



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 29, 2021 – 12:17 pm BST

PDB ID : 7NR4
Title : X-RAY STRUCTURE OF PRMT6 IN COMPLEX WITH indazole type inhibitor
Authors : Steuber, H.
Deposited on : 2021-03-02
Resolution : 2.03 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.18
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) : 2.18

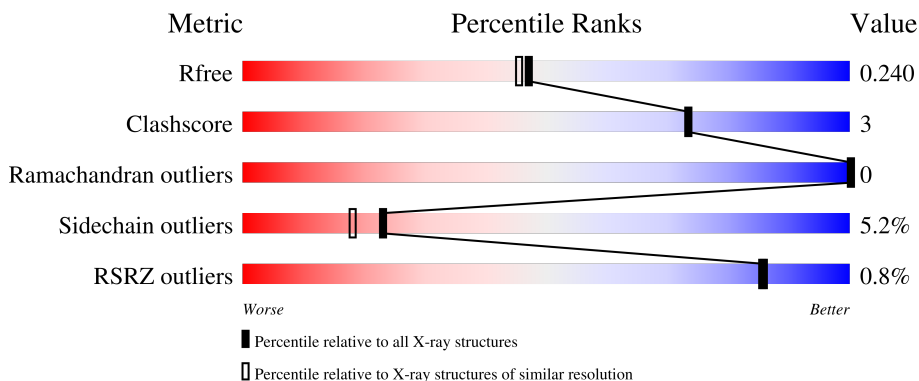
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



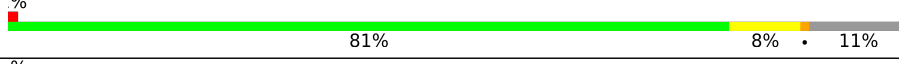

The reported resolution of this entry is 2.03 Å.

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	10434 (2.04-2.00)
Clashscore	141614	11643 (2.04-2.00)
Ramachandran outliers	138981	11493 (2.04-2.00)
Sidechain outliers	138945	11492 (2.04-2.00)
RSRZ outliers	127900	10220 (2.04-2.00)

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	376	 80% 8% • 11%
1	B	376	 80% 9% • 10%
1	C	376	 81% 8% • 11%
1	D	376	 78% 10% • 11%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11308 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.

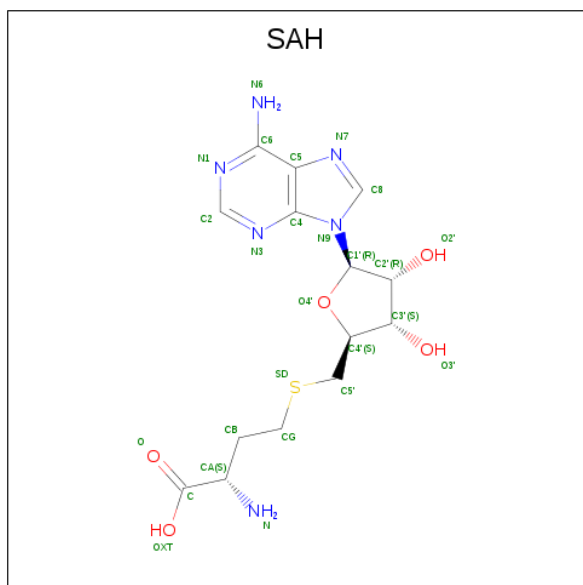
- Molecule 1 is a protein called Protein arginine N-methyltransferase 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	334	2659	1687	470	488	14	0	2	0
1	B	338	2687	1700	476	497	14	0	1	0
1	C	335	2654	1684	470	486	14	0	2	0
1	D	335	2663	1688	473	488	14	0	1	0

There are 8 discrepancies between the modelled and reference sequences:

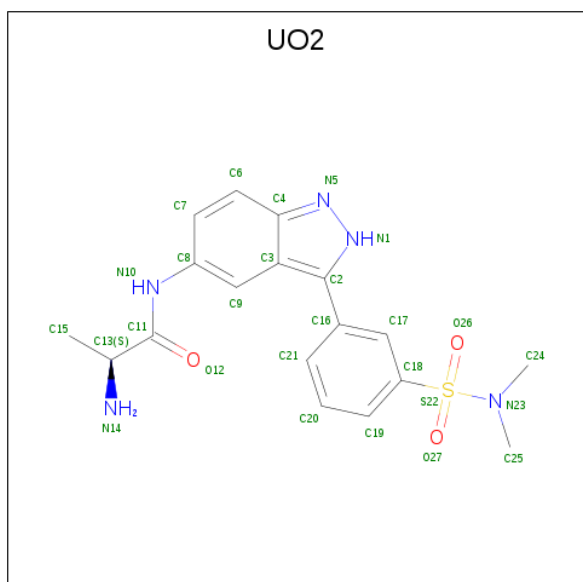
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q96LA8
A	194	VAL	ALA	conflict	UNP Q96LA8
B	0	GLY	-	expression tag	UNP Q96LA8
B	194	VAL	ALA	conflict	UNP Q96LA8
C	0	GLY	-	expression tag	UNP Q96LA8
C	194	VAL	ALA	conflict	UNP Q96LA8
D	0	GLY	-	expression tag	UNP Q96LA8
D	194	VAL	ALA	conflict	UNP Q96LA8

- 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		

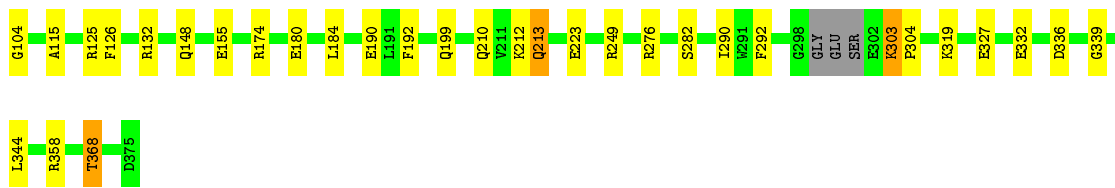
- Molecule 3 is (2 {S})-2-azanyl- {N}-[3-[3-(dimethylsulfamoyl)phenyl]-2 {H}-indazol-5-yl]propanamide (three-letter code: UO2) (formula: C₁₈H₂₁N₅O₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			27	18	5	3	1		
3	B	1	Total	C	N	O	S	0	0
			27	18	5	3	1		
3	C	1	Total	C	N	O	S	0	0
			27	18	5	3	1		
3	D	1	Total	C	N	O	S	0	0
			27	18	5	3	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	110	Total	O	0	0
			110	110		
4	B	122	Total	O	0	0
			122	122		
4	C	109	Total	O	0	0
			109	109		
4	D	92	Total	O	0	0
			92	92		



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	77.94Å 135.25Å 83.20Å 90.00° 98.28° 90.00°	Depositor
Resolution (Å)	49.05 – 2.03 49.05 – 2.03	Depositor EDS
% Data completeness (in resolution range)	97.8 (49.05-2.03) 97.8 (49.05-2.03)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 2.03Å)	Xtrriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.198 , 0.235 0.205 , 0.240	Depositor DCC
R_{free} test set	2062 reflections (1.92%)	wwPDB-VP
Wilson B-factor (Å ²)	33.2	Xtrriage
Anisotropy	0.228	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 29.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11308	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% of the height of the origin peak. No significant pseudotranslation is detected.*

