



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:35 AM UTC

PDB ID : 8BID / pdb_00008bid
Title : O-Methyltransferase Plu4890 (mutant H229N) in complex with SAH and AQ-270a
Authors : Huber, E.M.; Groll, M.
Deposited on : 2022-11-02
Resolution : 1.75 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

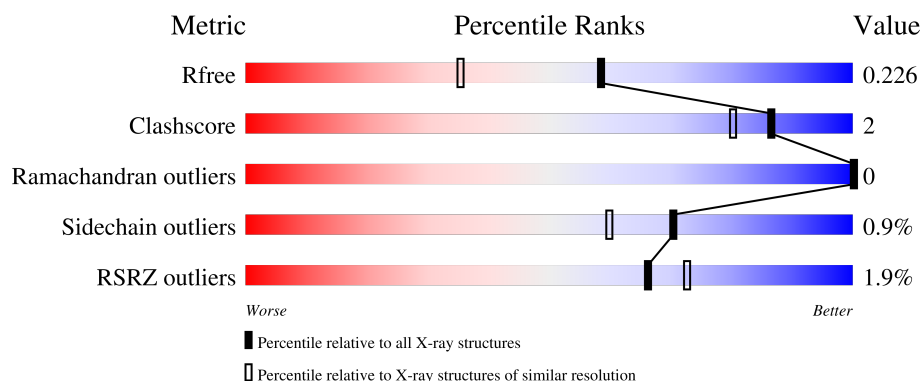
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

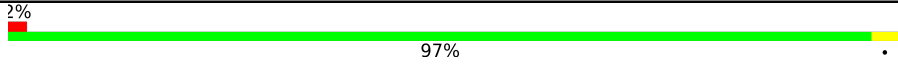
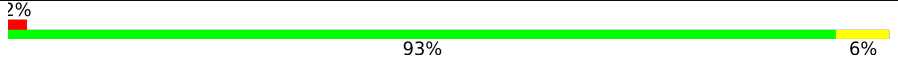
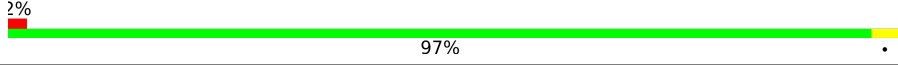
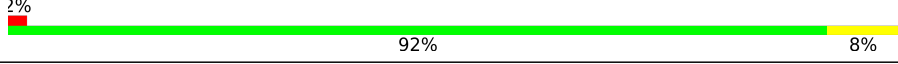
The reported resolution of this entry is 1.75 Å.

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}	180053	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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 $\leq 5\%$. 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	
1	B	319	
1	C	319	
1	D	319	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	CL	B	403	-	-	X	-
5	CL	D	403	-	-	X	-
5	CL	D	405	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11205 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.

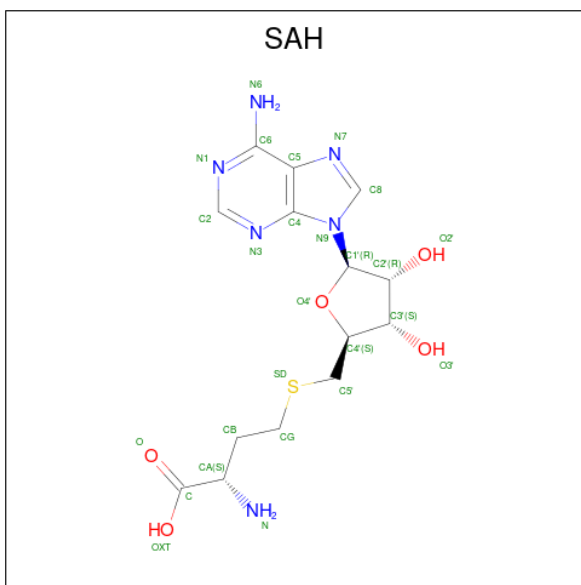
- Molecule 1 is a protein called methyltransferase Plu4890 H229N mutant.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	S	0	2	0
			2583	1657	425	489	12			
1	B	319	Total	C	N	O	S	0	5	0
			2611	1672	429	497	13			
1	C	319	Total	C	N	O	S	0	5	0
			2606	1666	430	497	13			
1	D	319	Total	C	N	O	S	0	5	0
			2614	1674	432	495	13			

There are 8 discrepancies between the modelled and reference sequences:

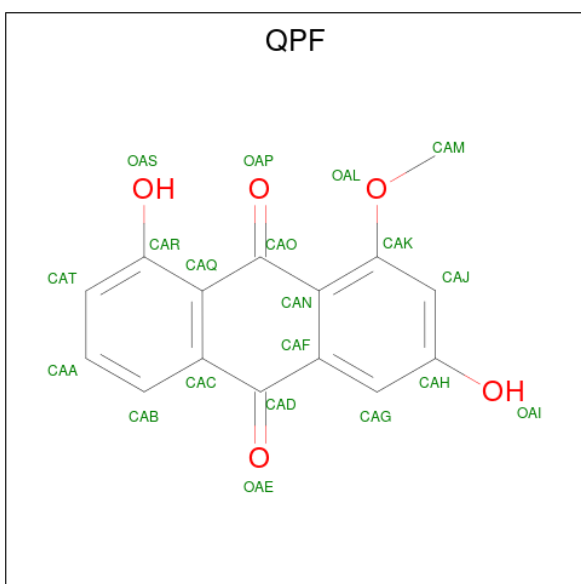
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP A0A6L9JR93
A	229	ASN	HIS	engineered mutation	UNP A0A6L9JR93
B	0	SER	-	expression tag	UNP A0A6L9JR93
B	229	ASN	HIS	engineered mutation	UNP A0A6L9JR93
C	0	SER	-	expression tag	UNP A0A6L9JR93
C	229	ASN	HIS	engineered mutation	UNP A0A6L9JR93
D	0	SER	-	expression tag	UNP A0A6L9JR93
D	229	ASN	HIS	engineered mutation	UNP A0A6L9JR93

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: C₁₄H₂₀N₆O₅S).



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		

- Molecule 3 is 1-methoxy-3,8-bis(oxidanyl)anthracene-9,10-dione (CCD ID: 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 (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Na	0	0
			2	2		
4	B	7	Total	Na	0	0
			7	7		
4	C	2	Total	Na	0	0
			2	2		
4	D	8	Total	Na	0	0
			8	8		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Cl	0	0
			1	1		
5	D	3	Total	Cl	0	0
			3	3		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	105	Total	O	0	0
			105	105		
7	B	172	Total	O	0	0
			172	172		
7	C	96	Total	O	0	0
			96	96		
7	D	175	Total	O	0	0
			175	175		

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 H229N mutant



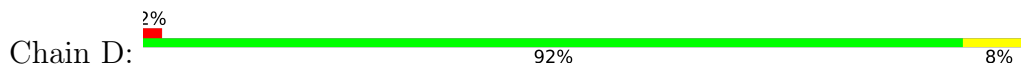
- Molecule 1: methyltransferase Plu4890 H229N mutant



- Molecule 1: methyltransferase Plu4890 H229N mutant



- Molecule 1: methyltransferase Plu4890 H229N mutant



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.40Å 77.67Å 167.33Å 90.00° 95.49° 90.00°	Depositor
Resolution (Å)	30.00 – 1.75 30.00 – 1.75	Depositor EDS
% Data completeness (in resolution range)	97.6 (30.00-1.75) 97.6 (30.00-1.75)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.180 , 0.217 0.192 , 0.226	Depositor DCC
R_{free} test set	7958 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	28.4	Xtriage
Anisotropy	0.280	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 48.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	11205	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.65 % 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 1.4792e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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: NA, SAH, CL, GOL, QPF

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.03	0/2637	1.33	0/3550
1	B	1.10	5/2665 (0.2%)	1.28	0/3587
1	C	1.03	0/2659	1.31	0/3579
1	D	1.09	1/2668 (0.0%)	1.29	0/3591
All	All	1.06	6/10629 (0.1%)	1.31	0/14307

