



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2024 – 07:54 PM EDT

PDB ID : 8BGX  
Title : O-Methyltransferase Plu4890 in complex with SAH and AQ-270a  
Authors : Huber, E.M.; Groll, M.  
Deposited on : 2022-10-28  
Resolution : 1.90 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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 : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 1.20.1  
EDS : 2.37.1  
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) : 2.37.1

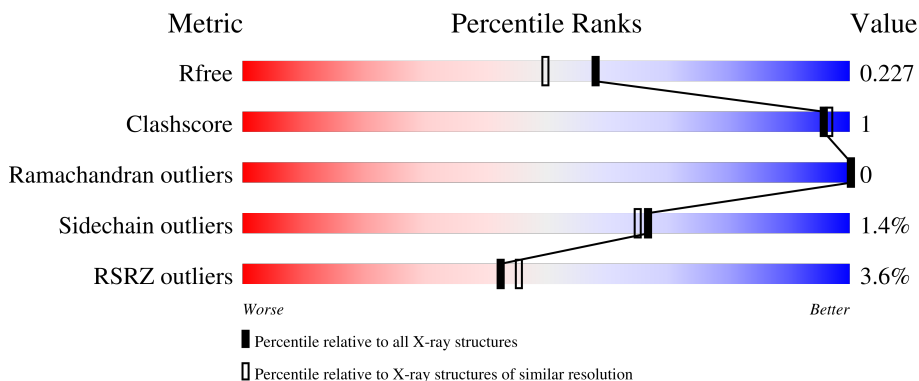
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

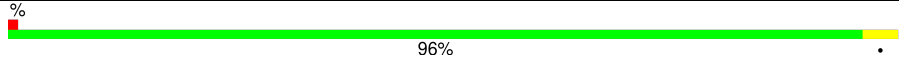
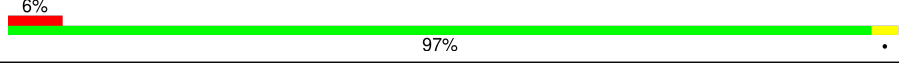
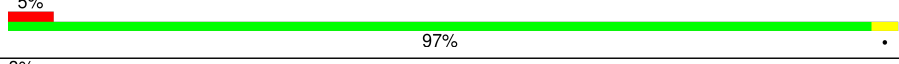
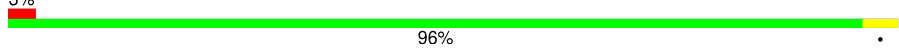
The reported resolution of this entry is 1.90 Å.

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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	319	 96%
1	B	319	 97%
1	C	319	 97%
1	D	319	 96%

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11093 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.

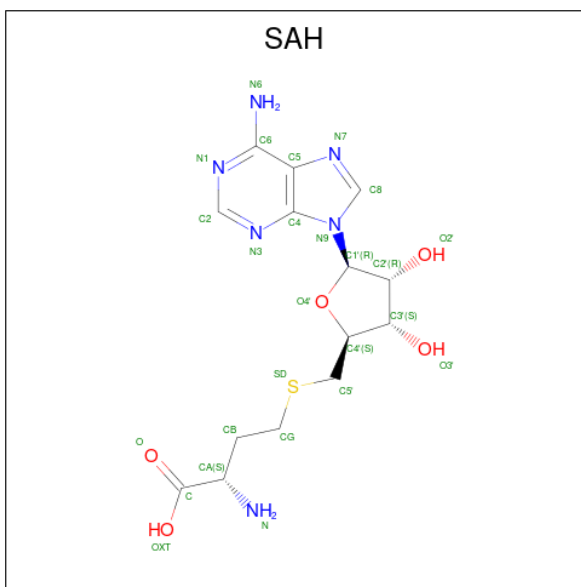
- Molecule 1 is a protein called Methyltransferase Plu4890.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	319	2601	1664	429	496	12	0	4	0
1	B	319	2607	1671	434	490	12	0	3	0
1	C	319	2580	1653	426	489	12	0	1	0
1	D	319	2615	1671	432	500	12	0	6	0

There are 4 discrepancies between the modelled and reference sequences:

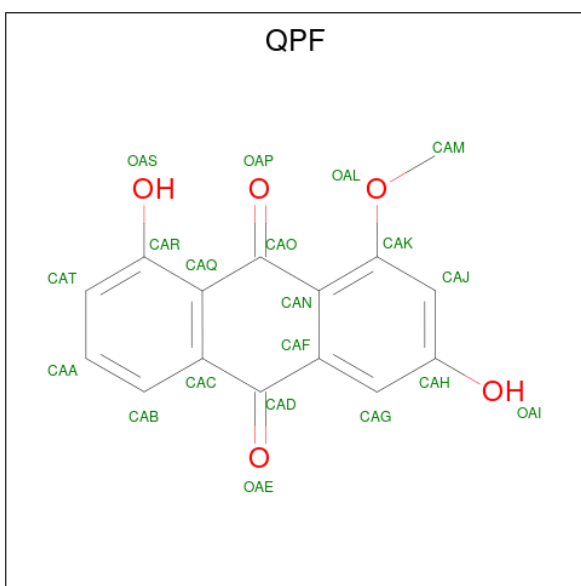
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP A0A6L9JR93
B	0	SER	-	expression tag	UNP A0A6L9JR93
C	0	SER	-	expression tag	UNP A0A6L9JR93
D	0	SER	-	expression tag	UNP A0A6L9JR93

- 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
			Total	C	N	O	S		
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		

- Molecule 3 is 1-methoxy-3,8-bis(oxidanyl)anthracene-9,10-dione (three-letter code: QPF) (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	0	0
			20	15	5		
3	B	1	Total	C	O	0	0
			20	15	5		
3	C	1	Total	C	O	0	0
			20	15	5		
3	D	1	Total	C	O	0	0
			20	15	5		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Na	0	0
			3	3		
4	C	1	Total	Na	0	0
			1	1		
4	D	1	Total	Na	0	0
			1	1		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Cl	0	0
			2	2		
5	B	1	Total	Cl	0	0
			1	1		
5	C	1	Total	Cl	0	0
			1	1		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0

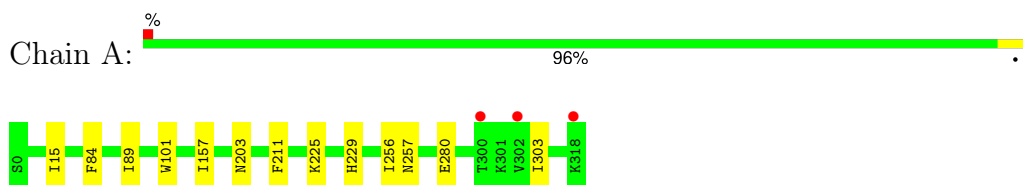
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	170	Total O 170 170	0	0
7	B	75	Total O 75 75	0	0
7	C	70	Total O 70 70	0	0
7	D	164	Total O 164 164	0	0

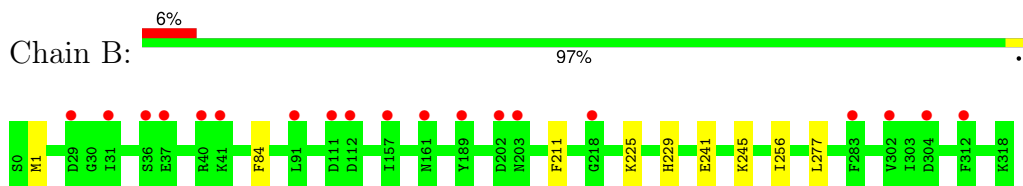
### 3 Residue-property plots i

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.

