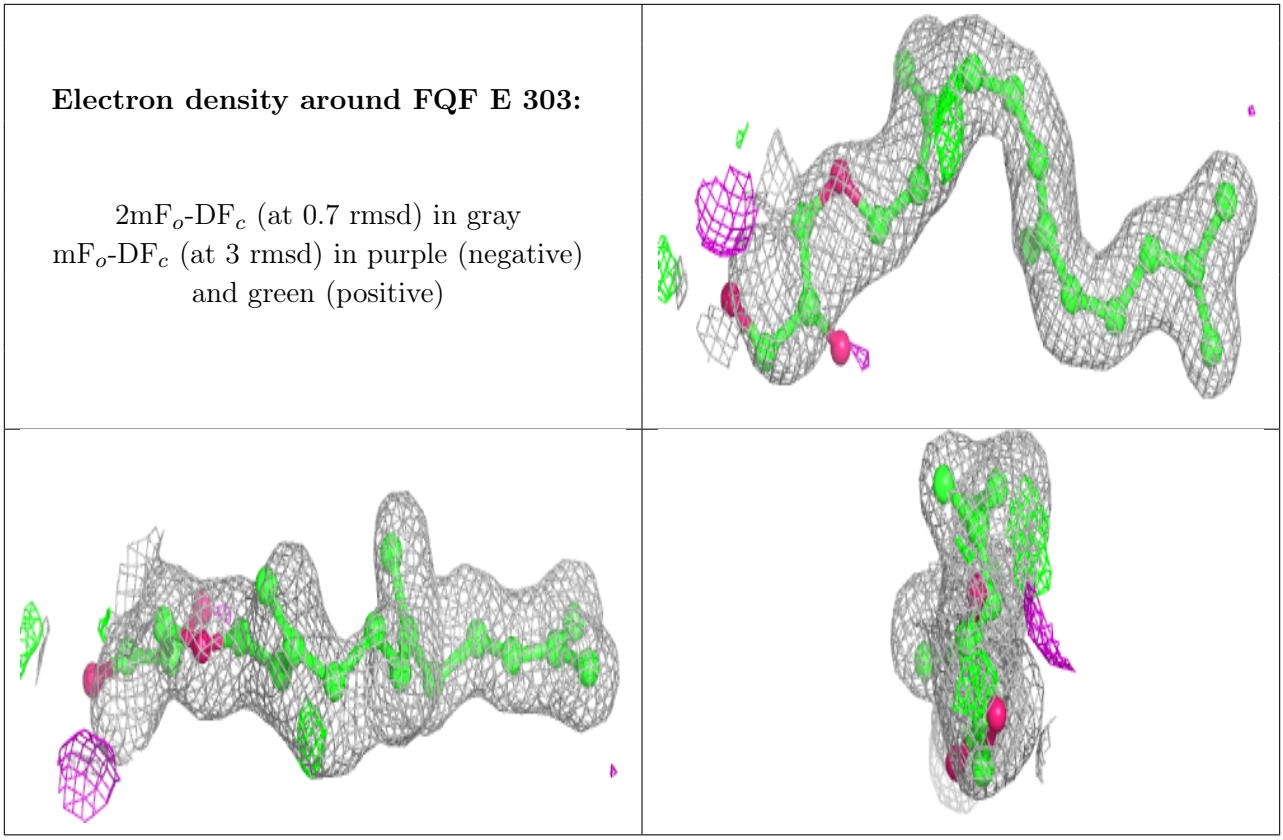
Electron density around FQF A 303:

