Full wwPDB X-ray Structure Validation Report ⓘ

Nov 11, 2023 – 06:35 pm GMT

PDB ID	:	8BH0
Title	:	O-Methyltransferase Plu4890 in complex with SAH and AQ-270b
Authors	:	Huber, E.M.; Groll, M.
Deposited on	:	2022-10-28
Resolution	:	1.70 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:

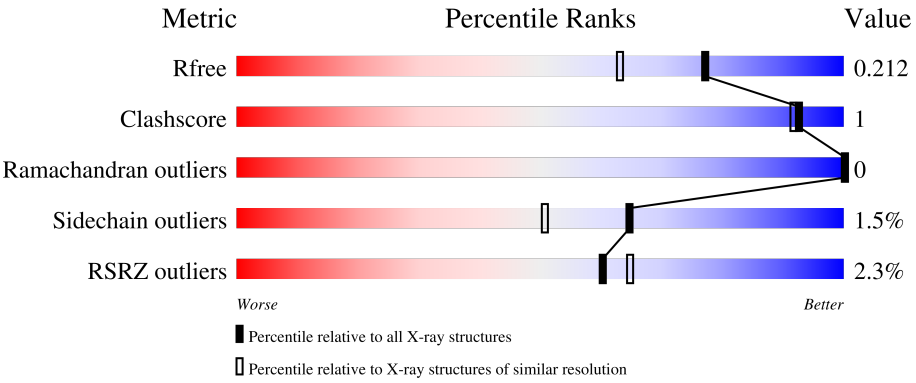
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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	319	93% 7%
1	B	319	96%
1	C	319	4% 95% 5%
1	D	319	95% 5%
1	E	319	93% 7%

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Mol	Chain	Length	Quality of chain
1	F	319	2% 95% 5%
1	G	319	3% 96%
1	H	319	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
4	CL	A	403	-	-	X	-
4	CL	D	404	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 21996 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.

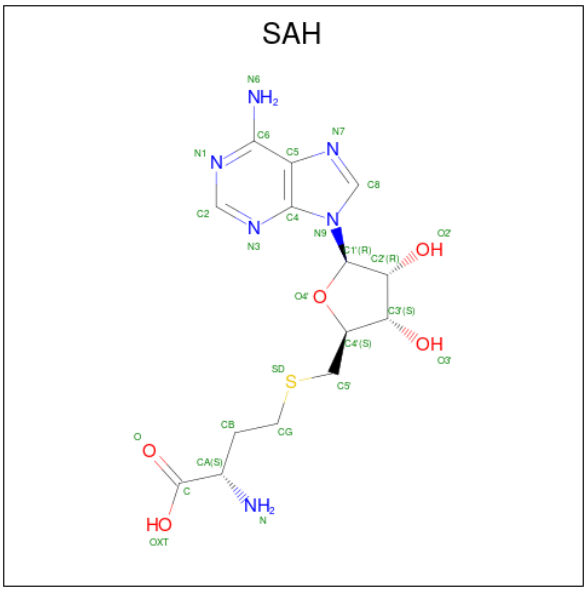
- Molecule 1 is a protein called Methyltransferase Plu4890.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	319	Total	C	N	O	S	0	2	0
			2590	1658	428	492	12			
1	B	319	Total	C	N	O	S	0	1	0
			2580	1653	426	489	12			
1	C	319	Total	C	N	O	S	0	2	0
			2591	1659	428	492	12			
1	D	319	Total	C	N	O	S	0	2	0
			2588	1658	427	490	13			
1	E	319	Total	C	N	O	S	0	4	0
			2602	1664	430	496	12			
1	F	319	Total	C	N	O	S	0	4	0
			2603	1665	432	494	12			
1	G	319	Total	C	N	O	S	0	7	0
			2626	1680	434	500	12			
1	H	319	Total	C	N	O	S	0	1	0
			2585	1656	429	488	12			

There are 8 discrepancies between the modelled and reference sequences:

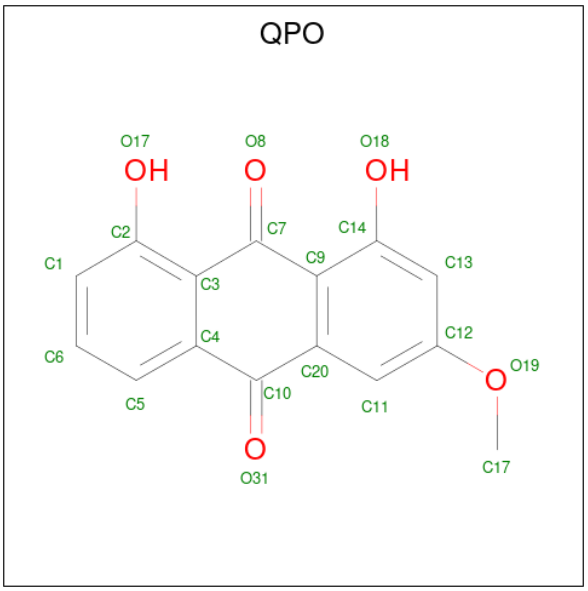
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP A0A6L9JR93
B	0	SER	-	expression tag	UNP A0A6L9JR93
C	0	SER	-	expression tag	UNP A0A6L9JR93
D	0	SER	-	expression tag	UNP A0A6L9JR93
E	0	SER	-	expression tag	UNP A0A6L9JR93
F	0	SER	-	expression tag	UNP A0A6L9JR93
G	0	SER	-	expression tag	UNP A0A6L9JR93
H	0	SER	-	expression tag	UNP A0A6L9JR93

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	B	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	C	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	D	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	E	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	F	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	G	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	H	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

- Molecule 3 is 3-methoxy-1,8-bis(oxidanyl)anthracene-9,10-dione (three-letter code: QPO) (formula: $C_{15}H_{10}O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 20 15 5	0	0
3	B	1	Total C O 20 15 5	0	0
3	C	1	Total C O 20 15 5	0	0
3	D	1	Total C O 20 15 5	0	0
3	E	1	Total C O 20 15 5	0	0
3	F	1	Total C O 20 15 5	0	0
3	G	1	Total C O 20 15 5	0	0
3	H	1	Total C O 20 15 5	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cl 1 1	0	0
4	D	1	Total Cl 1 1	0	0
4	F	1	Total Cl 1 1	0	0

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	2	Total Na 2 2	0	0
5	C	1	Total Na 1 1	0	0
5	D	1	Total Na 1 1	0	0
5	F	1	Total Na 1 1	0	0
5	G	1	Total Na 1 1	0	0

- Molecule 6 is water.

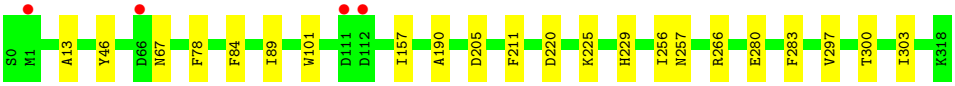
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	121	Total O 121 121	0	0
6	B	118	Total O 118 118	0	0
6	C	106	Total O 106 106	0	0
6	D	112	Total O 112 112	0	0
6	E	120	Total O 120 120	0	0
6	F	92	Total O 92 92	0	0
6	G	86	Total O 86 86	0	0
6	H	99	Total O 99 99	0	0

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.

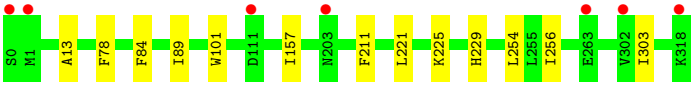
• Molecule 1: Methyltransferase Plu4890

Chain A:



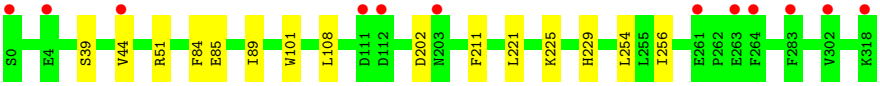
• Molecule 1: Methyltransferase Plu4890

Chain B:



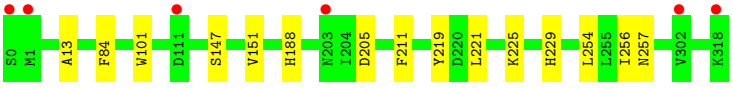
• Molecule 1: Methyltransferase Plu4890

Chain C:



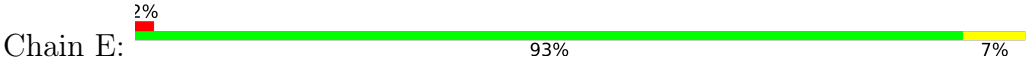
• Molecule 1: Methyltransferase Plu4890

Chain D:



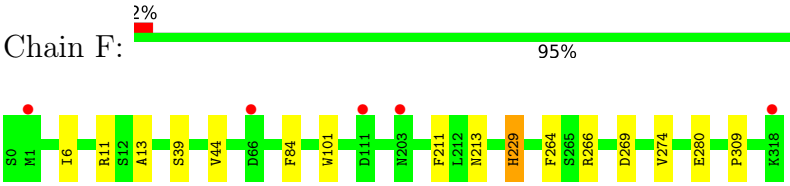
• Molecule 1: Methyltransferase Plu4890

Chain E:



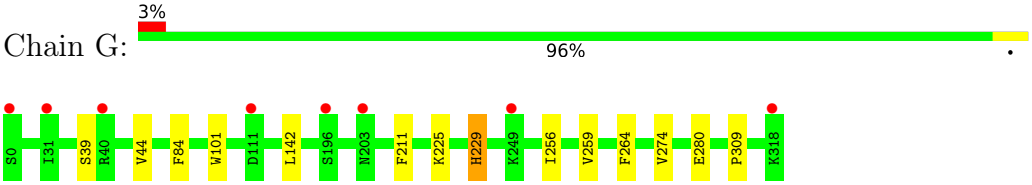
• Molecule 1: Methyltransferase Plu4890

Chain F:



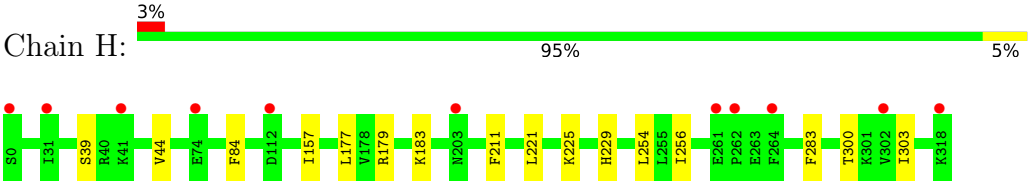
• Molecule 1: Methyltransferase Plu4890

Chain G:



• Molecule 1: Methyltransferase Plu4890

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	56.94Å 105.62Å 124.47Å 94.37° 90.22° 104.97°	Depositor
Resolution (Å)	30.00 – 1.70 49.83 – 1.70	Depositor EDS
% Data completeness (in resolution range)	94.8 (30.00-1.70) 91.5 (49.83-1.70)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.76 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.178 , 0.205 0.187 , 0.212	Depositor DCC
R_{free} test set	14567 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	28.7	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 22.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.379 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	21996	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% 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: CL, QPO, NA, SAH

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	0.65	0/2644	0.68	0/3560
1	B	0.65	0/2634	0.68	0/3546
1	C	0.65	0/2645	0.68	0/3561
1	D	0.65	0/2642	0.68	0/3556
1	E	0.65	0/2656	0.68	0/3576
1	F	0.66	0/2657	0.69	0/3576
1	G	0.66	0/2680	0.69	0/3609
1	H	0.65	0/2639	0.68	0/3552
All	All	0.65	0/21197	0.68	0/28536

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	2590	0	2539	13	0
1	B	2580	0	2535	6	0
1	C	2591	0	2540	9	0
1	D	2588	0	2542	8	0
1	E	2602	0	2547	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2603	0	2555	11	0
1	G	2626	0	2572	7	0
1	H	2585	0	2543	7	0
2	A	26	0	19	0	0
2	B	26	0	19	0	0
2	C	26	0	19	0	0
2	D	26	0	19	0	0
2	E	26	0	19	0	0
2	F	26	0	19	0	0
2	G	26	0	19	0	0
2	H	26	0	19	0	0
3	A	20	0	0	0	0
3	B	20	0	0	0	0
3	C	20	0	0	0	0
3	D	20	0	0	0	0
3	E	20	0	0	0	0
3	F	20	0	0	0	0
3	G	20	0	0	0	0
3	H	20	0	0	0	0
4	A	1	0	0	2	0
4	D	1	0	0	3	0
4	F	1	0	0	0	0
5	B	2	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
6	A	121	0	0	0	0
6	B	118	0	0	0	0
6	C	106	0	0	0	0
6	D	112	0	0	0	0
6	E	120	0	0	0	0
6	F	92	0	0	0	0
6	G	86	0	0	0	0
6	H	99	0	0	0	0
All	All	21996	0	20525	61	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (61) 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:G:39:SER:HA	1:G:44[A]:VAL:HG12	1.66	0.77
1:D:188:HIS:NE2	4:D:404:CL:CL	2.51	0.73
1:A:46:TYR:CZ	4:A:403:CL:CL	2.82	0.69
1:F:266[B]:ARG:HG2	1:F:269:ASP:HB3	1.75	0.68
1:G:229:HIS:HD2	1:G:280:GLU:OE1	1.77	0.67
1:F:229:HIS:HD2	1:F:280:GLU:OE2	1.79	0.65
1:F:39:SER:HA	1:F:44:VAL:HG12	1.81	0.62
1:C:89:ILE:HD13	1:F:6:ILE:HG23	1.82	0.61
1:H:39:SER:HA	1:H:44:VAL:HG12	1.84	0.58
1:A:46:TYR:OH	4:A:403:CL:CL	2.56	0.58
1:E:78:PHE:CE1	1:E:89:ILE:HD11	2.38	0.58
1:C:51:ARG:HG2	1:F:266[B]:ARG:NH1	2.23	0.54
1:C:39:SER:HA	1:C:44:VAL:HG12	1.90	0.54
1:A:157:ILE:HD11	1:A:303:ILE:HD11	1.90	0.53
1:A:101:TRP:CE3	1:D:13:ALA:HB1	2.43	0.53
1:C:89:ILE:HD11	1:F:6:ILE:HG12	1.91	0.52
1:G:142[A]:LEU:O	1:G:142[A]:LEU:HD23	2.10	0.52
1:A:266:ARG:NE	1:A:280:GLU:OE1	2.42	0.51
1:B:225:LYS:HA	1:B:256:ILE:O	2.10	0.51
1:B:13:ALA:HB1	1:E:101:TRP:CE3	2.46	0.51
1:A:225:LYS:HA	1:A:256:ILE:O	2.12	0.50
1:D:225:LYS:HA	1:D:256:ILE:O	2.12	0.50
1:D:219:TYR:OH	4:D:404:CL:CL	2.59	0.49
1:H:225:LYS:HA	1:H:256:ILE:O	2.13	0.49
1:E:225:LYS:HA	1:E:256:ILE:O	2.14	0.48
1:A:78:PHE:CE1	1:A:89:ILE:HD11	2.48	0.48
1:G:101:TRP:CZ3	1:G:274:VAL:HG21	2.49	0.47
1:B:78:PHE:CE1	1:B:89:ILE:HD11	2.49	0.47
1:A:283:PHE:CZ	1:A:300:THR:HG21	2.50	0.47
1:C:85:GLU:O	1:C:89:ILE:HG12	2.13	0.47
1:E:221:LEU:HD11	1:E:254:LEU:HG	1.97	0.47
1:C:225:LYS:HA	1:C:256:ILE:O	2.16	0.46
1:A:297:VAL:CG1	1:A:300:THR:HG23	2.46	0.46
1:B:101:TRP:CE3	1:E:13:ALA:HB1	2.51	0.46
1:C:221:LEU:HD11	1:C:254:LEU:HG	1.98	0.45
1:F:264:PHE:CE1	1:F:309:PRO:HG3	2.52	0.45
1:A:13:ALA:HB1	1:D:101:TRP:CE3	2.52	0.44
1:H:283:PHE:CE2	1:H:300:THR:HG21	2.51	0.44
1:B:157:ILE:HD11	1:B:303:ILE:HD11	1.99	0.43
1:D:205:ASP:OD2	4:D:404:CL:CL	2.73	0.43
1:F:101:TRP:CZ3	1:F:274:VAL:HG21	2.53	0.43
1:A:190:ALA:HA	1:A:205[B]:ASP:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:264:PHE:CE1	1:G:309:PRO:HG3	2.54	0.43
1:H:221:LEU:HD11	1:H:254:LEU:HG	2.01	0.43
1:E:36:SER:O	1:E:40:ARG:HG3	2.18	0.42
1:C:101:TRP:CE3	1:F:13:ALA:HB1	2.53	0.42
1:A:297:VAL:HG11	1:A:300:THR:HG23	2.01	0.42
1:A:283:PHE:CE2	1:A:300:THR:HG21	2.54	0.42
1:E:157:ILE:HD11	1:E:303:ILE:HD11	2.01	0.42
1:H:179:ARG:O	1:H:183:LYS:HD2	2.20	0.42
1:H:157:ILE:HD11	1:H:303:ILE:HD11	2.01	0.42
1:D:147:SER:O	1:D:151:VAL:HG23	2.20	0.42
1:E:283:PHE:CE1	1:E:300:THR:HG21	2.55	0.41
1:G:225:LYS:HA	1:G:256:ILE:O	2.19	0.41
1:D:221:LEU:HD11	1:D:254:LEU:HG	2.02	0.41
1:E:190:ALA:HA	1:E:205[A]:ASP:O	2.21	0.41
1:H:177:LEU:HD23	1:H:177:LEU:HA	1.85	0.41
1:F:266[B]:ARG:CG	1:F:269:ASP:HB3	2.49	0.40
1:B:221:LEU:HD11	1:B:254:LEU:HG	2.03	0.40
1:C:108:LEU:HB3	1:F:44:VAL:CG2	2.51	0.40
1:G:259:VAL:HB	1:G:309:PRO:HG2	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	319/319 (100%)	318 (100%)	1 (0%)	0	100	100
1	B	318/319 (100%)	317 (100%)	1 (0%)	0	100	100
1	C	319/319 (100%)	318 (100%)	1 (0%)	0	100	100
1	D	319/319 (100%)	317 (99%)	2 (1%)	0	100	100
1	E	321/319 (101%)	320 (100%)	1 (0%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	321/319 (101%)	320 (100%)	1 (0%)	0	100	100
1	G	324/319 (102%)	323 (100%)	1 (0%)	0	100	100
1	H	318/319 (100%)	316 (99%)	2 (1%)	0	100	100
All	All	2559/2552 (100%)	2549 (100%)	10 (0%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	289/287 (101%)	283 (98%)	6 (2%)	53	36
1	B	288/287 (100%)	285 (99%)	3 (1%)	76	67
1	C	289/287 (101%)	285 (99%)	4 (1%)	67	53
1	D	289/287 (101%)	285 (99%)	4 (1%)	67	53
1	E	291/287 (101%)	285 (98%)	6 (2%)	53	36
1	F	291/287 (101%)	286 (98%)	5 (2%)	60	46
1	G	294/287 (102%)	291 (99%)	3 (1%)	76	67
1	H	288/287 (100%)	285 (99%)	3 (1%)	76	67
All	All	2319/2296 (101%)	2285 (98%)	34 (2%)	65	51