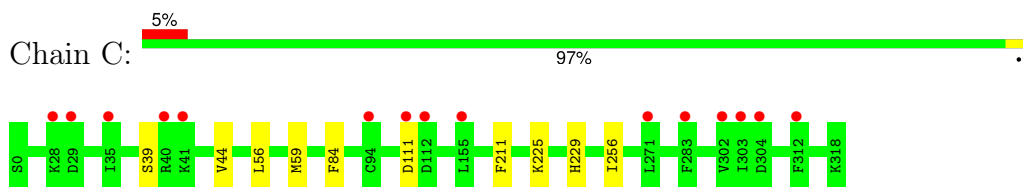
- Molecule 1: Methyltransferase Plu4890



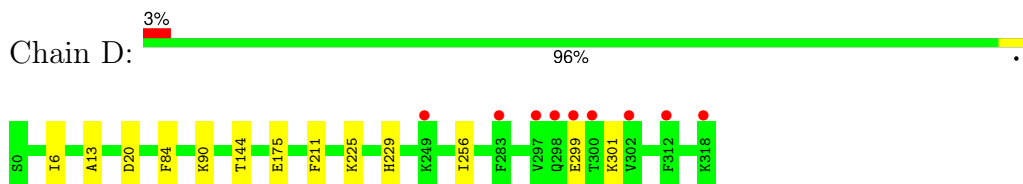
- Molecule 1: Methyltransferase Plu4890



- Molecule 1: Methyltransferase Plu4890



- Molecule 1: Methyltransferase Plu4890



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.14Å 78.37Å 167.73Å 90.00° 96.31° 90.00°	Depositor
Resolution (Å)	30.00 – 1.90 47.68 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.4 (30.00-1.90) 97.4 (47.68-1.90)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.92 (at 1.90Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.179 , 0.220 0.187 , 0.227	Depositor DCC
$R_{free}$ test set	6245 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.6	Xtrriage
Anisotropy	0.310	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 41.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11093	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.58 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.7271e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CL, QPF, SAH, NA

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	0/2655	0.67	0/3574
1	B	0.66	0/2662	0.68	0/3583
1	C	0.65	0/2634	0.68	0/3546
1	D	0.65	0/2669	0.68	0/3593
All	All	0.65	0/10620	0.68	0/14296

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 [i](#)

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	2601	0	2547	7	0
1	B	2607	0	2564	3	0
1	C	2580	0	2535	3	0
1	D	2615	0	2557	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
3	A	20	0	0	1	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	20	0	0	1	0
3	C	20	0	0	1	0
3	D	20	0	0	2	0
4	A	3	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	2	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
6	A	6	0	8	0	0
6	B	12	0	16	0	0
7	A	170	0	0	1	0
7	B	75	0	0	0	0
7	C	70	0	0	0	0
7	D	164	0	0	0	0
All	All	11093	0	10303	22	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 (22) 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:A:89:ILE:HD13	1:D:6:ILE:HG23	1.77	0.67
1:C:225:LYS:HA	1:C:256:ILE:O	2.04	0.58
1:C:56:LEU:HA	1:C:59:MET:HE3	1.88	0.56
1:A:89:ILE:HD11	1:D:6:ILE:HG12	1.87	0.55
1:D:225:LYS:HA	1:D:256:ILE:O	2.08	0.53
1:D:299:GLU:OE2	1:D:301:LYS:NZ	2.37	0.53
1:A:225:LYS:HA	1:A:256:ILE:O	2.10	0.51
1:B:225:LYS:HA	1:B:256:ILE:O	2.12	0.49
1:D:144:THR:HG23	1:D:175[B]:GLU:HG3	1.97	0.47
3:D:402:QPF:OAP	3:D:402:QPF:OAL	2.34	0.45
1:B:241:GLU:O	1:B:245:LYS:HG3	2.18	0.44
1:A:280[B]:GLU:CD	7:A:508:HOH:O	2.56	0.43
1:A:15:ILE:HG22	1:A:89:ILE:HD12	2.01	0.43
1:C:39:SER:HA	1:C:44:VAL:HG12	2.00	0.43
3:A:402:QPF:OAL	3:A:402:QPF:OAP	2.36	0.42
1:D:20:ASP:OD1	1:D:90:LYS:HG2	2.19	0.42
1:B:277:LEU:HD12	1:B:277:LEU:HA	1.96	0.41
3:B:402:QPF:OAP	3:B:402:QPF:OAL	2.37	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:ILE:HD11	1:A:303:ILE:HD11	2.03	0.41
3:D:402:QPF:OAP	3:D:402:QPF:OAS	2.38	0.40
1:A:101:TRP:CE3	1:D:13:ALA:HB1	2.55	0.40
3:C:402:QPF:OAP	3:C:402:QPF:OAS	2.38	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	321/319 (101%)	319 (99%)	2 (1%)	0	100	100
1	B	320/319 (100%)	319 (100%)	1 (0%)	0	100	100
1	C	318/319 (100%)	317 (100%)	1 (0%)	0	100	100
1	D	323/319 (101%)	322 (100%)	1 (0%)	0	100	100
All	All	1282/1276 (100%)	1277 (100%)	5 (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	291/287 (101%)	286 (98%)	5 (2%)	60	57
1	B	290/287 (101%)	286 (99%)	4 (1%)	67	65

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	288/287 (100%)	284 (99%)	4 (1%)	67	65
1	D	293/287 (102%)	290 (99%)	3 (1%)	76	76
All	All	1162/1148 (101%)	1146 (99%)	16 (1%)	67	65

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	PHE
1	A	203	ASN
1	A	211	PHE
1	A	229	HIS
1	A	257	ASN
1	B	1	MET
1	B	84	PHE
1	B	211	PHE
1	B	229	HIS
1	C	84	PHE
1	C	111	ASP
1	C	211	PHE
1	C	229	HIS
1	D	84	PHE
1	D	211	PHE
1	D	229	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	230	ASN
1	C	230	ASN
1	D	257	ASN
1	D	298	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 9 are monoatomic - leaving 11 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
3	QPF	B	402	-	22,22,22	1.62	4 (18%)	33,33,33	0.84	2 (6%)
6	GOL	A	408	-	5,5,5	0.08	0	5,5,5	0.25	0
3	QPF	A	402	4	22,22,22	1.62	4 (18%)	33,33,33	0.83	1 (3%)
2	SAH	A	401	-	23,28,28	0.73	1 (4%)	22,40,40	0.94	2 (9%)
2	SAH	D	401	-	23,28,28	0.74	1 (4%)	22,40,40	0.95	3 (13%)
3	QPF	D	402	-	22,22,22	1.59	4 (18%)	33,33,33	0.92	1 (3%)
6	GOL	B	405	-	5,5,5	0.09	0	5,5,5	0.27	0
6	GOL	B	404	-	5,5,5	0.10	0	5,5,5	0.30	0
3	QPF	C	402	-	22,22,22	1.60	4 (18%)	33,33,33	0.76	2 (6%)
2	SAH	B	401	-	23,28,28	0.75	1 (4%)	22,40,40	0.99	3 (13%)
2	SAH	C	401	-	23,28,28	0.74	1 (4%)	22,40,40	0.95	3 (13%)

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
3	QPF	B	402	-	-	0/2/18/18	0/3/3/3
6	GOL	A	408	-	-	0/4/4/4	-
3	QPF	A	402	4	-	0/2/18/18	0/3/3/3
2	SAH	A	401	-	-	0/11/31/31	0/3/3/3
2	SAH	D	401	-	-	1/11/31/31	0/3/3/3
3	QPF	D	402	-	-	0/2/18/18	0/3/3/3
6	GOL	B	405	-	-	0/4/4/4	-

*Continued on next page...*

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	B	404	-	-	0/4/4/4	-
3	QPF	C	402	-	-	0/2/18/18	0/3/3/3
2	SAH	B	401	-	-	0/11/31/31	0/3/3/3
2	SAH	C	401	-	-	0/11/31/31	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	QPF	CAC-CAD	-4.30	1.39	1.48
3	B	402	QPF	CAC-CAD	-4.25	1.39	1.48
3	C	402	QPF	CAC-CAD	-4.21	1.40	1.48
3	D	402	QPF	CAC-CAD	-4.21	1.40	1.48
3	B	402	QPF	CAF-CAD	-4.20	1.40	1.48
3	D	402	QPF	CAF-CAD	-4.05	1.40	1.48
3	C	402	QPF	CAF-CAD	-4.02	1.40	1.48
3	A	402	QPF	CAF-CAD	-4.01	1.40	1.48
3	B	402	QPF	CAQ-CAO	-3.14	1.40	1.47
3	C	402	QPF	CAN-CAO	-3.12	1.40	1.47
3	C	402	QPF	CAQ-CAO	-3.11	1.40	1.47
3	D	402	QPF	CAQ-CAO	-3.09	1.40	1.47
3	A	402	QPF	CAN-CAO	-3.08	1.40	1.47
3	A	402	QPF	CAQ-CAO	-3.08	1.40	1.47
3	B	402	QPF	CAN-CAO	-2.99	1.40	1.47
3	D	402	QPF	CAN-CAO	-2.93	1.40	1.47
2	B	401	SAH	OXT-C	-2.19	1.23	1.30
2	C	401	SAH	OXT-C	-2.14	1.23	1.30
2	D	401	SAH	OXT-C	-2.11	1.23	1.30
2	A	401	SAH	OXT-C	-2.06	1.24	1.30