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	14	ALA	C-O	5.77	1.30	1.24
1	D	103	MET	C-O	5.73	1.31	1.24
1	B	10	ARG	C-O	5.39	1.30	1.24
1	B	96	HIS	C-O	5.34	1.30	1.24
1	B	103	MET	C-O	5.08	1.30	1.24
1	B	105	GLY	C-O	5.02	1.29	1.23

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	2583	0	2537	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2611	0	2554	12	0
1	C	2606	0	2556	5	0
1	D	2614	0	2565	23	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
3	B	20	0	0	2	0
3	C	20	0	0	1	0
3	D	20	0	0	3	0
4	A	2	0	0	0	0
4	B	7	0	0	0	0
4	C	2	0	0	0	0
4	D	8	0	0	0	0
5	B	1	0	0	2	0
5	D	3	0	0	5	0
6	B	6	0	8	1	0
6	C	12	0	16	0	0
6	D	18	0	24	4	0
7	A	105	0	0	0	0
7	B	172	0	0	0	0
7	C	96	0	0	0	0
7	D	175	0	0	0	0
All	All	11205	0	10336	45	0

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

All (45) 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:B:307:TYR:HA	1:D:0:SER:CB	2.09	0.82
1:D:75:CYS:SG	6:D:416:GOL:H12	2.23	0.79
1:B:307:TYR:HA	1:D:0:SER:HB2	1.68	0.74
1:D:188:HIS:NE2	5:D:403:CL:CL	2.57	0.71
1:D:179:ARG:NH1	5:D:405:CL:CL	2.66	0.66
1:B:307:TYR:HA	1:D:0:SER:HB3	1.78	0.64
1:B:0:SER:HB3	1:D:307:TYR:HA	1.78	0.64
1:D:219:TYR:OH	5:D:403:CL:CL	2.49	0.60
1:B:205:ASP:OD2	5:B:403:CL:CL	2.57	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:TYR:OH	5:B:403:CL:CL	2.54	0.58
1:D:139:PHE:HE1	3:D:402:QPF:CAM	2.17	0.58
1:B:10:ARG:NH2	6:B:411:GOL:O1	2.36	0.56
1:D:1:MET:HE2	1:D:1:MET:HA	1.86	0.56
1:D:90:LYS:NZ	6:D:415:GOL:H11	2.23	0.54
1:D:175:GLU:OE2	5:D:405:CL:CL	2.64	0.51
1:D:205:ASP:OD2	5:D:403:CL:CL	2.66	0.51
3:B:402:QPF:OAL	3:B:402:QPF:OAP	2.27	0.51
3:D:402:QPF:OAL	3:D:402:QPF:OAP	2.29	0.51
1:C:266:ARG:HH11	1:C:266:ARG:HB3	1.77	0.50
1:D:225:LYS:HA	1:D:256:ILE:O	2.11	0.50
1:B:221:LEU:HD11	1:B:254:LEU:HG	1.95	0.49
1:B:283[B]:PHE:CE1	1:B:300:THR:HG21	2.48	0.48
1:A:151:VAL:HG12	1:A:176:LEU:HD12	1.94	0.47
1:B:225:LYS:HA	1:B:256:ILE:O	2.15	0.47
1:C:225:LYS:HA	1:C:256:ILE:O	2.15	0.47
1:B:32:TYR:CE1	1:B:70:ARG:HG2	2.50	0.46
3:C:402:QPF:OAL	3:C:402:QPF:OAP	2.33	0.46
3:A:402:QPF:OAP	3:A:402:QPF:OAL	2.31	0.46
1:D:283[B]:PHE:CE1	1:D:300:THR:HG21	2.51	0.46
1:D:15:ILE:HG13	1:D:59[B]:MET:HE1	1.97	0.46
1:A:148:ASN:O	1:A:151:VAL:HG22	2.16	0.46
1:D:142:LEU:HG	1:D:143:MET:HE2	2.00	0.44
1:A:142:LEU:HG	1:A:143:MET:HE2	2.00	0.44
1:D:31:ILE:HD12	1:D:33:VAL:HG23	1.99	0.43
1:C:148:ASN:O	1:C:151:VAL:HG12	2.20	0.42
1:D:258:MET:HE3	1:D:268:PHE:CE2	2.55	0.42
3:B:402:QPF:OAP	3:B:402:QPF:OAS	2.35	0.41
1:D:31:ILE:CD1	1:D:33:VAL:CG2	2.98	0.41
1:D:75:CYS:SG	6:D:416:GOL:C1	3.02	0.41
1:B:141:ALA:O	1:B:145:ARG:HG2	2.20	0.41
1:C:15:ILE:HG13	1:C:59[B]:MET:HE1	2.02	0.41
1:C:15:ILE:HG22	1:C:89:ILE:HG12	2.02	0.41
1:D:81:PRO:HB3	6:D:415:GOL:O3	2.21	0.41
3:D:402:QPF:OAP	3:D:402:QPF:OAS	2.38	0.41
1:D:229:ASN:OD1	1:D:229:ASN:N	2.45	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	318/319 (100%)	317 (100%)	1 (0%)	0	100	100
1	B	322/319 (101%)	319 (99%)	3 (1%)	0	100	100
1	C	322/319 (101%)	321 (100%)	1 (0%)	0	100	100
1	D	322/319 (101%)	320 (99%)	2 (1%)	0	100	100
All	All	1284/1276 (101%)	1277 (100%)	7 (0%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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	288/287 (100%)	284 (99%)	4 (1%)	59	44
1	B	292/287 (102%)	290 (99%)	2 (1%)	76	67
1	C	292/287 (102%)	289 (99%)	3 (1%)	68	56
1	D	292/287 (102%)	291 (100%)	1 (0%)	86	83
All	All	1164/1148 (101%)	1154 (99%)	10 (1%)	70	60

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	211	PHE

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Mol	Chain	Res	Type
1	A	213	ASN
1	A	258	MET
1	B	84	PHE
1	B	260	LYS
1	C	161	ASN
1	C	211	PHE
1	C	266	ARG
1	D	84	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	ASN
1	A	230	ASN
1	B	161	ASN
1	C	250	ASN
1	C	316	GLN
1	D	148	ASN
1	D	161	ASN
1	D	230	ASN
1	D	257	ASN
1	D	292	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 37 ligands modelled in this entry, 23 are monoatomic - leaving 14 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	4	22,22,22	1.71	4 (18%)	33,33,33	1.10	1 (3%)
3	QPF	C	402	-	22,22,22	1.57	4 (18%)	33,33,33	0.83	2 (6%)
6	GOL	C	406	-	5,5,5	0.10	0	5,5,5	0.22	0
6	GOL	D	415	-	5,5,5	0.08	0	5,5,5	0.26	0
3	QPF	A	402	4	22,22,22	1.63	4 (18%)	33,33,33	0.80	1 (3%)
6	GOL	D	416	-	5,5,5	0.13	0	5,5,5	0.41	0
2	SAH	B	401	-	27,28,28	0.54	1 (3%)	36,40,40	0.56	1 (2%)
2	SAH	A	401	-	27,28,28	0.54	1 (3%)	36,40,40	0.58	1 (2%)
3	QPF	D	402	4	22,22,22	1.71	4 (18%)	33,33,33	1.11	3 (9%)
2	SAH	C	401	-	27,28,28	0.48	1 (3%)	36,40,40	0.54	1 (2%)
6	GOL	D	414	-	5,5,5	0.06	0	5,5,5	0.18	0
2	SAH	D	401	-	27,28,28	0.56	1 (3%)	36,40,40	0.57	0
6	GOL	B	411	-	5,5,5	0.10	0	5,5,5	0.23	0
6	GOL	C	405	-	5,5,5	0.10	0	5,5,5	0.16	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
3	QPF	B	402	4	-	0/2/18/18	0/3/3/3
3	QPF	C	402	-	-	0/2/18/18	0/3/3/3
6	GOL	C	406	-	-	2/4/4/4	-
6	GOL	D	415	-	-	2/4/4/4	-
3	QPF	A	402	4	-	0/2/18/18	0/3/3/3
6	GOL	D	416	-	-	4/4/4/4	-
2	SAH	B	401	-	-	1/15/31/31	0/3/3/3
2	SAH	A	401	-	-	0/15/31/31	0/3/3/3
3	QPF	D	402	4	-	2/2/18/18	0/3/3/3
2	SAH	C	401	-	-	1/15/31/31	0/3/3/3
6	GOL	D	414	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SAH	D	401	-	-	0/15/31/31	0/3/3/3
6	GOL	B	411	-	-	1/4/4/4	-
6	GOL	C	405	-	-	0/4/4/4	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	QPF	CAF-CAD	-4.37	1.39	1.48
3	A	402	QPF	CAC-CAD	-4.13	1.40	1.48
3	C	402	QPF	CAC-CAD	-4.07	1.40	1.48
3	D	402	QPF	CAC-CAD	-4.04	1.40	1.48
3	C	402	QPF	CAF-CAD	-4.04	1.40	1.48
3	B	402	QPF	CAC-CAD	-3.82	1.40	1.48
3	B	402	QPF	CAQ-CAO	-3.43	1.39	1.47
3	D	402	QPF	CAQ-CAO	-3.35	1.39	1.47
3	B	402	QPF	CAF-CAD	-3.17	1.42	1.48
3	D	402	QPF	CAF-CAD	-3.15	1.42	1.48
3	A	402	QPF	CAN-CAO	-3.06	1.40	1.47
3	D	402	QPF	CAN-CAO	-2.97	1.40	1.47
3	C	402	QPF	CAQ-CAO	-2.95	1.40	1.47
3	A	402	QPF	CAQ-CAO	-2.86	1.41	1.47
3	C	402	QPF	CAN-CAO	-2.80	1.41	1.47
3	B	402	QPF	CAN-CAO	-2.74	1.41	1.47
2	B	401	SAH	OXT-C	-2.35	1.23	1.30
2	D	401	SAH	OXT-C	-2.33	1.23	1.30
2	A	401	SAH	OXT-C	-2.29	1.23	1.30
2	C	401	SAH	OXT-C	-2.17	1.23	1.30

