



Full wwPDB X-ray Structure Validation Report ⓘ

May 27, 2026 – 12:11 PM EDT

PDB ID : 9P3C / pdb_00009p3c
Title : Structure of radical S-adenosylmethionine methyltransferase, NocN, from *Nocardia* with SAH and side-ring closed product analog bound
Authors : Wang, B.; Knox, H.L.; York, N.J.; Radle, M.I.; Silakov, A.; Booker, S.J.
Deposited on : 2025-06-13
Resolution : 1.78 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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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

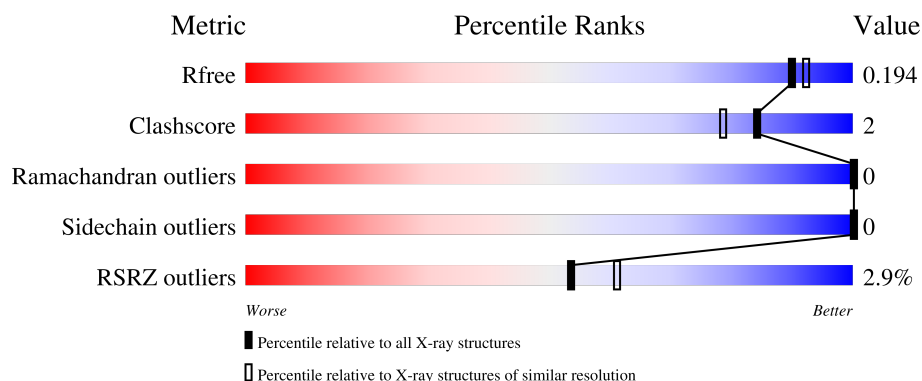
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

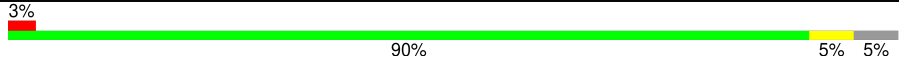

The reported resolution of this entry is 1.78 Å.

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	1365 (1.78-1.78)
Clashscore	190562	1395 (1.78-1.78)
Ramachandran outliers	187476	1382 (1.78-1.78)
Sidechain outliers	187428	1382 (1.78-1.78)
RSRZ outliers	180081	1365 (1.78-1.78)

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	420	
1	B	420	

2 Entry composition [i](#)

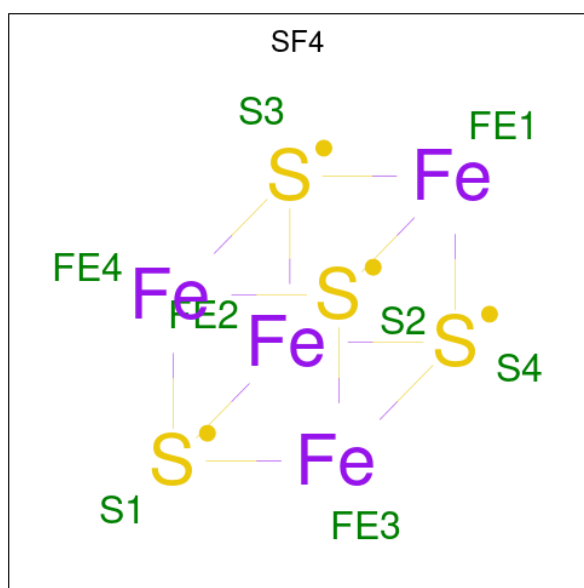
There are 7 unique types of molecules in this entry. The entry contains 7374 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 radical S-adenosylmethionine methyltransferase NocN.

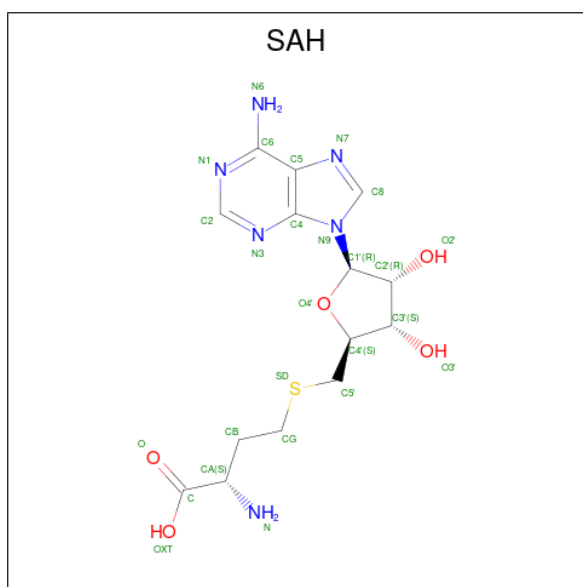
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	386	Total	C	N	O	S	0	5	0
			3049	1930	538	567	14			
1	A	397	Total	C	N	O	S	0	6	0
			3135	1986	551	582	16			