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	402	QPF	CAM-OAL-CAK	3.45	122.57	117.51
3	B	402	QPF	CAM-OAL-CAK	2.88	121.74	117.51
2	B	401	SAH	OXT-C-O	-2.72	117.92	124.08
2	C	401	SAH	OXT-C-O	-2.63	118.11	124.08
2	A	401	SAH	OXT-C-O	-2.60	118.18	124.08
3	A	402	QPF	CAM-OAL-CAK	2.51	121.20	117.51
2	D	401	SAH	OXT-C-O	-2.48	118.46	124.08
2	B	401	SAH	C5-C6-N6	2.32	123.85	120.31
2	A	401	SAH	C5-C6-N6	2.18	123.64	120.31
2	D	401	SAH	C4'-O4'-C1'	-2.17	107.94	109.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	SAH	C4'-O4'-C1'	-2.13	107.98	109.92
3	C	402	QPF	CAM-OAL-CAK	2.12	120.63	117.51
3	C	402	QPF	OAS-CAR-CAQ	-2.11	117.24	121.14
2	C	401	SAH	C5-C6-N6	2.09	123.50	120.31
2	D	401	SAH	C5-C6-N6	2.09	123.50	120.31
2	C	401	SAH	C4'-O4'-C1'	-2.06	108.04	109.92
3	B	402	QPF	OAS-CAR-CAQ	-2.01	117.42	121.14

There are no chirality outliers.

All (1) torsion outliers are listed below:

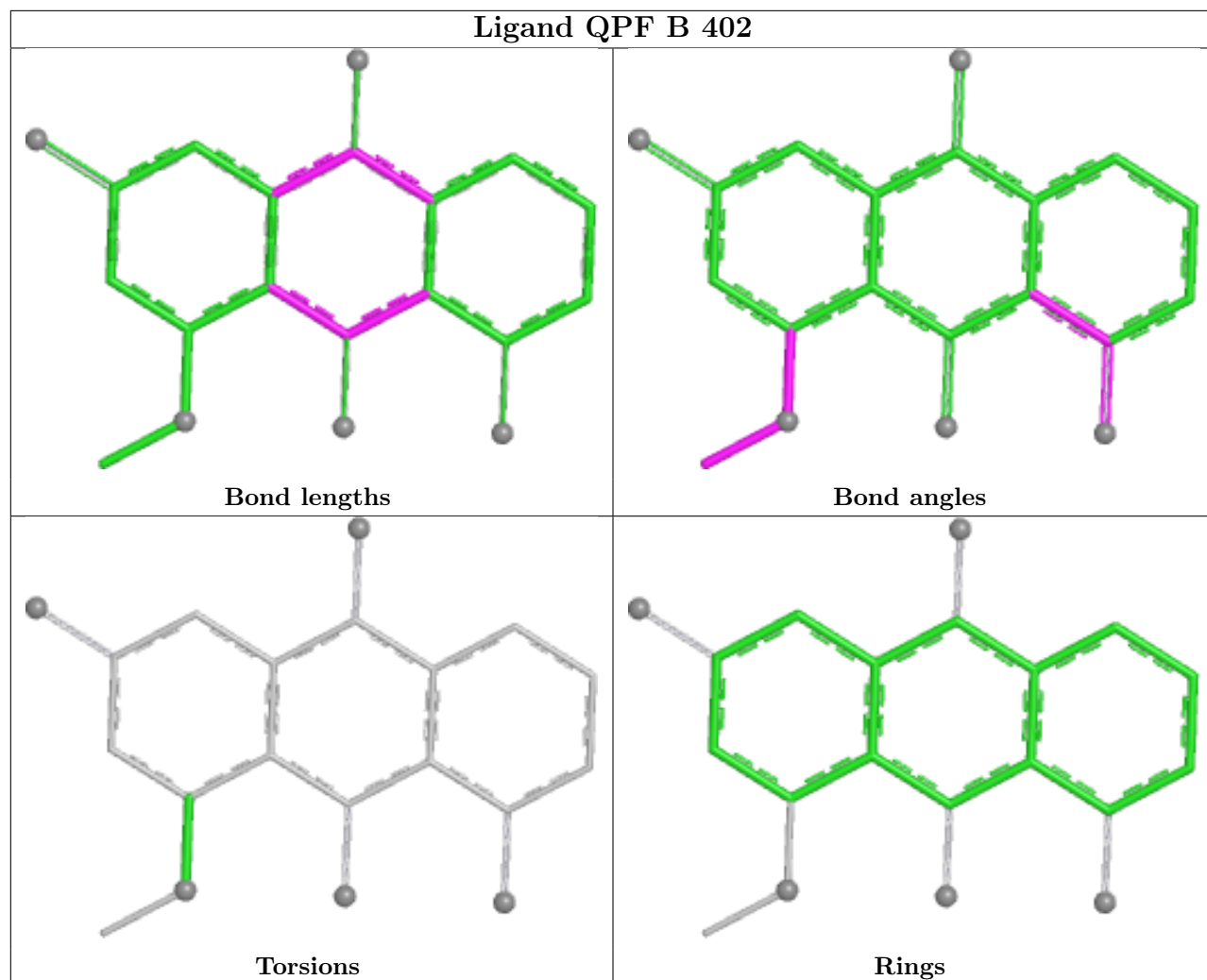
Mol	Chain	Res	Type	Atoms
2	D	401	SAH	OXT-C-CA-N

There are no ring outliers.