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: UO2, 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	0.69	0/2721	0.87	0/3686
1	B	0.70	0/2750	0.86	0/3723
1	C	0.68	0/2719	0.87	2/3681 (0.1%)
1	D	0.69	0/2725	0.86	0/3690
All	All	0.69	0/10915	0.87	2/14780 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	174	ARG	CB-CG-CD	5.08	124.81	111.60
1	C	174	ARG	CG-CD-NE	5.07	122.45	111.80

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	2659	0	2625	13	0
1	B	2687	0	2649	22	0
1	C	2654	0	2621	18	0
1	D	2663	0	2630	23	0
2	A	26	0	19	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	26	0	19	0	0
2	C	26	0	19	1	0
2	D	26	0	19	2	0
3	A	27	0	0	1	0
3	B	27	0	0	0	0
3	C	27	0	0	0	0
3	D	27	0	0	0	0
4	A	110	0	0	1	0
4	B	122	0	0	1	0
4	C	109	0	0	2	0
4	D	92	0	0	5	0
All	All	11308	0	10601	71	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 3.

All (71) 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:174[A]:ARG:HH11	1:B:174[A]:ARG:HG2	1.32	0.94
1:B:174[A]:ARG:HH11	1:B:174[A]:ARG:CG	1.80	0.94
1:B:174[A]:ARG:HG2	1:B:174[A]:ARG:NH1	1.90	0.83
1:D:56:VAL:HG23	4:D:555:HOH:O	1.79	0.81
1:C:174:ARG:HH11	1:C:174:ARG:HG2	1.44	0.80
1:A:303:LYS:HG2	1:A:304:PRO:CD	2.13	0.79
1:A:303:LYS:HG2	1:A:304:PRO:HD2	1.62	0.79
1:A:174:ARG:HD3	4:A:599:HOH:O	1.83	0.76
1:C:174:ARG:HH11	1:C:174:ARG:CG	2.00	0.73
1:C:50:CYS:SG	1:C:56:VAL:HG11	2.32	0.70
1:B:174[A]:ARG:HH11	1:B:174[A]:ARG:CB	2.07	0.67
1:B:72:LEU:O	1:B:76:ARG:HB2	1.96	0.63
1:D:50:CYS:SG	1:D:56:VAL:HG21	2.39	0.63
1:B:213:GLN:NE2	1:D:210:GLN:OE1	2.32	0.62
1:B:219:MET:HE1	1:C:95:ILE:HD12	1.82	0.62
1:C:130:GLU:HG2	4:C:577:HOH:O	2.01	0.60
1:D:303:LYS:HG3	1:D:304:PRO:HD2	1.85	0.57
1:B:174[A]:ARG:HH11	1:B:174[A]:ARG:HB3	1.70	0.55
1:C:45:GLN:NE2	1:C:49:GLU:OE2	2.40	0.54
1:D:39:THR:HG23	1:D:42:GLU:HB2	1.89	0.54
1:B:367:LYS:HE2	4:B:615:HOH:O	2.07	0.54
1:B:71:ARG:HD3	1:B:99:PHE:CE1	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:ARG:O	1:C:75:LEU:HG	2.10	0.51
1:C:313:HIS:HB3	1:C:314:PRO:HD2	1.92	0.51
1:D:223:GLU:HG3	4:D:508:HOH:O	2.10	0.51
1:A:203:TRP:CZ2	1:B:314:PRO:HD3	2.46	0.51
1:A:184:LEU:HD13	1:A:258:LEU:HB3	1.93	0.50
1:B:80:ALA:O	1:B:84:LYS:HG3	2.12	0.50
1:D:303:LYS:CG	1:D:304:PRO:HD2	2.41	0.50
1:B:219:MET:CE	1:C:95:ILE:HD12	2.42	0.49
1:C:313:HIS:HB3	1:C:314:PRO:CD	2.42	0.49
1:D:39:THR:HG22	1:D:42:GLU:OE1	2.12	0.49
1:A:39:THR:HG23	1:A:42:GLU:HB2	1.94	0.49
1:D:125:ARG:NH1	4:D:504:HOH:O	2.46	0.48
1:A:50:CYS:SG	1:A:56[B]:VAL:HG11	2.55	0.47
1:D:190:GLU:O	1:D:292:PHE:HA	2.15	0.47
1:D:282:SER:OG	1:D:332:GLU:OE1	2.32	0.47
1:A:339:GLY:HA3	1:A:358:ARG:O	2.14	0.47
1:D:339:GLY:HA3	1:D:358:ARG:O	2.16	0.46
1:C:51:TYR:CD1	2:C:401:SAH:H3'	2.50	0.46
1:C:114:SER:OG	1:C:116:ILE:HG22	2.15	0.46
1:B:167:LEU:HD23	1:B:267:LEU:HD11	1.97	0.46
1:B:210:GLN:HE22	1:D:213:GLN:HE22	1.64	0.45
1:C:174:ARG:HG2	1:C:174:ARG:NH1	2.21	0.45
1:C:48:TYR:CE1	1:C:113:ALA:HB3	2.52	0.45
1:B:74:ILE:HD11	1:B:153:VAL:HG21	1.98	0.45
1:A:56[A]:VAL:HG13	3:A:402:UO2:C6	2.47	0.45
1:B:276:ARG:NH1	1:B:336:ASP:OD2	2.50	0.45
1:A:325:LEU:HD22	1:A:359:TYR:CZ	2.52	0.44
1:D:174[A]:ARG:HD2	1:D:184:LEU:HD11	1.99	0.44
1:D:60:MET:HE3	2:D:401:SAH:HG2	1.99	0.44
1:D:82:ARG:HG3	1:D:104:GLY:HA3	1.99	0.44
1:D:101:ALA:O	1:D:132:ARG:NH2	2.51	0.43
1:B:85:THR:HA	1:B:107:ARG:O	2.19	0.43
1:D:368:THR:HG23	4:D:588:HOH:O	2.17	0.43
1:D:60:MET:CE	2:D:401:SAH:HG2	2.48	0.43
1:B:365:GLU:OE2	1:B:367:LYS:HE3	2.19	0.43
1:A:107[A]:ARG:NH1	1:A:131:ASP:O	2.51	0.42
1:C:305:LEU:HD23	1:C:306:VAL:N	2.34	0.42
1:C:76:ARG:HH11	1:C:76:ARG:HG2	1.84	0.42
1:C:85:THR:OG1	1:C:149:VAL:HA	2.20	0.42
1:C:175:THR:HB	4:C:533:HOH:O	2.20	0.41
1:D:344:LEU:N	1:D:344:LEU:HD23	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:TYR:CE1	1:A:155:GLU:HG2	2.55	0.41
1:B:325:LEU:HD22	1:B:359:TYR:CZ	2.56	0.41
1:D:192:PHE:O	1:D:290:ILE:HA	2.21	0.41
1:B:52:SER:HB2	1:B:115:ALA:HB3	2.03	0.41
1:B:192:PHE:O	1:B:290:ILE:HA	2.21	0.41
1:D:319:LYS:HA	4:D:587:HOH:O	2.21	0.40
1:D:52:SER:HB2	1:D:115:ALA:HB3	2.03	0.40
1:A:313:HIS:HB3	1:A:314:PRO:CD	2.52	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	332/376 (88%)	325 (98%)	7 (2%)	0	100	100
1	B	337/376 (90%)	331 (98%)	6 (2%)	0	100	100
1	C	333/376 (89%)	325 (98%)	8 (2%)	0	100	100
1	D	332/376 (88%)	324 (98%)	8 (2%)	0	100	100
All	All	1334/1504 (89%)	1305 (98%)	29 (2%)	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	282/310 (91%)	266 (94%)	16 (6%)	20	15
1	B	285/310 (92%)	272 (95%)	13 (5%)	27	22
1	C	280/310 (90%)	267 (95%)	13 (5%)	27	22
1	D	282/310 (91%)	264 (94%)	18 (6%)	17	12
All	All	1129/1240 (91%)	1069 (95%)	60 (5%)	23	17