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	ASN
1	A	84	PHE
1	A	211	PHE
1	A	220	ASP
1	A	229	HIS
1	A	257	ASN
1	B	84	PHE
1	B	211	PHE

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Mol	Chain	Res	Type
1	B	229	HIS
1	C	84	PHE
1	C	202	ASP
1	C	211	PHE
1	C	229	HIS
1	D	84	PHE
1	D	211	PHE
1	D	229	HIS
1	D	257	ASN
1	E	84	PHE
1	E	203	ASN
1	E	211	PHE
1	E	220	ASP
1	E	229	HIS
1	E	257	ASN
1	F	11	ARG
1	F	84	PHE
1	F	211	PHE
1	F	213	ASN
1	F	229	HIS
1	G	84	PHE
1	G	211	PHE
1	G	229	HIS
1	H	84	PHE
1	H	211	PHE
1	H	229	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	229	HIS
1	A	292	GLN
1	B	161	ASN
1	C	229	HIS
1	E	292	GLN
1	F	229	HIS
1	G	229	HIS
1	G	250	ASN
1	H	229	HIS

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 25 ligands modelled in this entry, 9 are monoatomic - leaving 16 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SAH	G	401	-	24,28,28	0.69	1 (4%)	25,40,40	0.97	3 (12%)
3	QPO	C	402	-	22,22,22	1.59	4 (18%)	33,33,33	0.68	0
3	QPO	B	402	-	22,22,22	1.60	4 (18%)	33,33,33	0.68	0
3	QPO	F	402	-	22,22,22	1.58	4 (18%)	33,33,33	0.72	0
2	SAH	A	401	-	24,28,28	0.69	1 (4%)	25,40,40	0.99	3 (12%)
2	SAH	F	401	-	24,28,28	0.69	1 (4%)	25,40,40	0.99	3 (12%)
2	SAH	D	401	-	24,28,28	0.71	1 (4%)	25,40,40	0.97	3 (12%)
2	SAH	B	401	-	24,28,28	0.70	1 (4%)	25,40,40	0.96	3 (12%)
3	QPO	D	402	-	22,22,22	1.58	4 (18%)	33,33,33	0.67	0
2	SAH	H	401	-	24,28,28	0.70	1 (4%)	25,40,40	0.97	3 (12%)
3	QPO	G	402	-	22,22,22	1.60	4 (18%)	33,33,33	0.72	0
3	QPO	A	402	-	22,22,22	1.62	4 (18%)	33,33,33	0.69	1 (3%)
3	QPO	E	402	-	22,22,22	1.62	4 (18%)	33,33,33	0.73	1 (3%)
2	SAH	E	401	-	24,28,28	0.69	1 (4%)	25,40,40	0.99	3 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SAH	C	401	-	24,28,28	0.70	1 (4%)	25,40,40	0.99	3 (12%)
3	QPO	H	402	-	22,22,22	1.58	4 (18%)	33,33,33	0.68	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SAH	G	401	-	-	0/11/31/31	0/3/3/3
3	QPO	C	402	-	-	0/2/18/18	0/3/3/3
3	QPO	B	402	-	-	0/2/18/18	0/3/3/3
3	QPO	F	402	-	-	0/2/18/18	0/3/3/3
2	SAH	A	401	-	-	0/11/31/31	0/3/3/3
2	SAH	F	401	-	-	0/11/31/31	0/3/3/3
2	SAH	D	401	-	-	0/11/31/31	0/3/3/3
2	SAH	B	401	-	-	0/11/31/31	0/3/3/3
3	QPO	D	402	-	-	0/2/18/18	0/3/3/3
2	SAH	H	401	-	-	0/11/31/31	0/3/3/3
3	QPO	G	402	-	-	0/2/18/18	0/3/3/3
3	QPO	A	402	-	-	0/2/18/18	0/3/3/3
3	QPO	E	402	-	-	0/2/18/18	0/3/3/3
2	SAH	E	401	-	-	0/11/31/31	0/3/3/3
2	SAH	C	401	-	-	0/11/31/31	0/3/3/3
3	QPO	H	402	-	-	0/2/18/18	0/3/3/3

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	402	QPO	C4-C10	-4.29	1.39	1.48
3	B	402	QPO	C4-C10	-4.25	1.39	1.48
3	E	402	QPO	C4-C10	-4.24	1.39	1.48
3	A	402	QPO	C4-C10	-4.23	1.39	1.48
3	F	402	QPO	C4-C10	-4.22	1.39	1.48
3	A	402	QPO	C20-C10	-4.21	1.39	1.48
3	E	402	QPO	C20-C10	-4.17	1.39	1.48
3	C	402	QPO	C4-C10	-4.15	1.39	1.48
3	D	402	QPO	C4-C10	-4.14	1.39	1.48
3	D	402	QPO	C20-C10	-4.14	1.39	1.48
3	H	402	QPO	C4-C10	-4.12	1.39	1.48
3	B	402	QPO	C20-C10	-4.12	1.39	1.48
3	H	402	QPO	C20-C10	-4.10	1.39	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	402	QPO	C20-C10	-4.07	1.39	1.48
3	G	402	QPO	C20-C10	-4.03	1.39	1.48
3	F	402	QPO	C20-C10	-4.01	1.40	1.48
3	A	402	QPO	C3-C7	-3.05	1.40	1.47
3	C	402	QPO	C9-C7	-3.04	1.40	1.47
3	H	402	QPO	C3-C7	-3.04	1.40	1.47
3	G	402	QPO	C9-C7	-3.03	1.40	1.47
3	E	402	QPO	C3-C7	-3.03	1.40	1.47
3	C	402	QPO	C3-C7	-3.01	1.40	1.47
3	E	402	QPO	C9-C7	-3.00	1.40	1.47
3	D	402	QPO	C3-C7	-3.00	1.40	1.47
3	B	402	QPO	C9-C7	-3.00	1.40	1.47
3	A	402	QPO	C9-C7	-2.97	1.40	1.47
3	D	402	QPO	C9-C7	-2.97	1.40	1.47
3	B	402	QPO	C3-C7	-2.95	1.40	1.47
3	H	402	QPO	C9-C7	-2.94	1.40	1.47
3	F	402	QPO	C3-C7	-2.94	1.40	1.47
3	F	402	QPO	C9-C7	-2.91	1.40	1.47
3	G	402	QPO	C3-C7	-2.90	1.40	1.47
2	C	401	SAH	OXT-C	-2.12	1.23	1.30
2	D	401	SAH	OXT-C	-2.11	1.23	1.30
2	H	401	SAH	OXT-C	-2.10	1.23	1.30
2	B	401	SAH	OXT-C	-2.10	1.23	1.30
2	E	401	SAH	OXT-C	-2.07	1.23	1.30
2	F	401	SAH	OXT-C	-2.06	1.23	1.30
2	A	401	SAH	OXT-C	-2.04	1.23	1.30
2	G	401	SAH	OXT-C	-2.02	1.23	1.30

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	401	SAH	OXT-C-O	-2.60	118.18	124.09
2	F	401	SAH	OXT-C-O	-2.55	118.30	124.09
2	C	401	SAH	OXT-C-O	-2.55	118.30	124.09
2	E	401	SAH	OXT-C-O	-2.54	118.31	124.09
2	G	401	SAH	OXT-C-O	-2.52	118.37	124.09
2	H	401	SAH	OXT-C-O	-2.49	118.43	124.09
2	B	401	SAH	OXT-C-O	-2.48	118.45	124.09
2	A	401	SAH	OXT-C-O	-2.44	118.54	124.09
2	F	401	SAH	OXT-C-CA	2.37	121.45	113.38
2	C	401	SAH	OXT-C-CA	2.30	121.20	113.38
2	H	401	SAH	OXT-C-CA	2.27	121.11	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	401	SAH	C5-C6-N6	2.25	123.77	120.35
2	E	401	SAH	OXT-C-CA	2.23	120.99	113.38
2	A	401	SAH	C5-C6-N6	2.22	123.73	120.35
2	A	401	SAH	OXT-C-CA	2.22	120.94	113.38
2	H	401	SAH	C5-C6-N6	2.21	123.70	120.35
2	G	401	SAH	OXT-C-CA	2.19	120.86	113.38
2	B	401	SAH	C5-C6-N6	2.18	123.66	120.35
3	E	402	QPO	O17-C2-C3	-2.17	117.08	121.14
2	E	401	SAH	C5-C6-N6	2.16	123.63	120.35
2	G	401	SAH	C5-C6-N6	2.15	123.61	120.35
2	D	401	SAH	OXT-C-CA	2.14	120.68	113.38
2	F	401	SAH	C5-C6-N6	2.11	123.56	120.35
2	D	401	SAH	C5-C6-N6	2.08	123.51	120.35
2	B	401	SAH	OXT-C-CA	2.07	120.43	113.38
3	A	402	QPO	O18-C14-C9	-2.02	117.37	121.14

There are no chirality outliers.

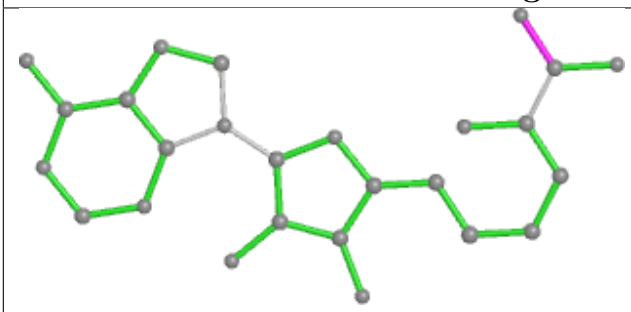
There are no torsion outliers.

There are no ring outliers.

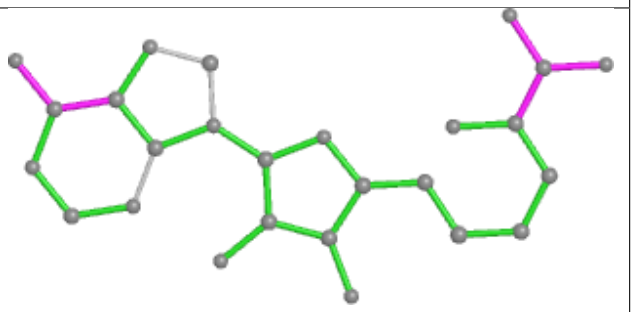
No monomer is involved in short contacts.

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.