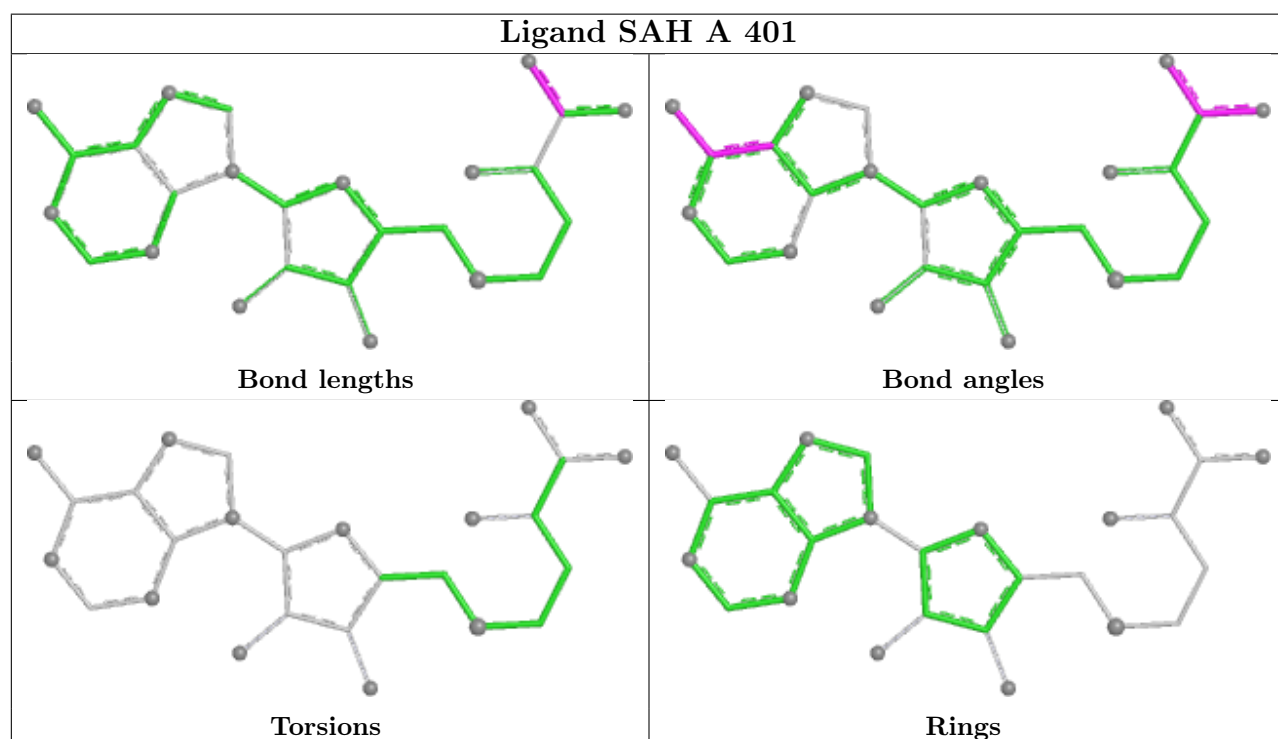
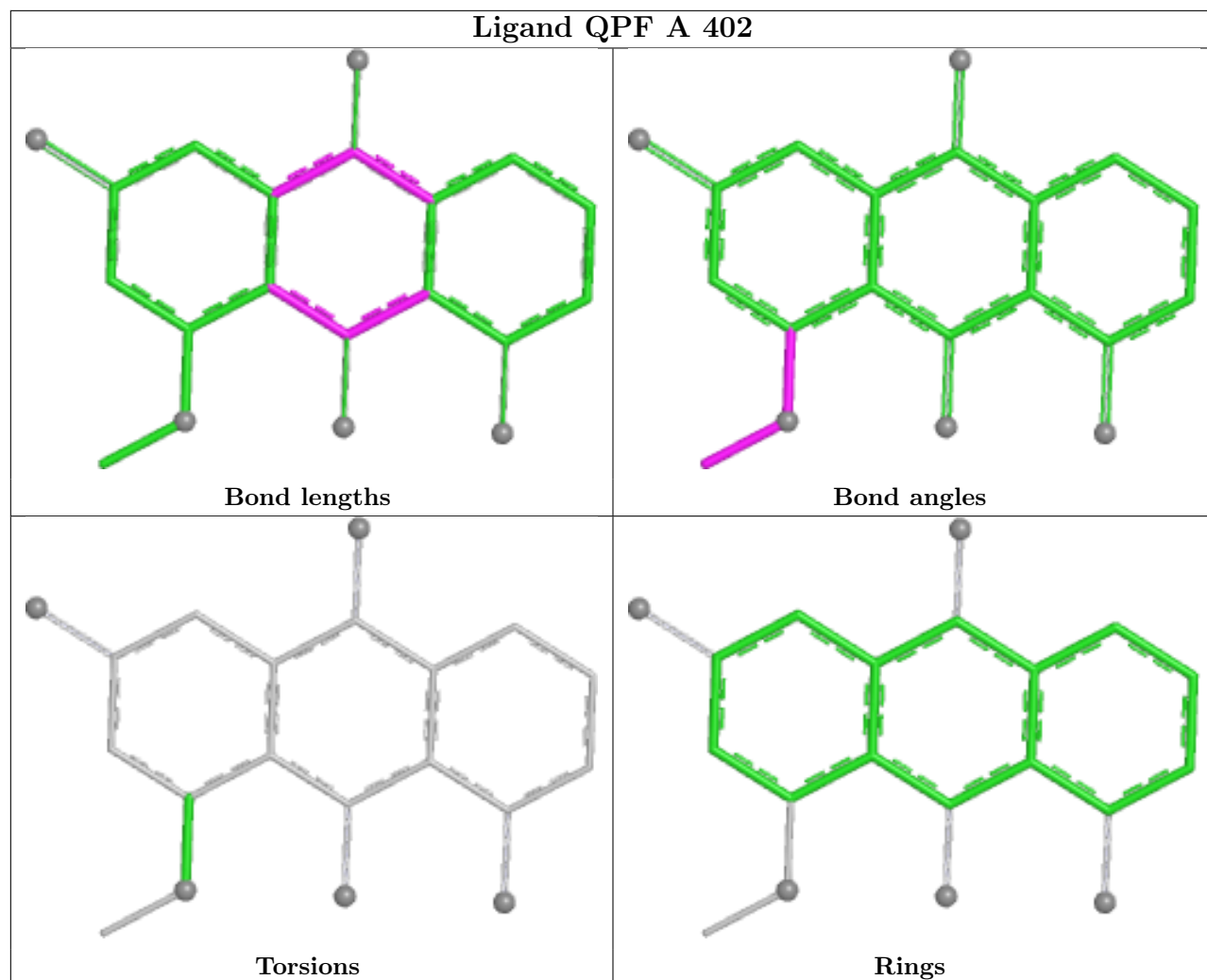
4 monomers are involved in 5 short contacts:

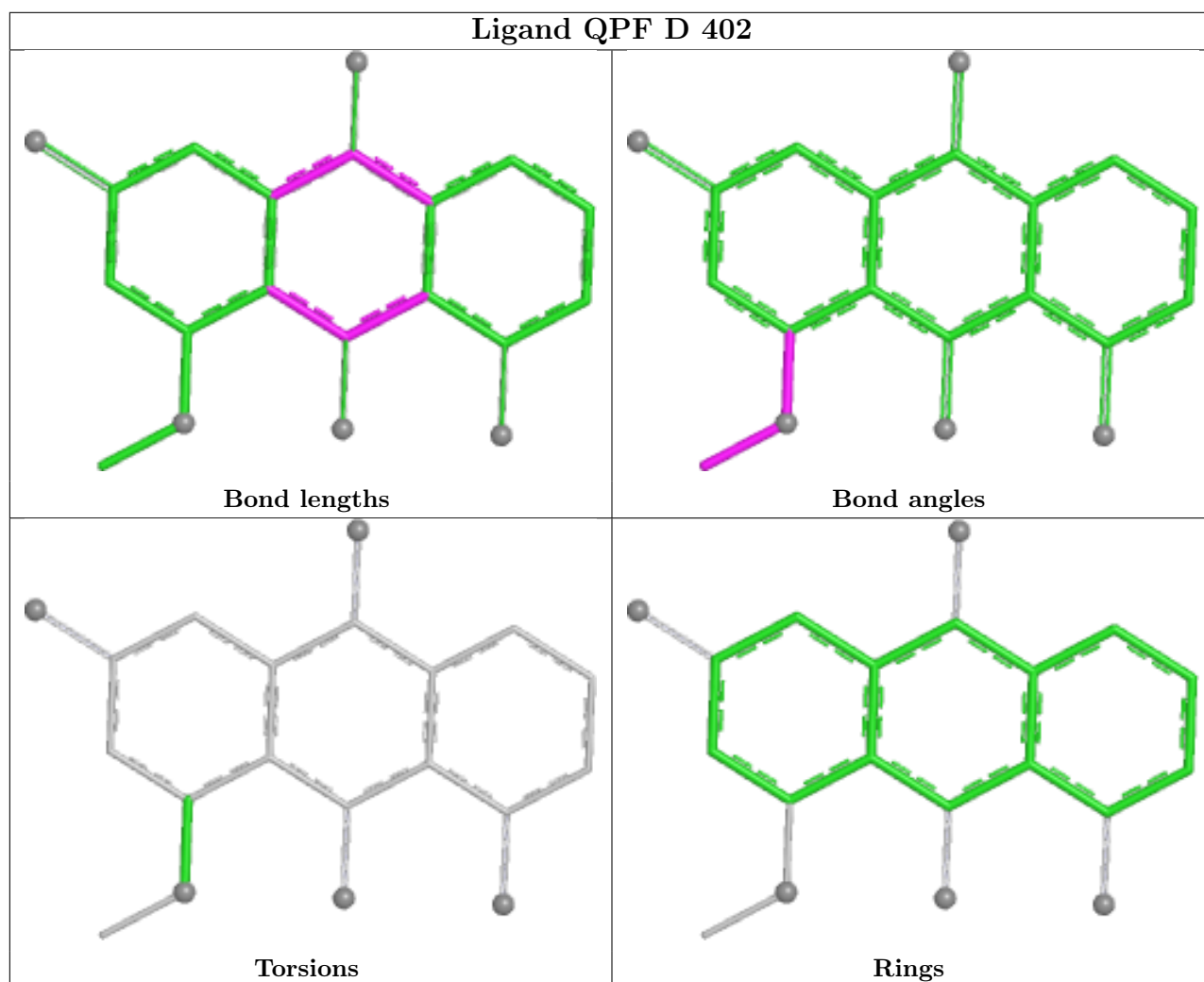
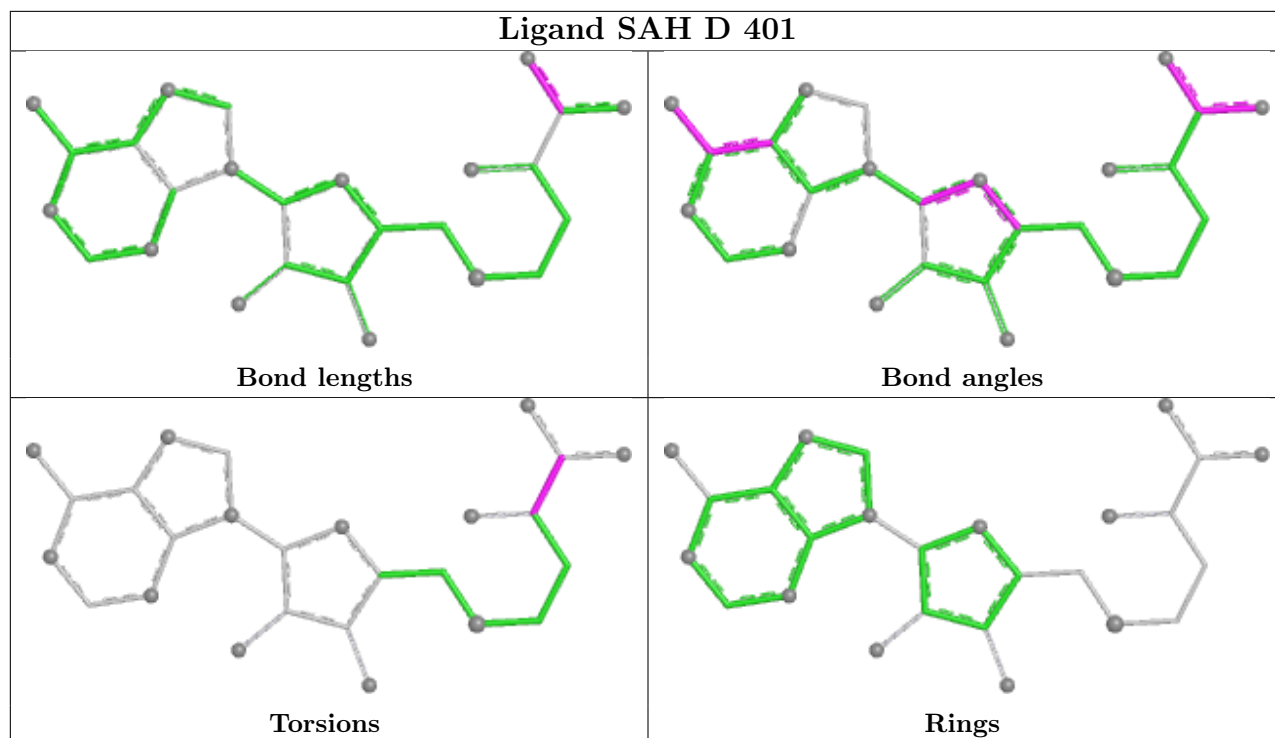
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	402	QPF	1	0
3	A	402	QPF	1	0
3	D	402	QPF	2	0
3	C	402	QPF	1	0