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	THR
1	A	40	LYS
1	A	45	GLN
1	A	49	GLU
1	A	72	LEU
1	A	106	ARG
1	A	107[A]	ARG
1	A	107[B]	ARG
1	A	114	SER
1	A	125	ARG
1	A	155	GLU
1	A	202	GLU
1	A	239	GLN
1	A	327	GLU
1	A	347	ARG
1	A	368	THR
1	B	39	THR
1	B	45	GLN
1	B	76	ARG
1	B	106	ARG
1	B	155	GLU
1	B	174[A]	ARG
1	B	174[B]	ARG
1	B	303	LYS
1	B	305	LEU
1	B	327	GLU
1	B	365	GLU
1	B	368	THR
1	B	375	ASP
1	C	41	ARG
1	C	45	GLN
1	C	72	LEU
1	C	125	ARG

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Mol	Chain	Res	Type
1	C	130	GLU
1	C	143	VAL
1	C	155	GLU
1	C	174	ARG
1	C	180	GLU
1	C	200	MET
1	C	327	GLU
1	C	336	ASP
1	C	374	GLU
1	D	39	THR
1	D	41	ARG
1	D	42	GLU
1	D	45	GLN
1	D	76	ARG
1	D	126	PHE
1	D	148	GLN
1	D	155	GLU
1	D	180	GLU
1	D	199	GLN
1	D	212	LYS
1	D	213	GLN
1	D	249	ARG
1	D	276	ARG
1	D	303	LYS
1	D	327	GLU
1	D	336	ASP
1	D	368	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	199	GLN
1	A	210	GLN
1	B	210	GLN
1	B	213	GLN
1	C	330	GLN
1	D	45	GLN
1	D	213	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](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SAH	D	401	-	21,28,28	0.77	0	20,40,40	0.87	0
2	SAH	B	401	-	21,28,28	0.76	0	20,40,40	0.85	0
3	UO2	B	402	-	26,29,29	2.64	5 (19%)	35,43,43	2.12	8 (22%)
3	UO2	C	402	-	26,29,29	2.72	7 (26%)	35,43,43	2.01	8 (22%)
3	UO2	A	402	-	26,29,29	2.68	8 (30%)	35,43,43	1.58	6 (17%)
3	UO2	D	402	-	26,29,29	2.68	7 (26%)	35,43,43	2.00	9 (25%)
2	SAH	A	401	-	21,28,28	0.77	1 (4%)	20,40,40	0.84	0
2	SAH	C	401	-	21,28,28	0.73	1 (4%)	20,40,40	0.90	2 (10%)

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	D	401	-	-	2/7/31/31	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SAH	B	401	-	-	0/7/31/31	0/3/3/3
3	UO2	B	402	-	-	5/24/24/24	0/3/3/3
3	UO2	C	402	-	-	6/24/24/24	0/3/3/3
3	UO2	A	402	-	-	8/24/24/24	0/3/3/3
3	UO2	D	402	-	-	6/24/24/24	0/3/3/3
2	SAH	A	401	-	-	0/7/31/31	0/3/3/3
2	SAH	C	401	-	-	0/7/31/31	0/3/3/3

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	402	UO2	O26-S22	7.47	1.51	1.43
3	D	402	UO2	N5-N1	-7.11	1.24	1.37
3	C	402	UO2	N5-N1	-7.00	1.24	1.37
3	B	402	UO2	N5-N1	-6.73	1.24	1.37
3	B	402	UO2	O27-S22	6.68	1.50	1.43
3	A	402	UO2	N5-N1	-6.58	1.25	1.37
3	A	402	UO2	C16-C2	-6.53	1.40	1.49
3	C	402	UO2	C16-C2	-6.37	1.40	1.49
3	C	402	UO2	O26-S22	5.91	1.50	1.43
3	B	402	UO2	O26-S22	5.88	1.50	1.43
3	A	402	UO2	O26-S22	5.72	1.49	1.43
3	A	402	UO2	O27-S22	5.45	1.49	1.43
3	C	402	UO2	O27-S22	5.24	1.49	1.43
3	D	402	UO2	O27-S22	5.06	1.49	1.43
3	B	402	UO2	C16-C2	-4.54	1.43	1.49
3	D	402	UO2	C16-C2	-3.66	1.44	1.49
3	D	402	UO2	C8-N10	-3.63	1.34	1.41
3	B	402	UO2	C8-N10	-3.48	1.34	1.41
3	C	402	UO2	C6-C4	-3.33	1.36	1.41
3	A	402	UO2	S22-N23	3.15	1.72	1.62
3	A	402	UO2	C6-C4	-2.56	1.37	1.41
3	C	402	UO2	C18-S22	2.45	1.79	1.76
3	D	402	UO2	C6-C4	-2.42	1.37	1.41
3	A	402	UO2	C8-N10	-2.39	1.36	1.41
3	C	402	UO2	C8-N10	-2.32	1.36	1.41
3	A	402	UO2	C9-C3	-2.32	1.37	1.42
2	C	401	SAH	C8-N7	-2.22	1.30	1.34
2	A	401	SAH	C8-N7	-2.12	1.30	1.34
3	D	402	UO2	S22-N23	2.10	1.69	1.62