- Molecule 2 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



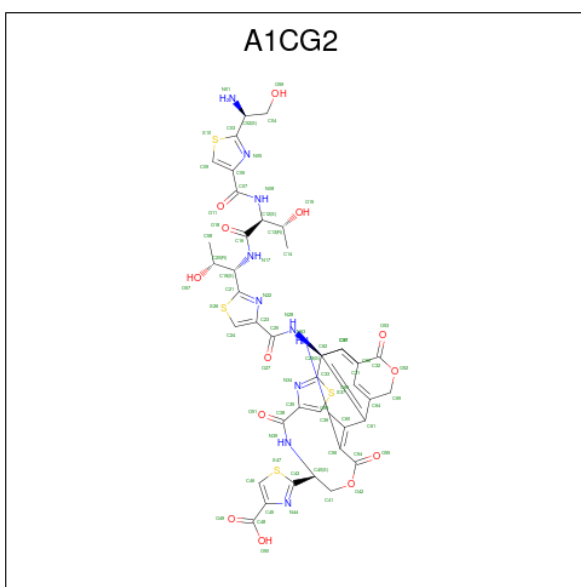
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	A	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 3 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: C₁₄H₂₀N₆O₅S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	B	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	A	1	Total	C	N	O	S	0	1
			52	28	12	10	2		

- Molecule 4 is 2-[(6S,13S)-6-[(2-{(1S,2R)-1-[(N-{2-[(1S)-1-amino-2-hydroxyethyl]-1,3-thiazole-4-carbonyl})-L-threonyl)amino]-2-hydroxypropyl}-1,3-thiazole-4-carbonyl)amino]-18-methyl-3,11,16-trioxo-1,3,4,5,6,11,12,13,14,16-decahydro-10,7-(azeno)-17,19-epimino-2,15,8,12-benzodioxathiazacycloicosin-13-yl]-1,3-thiazole-4-carboxylic acid (CCD ID: A1CG2) (formula: C₄₂H₄₄N₁₀O₁₃S₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total 69	C 42	N 10	O 13	S 4	0	0
4	B	1	Total 69	C 42	N 10	O 13	S 4	0	0
4	A	1	Total 69	C 42	N 10	O 13	S 4	0	0
4	A	1	Total 69	C 42	N 10	O 13	S 4	0	0

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Ca	0	0
			1	1		
5	A	1	Total	Ca	0	0
			1	1		

- Molecule 6 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Ni	0	0
			1	1		

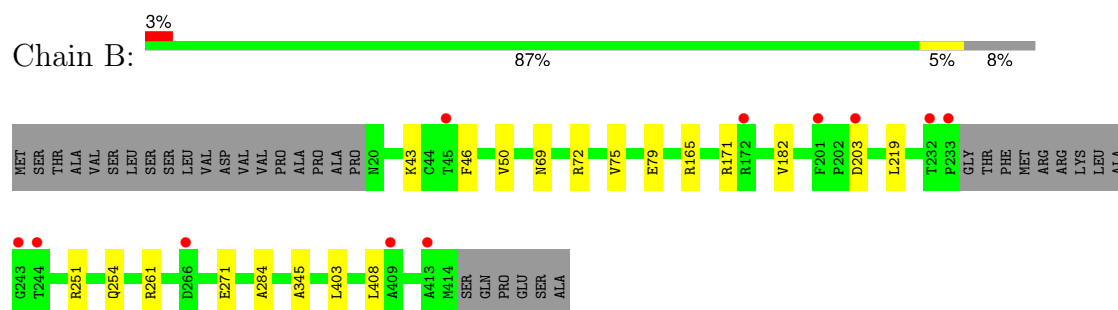
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	373	Total 373	O 373	0	0
7	A	392	Total 392	O 392	0	0