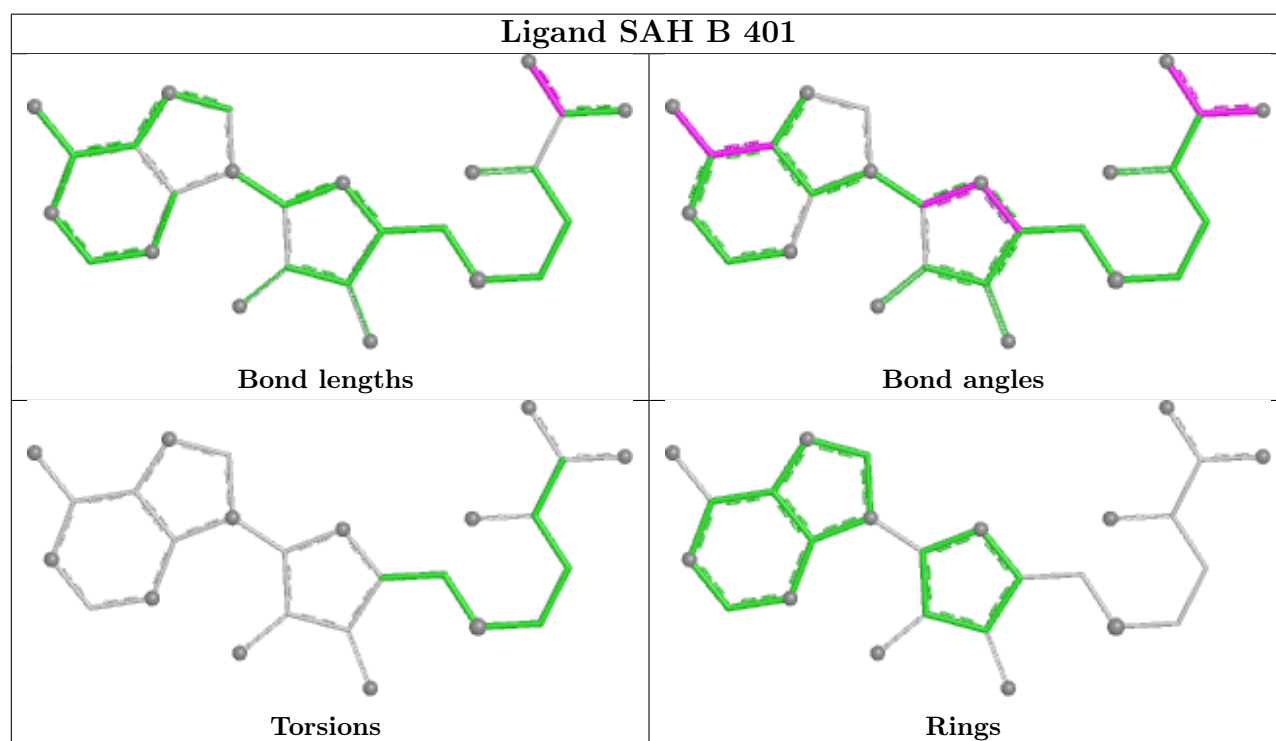
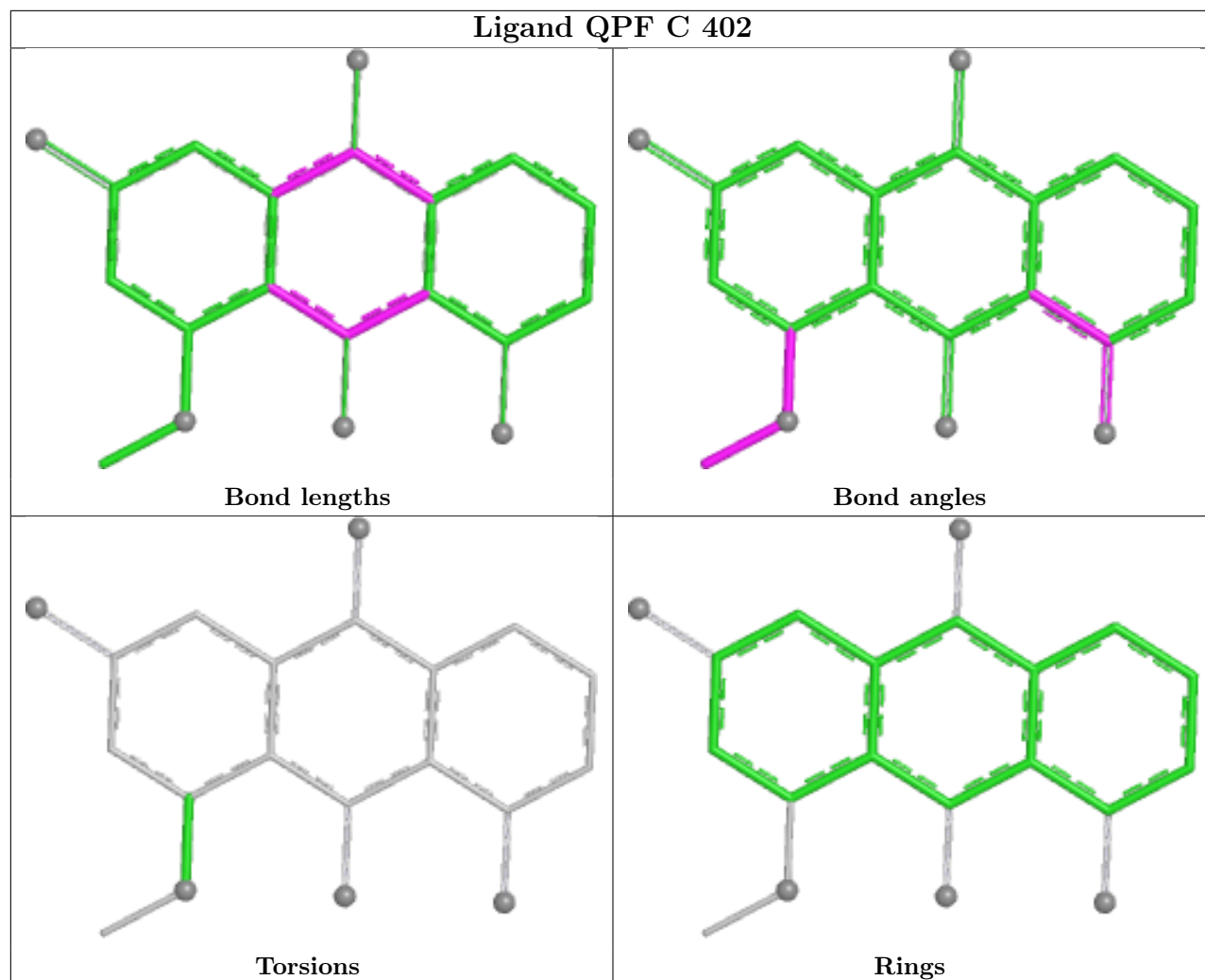
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