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	UO2	O27-S22-O26	-6.41	109.13	119.52
3	C	402	UO2	O26-S22-C18	6.27	115.97	108.05
3	B	402	UO2	O27-S22-C18	6.19	115.88	108.05
3	D	402	UO2	O27-S22-C18	5.69	115.24	108.05
3	D	402	UO2	O27-S22-O26	-5.07	111.30	119.52
3	B	402	UO2	C25-N23-C24	4.49	123.87	114.79
3	D	402	UO2	C25-N23-C24	4.35	123.58	114.79
3	A	402	UO2	O27-S22-C18	4.26	113.44	108.05
3	D	402	UO2	O26-S22-N23	4.12	115.58	106.85
3	A	402	UO2	C25-N23-C24	4.05	122.98	114.79
3	C	402	UO2	C21-C16-C2	-3.94	114.21	120.65
3	A	402	UO2	O26-S22-N23	3.90	115.12	106.85
3	C	402	UO2	O27-S22-O26	-3.38	114.05	119.52
3	C	402	UO2	C17-C16-C2	3.27	126.33	120.16
3	B	402	UO2	O26-S22-N23	3.09	113.41	106.85
3	C	402	UO2	C16-C2-N1	3.08	126.06	120.78
3	C	402	UO2	C19-C18-S22	-3.03	116.57	119.76
3	A	402	UO2	C17-C16-C2	2.87	125.57	120.16
3	C	402	UO2	C25-N23-C24	2.83	120.52	114.79
3	B	402	UO2	C17-C18-S22	-2.69	116.34	119.34
3	B	402	UO2	C16-C2-N1	2.69	125.39	120.78
3	A	402	UO2	C15-C13-C11	2.65	115.17	110.14
3	D	402	UO2	C17-C16-C2	2.64	125.14	120.16
3	C	402	UO2	C17-C18-S22	2.62	122.25	119.34
3	D	402	UO2	C16-C2-N1	2.45	124.98	120.78
3	D	402	UO2	C16-C17-C18	2.40	121.86	119.96
3	A	402	UO2	C21-C16-C2	-2.40	116.73	120.65
3	D	402	UO2	C15-C13-C11	2.36	114.61	110.14
2	C	401	SAH	C5-C6-N6	2.36	123.93	120.35
3	B	402	UO2	O27-S22-N23	2.33	111.80	106.85
3	B	402	UO2	C20-C21-C16	2.33	123.49	120.56
2	C	401	SAH	O4'-C1'-C2'	-2.06	103.92	106.93
3	D	402	UO2	C20-C21-C16	2.04	123.13	120.56

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	401	SAH	N-CA-CB-CG
2	D	401	SAH	C-CA-CB-CG
3	A	402	UO2	O12-C11-C13-N14

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Mol	Chain	Res	Type	Atoms
3	A	402	UO2	C17-C16-C2-C3
3	B	402	UO2	C17-C16-C2-C3
3	A	402	UO2	C21-C16-C2-C3
3	B	402	UO2	C21-C16-C2-C3
3	D	402	UO2	C17-C16-C2-C3
3	D	402	UO2	C21-C16-C2-C3
3	C	402	UO2	O12-C11-C13-N14
3	C	402	UO2	C17-C16-C2-C3
3	D	402	UO2	O12-C11-C13-N14
3	D	402	UO2	N10-C11-C13-N14
3	B	402	UO2	C24-N23-S22-O27
3	B	402	UO2	C25-N23-S22-O26
3	C	402	UO2	C25-N23-S22-O27
3	D	402	UO2	C24-N23-S22-O26
3	A	402	UO2	C24-N23-S22-O26
3	A	402	UO2	C24-N23-S22-O27
3	D	402	UO2	C25-N23-S22-O27
3	C	402	UO2	N10-C11-C13-N14
3	A	402	UO2	O12-C11-C13-C15
3	A	402	UO2	C25-N23-S22-O26
3	A	402	UO2	C25-N23-S22-O27
3	C	402	UO2	C24-N23-S22-O26
3	C	402	UO2	C25-N23-S22-O26
3	B	402	UO2	C7-C8-N10-C11

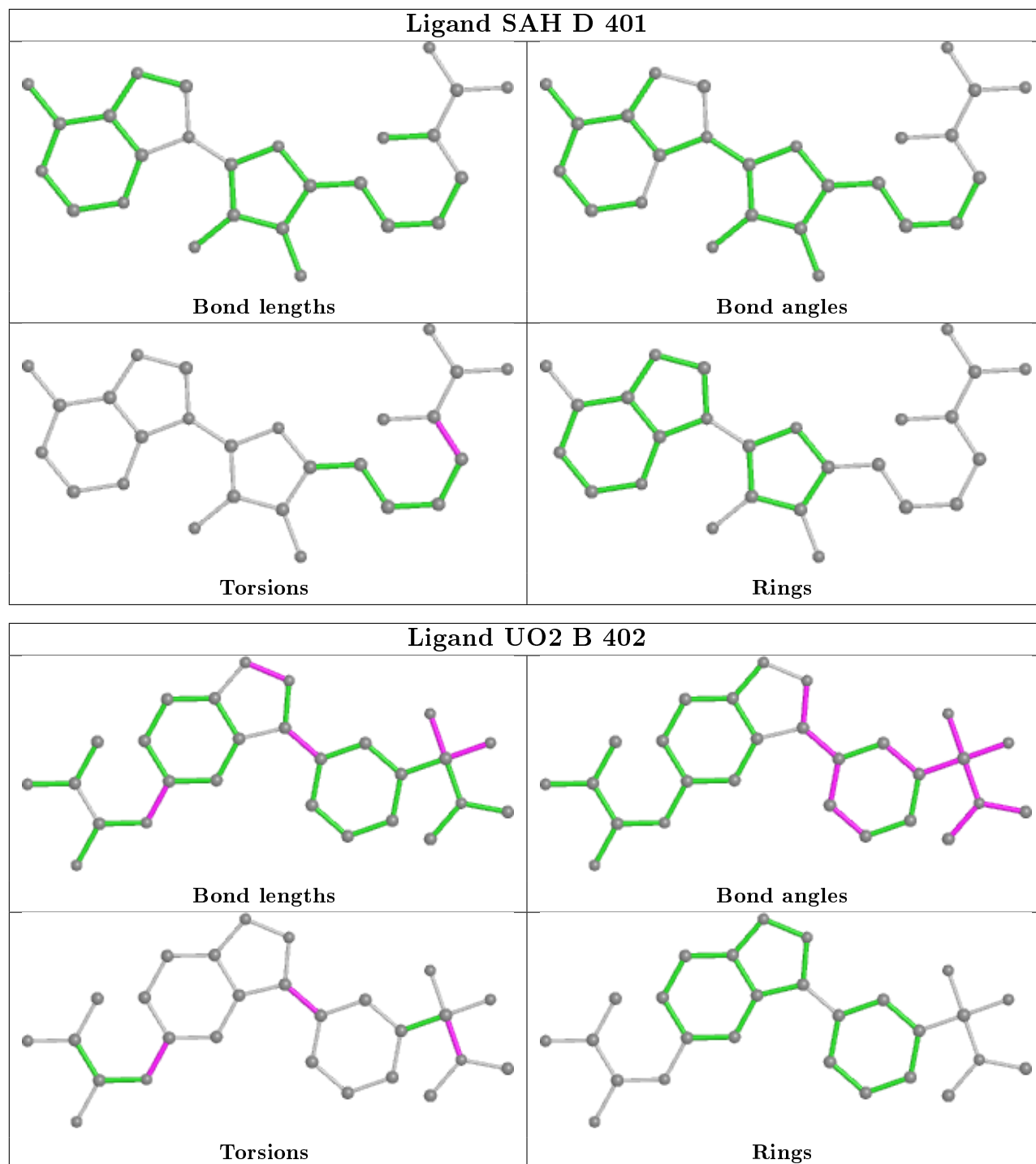
There are no ring outliers.