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



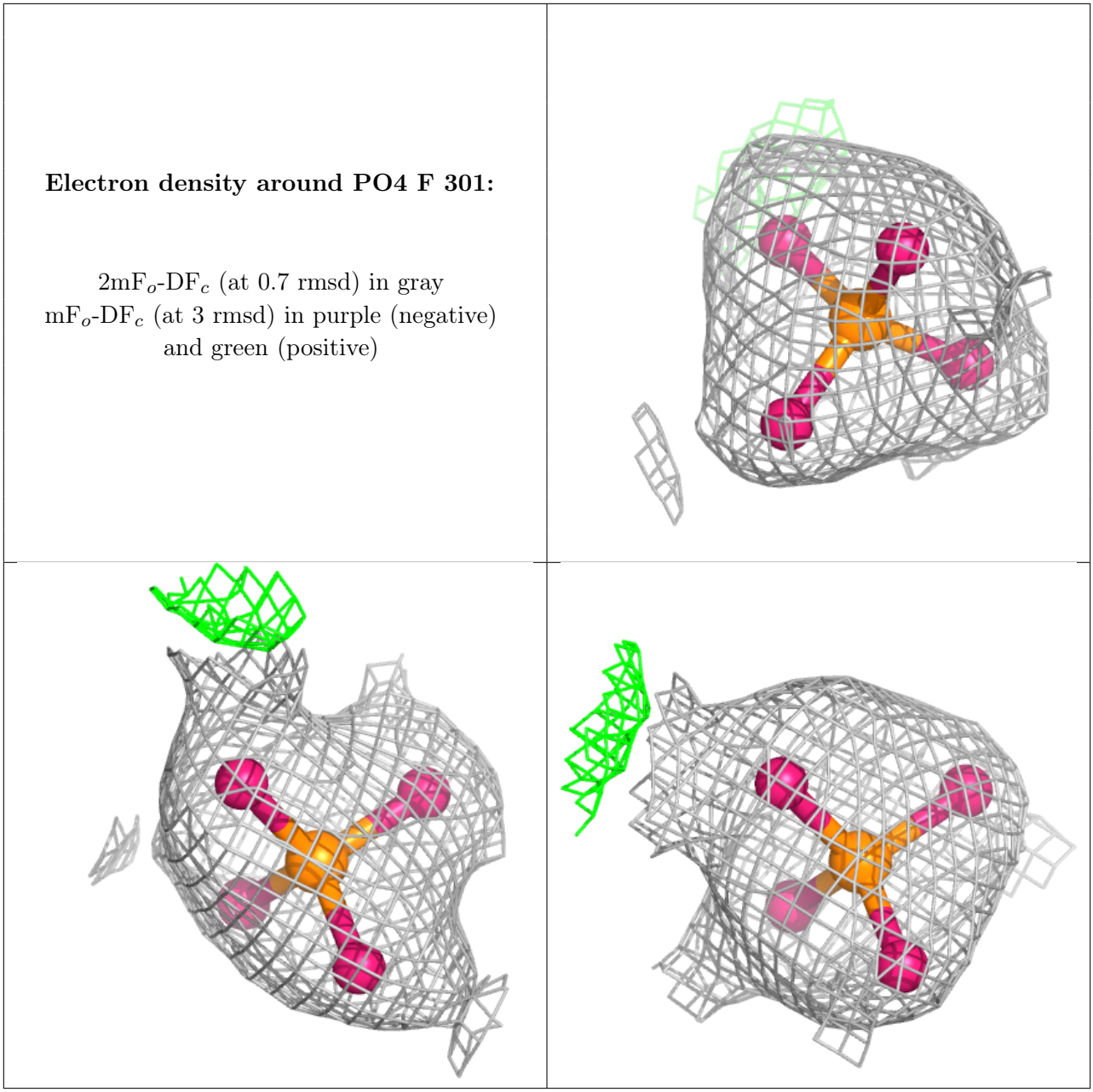
Electron density around FQF E 303:

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



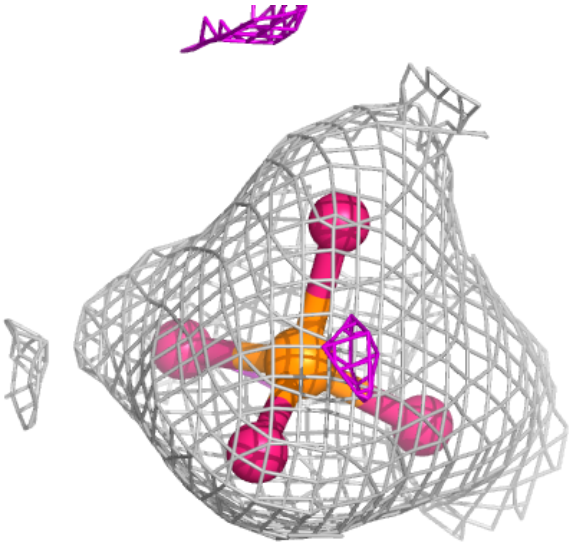
Electron density around PO4 F 301:

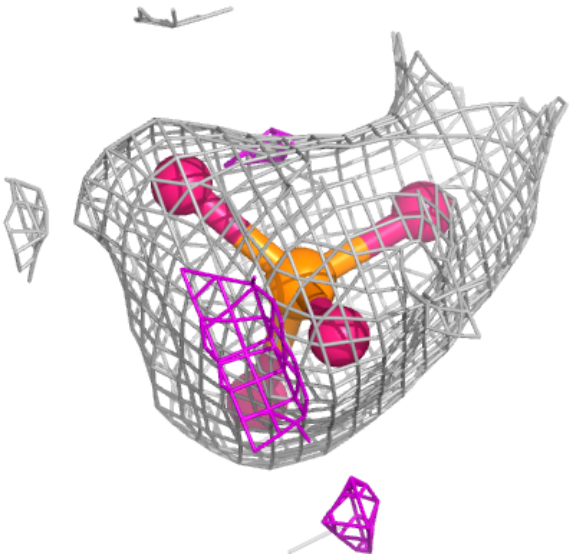
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

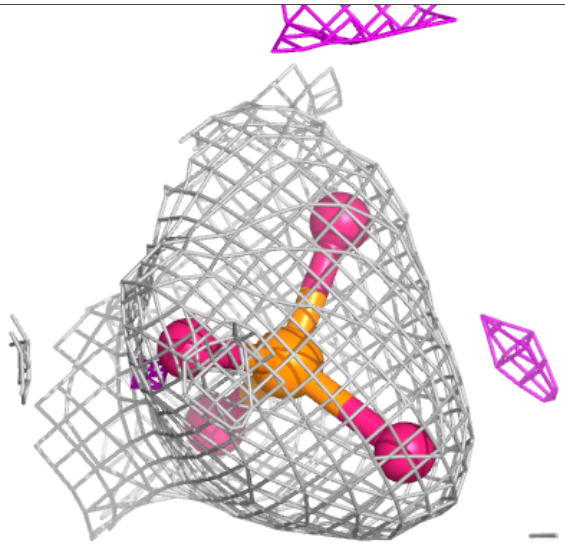


Electron density around PO4 H 301:

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

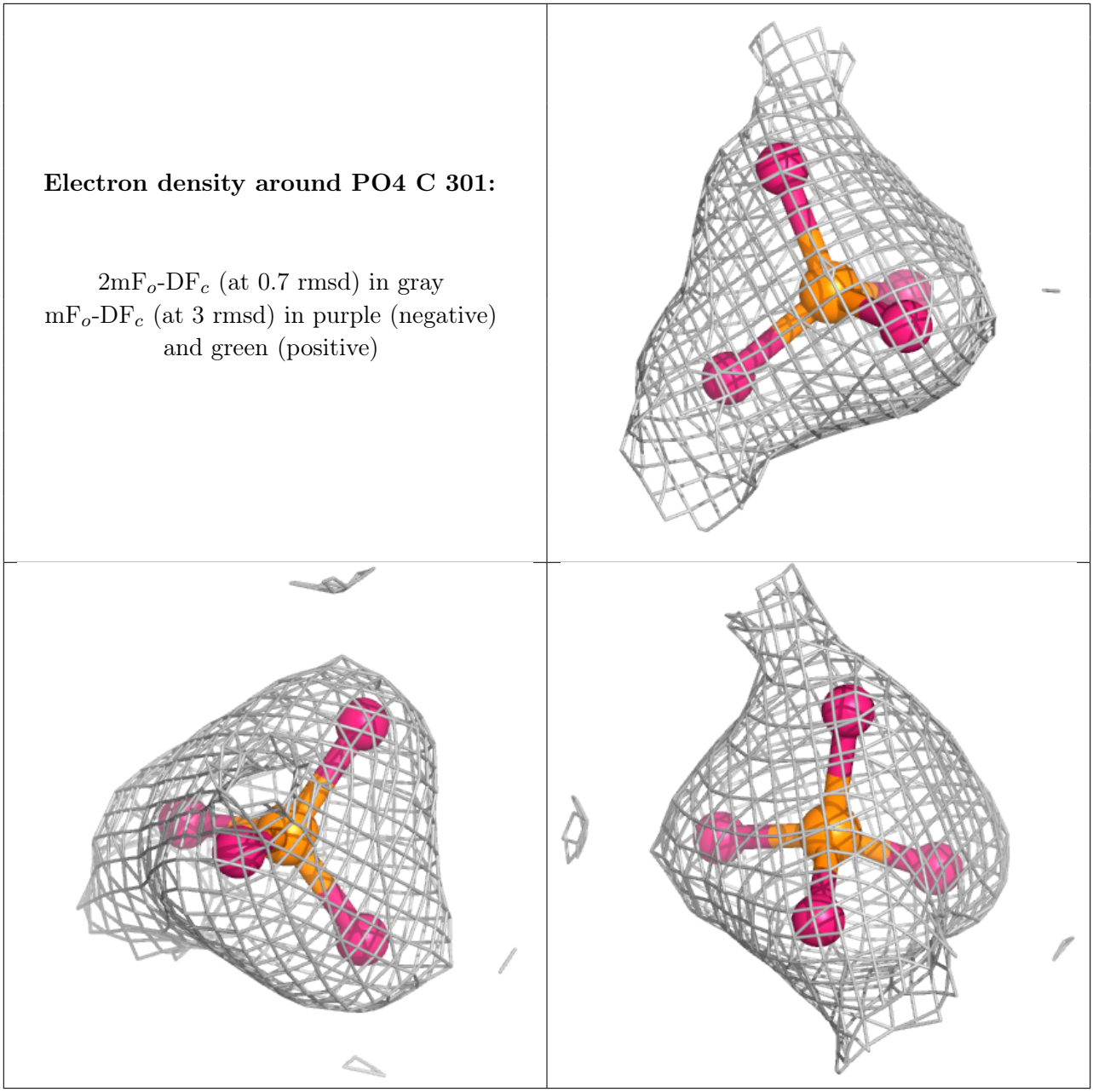






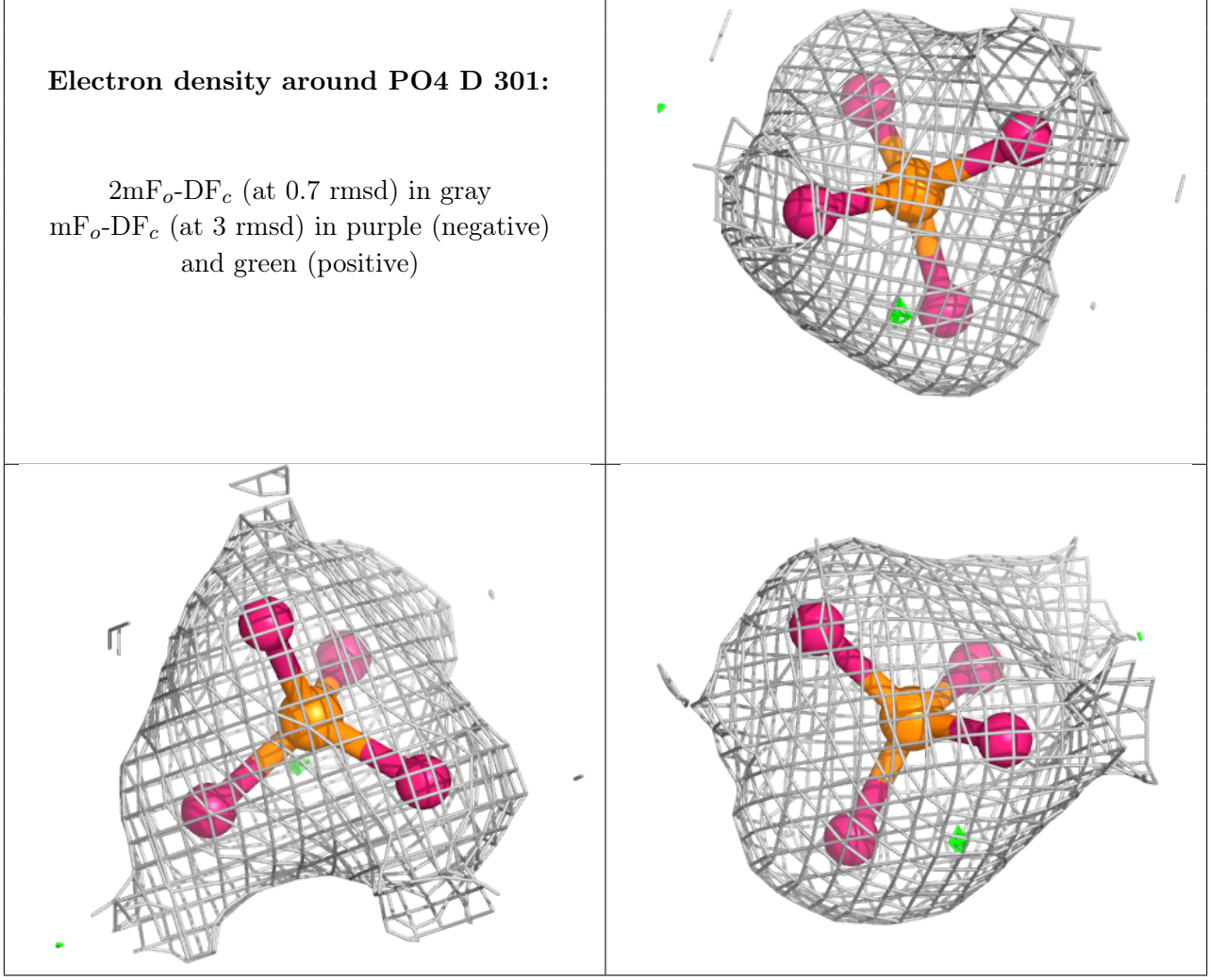
Electron density around PO4 C 301:

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



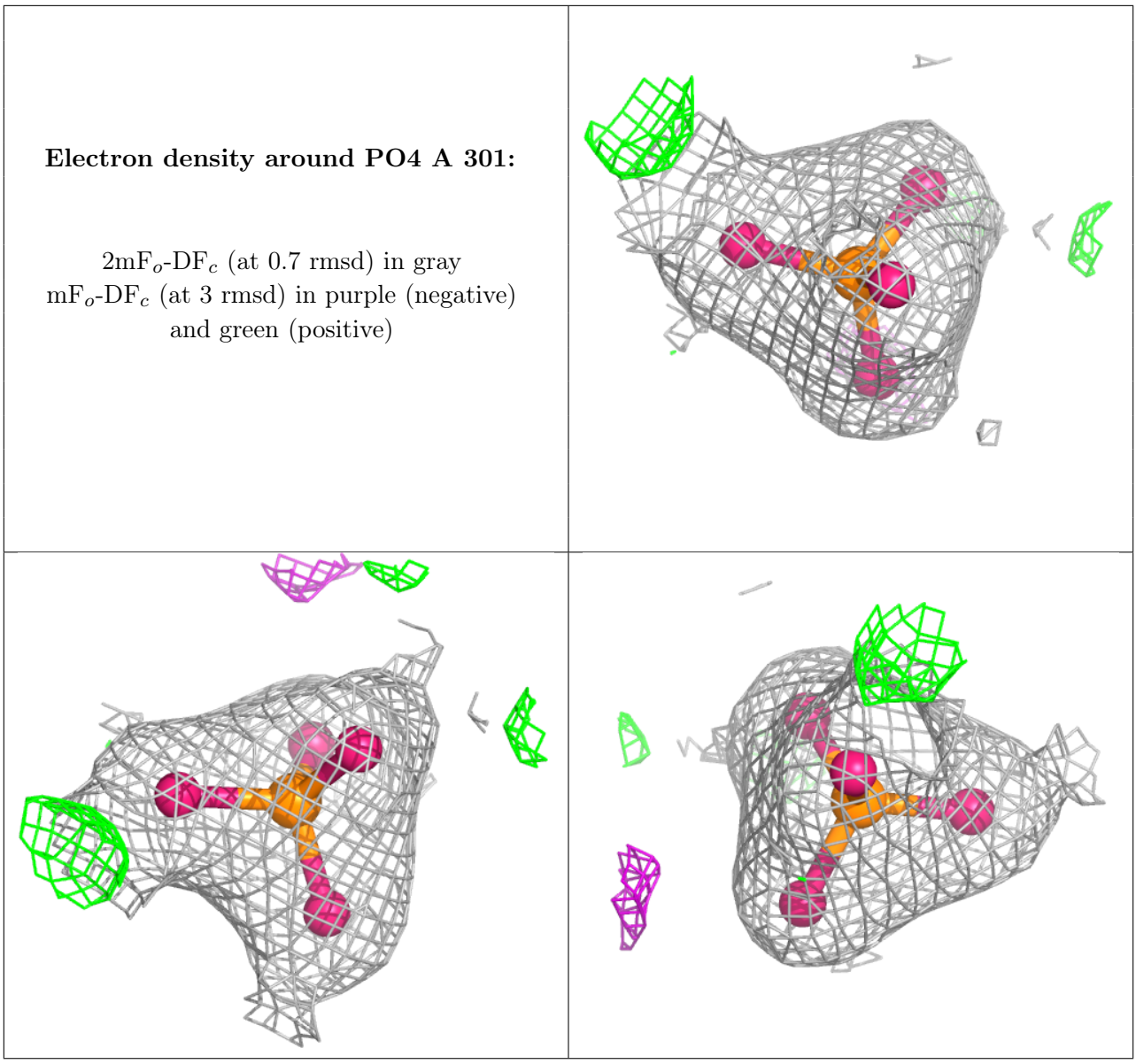
Electron density around PO4 D 301:

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



Electron density around PO4 A 301:

$2mF_o$-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.