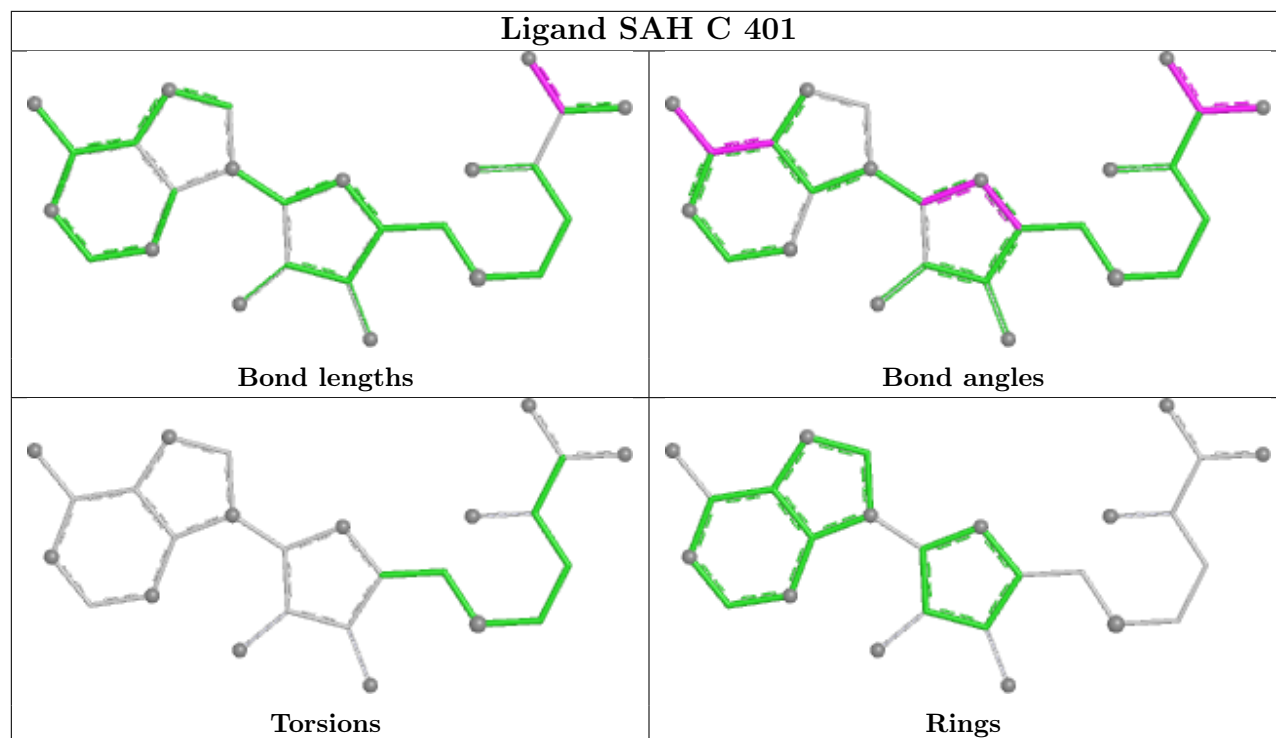












## 5.7 Other polymers [i](#)

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	319/319 (100%)	0.03	3 (0%) 84 85	22, 35, 56, 74	0
1	B	319/319 (100%)	0.33	19 (5%) 21 24	34, 46, 67, 80	0
1	C	319/319 (100%)	0.36	15 (4%) 31 34	33, 46, 65, 81	0
1	D	319/319 (100%)	0.13	9 (2%) 53 56	22, 36, 60, 74	0
All	All	1276/1276 (100%)	0.21	46 (3%) 42 45	22, 42, 63, 81	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	283	PHE	5.0
1	B	40	ARG	4.0
1	B	302	VAL	3.6
1	C	302	VAL	3.5
1	D	318	LYS	3.5
1	D	302	VAL	3.3
1	B	202	ASP	3.2
1	B	304	ASP	3.2
1	B	157	ILE	3.1
1	A	318	LYS	3.0
1	C	155	LEU	3.0
1	B	41	LYS	3.0
1	B	29	ASP	3.0
1	B	283[A]	PHE	2.8
1	B	312	PHE	2.7
1	D	312	PHE	2.6
1	C	303	ILE	2.6
1	C	112	ASP	2.6
1	A	300	THR	2.5
1	D	298	GLN	2.5
1	C	29	ASP	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	299	GLU	2.5
1	C	28	LYS	2.4
1	B	218	GLY	2.4
1	A	302	VAL	2.4
1	C	94	CYS	2.3
1	B	203	ASN	2.3
1	C	41	LYS	2.3
1	D	297	VAL	2.3
1	B	111	ASP	2.3
1	B	37	GLU	2.3
1	B	112	ASP	2.3
1	C	40	ARG	2.2
1	C	304	ASP	2.2
1	B	31	ILE	2.2
1	C	111	ASP	2.2
1	B	91	LEU	2.2
1	C	271	LEU	2.1
1	D	300	THR	2.1
1	B	189	TYR	2.1
1	C	312	PHE	2.1
1	D	283	PHE	2.1
1	B	161	ASN	2.1
1	D	249	LYS	2.1
1	C	35	ILE	2.0
1	B	36	SER	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](#)