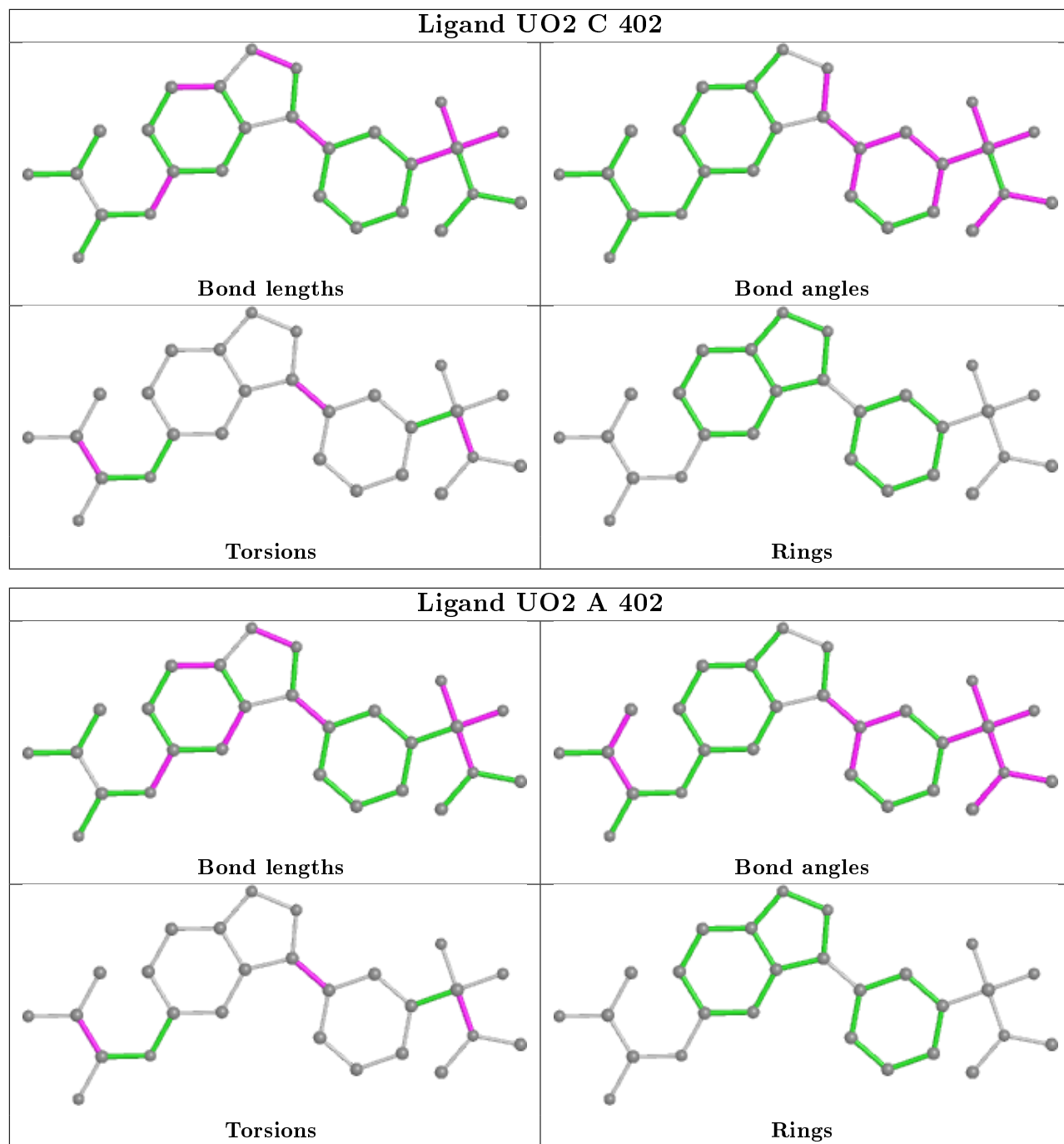
3 monomers are involved in 4 short contacts:

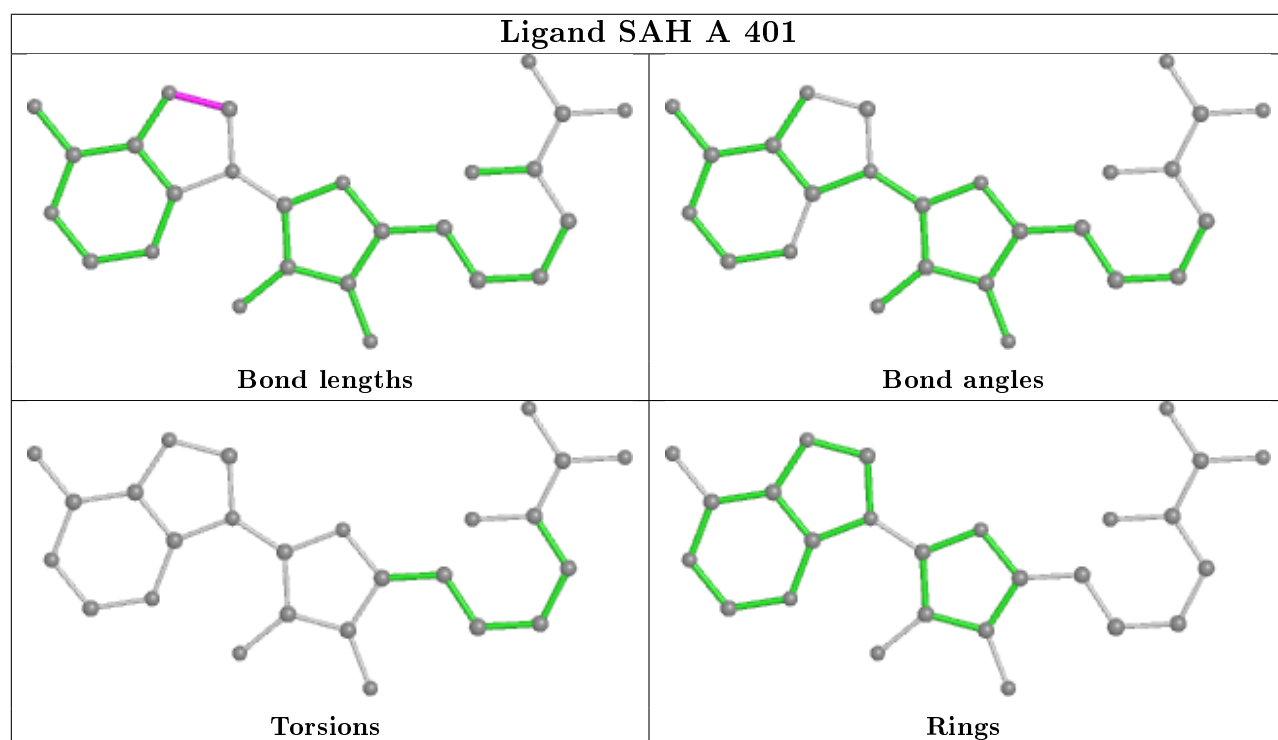
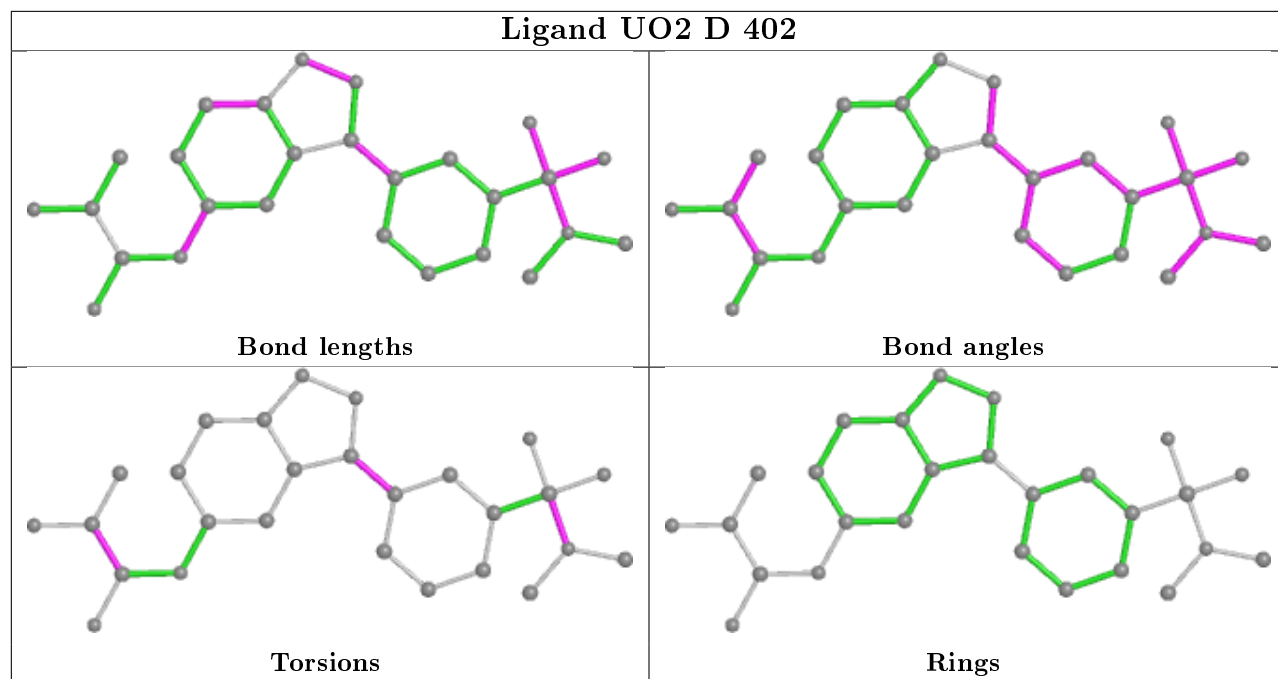
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	SAH	2	0
3	A	402	UO2	1	0
2	C	401	SAH	1	0