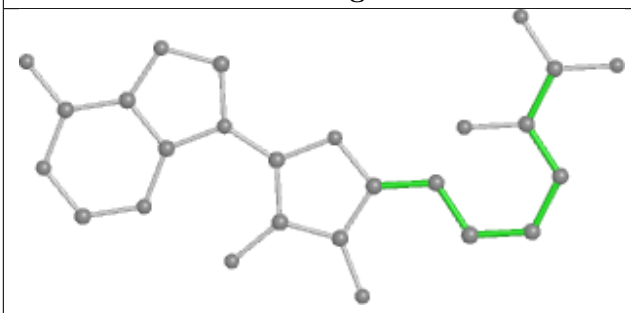
Ligand SAH G 401



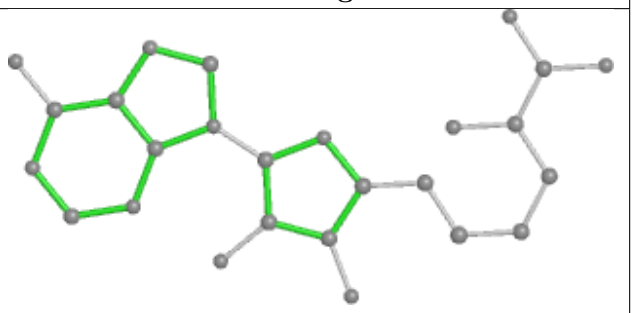
Bond lengths



Bond angles

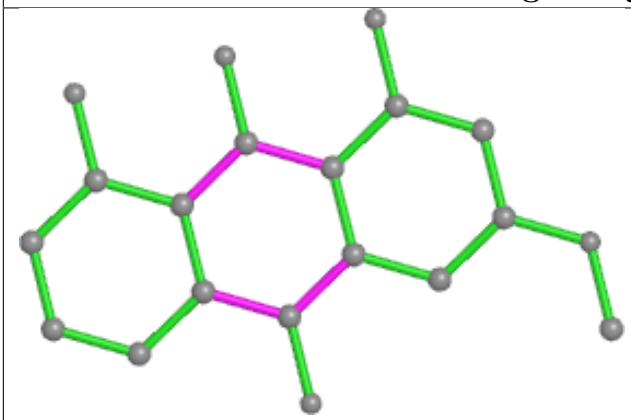


Torsions

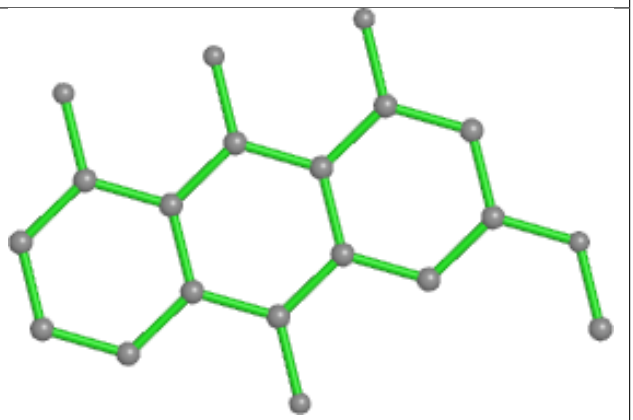


Rings

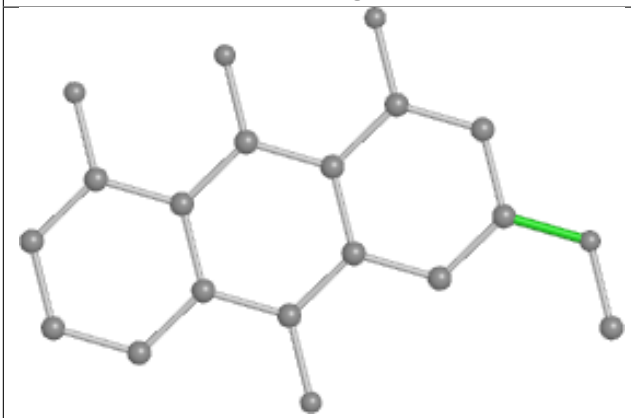
Ligand QPO C 402



Bond lengths



Bond angles



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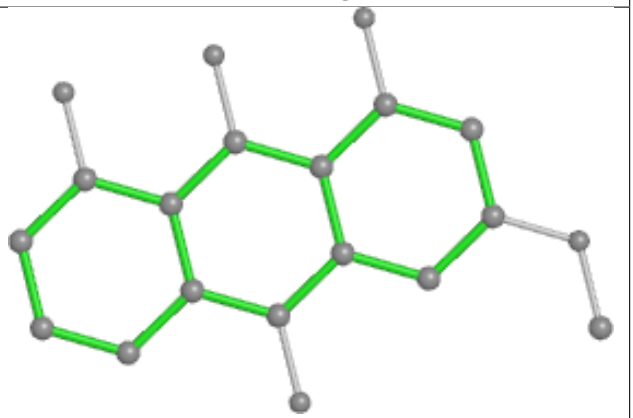
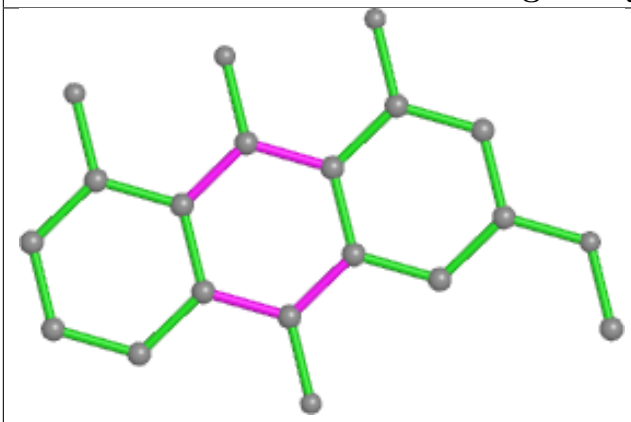
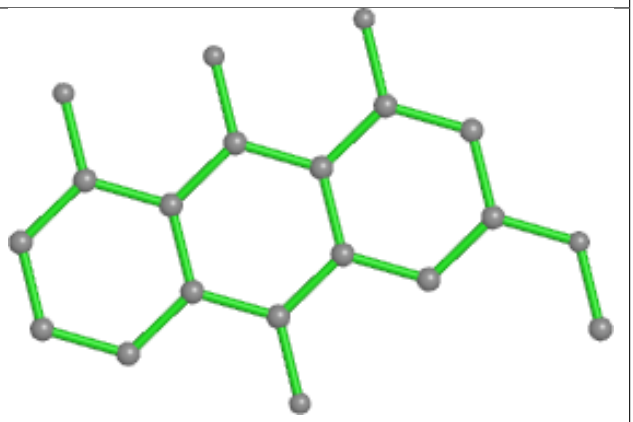


Rings

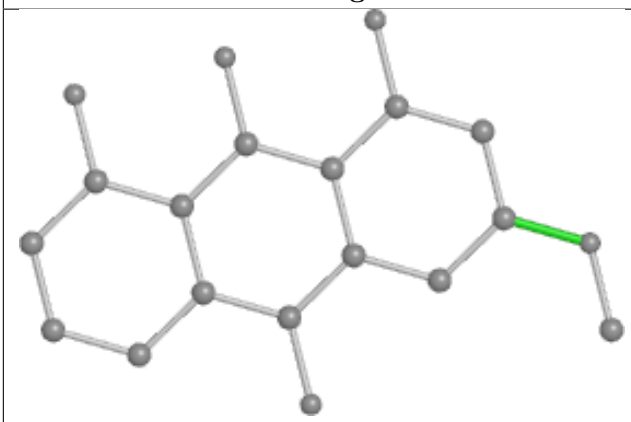
Ligand QPO B 402



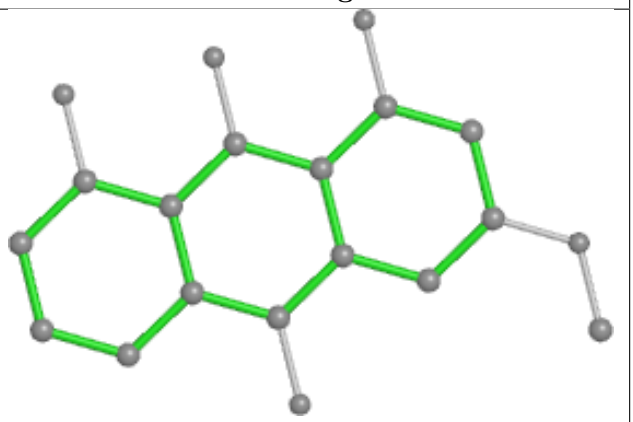
Bond lengths



Bond angles

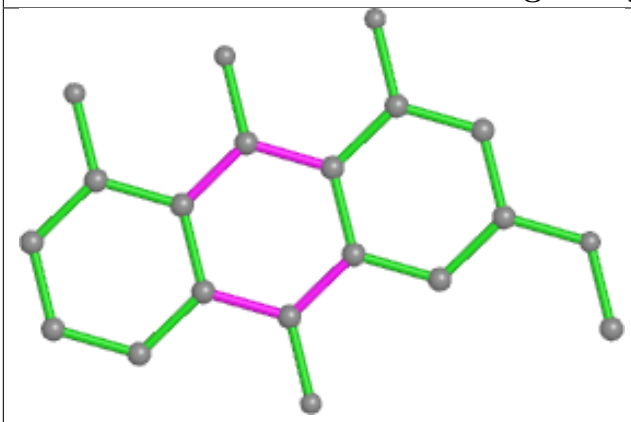


Torsions

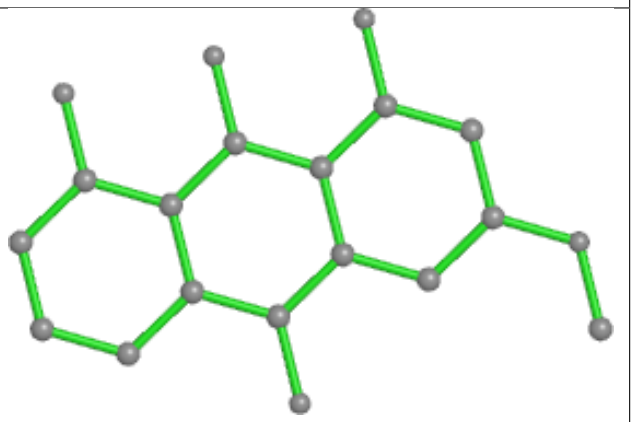


Rings

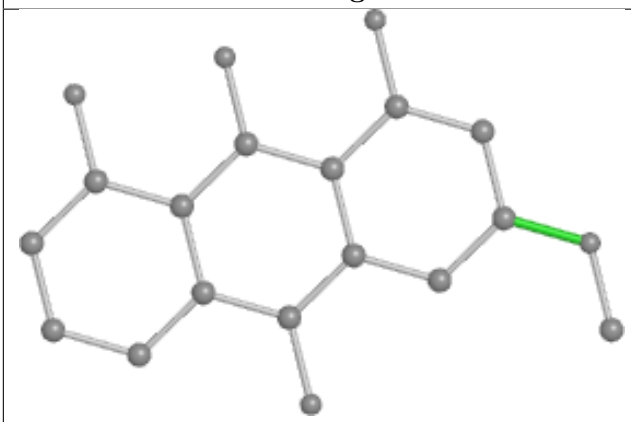
Ligand QPO F 402



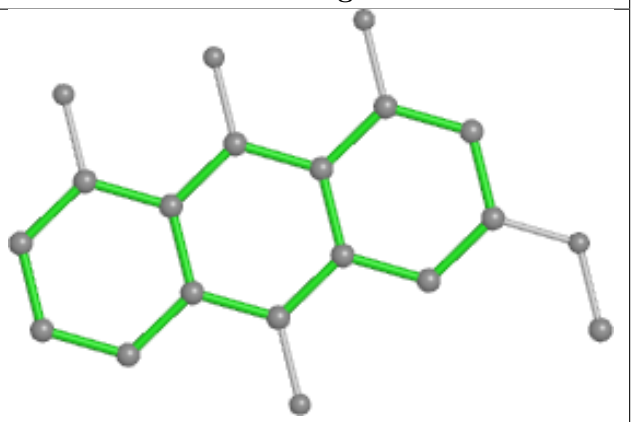
Bond lengths



Bond angles

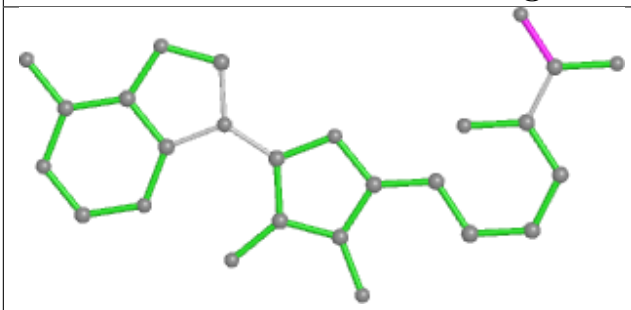


Torsions

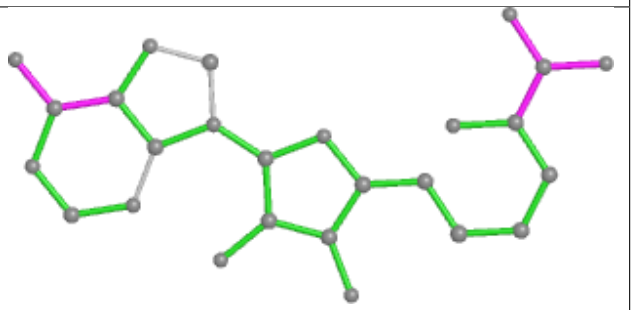


Rings

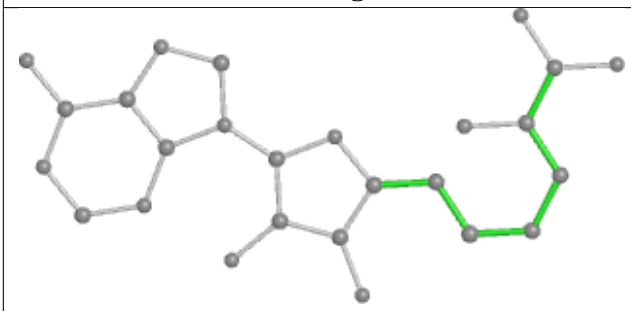
Ligand SAH A 401



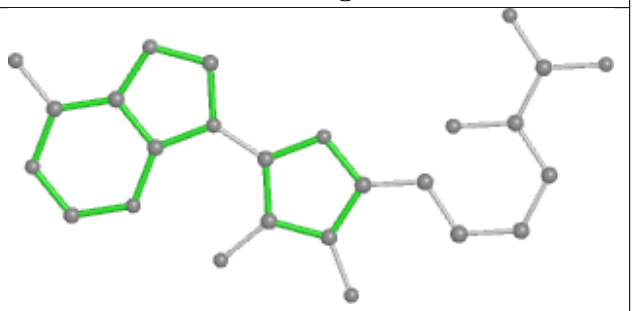
Bond lengths



Bond angles

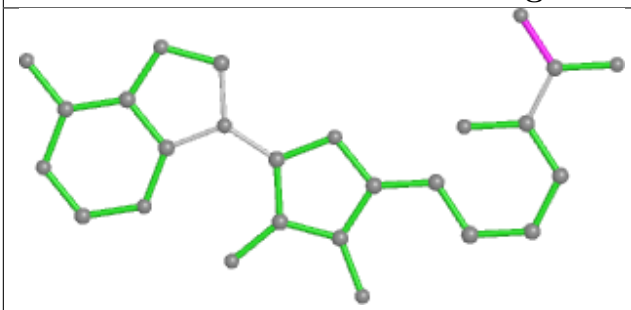


Torsions

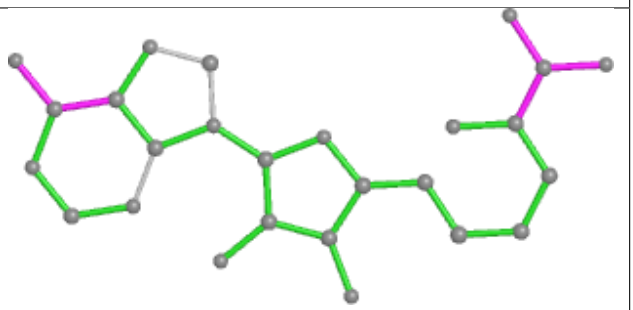


Rings

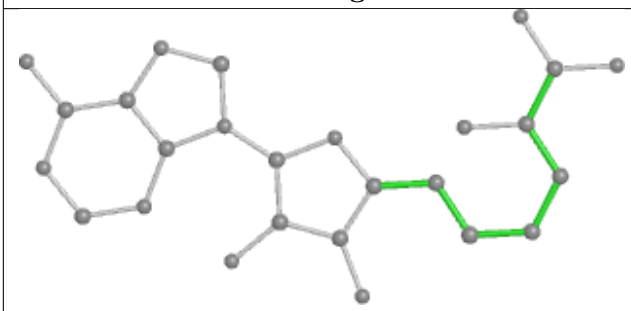
Ligand SAH F 401



Bond lengths



Bond angles



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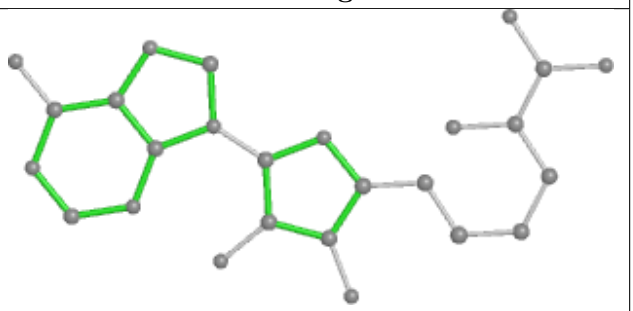
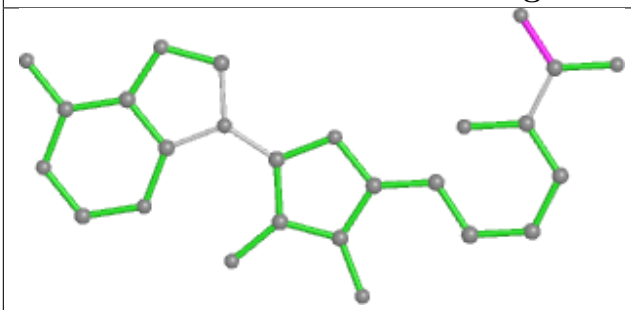


Rings

Ligand SAH D 401



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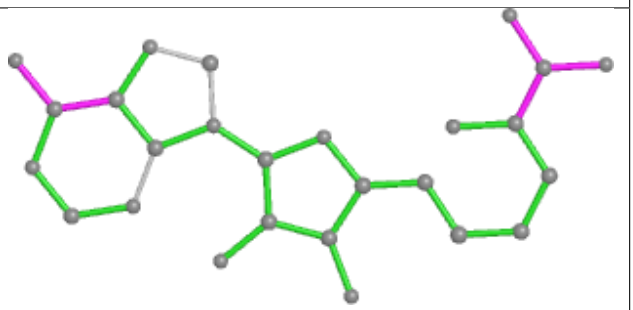
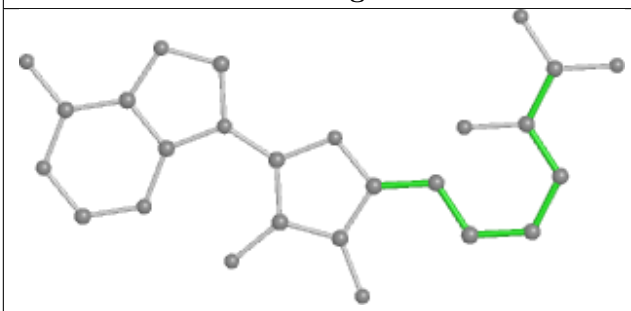