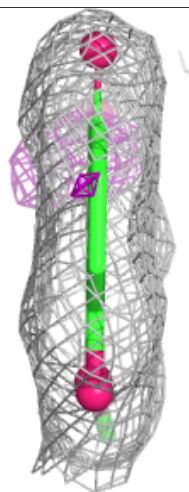
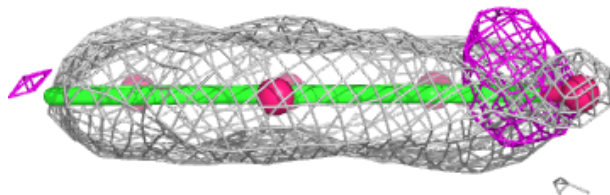
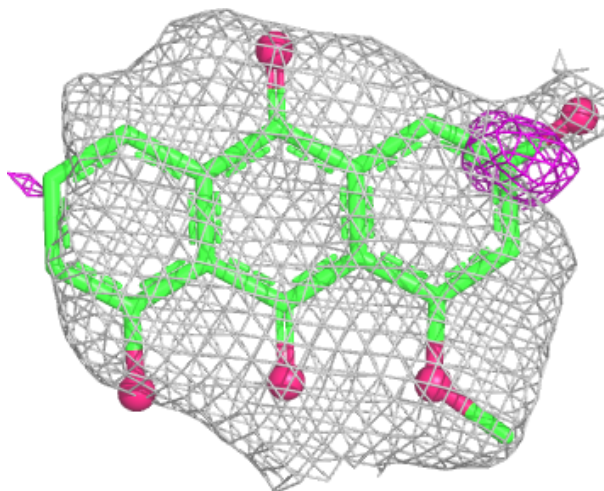
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NA	A	403	1/1	0.68	0.17	68,68,68,68	0
6	GOL	B	405	6/6	0.73	0.20	71,72,75,77	0
3	QPF	D	402	20/20	0.86	0.16	56,62,68,69	0
3	QPF	C	402	20/20	0.88	0.15	59,66,75,81	0
5	CL	C	404	1/1	0.88	0.07	62,62,62,62	0
3	QPF	A	402	20/20	0.88	0.16	54,58,68,73	0
6	GOL	B	404	6/6	0.89	0.19	55,67,69,70	0
5	CL	B	403	1/1	0.89	0.07	62,62,62,62	0
5	CL	A	407	1/1	0.90	0.08	59,59,59,59	0
3	QPF	B	402	20/20	0.91	0.16	62,66,73,74	0
4	NA	C	403	1/1	0.92	0.14	60,60,60,60	0
6	GOL	A	408	6/6	0.92	0.13	65,67,67,70	0
4	NA	A	405	1/1	0.94	0.15	55,55,55,55	0
2	SAH	C	401	26/26	0.95	0.14	38,39,44,48	0
5	CL	A	406	1/1	0.95	0.14	67,67,67,67	0
2	SAH	A	401	26/26	0.96	0.10	28,29,36,37	0
2	SAH	B	401	26/26	0.96	0.13	37,39,42,47	0
4	NA	A	404	1/1	0.96	0.14	47,47,47,47	0
4	NA	D	403	1/1	0.97	0.11	37,37,37,37	0
2	SAH	D	401	26/26	0.97	0.09	30,32,40,43	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 QPF D 402:**

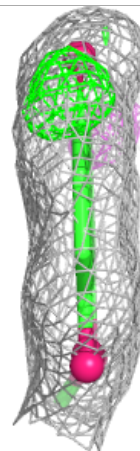
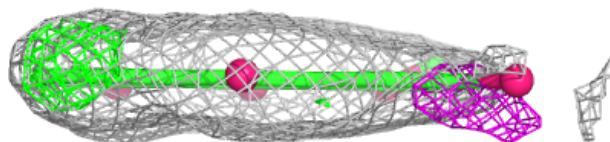
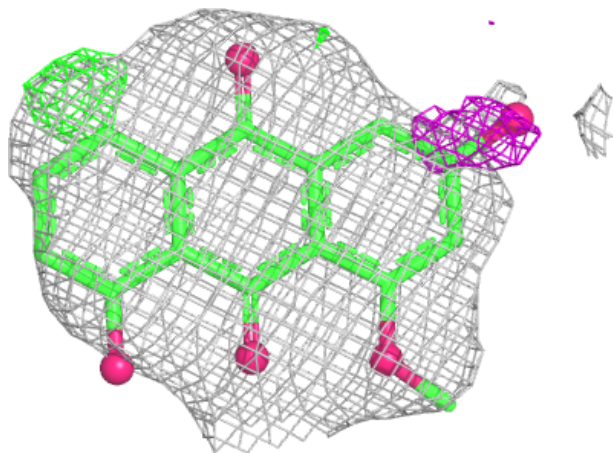
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

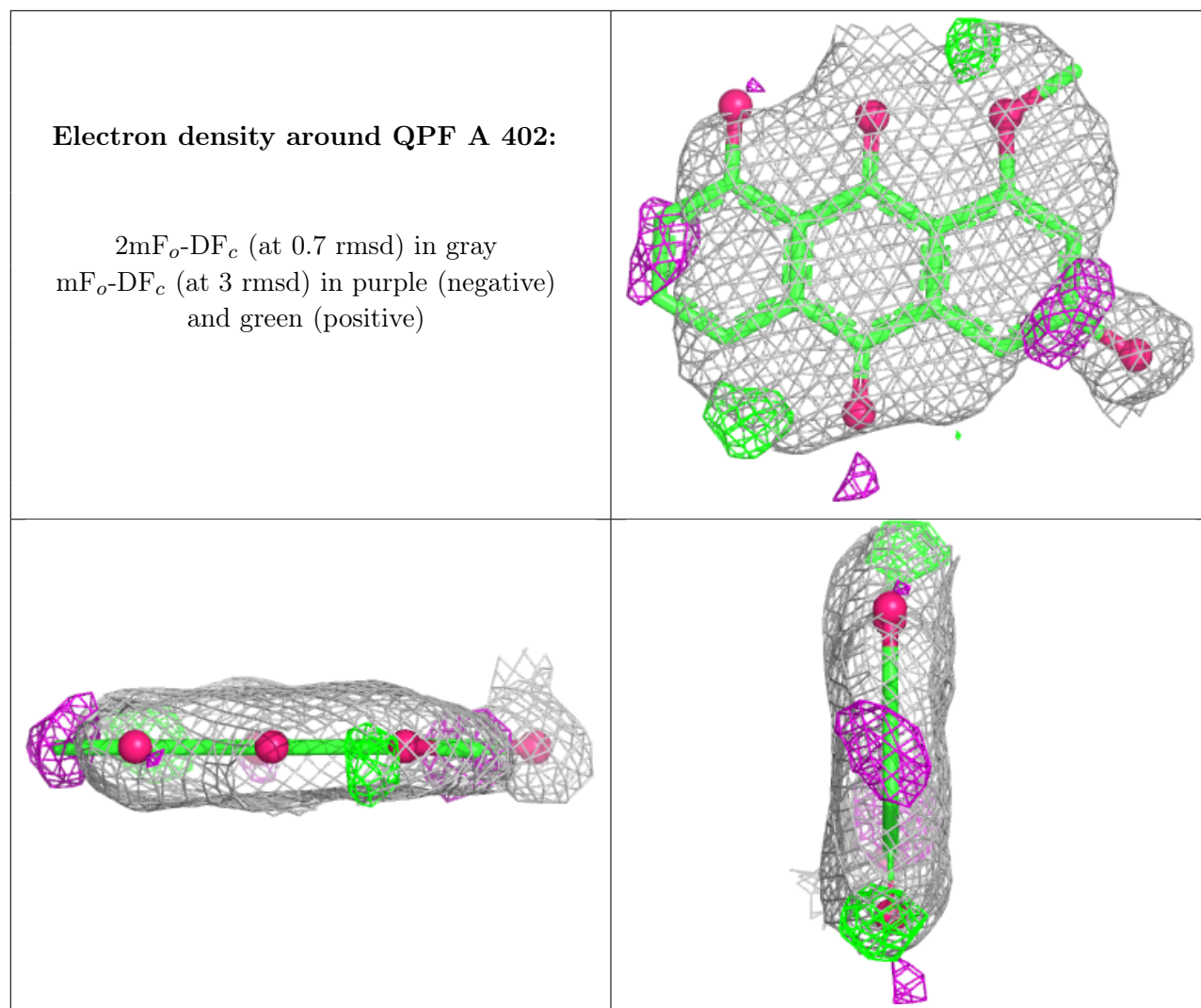




**Electron density around QPF C 402:**

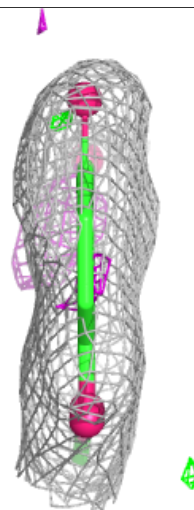
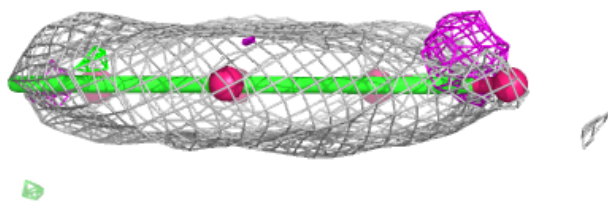
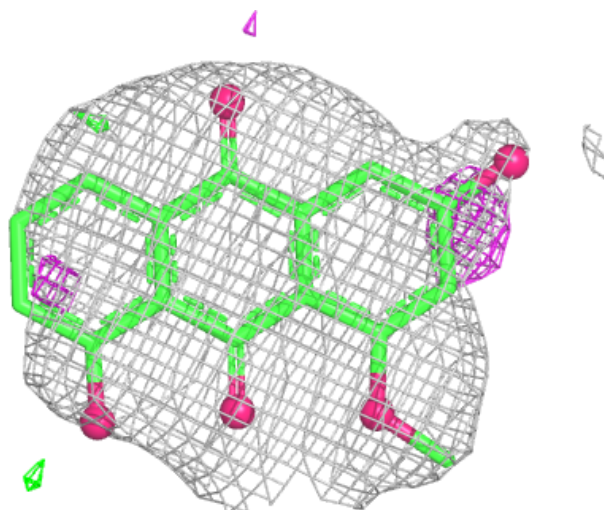
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