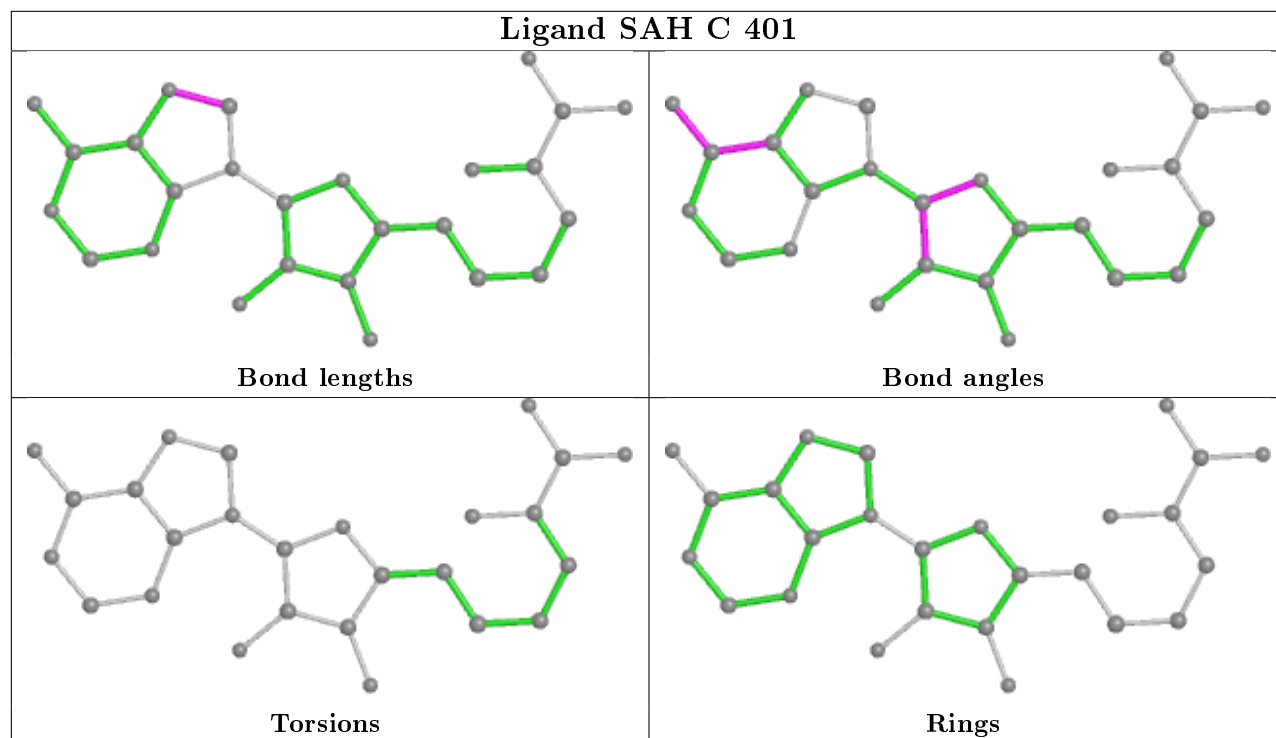
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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, 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	334/376 (88%)	-0.34	4 (1%) 79 78	24, 38, 62, 93	0
1	B	338/376 (89%)	-0.40	2 (0%) 89 89	23, 35, 59, 100	0
1	C	335/376 (89%)	-0.19	3 (0%) 84 83	25, 37, 62, 89	0
1	D	335/376 (89%)	-0.38	2 (0%) 89 89	26, 41, 70, 89	0
All	All	1342/1504 (89%)	-0.33	11 (0%) 86 85	23, 38, 64, 100	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	303	LYS	3.0
1	A	375	ASP	2.8
1	C	303	LYS	2.8
1	A	203	TRP	2.8
1	C	78	TRP	2.8
1	B	302	GLU	2.6
1	B	375	ASP	2.5
1	D	41	ARG	2.4
1	A	347	ARG	2.2
1	C	203	TRP	2.1
1	D	38	ARG	2.1

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](#)