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	402	QPF	CAK-CAN-CAO	-3.00	118.20	122.22
3	B	402	QPF	CAK-CAN-CAO	-2.77	118.50	122.22
3	A	402	QPF	OAS-CAR-CAQ	-2.34	116.81	121.14
2	A	401	SAH	OXT-C-O	-2.28	118.91	124.08
3	C	402	QPF	OAS-CAR-CAQ	-2.20	117.07	121.14
3	D	402	QPF	OAS-CAR-CAQ	-2.18	117.10	121.14
3	C	402	QPF	CAM-OAL-CAK	2.14	120.65	117.51
2	B	401	SAH	OXT-C-O	-2.12	119.28	124.08
2	C	401	SAH	OXT-C-O	-2.03	119.47	124.08
3	D	402	QPF	CAT-CAA-CAB	-2.02	117.64	120.24

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	416	GOL	O1-C1-C2-C3
3	D	402	QPF	CAJ-CAK-OAL-CAM
3	D	402	QPF	CAN-CAK-OAL-CAM
6	C	406	GOL	C1-C2-C3-O3
6	D	414	GOL	C1-C2-C3-O3
6	D	415	GOL	C1-C2-C3-O3
6	D	416	GOL	C1-C2-C3-O3
6	D	416	GOL	O1-C1-C2-O2
6	C	406	GOL	O2-C2-C3-O3
6	D	416	GOL	O2-C2-C3-O3
6	D	414	GOL	O2-C2-C3-O3
6	D	415	GOL	O2-C2-C3-O3
6	B	411	GOL	O2-C2-C3-O3
2	B	401	SAH	OXT-C-CA-N
2	C	401	SAH	OXT-C-CA-N

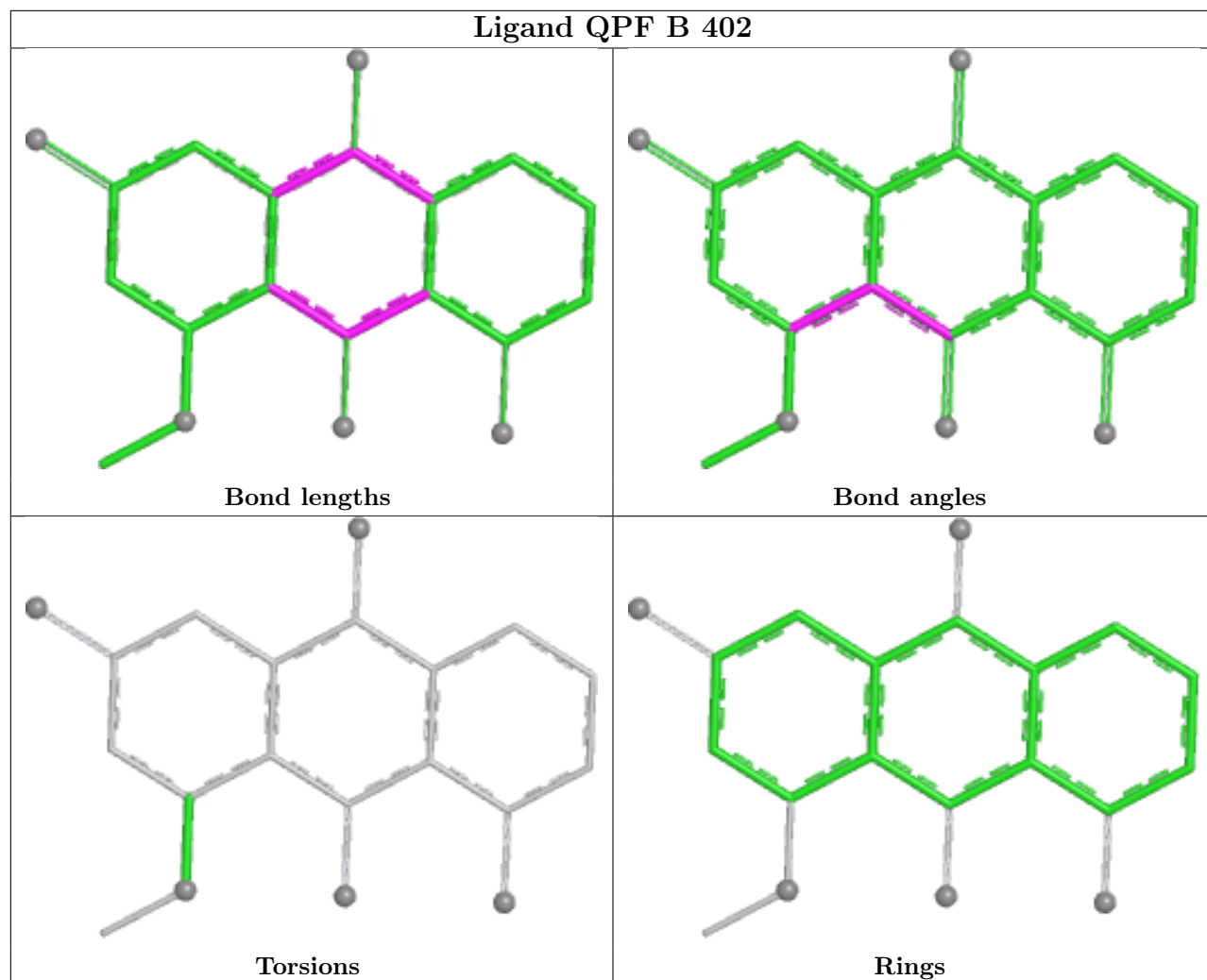
There are no ring outliers.