Bond angles



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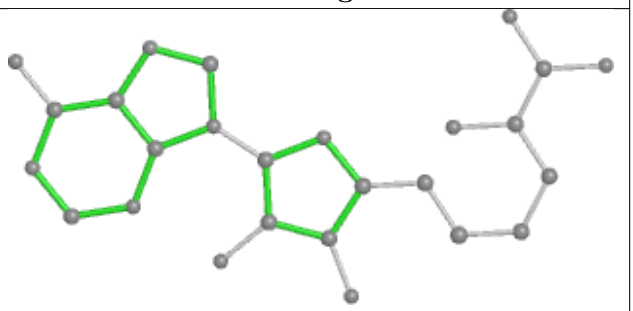

Rings

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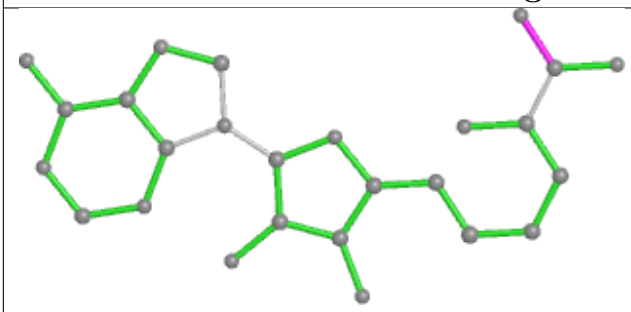
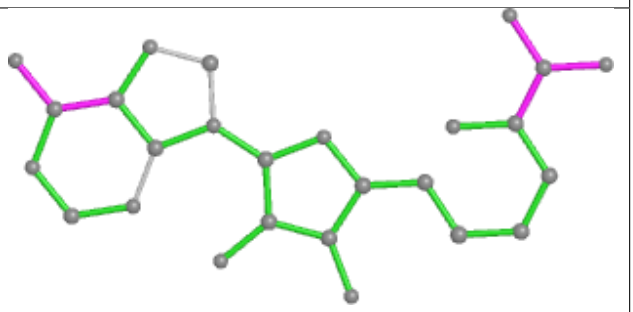
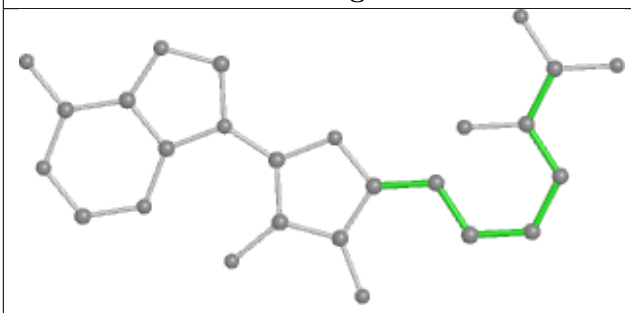


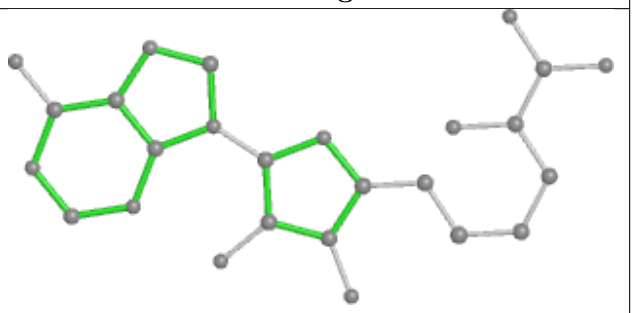
Bond lengths



Bond angles

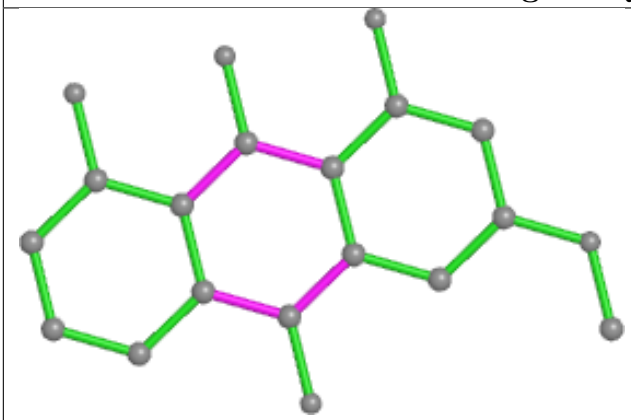


Torsions

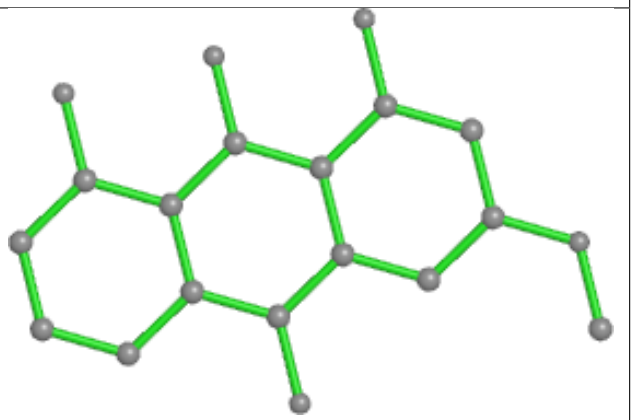


Rings

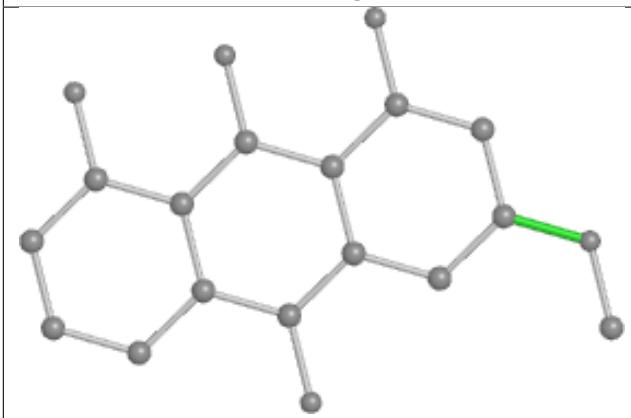
Ligand QPO D 402



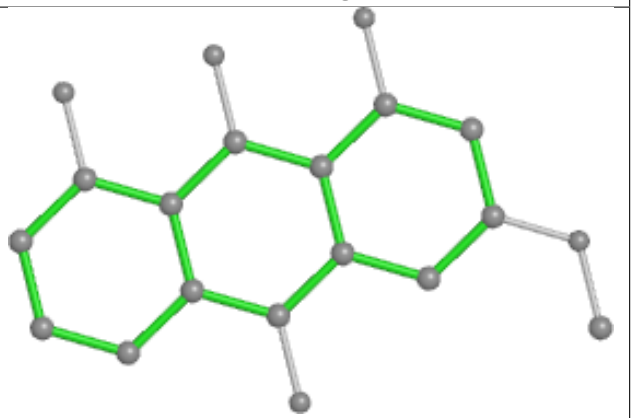
Bond lengths



Bond angles

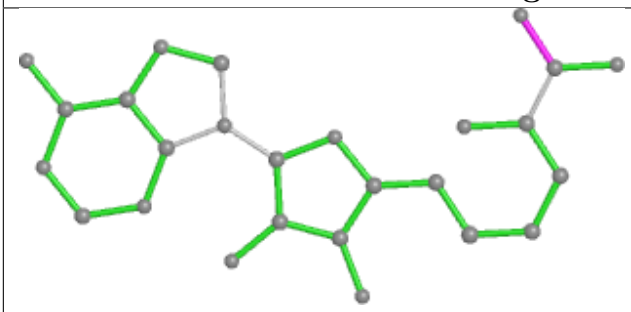


Torsions

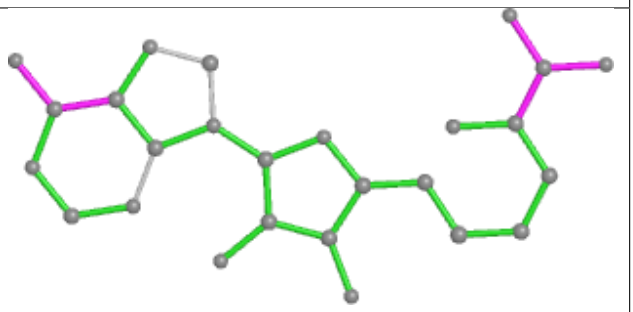


Rings

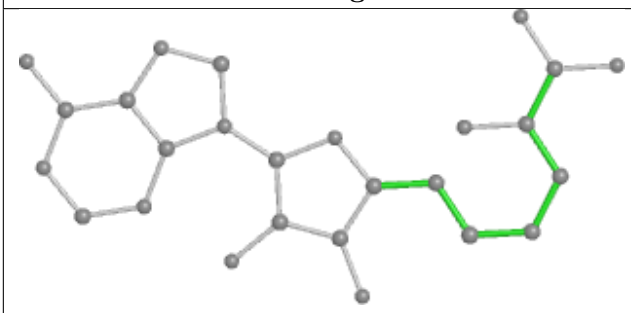
Ligand SAH H 401



Bond lengths



Bond angles



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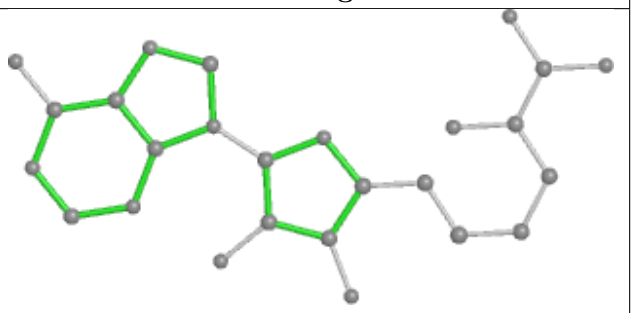
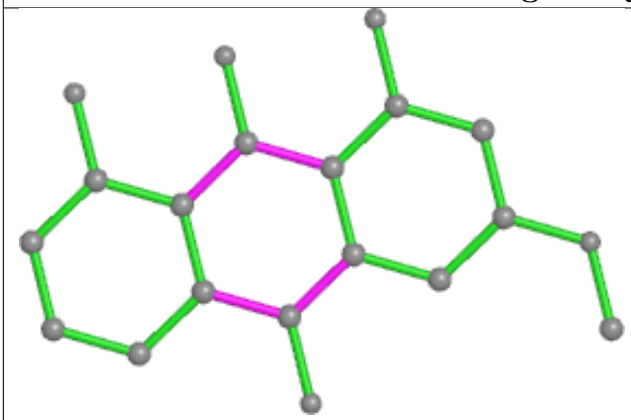
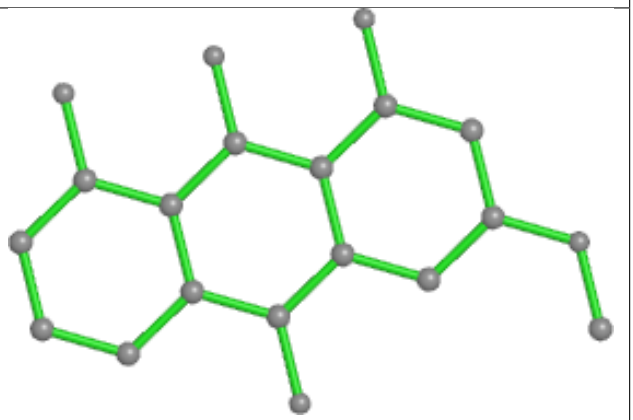


Rings

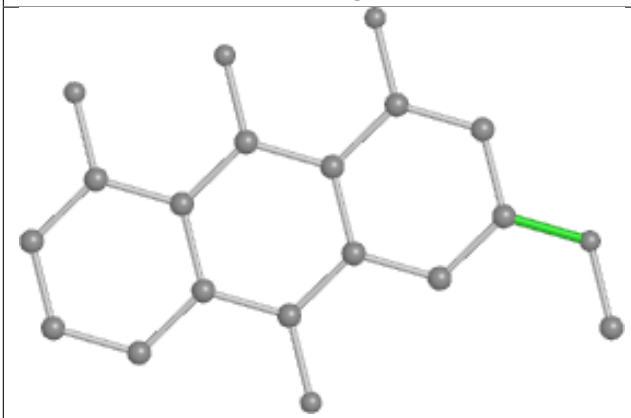
Ligand QPO G 402



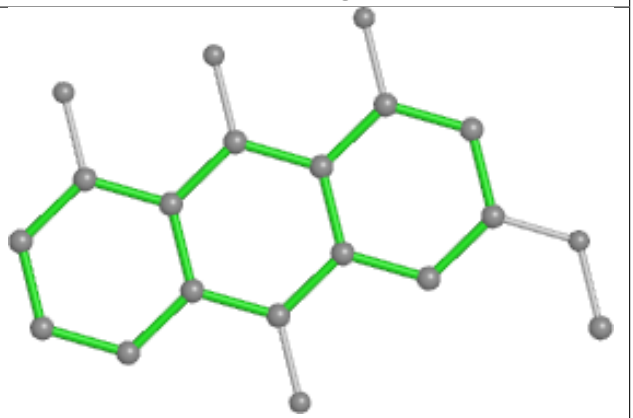
Bond lengths



Bond angles

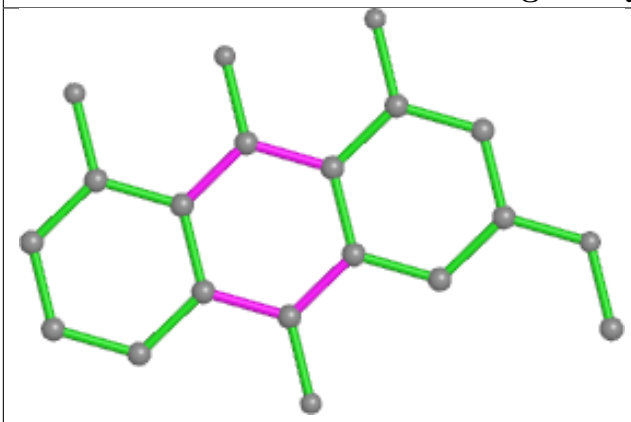


Torsions



Rings

Ligand QPO A 402



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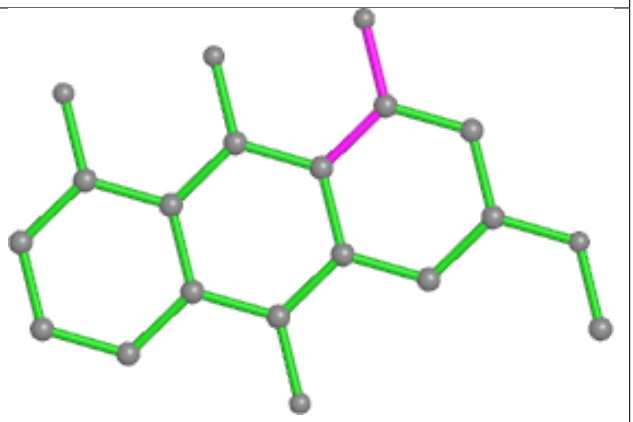
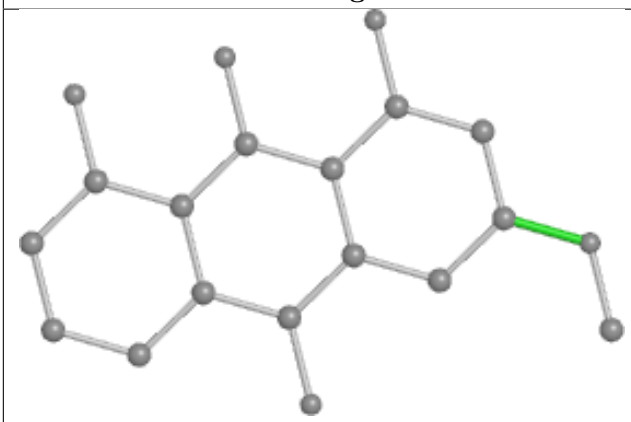