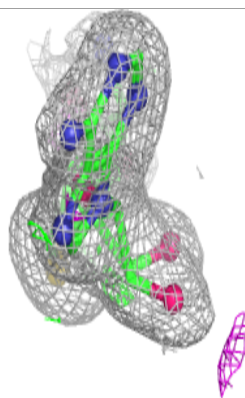
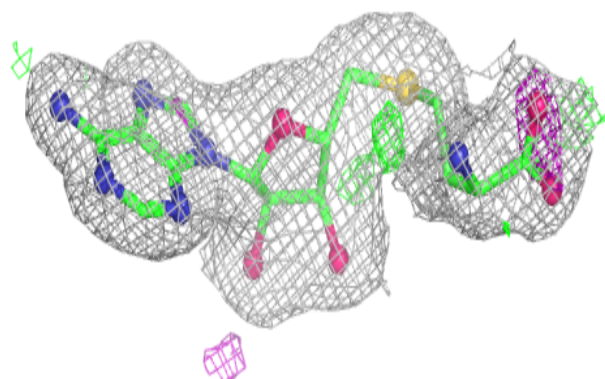
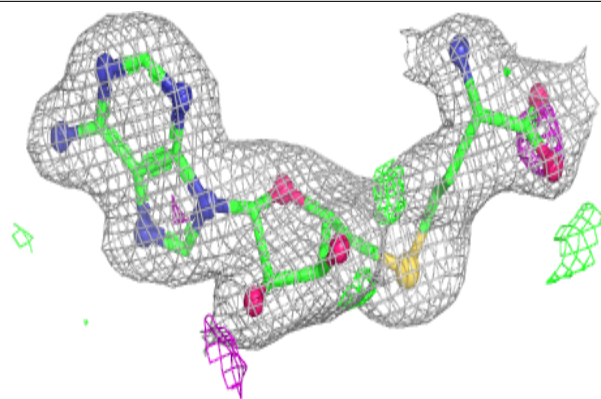
**Electron density around QPF B 402:**

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

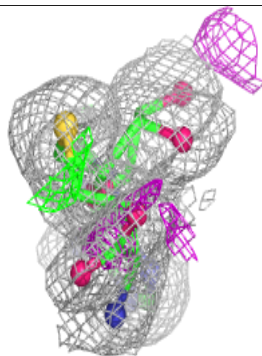
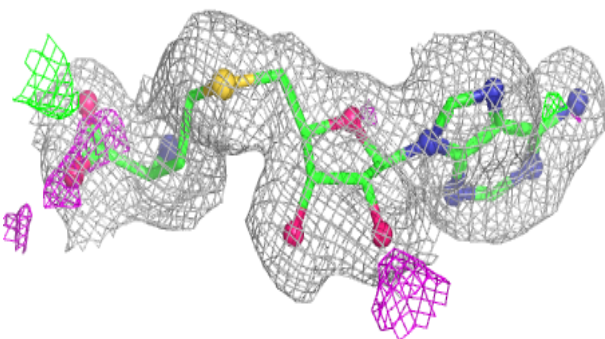
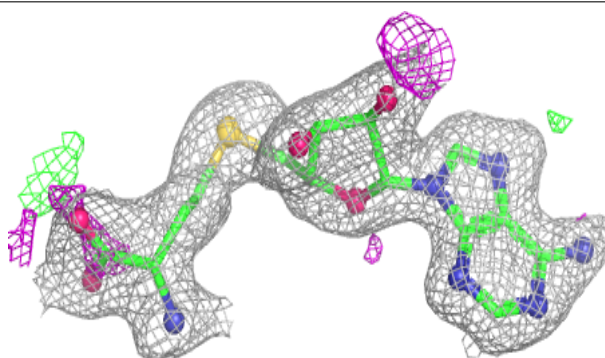


**Electron density around SAH C 401:**

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

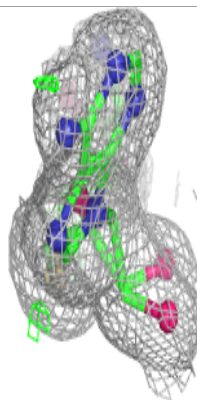
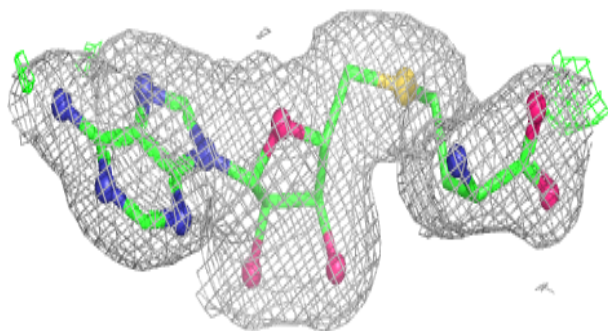
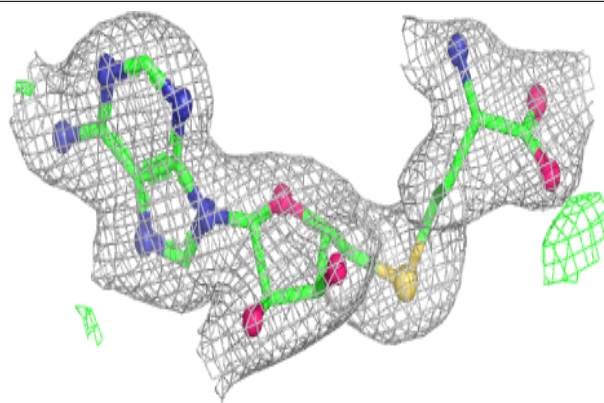
**Electron density around SAH A 401:**

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

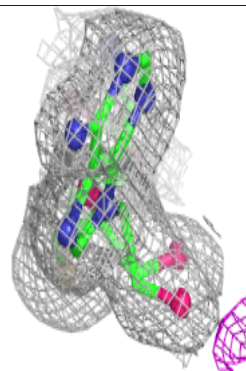
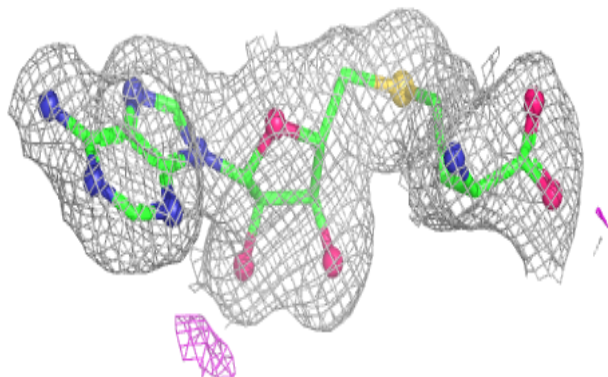
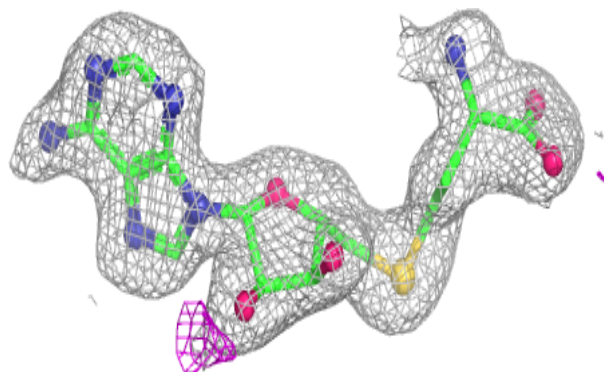


**Electron density around SAH B 401:**

$2mF_o-DF_c$  (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.