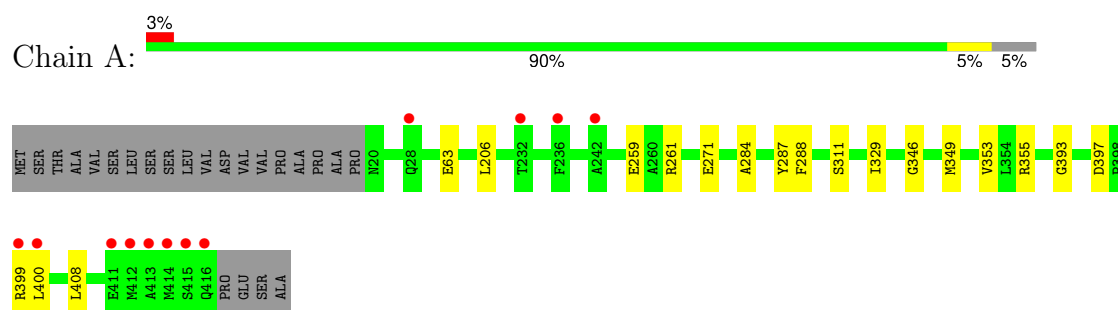
3 Residue-property plots [i](#)

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: radical S-adenosylmethionine methyltransferase NocN



- Molecule 1: radical S-adenosylmethionine methyltransferase NocN



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	59.93Å 88.03Å 146.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.50 – 1.78 29.50 – 1.78	Depositor EDS
% Data completeness (in resolution range)	81.1 (29.50-1.78) 99.0 (29.50-1.78)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 1.77Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.161 , 0.194 0.162 , 0.194	Depositor DCC
R_{free} test set	2149 reflections (2.02%)	wwPDB-VP
Wilson B-factor (Å ²)	18.2	Xtrriage
Anisotropy	0.110	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7374	wwPDB-VP
Average B, all atoms (Å ²)	26.0	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 36.77 % 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 4.7512e-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: SAH, CA, SF4, A1CG2, NI

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	0.27	0/3218	0.47	0/4352
1	B	0.28	0/3127	0.48	0/4230
All	All	0.27	0/6345	0.47	0/8582

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	3135	0	3119	15	0
1	B	3049	0	3023	14	0
2	A	8	0	0	0	0
2	B	8	0	0	0	0
3	A	78	0	57	0	0
3	B	52	0	38	0	0
4	A	138	0	0	3	0
4	B	138	0	0	4	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	392	0	0	0	0
7	B	373	0	0	0	0
All	All	7374	0	6237	29	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 (29) 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:408:LEU:HB2	4:B:504:A1CG2:N63	2.11	0.66
1:B:69:ASN:OD1	1:B:72:ARG:NH1	2.32	0.63
1:A:261:ARG:NE	1:A:271:GLU:OE1	2.33	0.58
1:A:399:ARG:HG3	1:A:400:LEU:HG	1.89	0.55
1:B:408:LEU:HB2	4:B:504:A1CG2:C56	2.37	0.54
1:A:397:ASP:OD2	1:A:399:ARG:NH1	2.41	0.54
1:B:43:LYS:HE2	1:B:50:VAL:HG22	1.91	0.54
1:A:284:ALA:HA	4:A:505:A1CG2:C66	2.39	0.53
1:B:75:VAL:O	1:B:79:GLU:HG3	2.08	0.53
1:A:288:PHE:HD2	1:A:349[B]:MET:HE2	1.73	0.53
1:A:206:LEU:HD11	1:A:259:GLU:HG2	1.89	0.53
1:A:397:ASP:OD1	1:A:399:ARG:HG2	2.13	0.49
1:A:63:GLU:H	1:A:63:GLU:CD	2.23	0.47
1:B:284:ALA:HA	4:B:505:A1CG2:C66	2.45	0.47
1:A:346:GLY:HA3	1:A:353:VAL:HG22	1.96	0.46
1:A:408:LEU:HB2	4:A:504:A1CG2:N63	2.30	0.46
1:B:254:GLN:HB3	1:B:403:LEU:HD22	1.97	0.46
1:B:165:ARG:NH1	1:B:203:ASP:OD1	2.45	0.46
1:B:345:ALA:HB2	4:B:505:A1CG2:C36	2.45	0.46
1:B:261:ARG:NE	1:B:271:GLU:OE1	2.48	0.43
1:B:182:VAL:HG11	1:B:219:LEU:HB3	2.00	0.43
1:A:353:VAL:O	1:A:393:GLY:HA3	2.19	0.43
1:A:311:SER:HB3	1:A:329:ILE:HB	2.01	0.43
1:B:46:PHE:CE1	1:B:171:ARG:HD3	2.54	0.42
1:A:287:TYR:OH	4:A:505:A1CG2:O51	2.28	0.42
1:A:349[B]:MET:HE2	1:A:349[B]:MET:HB2	1.85	0.41
1:A:355:ARG:HG3	1:A:393:GLY:HA2	2.02	0.41