Bond angles



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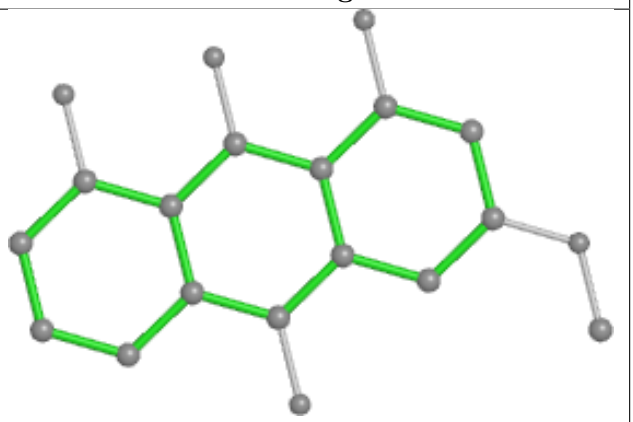
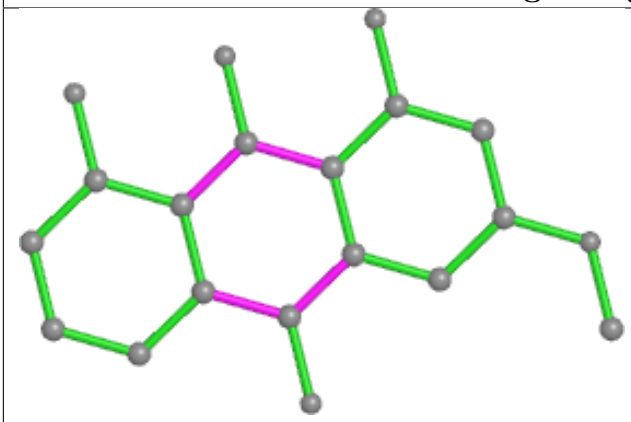
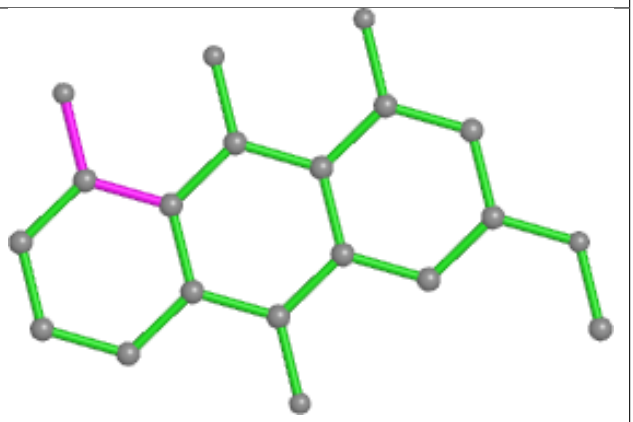


Rings

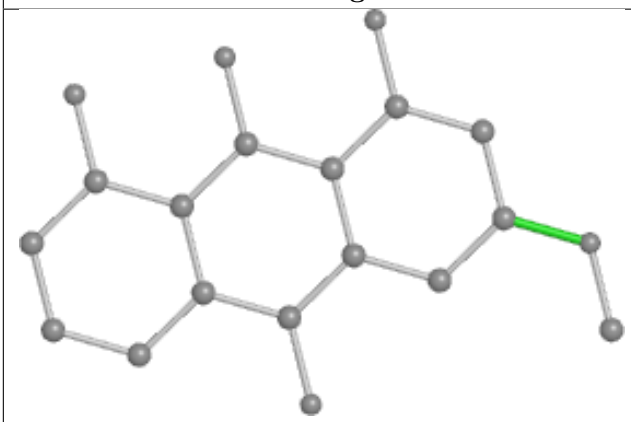
Ligand QPO E 402



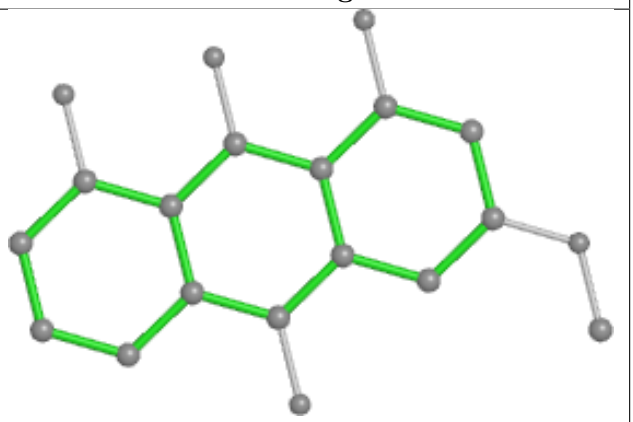
Bond lengths



Bond angles

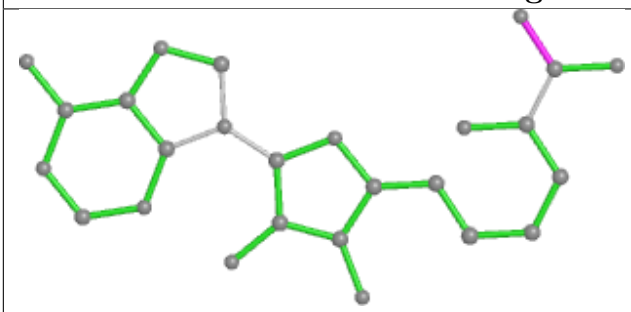


Torsions

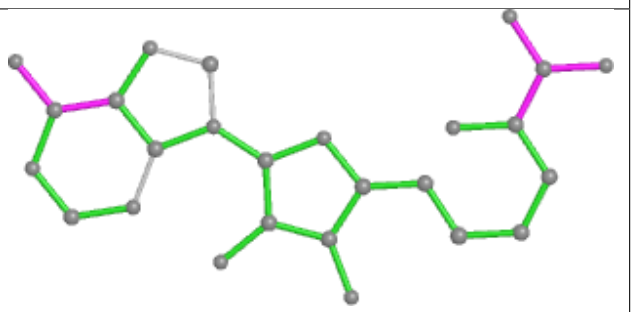


Rings

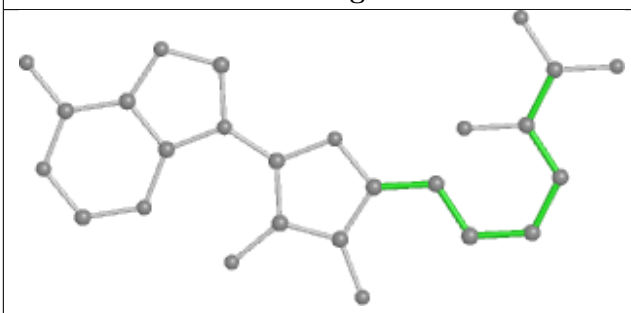
Ligand SAH E 401



Bond lengths



Bond angles



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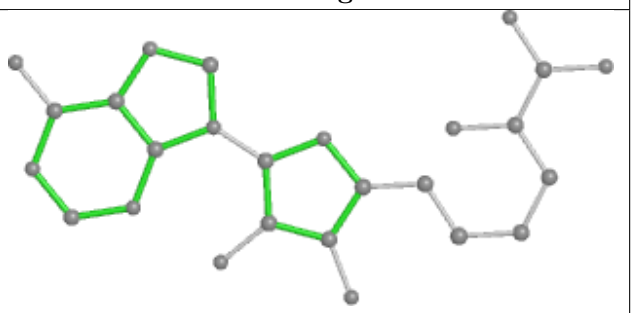
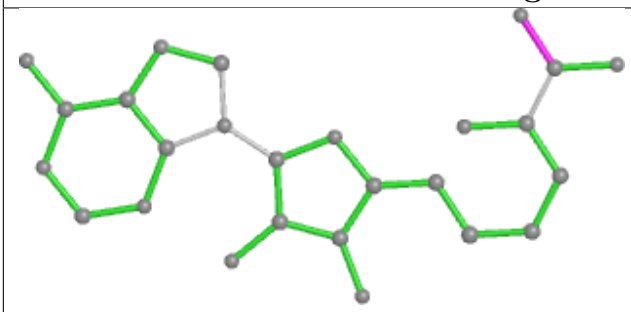
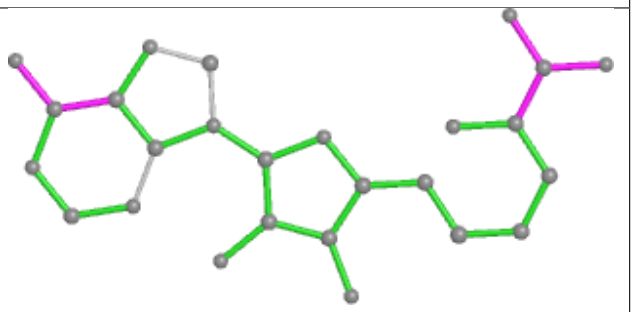


Rings

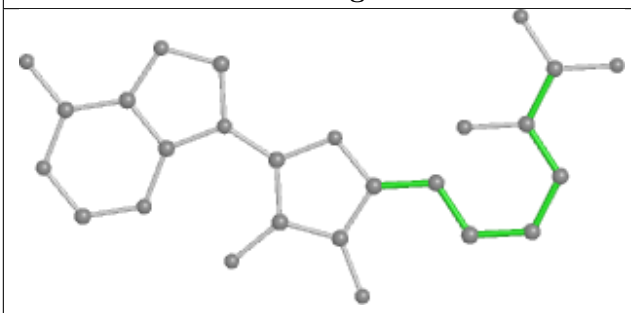
Ligand SAH C 401



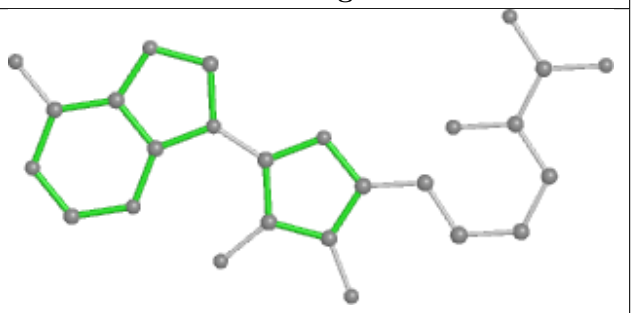
Bond lengths



Bond angles

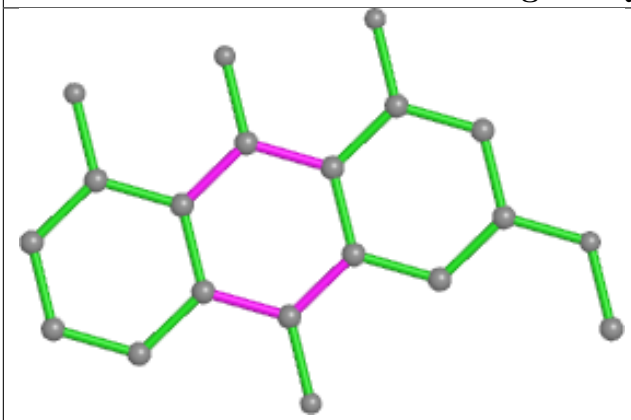


Torsions

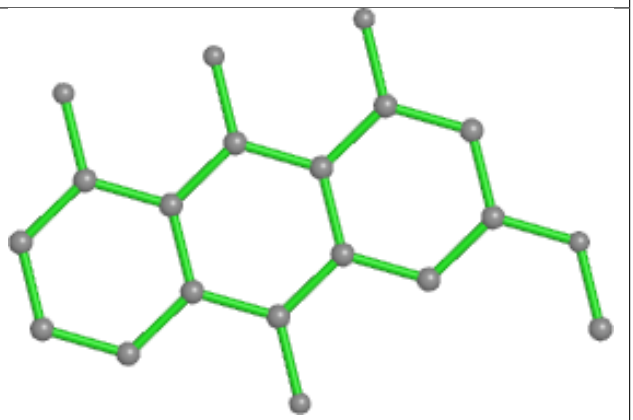


Rings

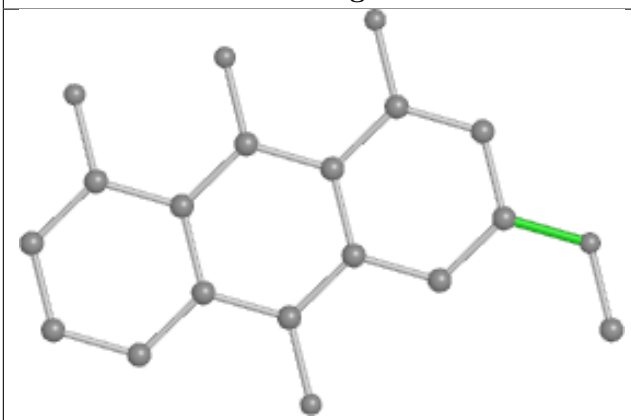
Ligand QPO H 402



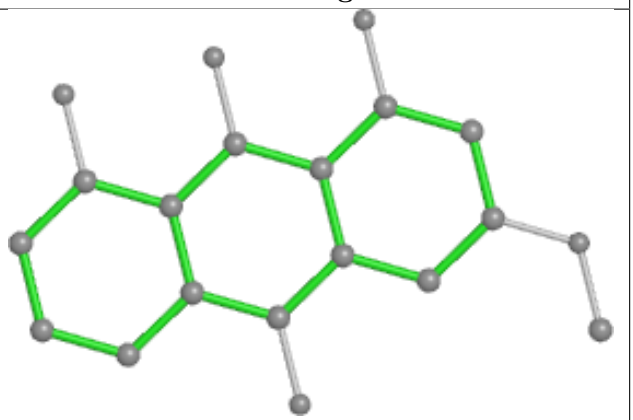
Bond lengths



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	319/319 (100%)	0.09	4 (1%)	77	81	20, 28, 42, 67	0
1	B	319/319 (100%)	0.09	7 (2%)	62	66	20, 30, 45, 54	0
1	C	319/319 (100%)	0.19	12 (3%)	40	45	23, 32, 47, 58	0
1	D	319/319 (100%)	0.09	6 (1%)	66	70	20, 31, 45, 55	0
1	E	319/319 (100%)	0.08	5 (1%)	72	76	20, 28, 43, 70	0
1	F	319/319 (100%)	0.18	5 (1%)	72	76	24, 33, 50, 61	0
1	G	319/319 (100%)	0.20	8 (2%)	57	61	24, 35, 50, 60	0
1	H	319/319 (100%)	0.20	11 (3%)	45	50	22, 32, 47, 62	0
All	All	2552/2552 (100%)	0.14	58 (2%)	60	65	20, 31, 47, 70	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	111	ASP	7.6
1	A	111	ASP	7.2
1	B	111	ASP	4.2
1	B	203	ASN	4.0
1	F	318	LYS	3.9
1	H	264	PHE	3.8
1	F	1	MET	3.7
1	A	1	MET	3.6
1	A	112	ASP	3.6
1	H	302	VAL	3.6
1	F	203	ASN	3.5
1	C	283	PHE	3.5
1	D	203	ASN	3.5
1	D	318	LYS	3.4
1	G	203	ASN	3.4
1	C	263	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	112	ASP	3.3
1	C	264	PHE	3.2
1	B	1	MET	3.1
1	E	0	SER	3.1
1	E	1	MET	3.0
1	B	263	GLU	3.0
1	H	112	ASP	3.0
1	C	302	VAL	2.9
1	B	318	LYS	2.9
1	B	302	VAL	2.9
1	E	112	ASP	2.8
1	D	1	MET	2.8
1	D	111	ASP	2.7
1	C	261	GLU	2.7
1	H	318	LYS	2.7
1	G	318	LYS	2.6
1	E	249	LYS	2.5
1	C	111	ASP	2.4
1	H	0	SER	2.4
1	F	66	ASP	2.4
1	H	41	LYS	2.4
1	G	31	ILE	2.3
1	C	318	LYS	2.3
1	C	0	SER	2.3
1	G	196	SER	2.3
1	G	111	ASP	2.3
1	A	66	ASP	2.2
1	C	44	VAL	2.2
1	H	74	GLU	2.2
1	B	0	SER	2.2
1	C	4[A]	GLU	2.2
1	F	111	ASP	2.2
1	C	203	ASN	2.1
1	H	31	ILE	2.1
1	G	40	ARG	2.1
1	H	262	PRO	2.1
1	G	0	SER	2.1
1	G	249	LYS	2.0
1	H	261	GLU	2.0
1	H	203	ASN	2.0
1	D	0	SER	2.0
1	D	302	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.