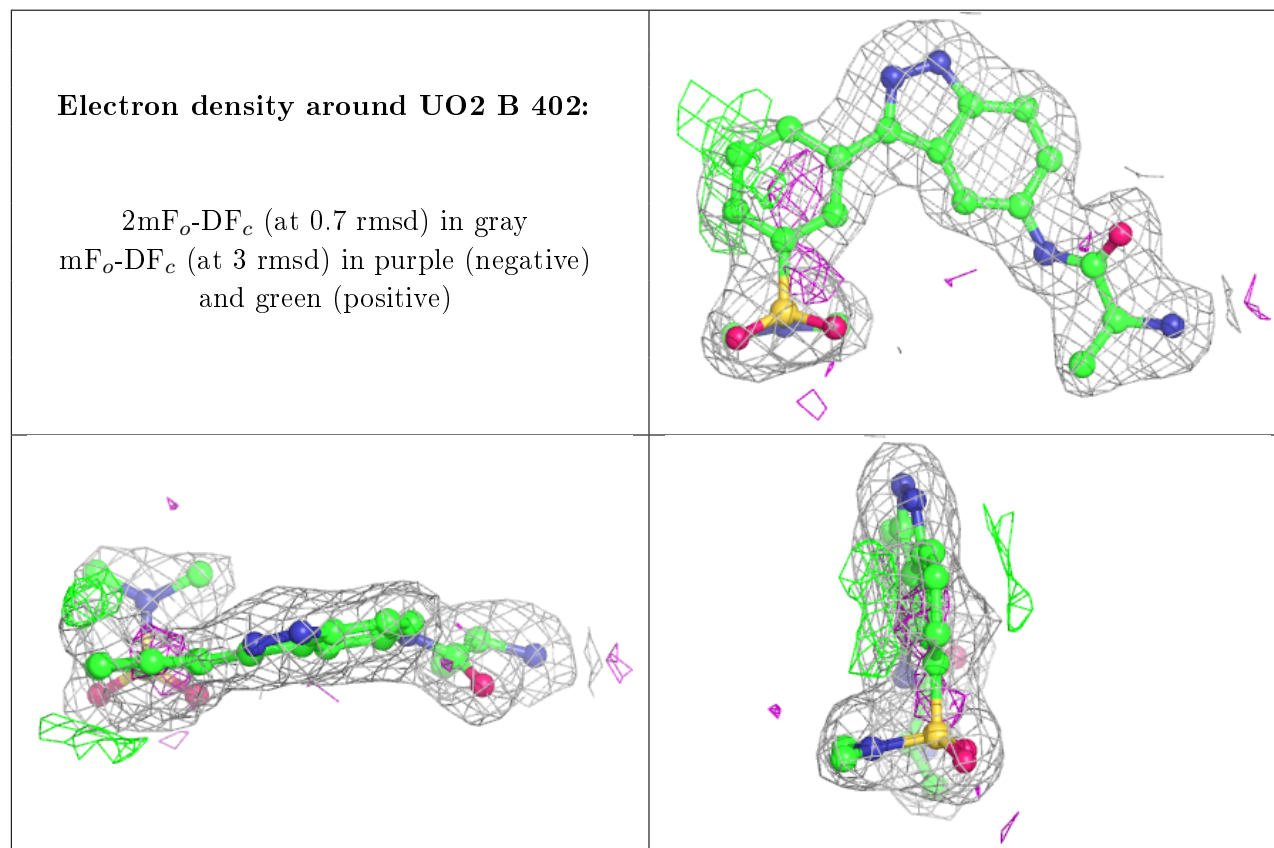
There are no monosaccharides in this entry.

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, 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.

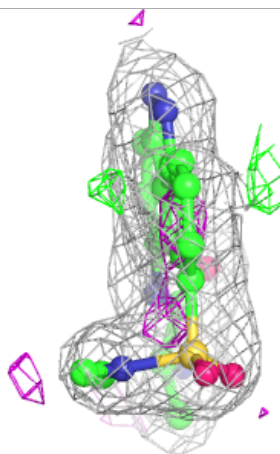
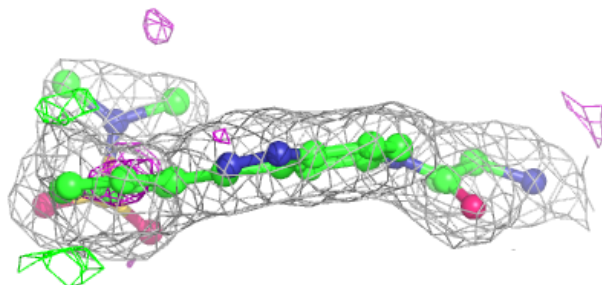
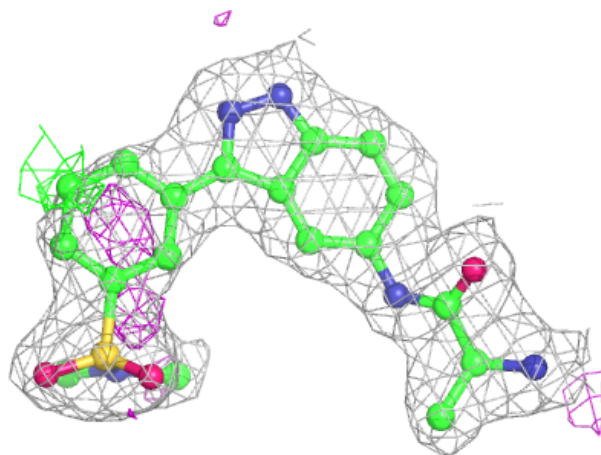
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	UO2	B	402	27/27	0.94	0.14	26,34,59,62	0
3	UO2	A	402	27/27	0.95	0.11	26,31,53,60	0
3	UO2	C	402	27/27	0.95	0.12	24,33,51,56	0
3	UO2	D	402	27/27	0.95	0.12	28,36,54,59	0
2	SAH	C	401	26/26	0.96	0.09	28,31,34,35	0
2	SAH	A	401	26/26	0.97	0.09	25,28,31,33	0
2	SAH	D	401	26/26	0.97	0.08	28,33,40,41	0
2	SAH	B	401	26/26	0.98	0.09	26,29,30,33	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.



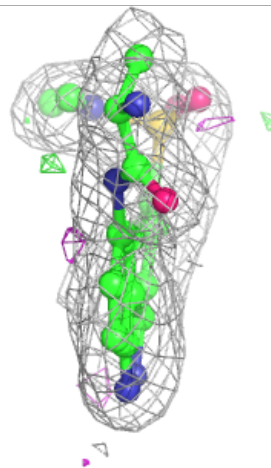
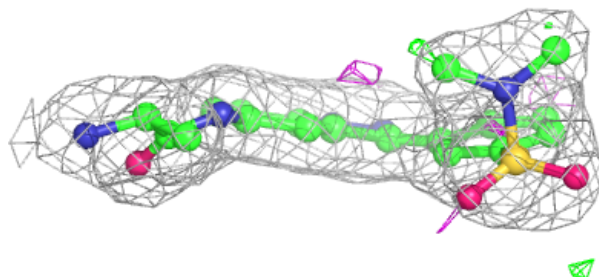
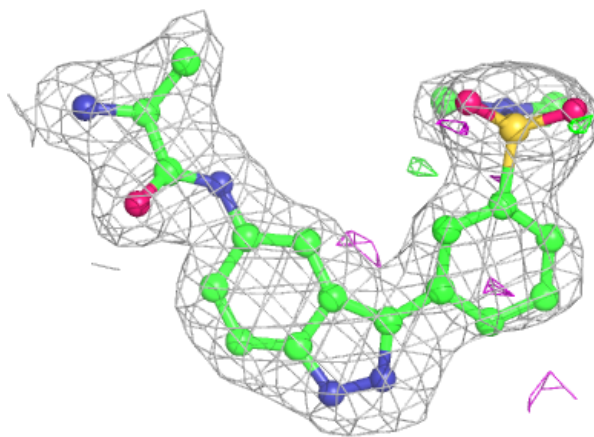
Electron density around UO2 A 402:

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



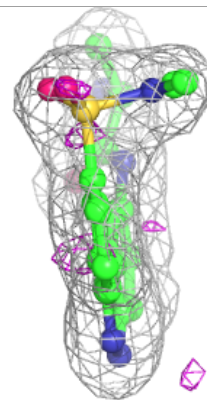
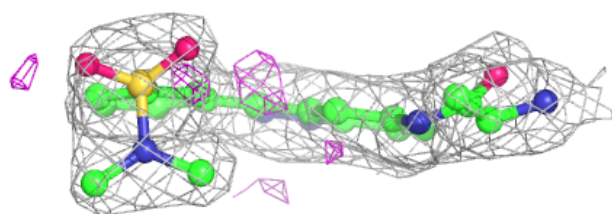
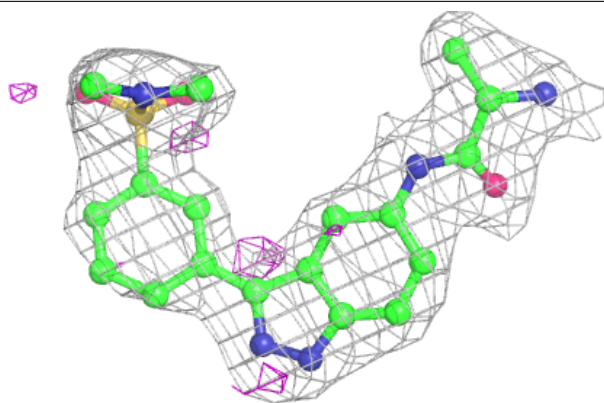
Electron density around UO2 C 402:

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

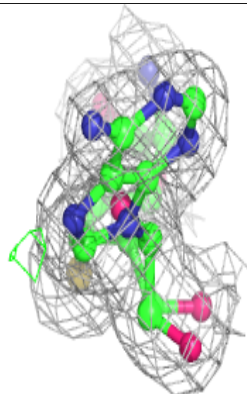
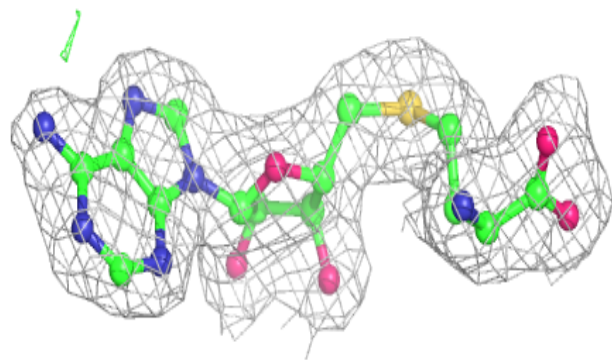
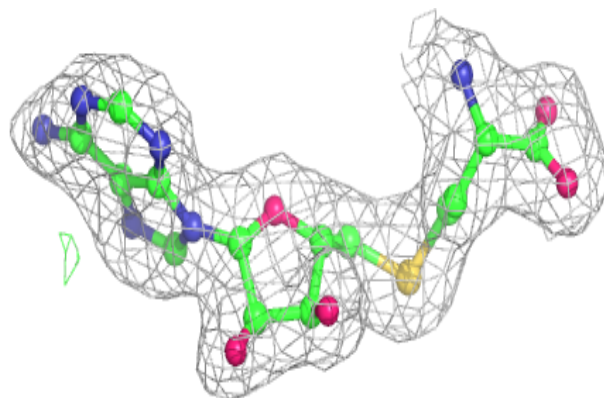


Electron density around UO2 D 402:

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

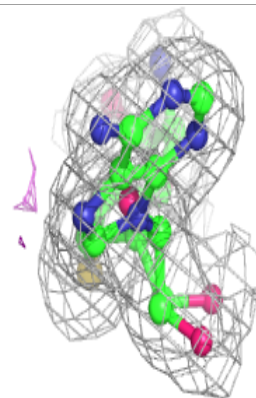
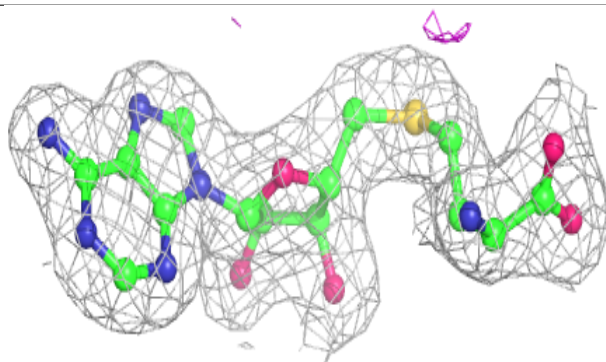
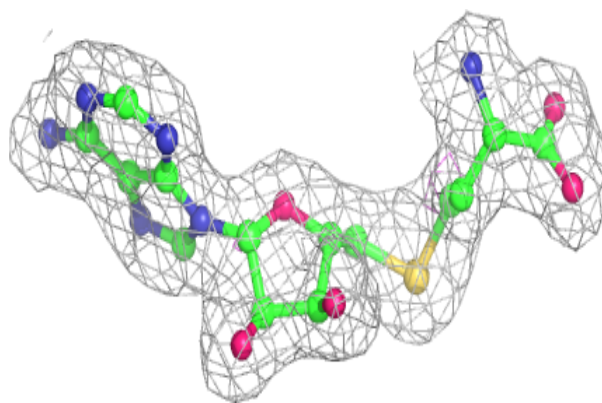
**Electron density around SAH C 401:**

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

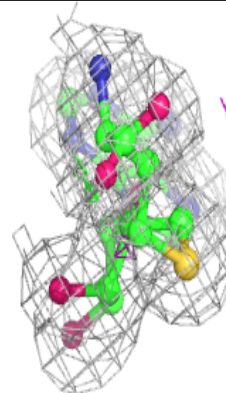
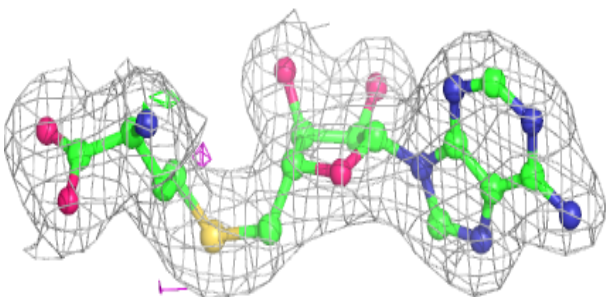
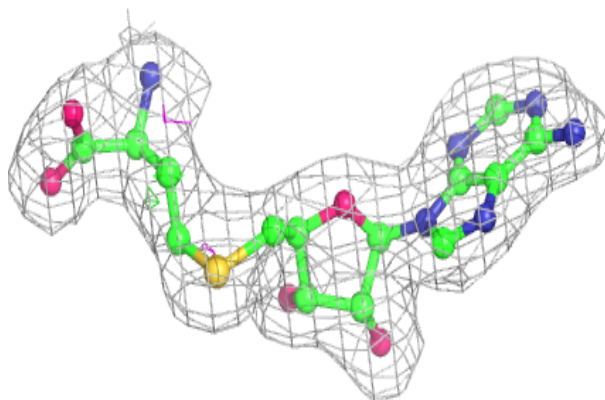


Electron density around SAH A 401:

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

**Electron density around SAH 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

There are no such residues in this entry.