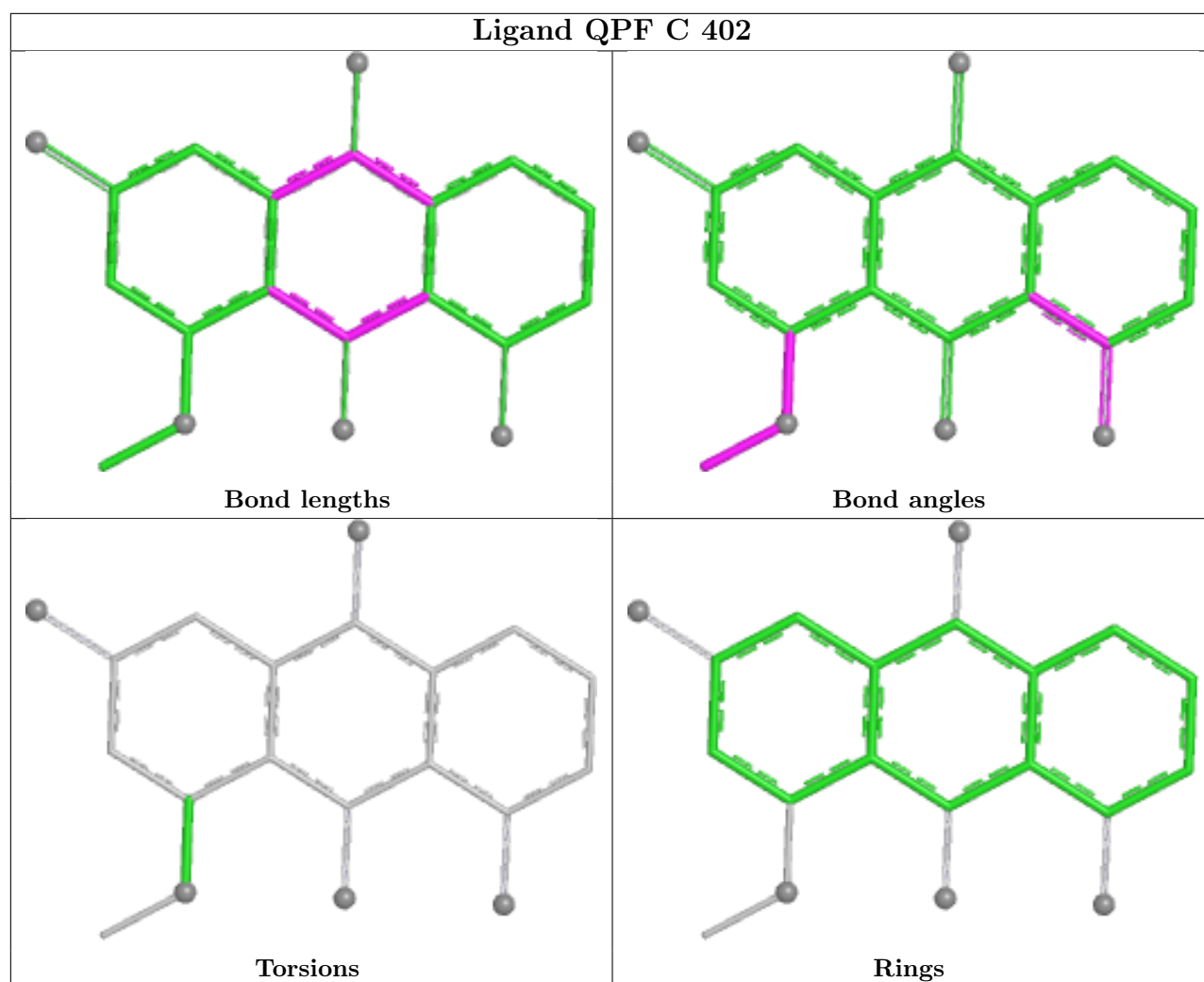
7 monomers are involved in 12 short contacts:

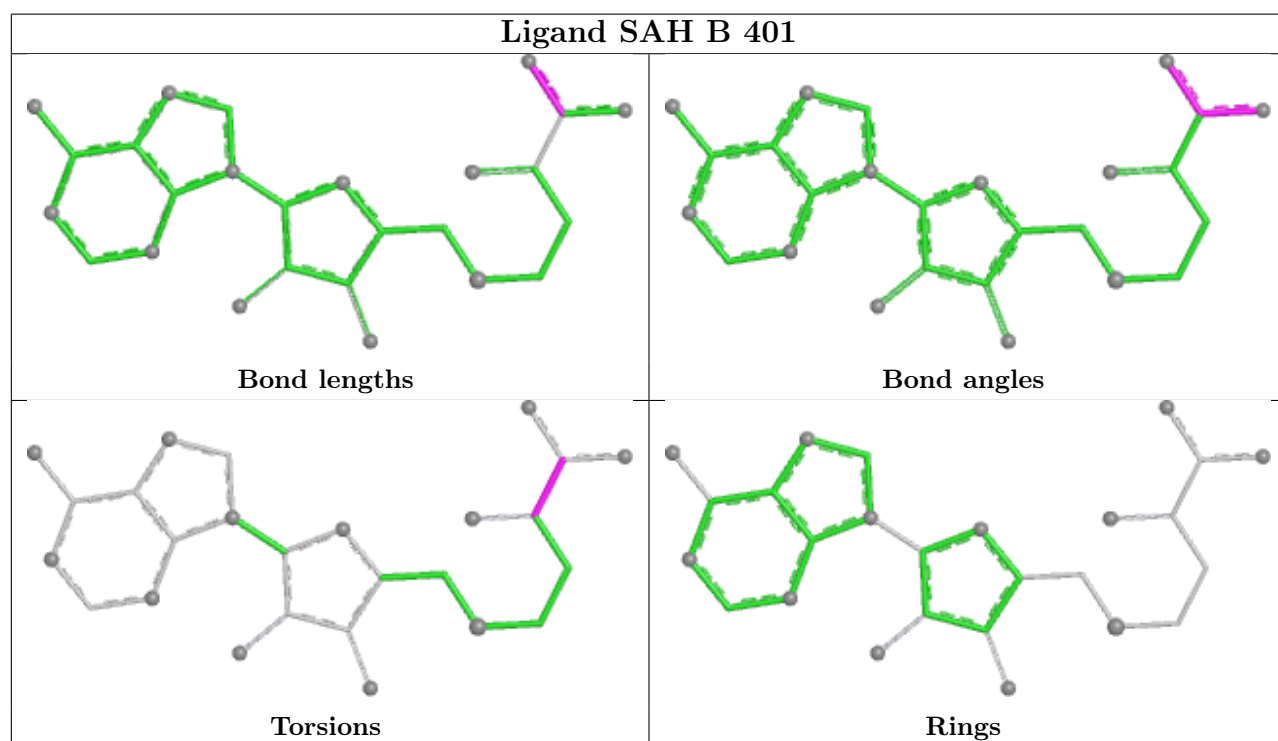
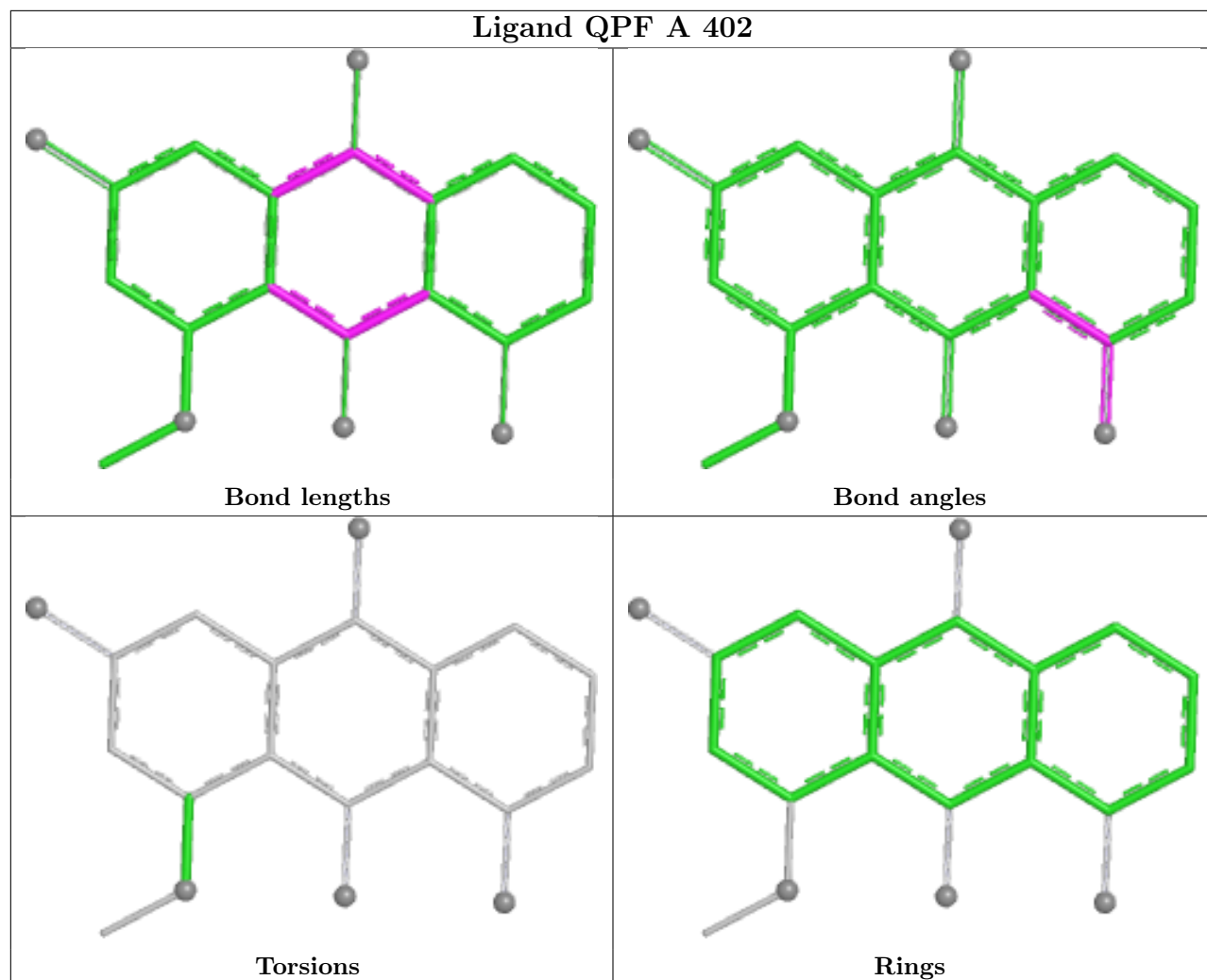
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	402	QPF	2	0
3	C	402	QPF	1	0
6	D	415	GOL	2	0
3	A	402	QPF	1	0
6	D	416	GOL	2	0
3	D	402	QPF	3	0
6	B	411	GOL	1	0