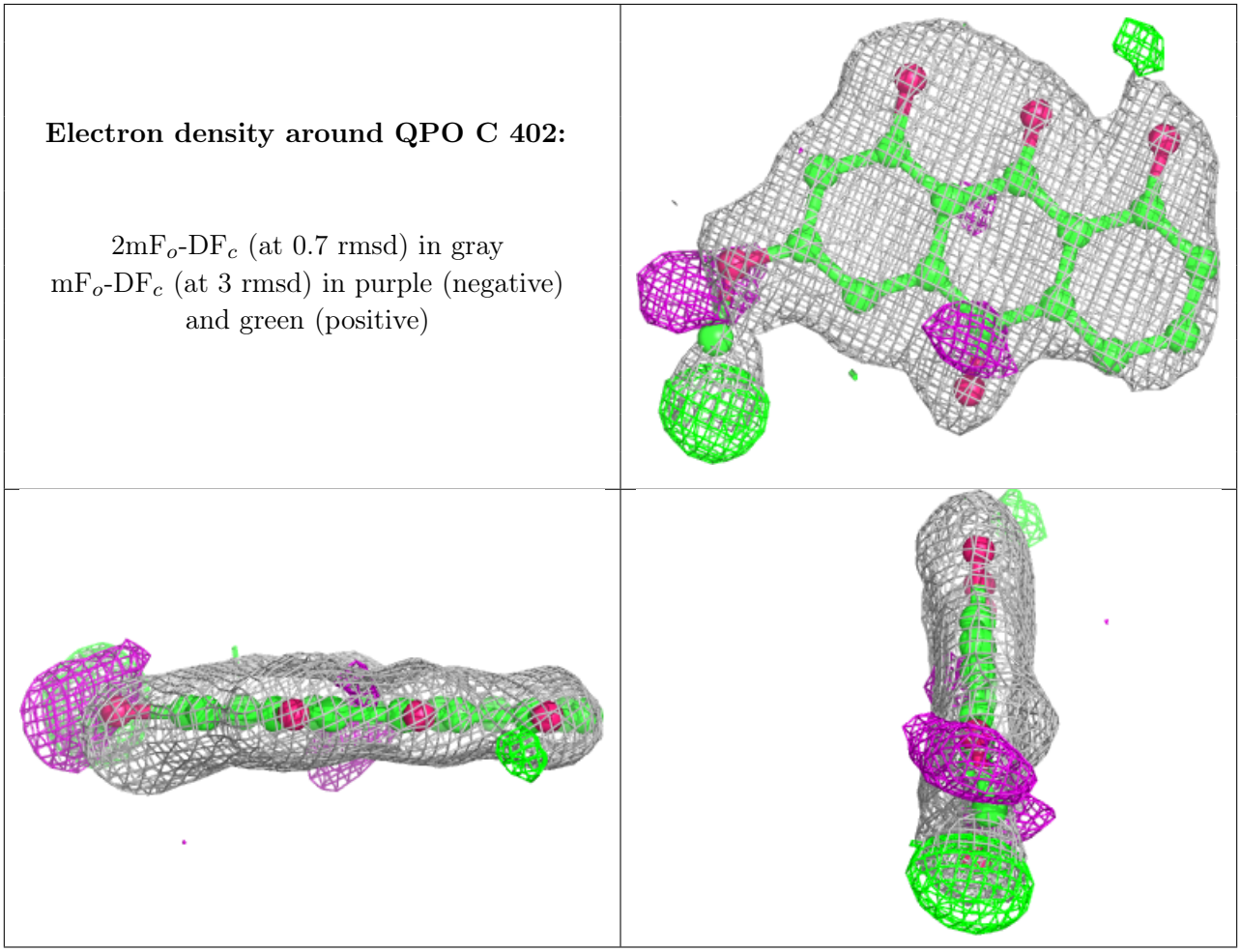
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NA	F	403	1/1	0.61	0.26	48,48,48,48	0
5	NA	C	403	1/1	0.64	0.22	48,48,48,48	0
4	CL	A	403	1/1	0.76	0.39	63,63,63,63	0
3	QPO	C	402	20/20	0.80	0.21	43,45,48,49	0
3	QPO	H	402	20/20	0.81	0.17	43,45,47,48	0
3	QPO	A	402	20/20	0.83	0.17	37,39,46,46	0
3	QPO	D	402	20/20	0.83	0.15	44,48,50,53	0
3	QPO	B	402	20/20	0.83	0.17	43,46,51,52	0
3	QPO	E	402	20/20	0.86	0.16	37,38,42,46	0
3	QPO	F	402	20/20	0.88	0.14	40,42,47,47	0
3	QPO	G	402	20/20	0.88	0.14	41,42,45,45	0
4	CL	D	404	1/1	0.89	0.22	52,52,52,52	0
5	NA	D	403	1/1	0.93	0.21	49,49,49,49	0
2	SAH	G	401	26/26	0.94	0.08	29,29,34,35	0
5	NA	G	403	1/1	0.94	0.12	41,41,41,41	0
2	SAH	A	401	26/26	0.95	0.09	21,22,29,30	0
2	SAH	H	401	26/26	0.95	0.08	24,26,32,35	0
2	SAH	C	401	26/26	0.95	0.09	26,27,33,34	0
4	CL	F	404	1/1	0.95	0.17	61,61,61,61	0
2	SAH	E	401	26/26	0.96	0.08	21,23,29,30	0
2	SAH	F	401	26/26	0.96	0.08	26,28,31,32	0
2	SAH	B	401	26/26	0.96	0.08	24,25,32,33	0
5	NA	B	404	1/1	0.96	0.06	34,34,34,34	0
5	NA	B	403	1/1	0.97	0.21	45,45,45,45	0
2	SAH	D	401	26/26	0.97	0.07	24,25,32,33	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.

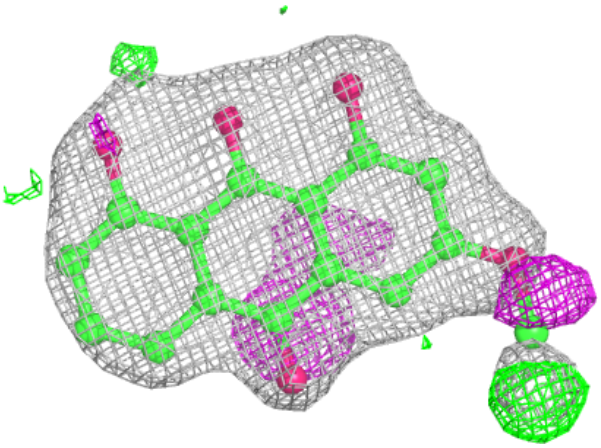
Electron density around QPO C 402:

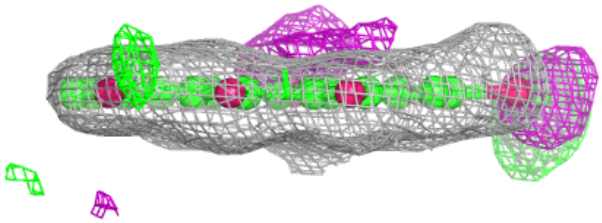
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

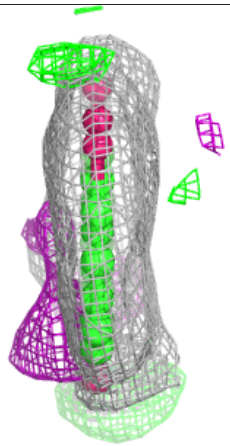


Electron density around QPO H 402:

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

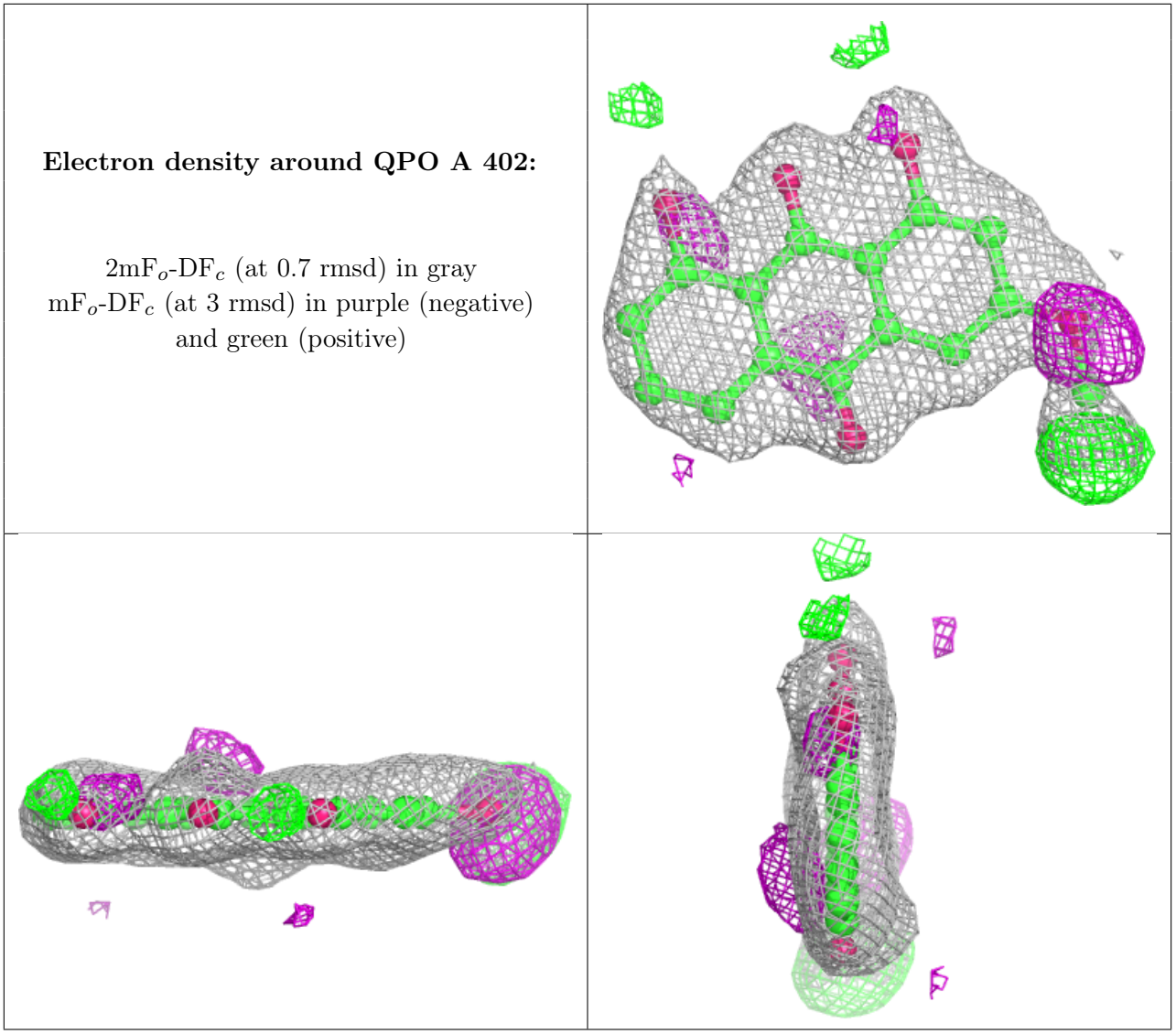






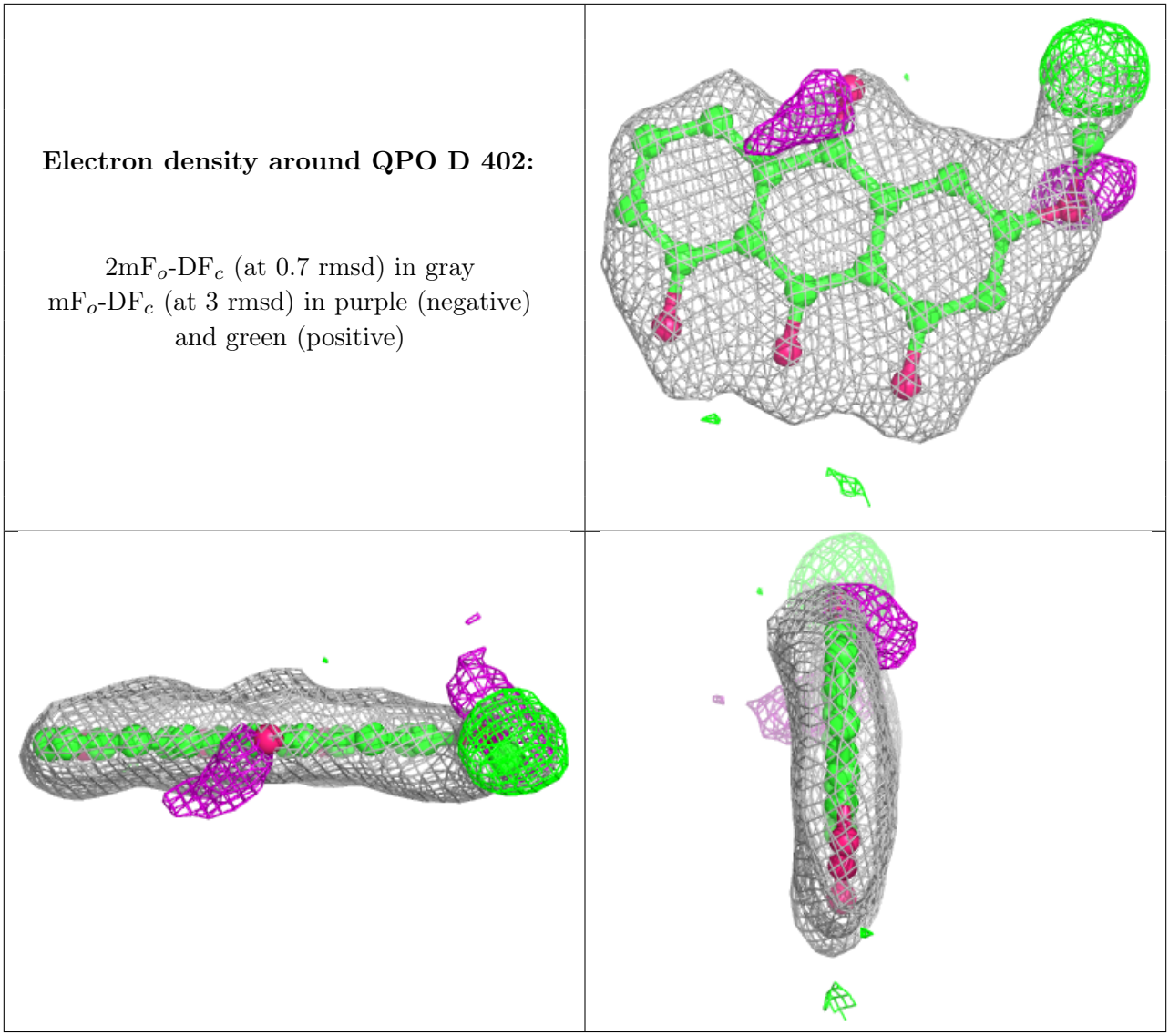
Electron density around QPO A 402:

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



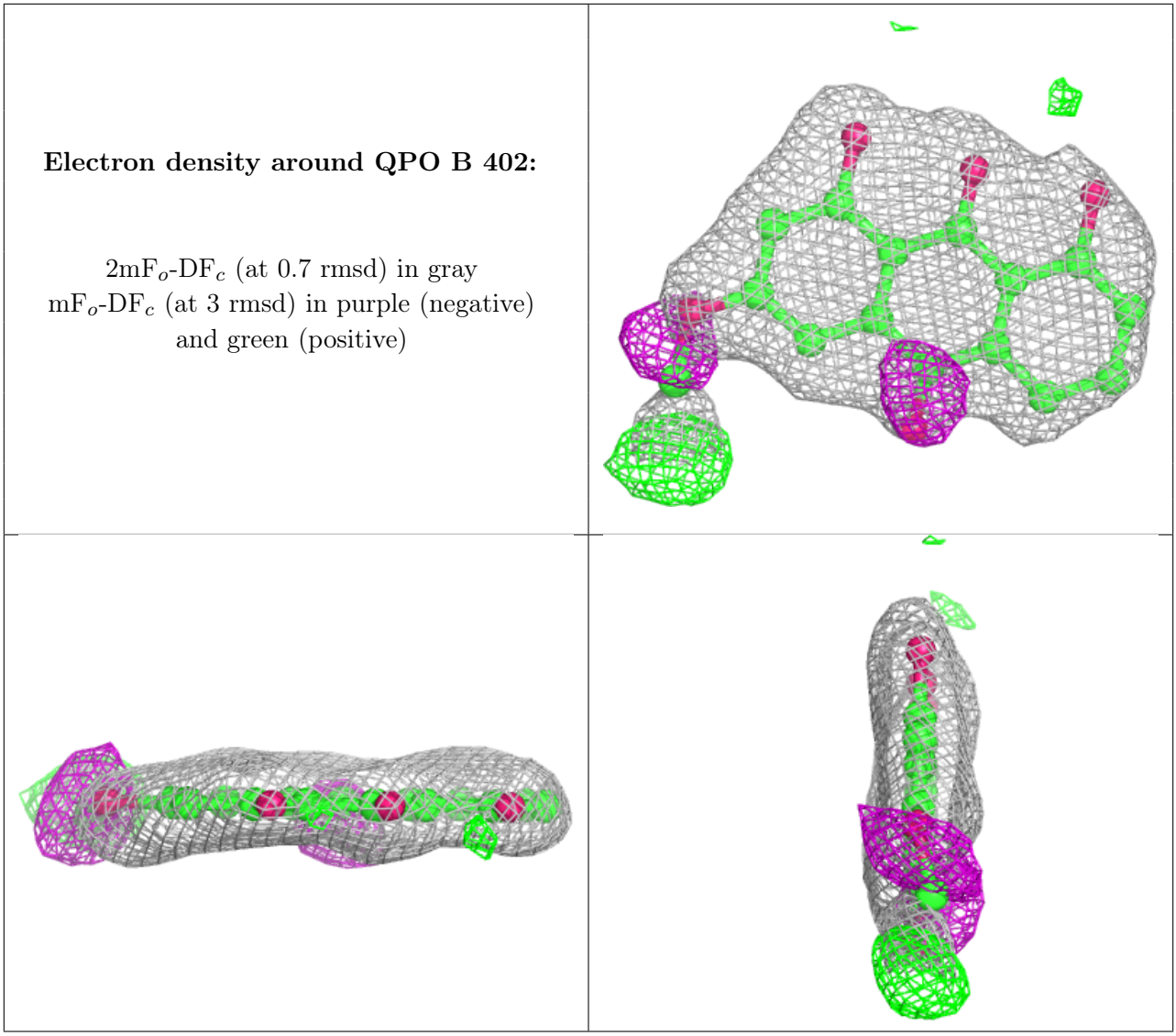
Electron density around QPO D 402:

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



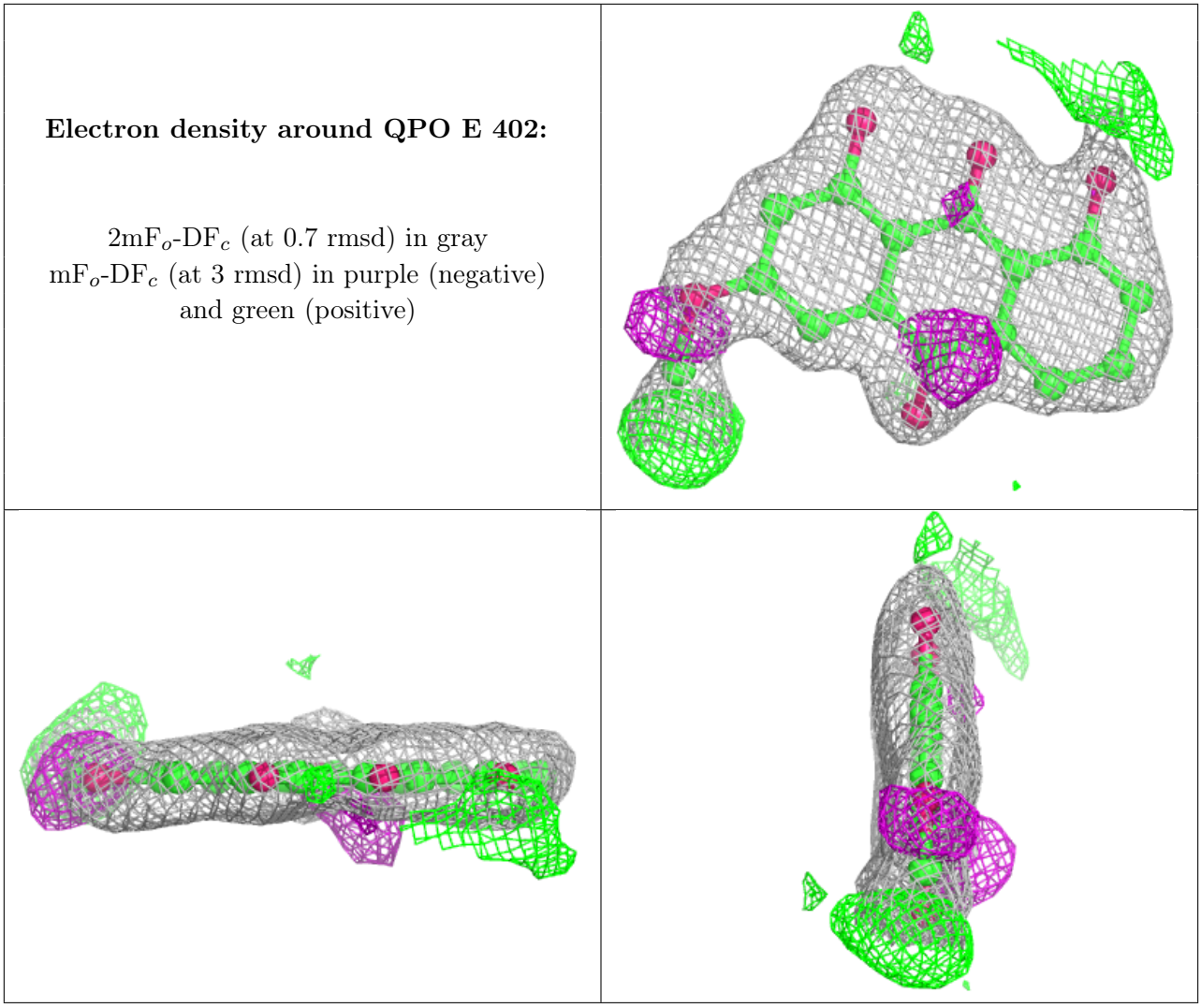
Electron density around QPO B 402:

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



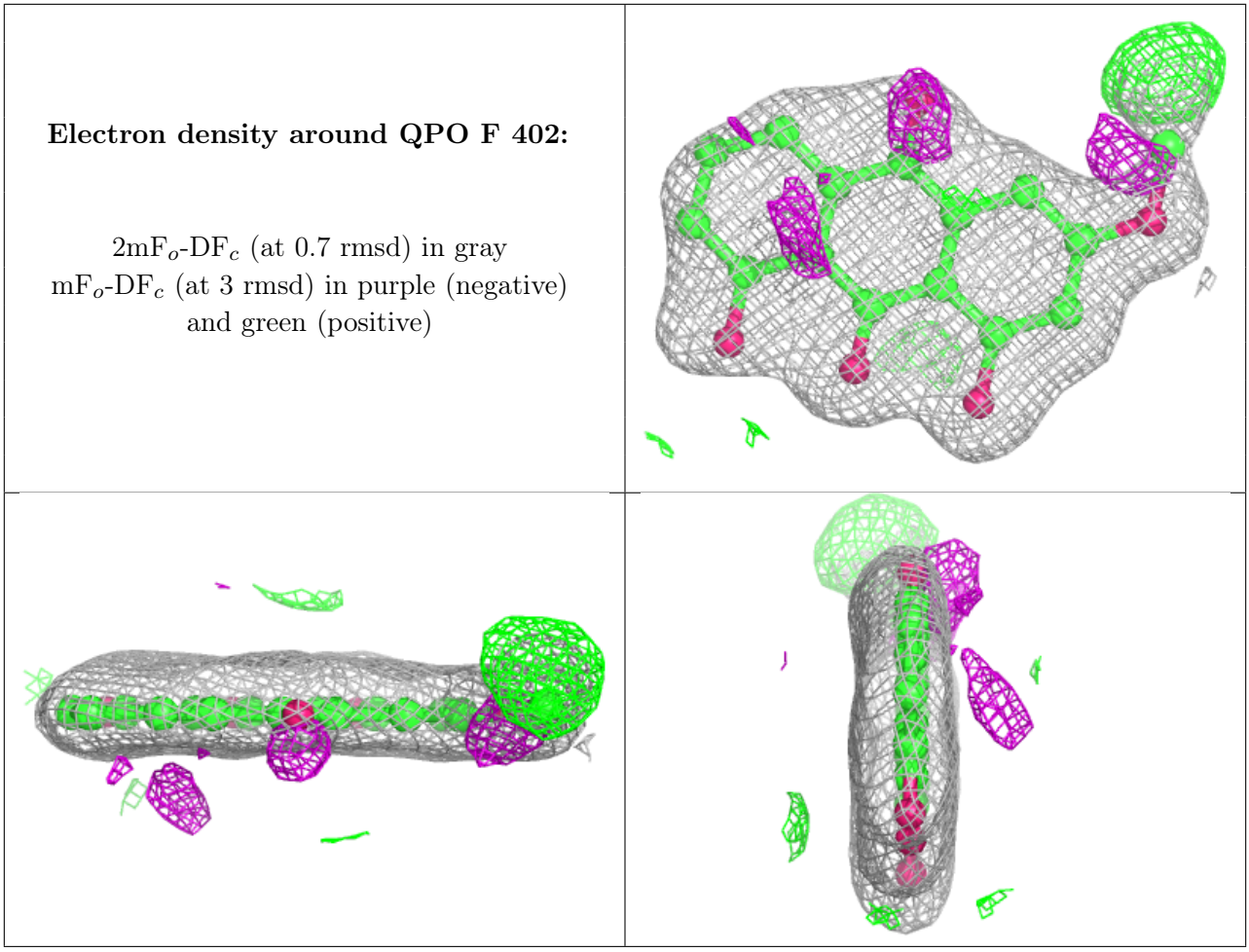
Electron density around QPO E 402:

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



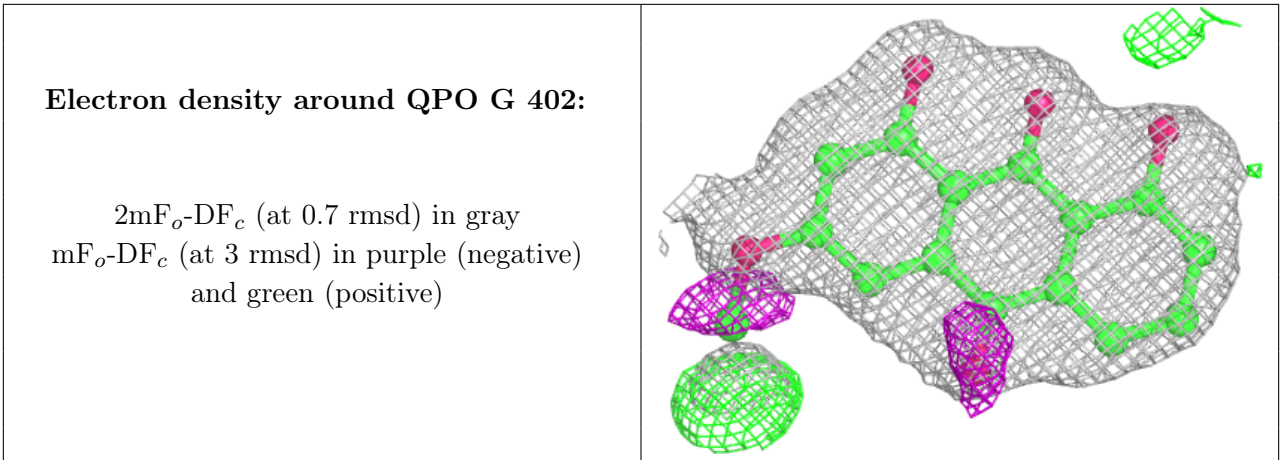
Electron density around QPO F 402:

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



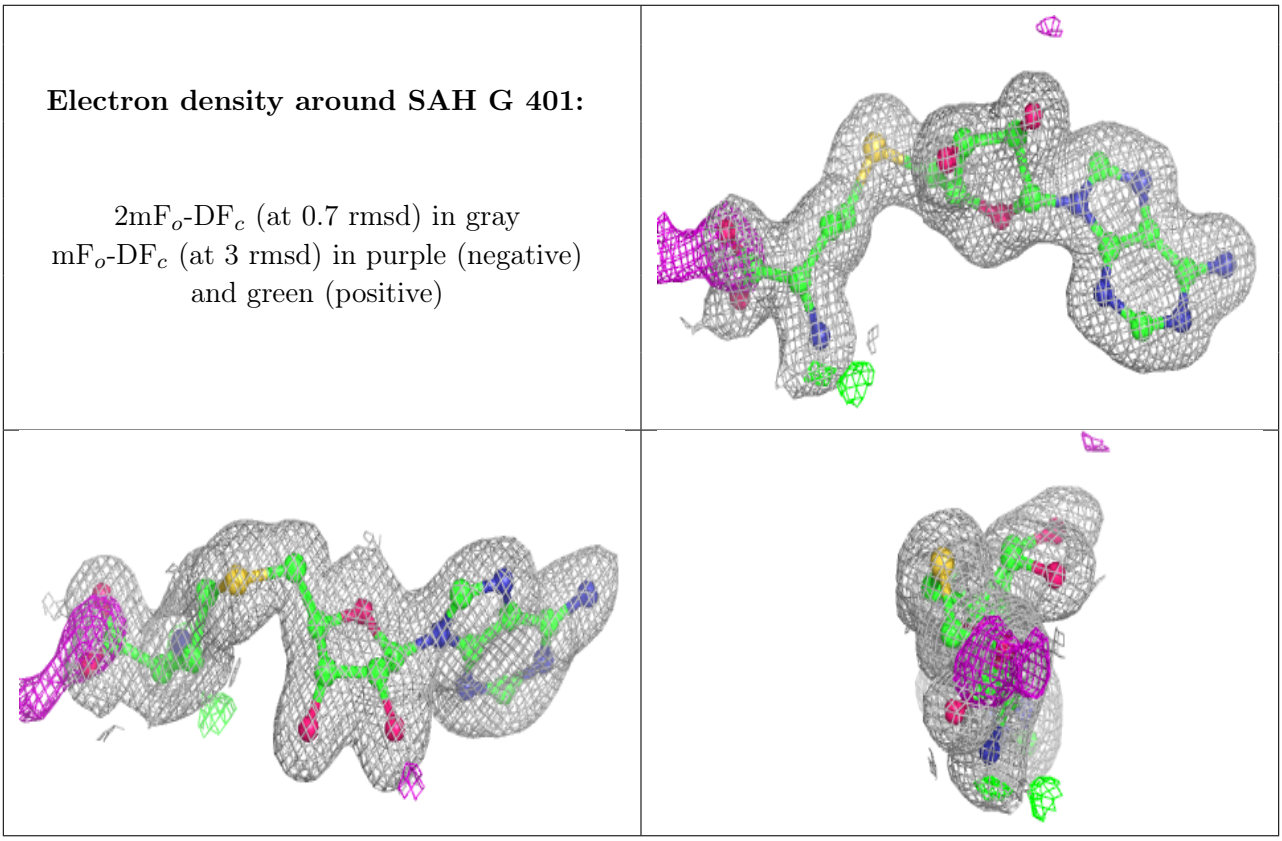
Electron density around QPO G 402:

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



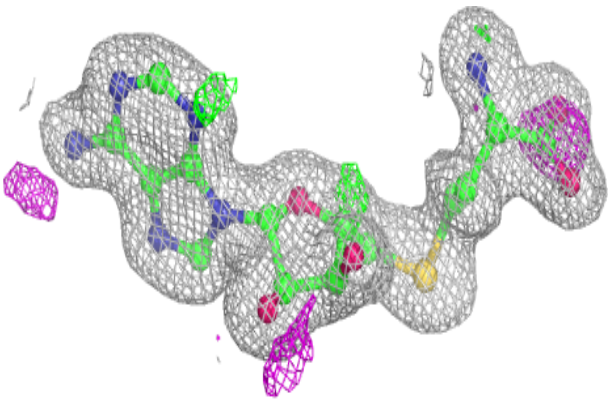
Electron density around SAH G 401:

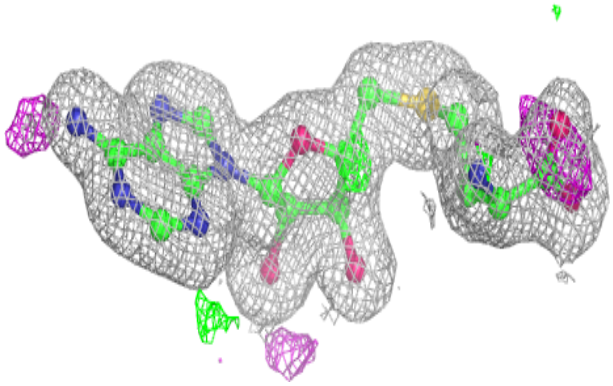
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

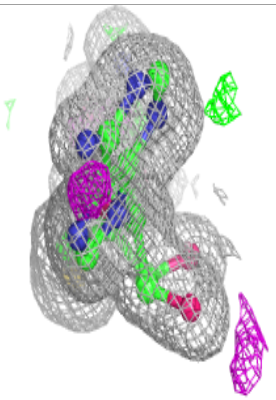


Electron density around SAH A 401:

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

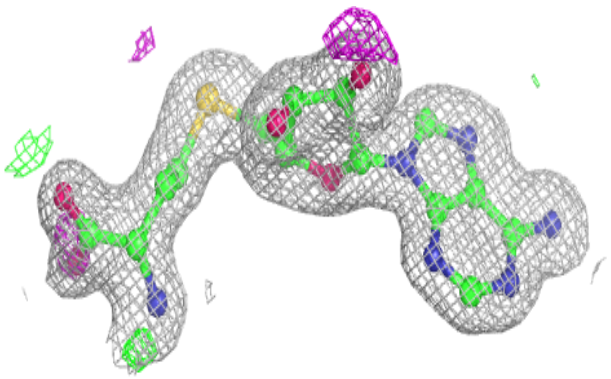


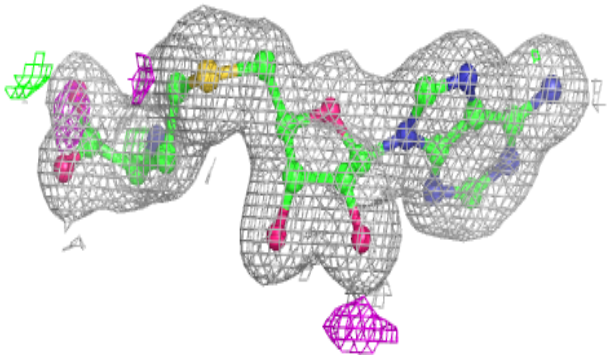


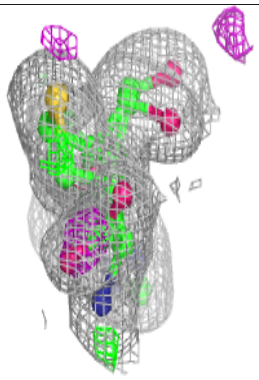


Electron density around SAH H 401:

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

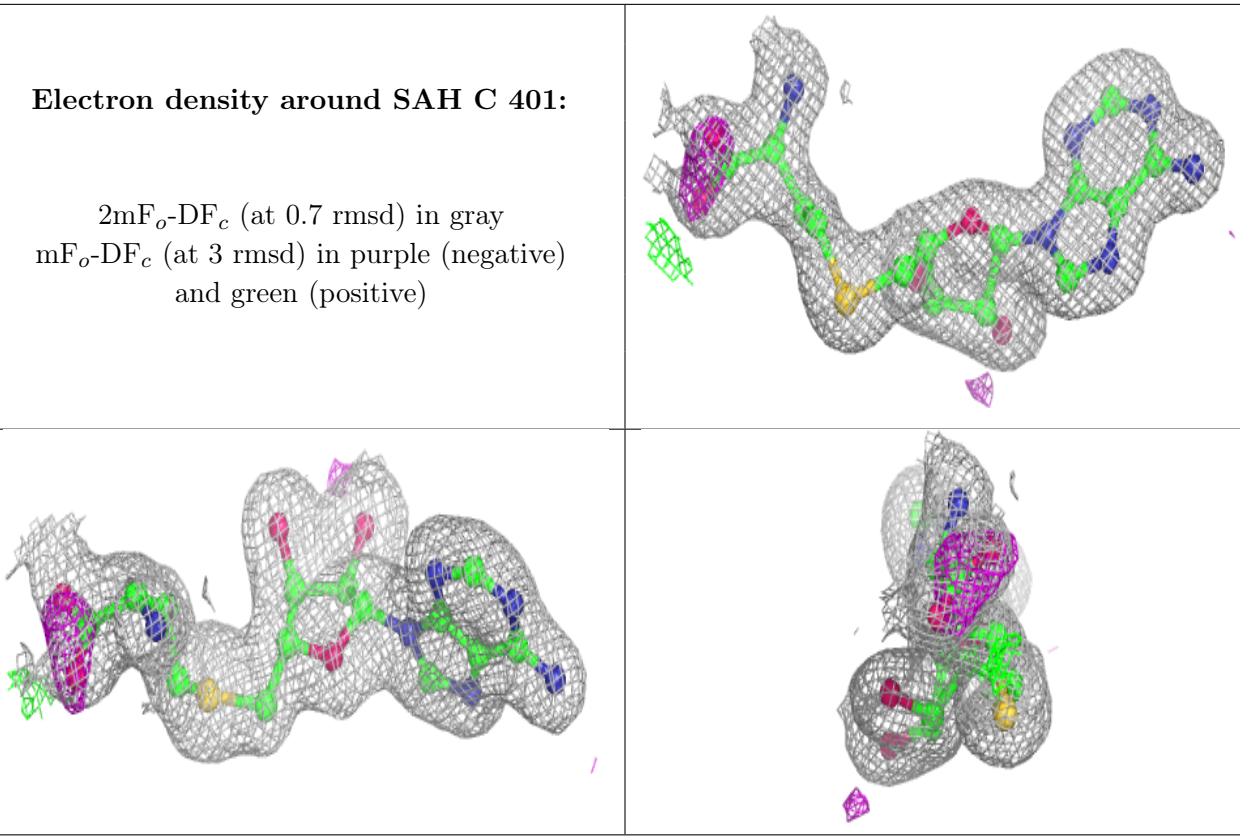






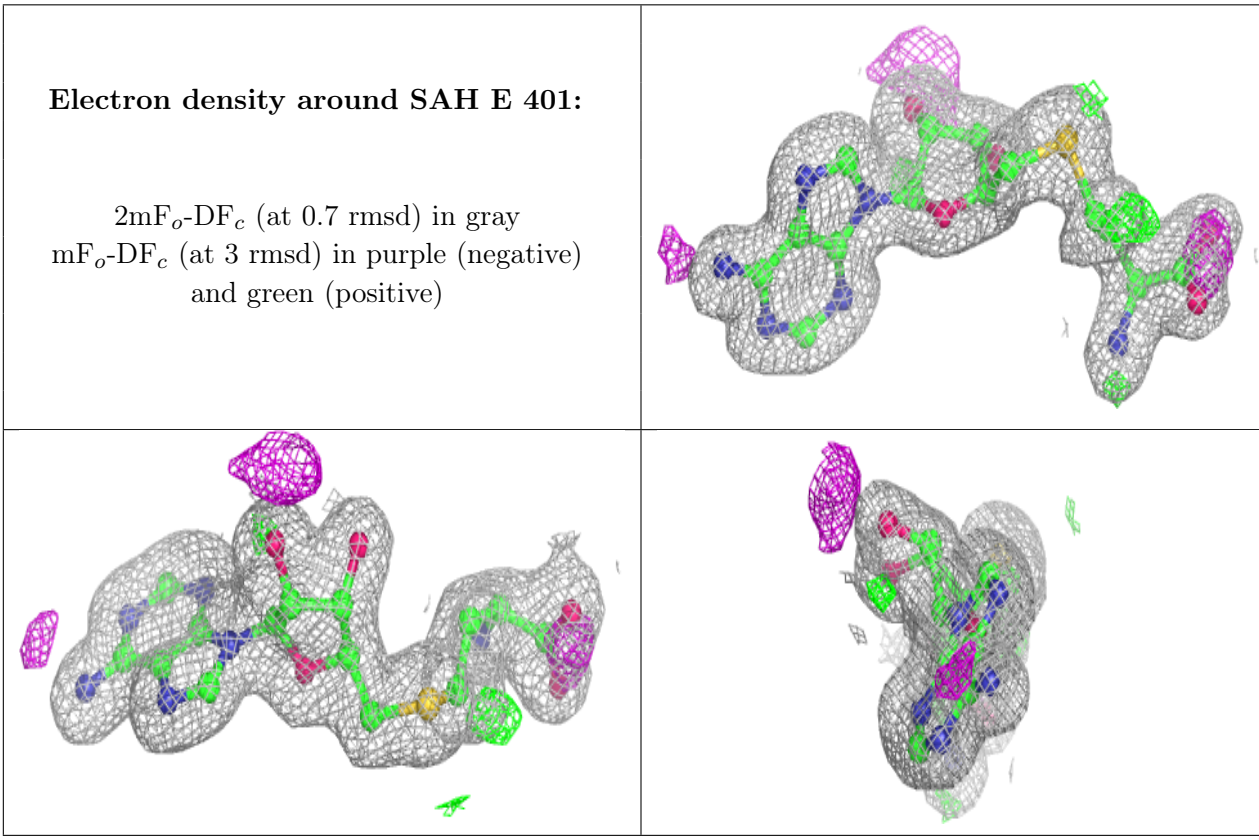
Electron density around SAH C 401:

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



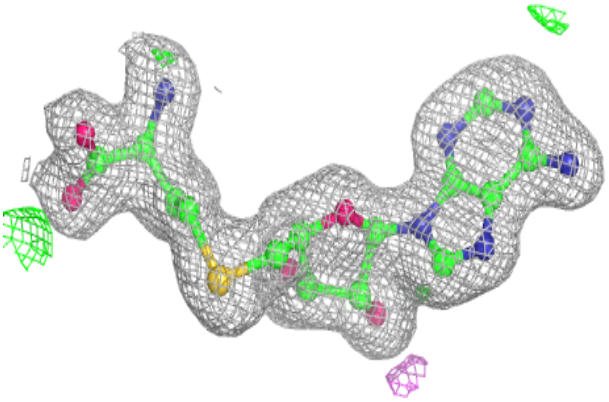
Electron density around SAH E 401:

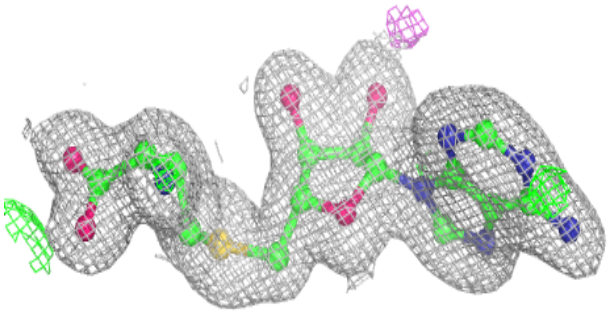
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

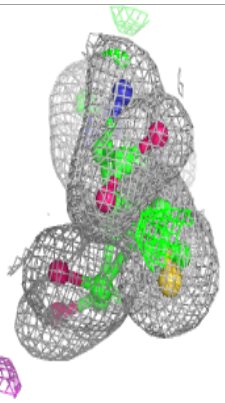


Electron density around SAH F 401:

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

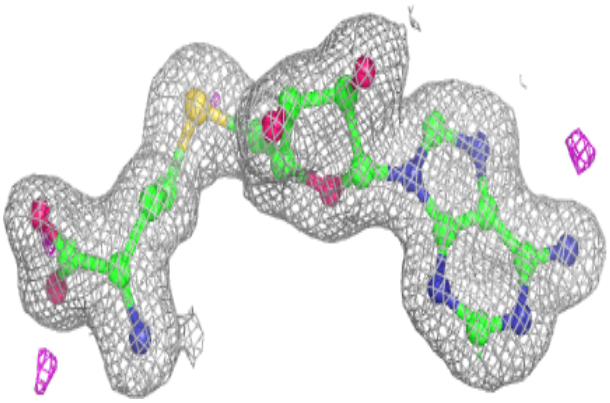


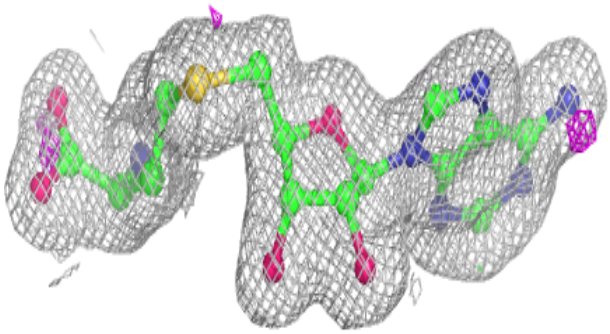


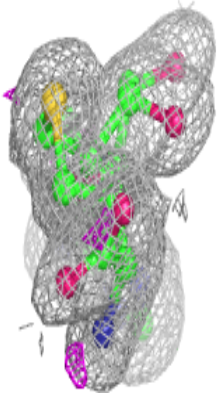


Electron density around SAH B 401:

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

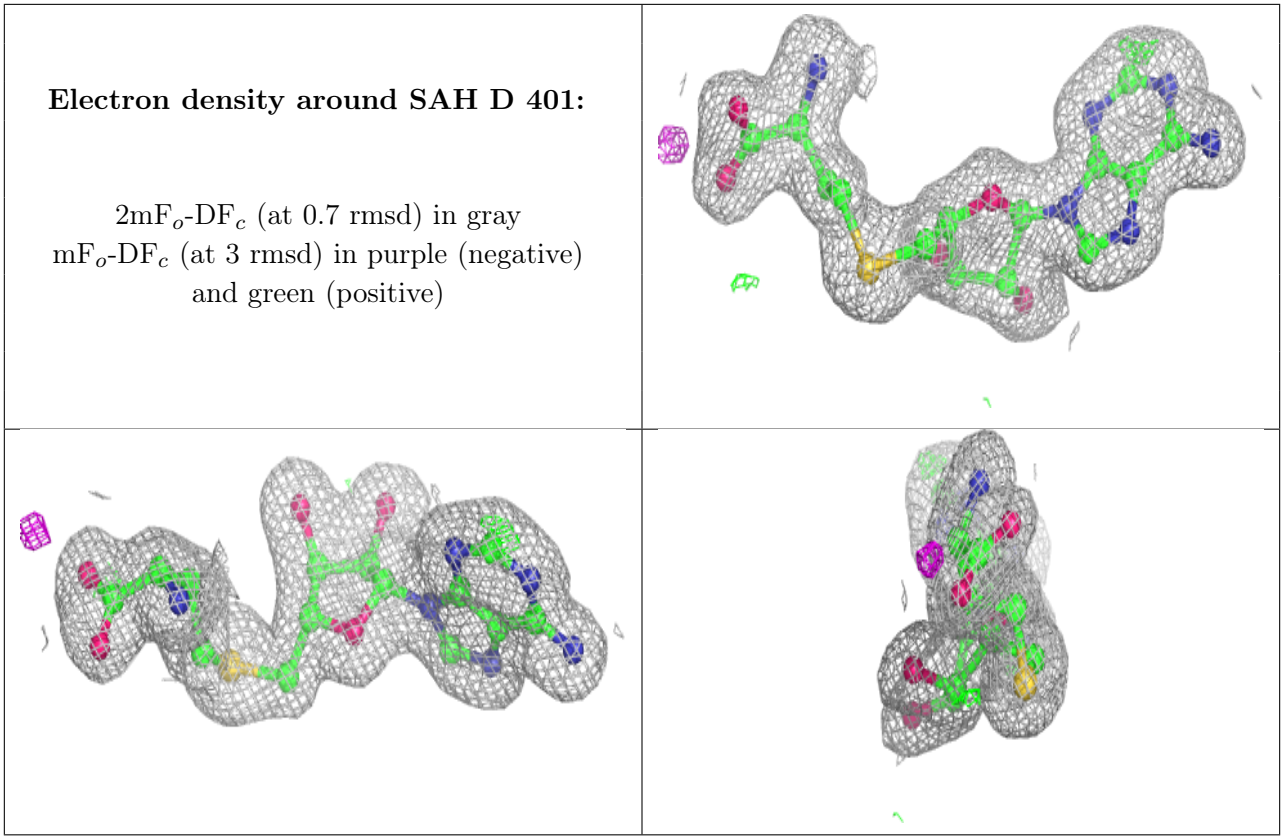






Electron density around SAH D 401:

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



6.5 Other polymers (i)

There are no such residues in this entry.