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	401/420 (96%)	394 (98%)	7 (2%)	0	100	100
1	B	387/420 (92%)	381 (98%)	6 (2%)	0	100	100
All	All	788/840 (94%)	775 (98%)	13 (2%)	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	330/343 (96%)	330 (100%)	0	100	100
1	B	320/343 (93%)	320 (100%)	0	100	100
All	All	650/686 (95%)	650 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

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 14 ligands modelled in this entry, 3 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	SAH	B	503	-	27,28,28	0.19	0	36,40,40	0.61	1 (2%)
2	SF4	A	501	1,3	0,12,12	-	-	-		
4	A1CG2	A	505	-	73,75,75	3.39	26 (35%)	104,108,108	2.89	46 (44%)
4	A1CG2	B	504	-	73,75,75	3.77	31 (42%)	104,108,108	2.92	47 (45%)
3	SAH	A	503[A]	2	27,28,28	0.15	0	36,40,40	0.34	0
4	A1CG2	A	504	-	73,75,75	3.24	18 (24%)	104,108,108	2.53	35 (33%)
3	SAH	A	502	-	27,28,28	0.28	0	36,40,40	0.59	1 (2%)
3	SAH	A	503[B]	2	27,28,28	0.17	0	36,40,40	0.48	0
3	SAH	B	502	2	27,28,28	0.17	0	36,40,40	0.63	1 (2%)
2	SF4	B	501	1,3	0,12,12	-	-	-		
4	A1CG2	B	505	-	73,75,75	3.93	34 (46%)	104,108,108	2.94	47 (45%)

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	SAH	B	503	-	-	1/15/31/31	0/3/3/3
2	SF4	A	501	1,3	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	A1CG2	A	505	-	-	19/79/81/81	0/6/7/7
4	A1CG2	B	504	-	-	6/79/81/81	0/6/7/7
3	SAH	A	503[A]	2	-	3/15/31/31	0/3/3/3
4	A1CG2	A	504	-	-	4/79/81/81	0/6/7/7
3	SAH	A	502	-	-	0/15/31/31	0/3/3/3
3	SAH	A	503[B]	2	-	2/15/31/31	0/3/3/3
3	SAH	B	502	2	-	2/15/31/31	0/3/3/3
4	A1CG2	B	505	-	-	18/79/81/81	0/6/7/7
2	SF4	B	501	1,3	-	-	0/6/5/5