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.

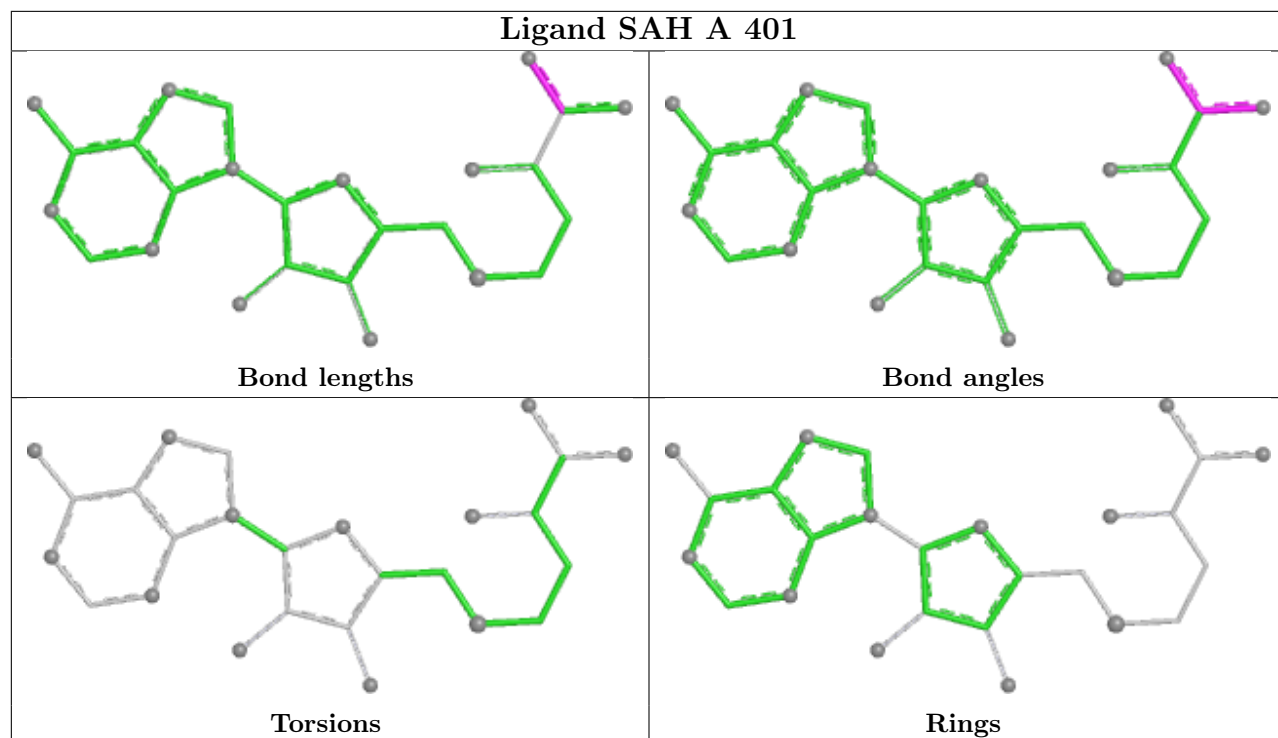
Ligand QPF B 402



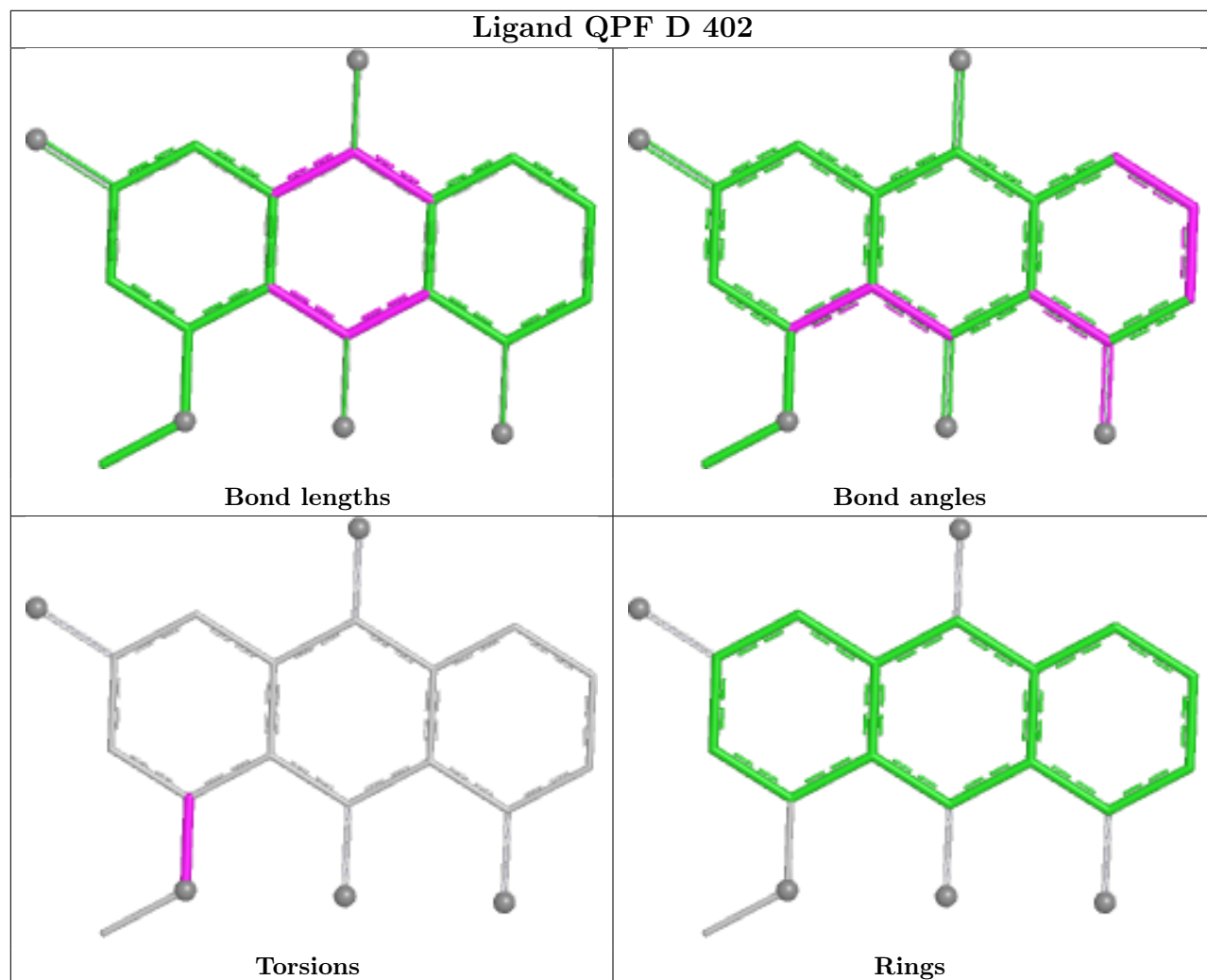


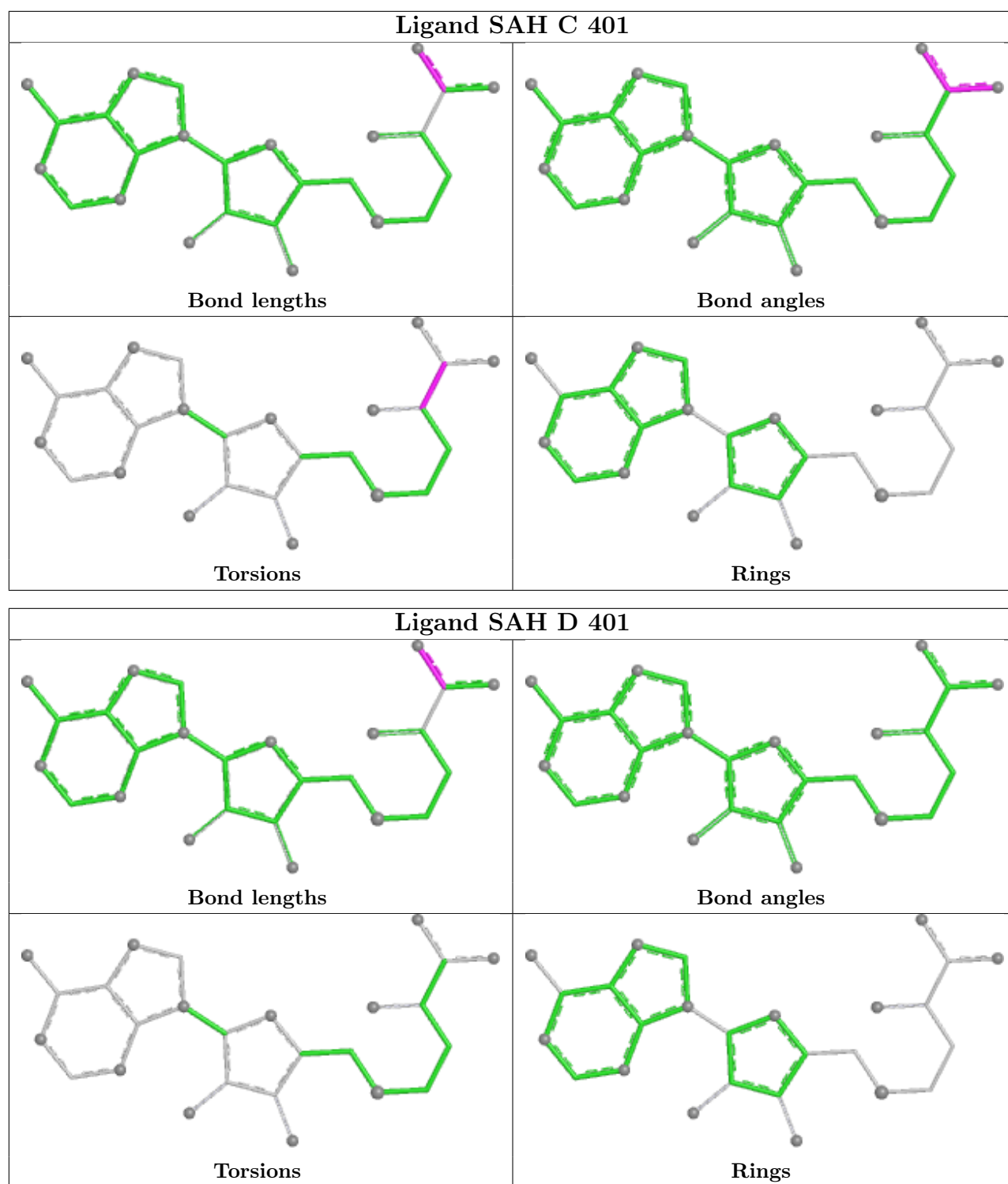


Ligand SAH A 401



Ligand QPF D 402





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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, 95th 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	318/319 (99%)	0.44	6 (1%) 66 73	21, 36, 57, 69	2 (0%)
1	B	319/319 (100%)	0.21	7 (2%) 62 69	11, 30, 52, 184	5 (1%)
1	C	319/319 (100%)	0.43	5 (1%) 70 77	15, 36, 57, 69	5 (1%)
1	D	319/319 (100%)	0.14	6 (1%) 66 73	10, 29, 51, 235	5 (1%)
All	All	1275/1276 (99%)	0.31	24 (1%) 66 73	10, 33, 55, 235	17 (1%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	40	ARG	7.1
1	B	40	ARG	6.8
1	A	283[A]	PHE	5.2
1	B	283[A]	PHE	5.0
1	D	283[A]	PHE	4.6
1	A	1	MET	2.9
1	B	50	SER	2.9
1	B	203	ASN	2.9
1	A	203	ASN	2.8
1	B	1	MET	2.7
1	B	186	GLY	2.6
1	D	1	MET	2.6
1	D	0	SER	2.5
1	C	189	TYR	2.3
1	B	47	ALA	2.3
1	A	189	TYR	2.3
1	C	31	ILE	2.3
1	A	31	ILE	2.2
1	D	112	ASP	2.2
1	C	112	ASP	2.1
1	C	1	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	198	LEU	2.0
1	D	249	LYS	2.0
1	A	200	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 oligosaccharides 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, 95th 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	GOL	D	415	6/6	0.77	0.15	42,46,47,49	0
6	GOL	D	416	6/6	0.79	0.22	24,28,30,31	6
6	GOL	C	406	6/6	0.81	0.24	35,38,40,48	6
3	QPF	C	402	20/20	0.86	0.15	51,54,65,73	0
4	NA	B	406	1/1	0.87	0.21	47,47,47,47	0
3	QPF	D	402	20/20	0.87	0.12	35,40,48,59	0
6	GOL	C	405	6/6	0.88	0.19	23,27,29,34	6
3	QPF	B	402	20/20	0.88	0.13	36,42,48,59	0
4	NA	B	410	1/1	0.89	0.12	45,45,45,45	0
3	QPF	A	402	20/20	0.90	0.12	48,55,61,64	0
6	GOL	B	411	6/6	0.90	0.14	28,31,35,37	0
5	CL	D	405	1/1	0.91	0.13	71,71,71,71	0
4	NA	C	403	1/1	0.91	0.19	64,64,64,64	0
4	NA	D	410	1/1	0.91	0.12	42,42,42,42	0
4	NA	A	404	1/1	0.92	0.22	58,58,58,58	0
4	NA	D	413	1/1	0.93	0.27	45,45,45,45	0
4	NA	B	404	1/1	0.94	0.23	57,57,57,57	0
4	NA	C	404	1/1	0.95	0.17	45,45,45,45	0
4	NA	A	403	1/1	0.95	0.12	48,48,48,48	0
2	SAH	A	401	26/26	0.95	0.07	27,30,32,33	0

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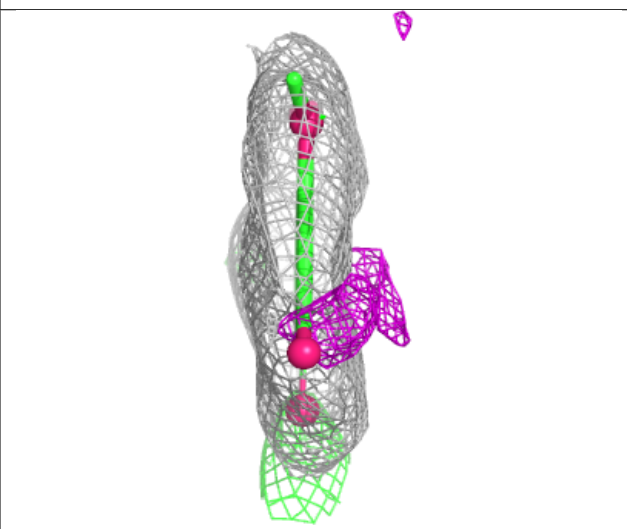
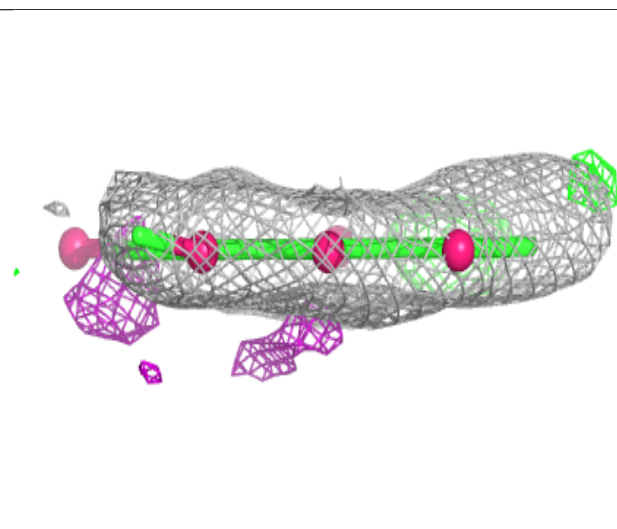
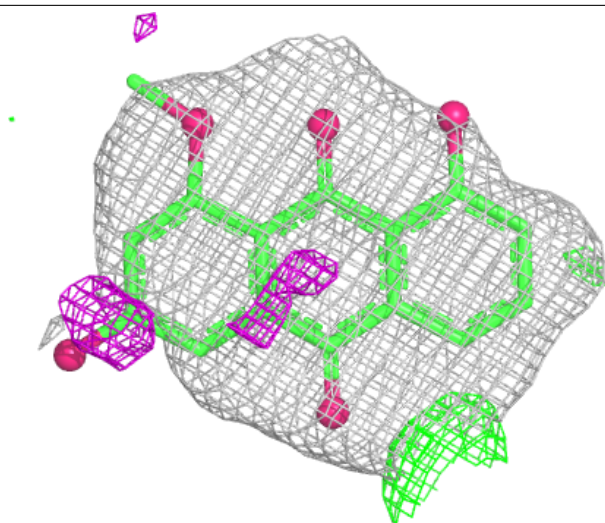
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SAH	C	401	26/26	0.96	0.07	27,31,34,37	0
4	NA	D	407	1/1	0.96	0.10	79,79,79,79	0
5	CL	D	404	1/1	0.97	0.07	53,53,53,53	0
4	NA	D	409	1/1	0.97	0.10	34,34,34,34	0
2	SAH	B	401	26/26	0.97	0.05	22,24,26,29	0
4	NA	D	412	1/1	0.97	0.10	44,44,44,44	0
2	SAH	D	401	26/26	0.97	0.06	22,23,25,27	0
6	GOL	D	414	6/6	0.97	0.07	26,30,34,41	0
5	CL	B	403	1/1	0.97	0.12	61,61,61,61	0
5	CL	D	403	1/1	0.97	0.29	62,62,62,62	0
4	NA	B	405	1/1	0.98	0.07	54,54,54,54	0
4	NA	B	407	1/1	0.98	0.06	49,49,49,49	0
4	NA	B	408	1/1	0.99	0.03	31,31,31,31	0
4	NA	D	406	1/1	0.99	0.12	38,38,38,38	0
4	NA	D	411	1/1	0.99	0.12	30,30,30,30	0
4	NA	B	409	1/1	0.99	0.07	36,36,36,36	0
4	NA	D	408	1/1	0.99	0.07	43,43,43,43	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.

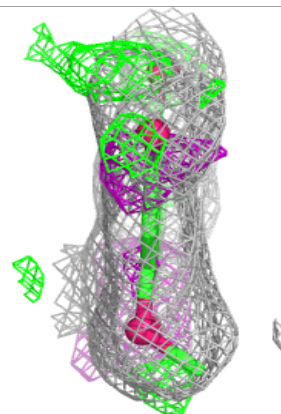
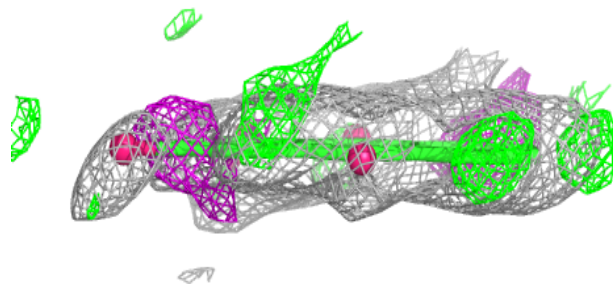
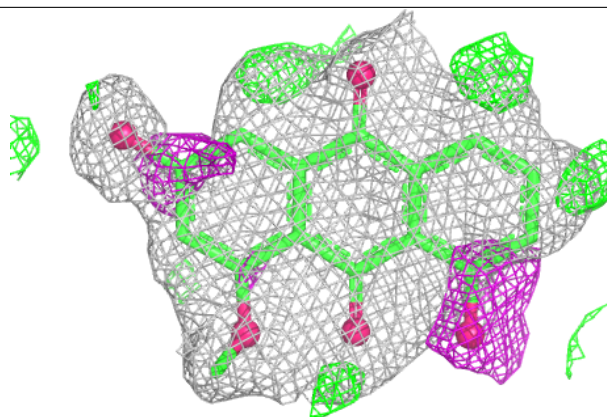
Electron density around QPF C 402:

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



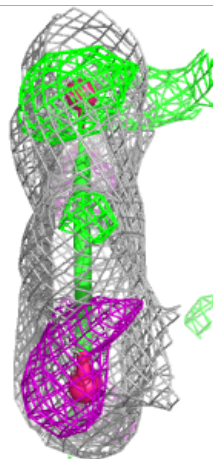
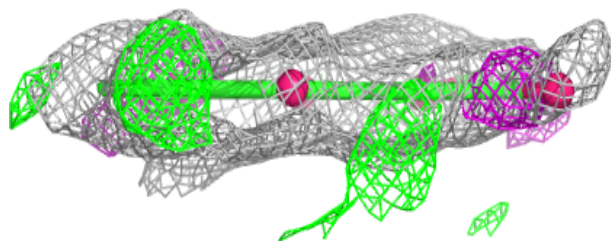
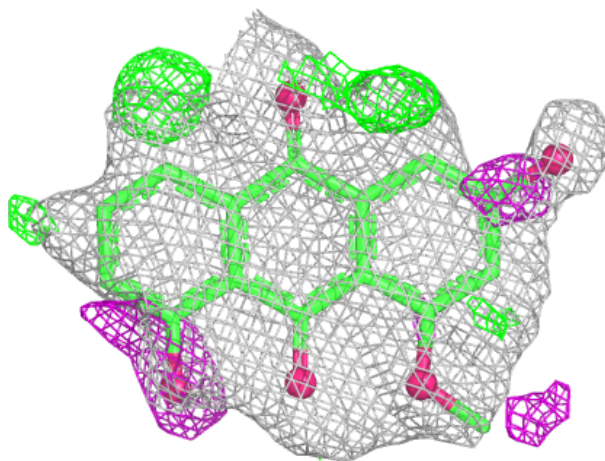
Electron density around QPF D 402:

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and green (positive)



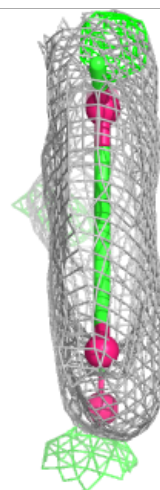
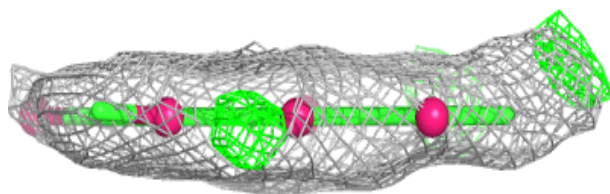
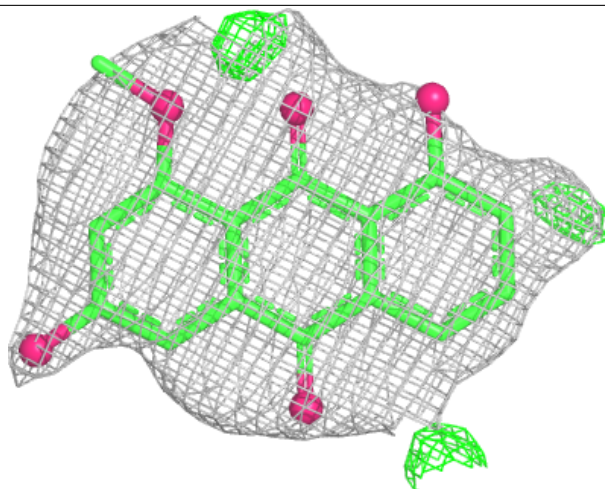
Electron density around QPF B 402:

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and green (positive)



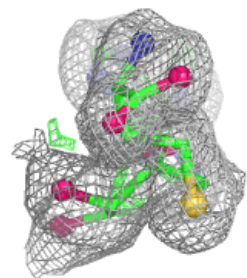
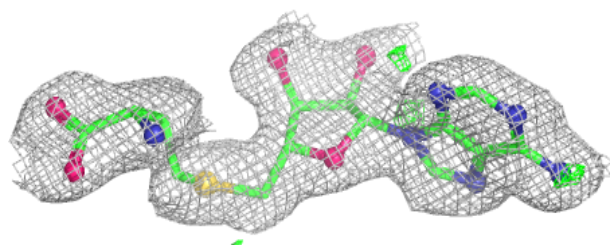
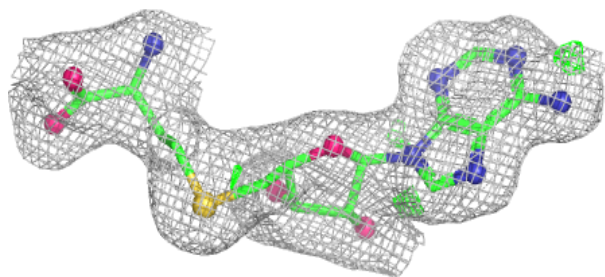
Electron density around QPF A 402:

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and green (positive)

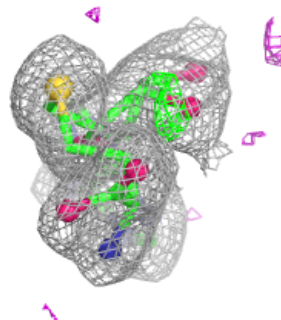
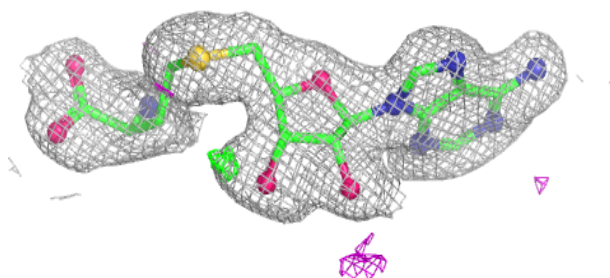
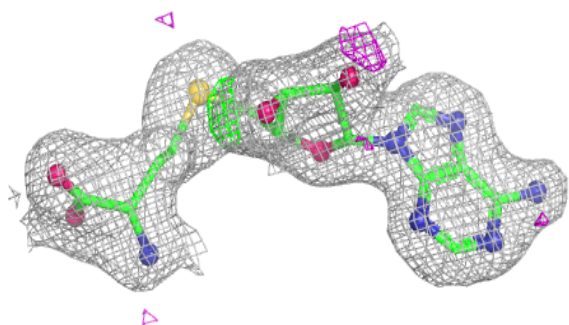


Electron density around SAH A 401:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

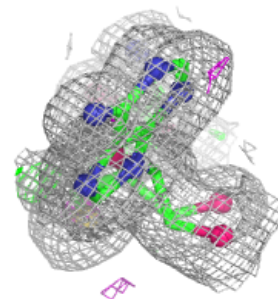
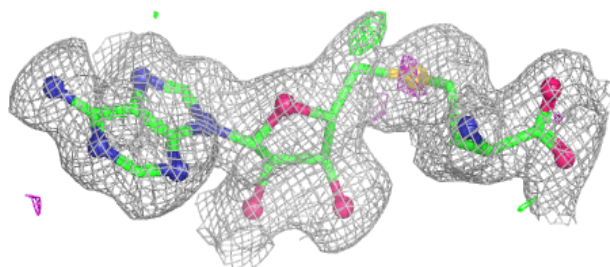
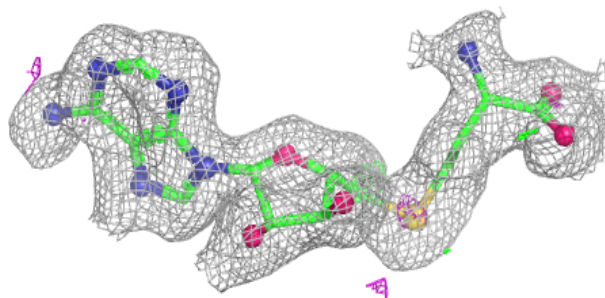
**Electron density around SAH C 401:**

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and green (positive)

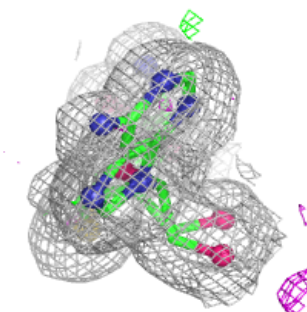
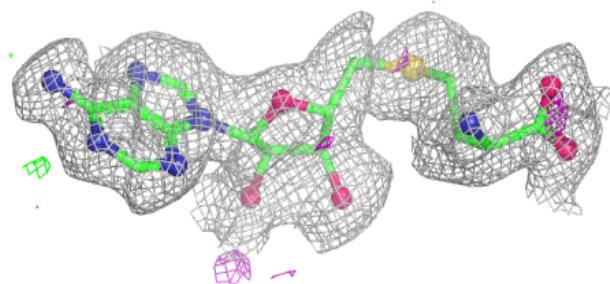
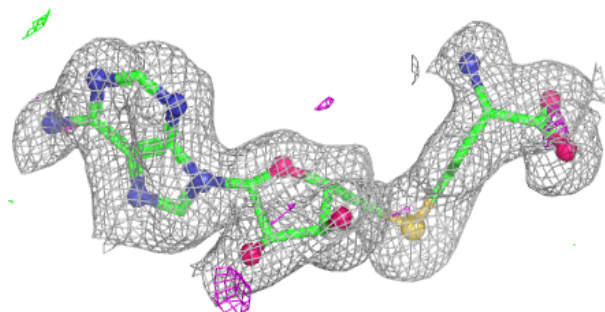


Electron density around SAH B 401:

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 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.