All (109) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	505	A1CG2	C45-C48	23.50	1.71	1.48
4	A	504	A1CG2	C45-C48	22.85	1.70	1.48
4	B	504	A1CG2	C45-C48	22.50	1.70	1.48
4	A	505	A1CG2	C45-C48	22.43	1.70	1.48
4	B	504	A1CG2	C67-C62	6.76	1.50	1.39
4	B	504	A1CG2	C02-C03	6.54	1.64	1.51
4	B	505	A1CG2	C07-N08	6.50	1.47	1.34
4	B	505	A1CG2	C19-C21	6.06	1.63	1.51
4	B	504	A1CG2	C06-C07	6.05	1.60	1.48
4	B	505	A1CG2	C06-C07	5.66	1.59	1.48
4	B	504	A1CG2	C07-N08	5.57	1.45	1.34
4	B	504	A1CG2	C66-C65	5.56	1.48	1.38
4	B	504	A1CG2	C06-N05	5.30	1.50	1.38
4	B	505	A1CG2	C02-C03	5.27	1.61	1.51
4	B	505	A1CG2	C56-N63	5.23	1.45	1.38
4	B	504	A1CG2	C16-N17	5.17	1.45	1.34
4	B	505	A1CG2	C23-N22	5.14	1.49	1.38
4	B	504	A1CG2	C19-C21	5.09	1.61	1.51
4	B	505	A1CG2	C67-C62	5.08	1.47	1.39
4	B	505	A1CG2	C16-N17	5.07	1.44	1.34
4	B	505	A1CG2	C66-C65	5.04	1.47	1.38
4	B	504	A1CG2	C56-N63	4.98	1.45	1.38
4	A	505	A1CG2	C67-C62	4.75	1.47	1.39
4	A	505	A1CG2	C61-C64	4.74	1.50	1.41
4	A	504	A1CG2	C02-C03	4.73	1.60	1.51
4	A	505	A1CG2	C02-C03	4.71	1.60	1.51
4	A	505	A1CG2	C07-N08	4.71	1.44	1.34
4	A	504	A1CG2	C66-C65	4.68	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	504	A1CG2	C61-C64	4.62	1.50	1.41
4	A	504	A1CG2	C69-C64	4.62	1.62	1.50
4	B	505	A1CG2	C06-N05	4.58	1.48	1.38
4	A	505	A1CG2	C66-C65	4.54	1.46	1.38
4	B	504	A1CG2	C69-C64	4.51	1.62	1.50
4	B	505	A1CG2	C12-N08	4.47	1.55	1.45
4	B	505	A1CG2	C61-C64	4.42	1.50	1.41
4	A	505	A1CG2	C06-N05	4.42	1.48	1.38
4	B	505	A1CG2	C25-N28	4.33	1.43	1.34
4	B	505	A1CG2	C69-C64	4.28	1.62	1.50
4	A	504	A1CG2	C67-C62	4.24	1.46	1.39
4	A	505	A1CG2	C25-N28	4.19	1.42	1.34
4	A	505	A1CG2	C56-N63	4.18	1.44	1.38
4	B	505	A1CG2	C23-C25	4.00	1.56	1.48
4	B	505	A1CG2	C12-C16	4.00	1.63	1.52
4	B	504	A1CG2	C23-N22	3.95	1.47	1.38
4	A	504	A1CG2	C06-N05	3.88	1.46	1.38
4	A	504	A1CG2	C23-C25	-3.81	1.41	1.48
4	B	505	A1CG2	C62-N63	3.76	1.45	1.38
4	A	504	A1CG2	C61-C64	3.68	1.48	1.41
4	B	505	A1CG2	C38-N39	3.60	1.41	1.34
4	B	504	A1CG2	C25-N28	3.56	1.41	1.34
4	A	505	A1CG2	C35-N34	3.49	1.46	1.38
4	B	505	A1CG2	C40-N39	3.43	1.53	1.45
4	A	505	A1CG2	C40-N39	3.38	1.52	1.45
4	B	505	A1CG2	C19-N17	3.31	1.52	1.45
4	B	504	A1CG2	C12-N08	3.27	1.52	1.45
4	A	505	A1CG2	C16-N17	3.26	1.41	1.34
4	B	504	A1CG2	C12-C16	3.23	1.61	1.52
4	B	504	A1CG2	C62-N63	3.20	1.44	1.38
4	B	504	A1CG2	C38-N39	3.16	1.40	1.34
4	A	505	A1CG2	C19-C21	3.10	1.57	1.51
4	B	505	A1CG2	C21-N22	3.06	1.37	1.30
4	B	504	A1CG2	C19-N17	3.01	1.52	1.45
4	A	505	A1CG2	C38-N39	2.99	1.40	1.34
4	B	504	A1CG2	C56-C54	2.98	1.53	1.46
4	B	504	A1CG2	C61-C60	2.90	1.52	1.45
4	B	504	A1CG2	C03-N05	2.84	1.36	1.30
4	B	505	A1CG2	C20-C19	2.82	1.61	1.53
4	A	504	A1CG2	C56-N63	2.79	1.42	1.38
4	B	505	A1CG2	C35-C38	2.75	1.54	1.48
4	A	504	A1CG2	C38-N39	2.75	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	505	A1CG2	C13-C12	2.74	1.61	1.53
4	A	504	A1CG2	C45-N44	2.74	1.44	1.38
4	A	504	A1CG2	C40-N39	2.70	1.51	1.45
4	A	505	A1CG2	O42-C54	2.68	1.38	1.33
4	B	504	A1CG2	C40-N39	2.65	1.51	1.45
4	A	505	A1CG2	C06-C07	2.63	1.53	1.48
4	A	505	A1CG2	C62-N63	2.57	1.43	1.38
4	B	505	A1CG2	C29-N28	2.52	1.51	1.45
4	B	505	A1CG2	C45-N44	2.51	1.44	1.38
4	B	504	A1CG2	O42-C54	2.49	1.38	1.33
4	A	504	A1CG2	C40-C43	2.49	1.57	1.50
4	A	505	A1CG2	C61-C60	2.46	1.51	1.45
4	A	505	A1CG2	C35-C38	2.45	1.53	1.48
4	A	505	A1CG2	C56-C54	2.44	1.52	1.46
4	B	505	A1CG2	C03-N05	2.42	1.35	1.30
4	B	505	A1CG2	C35-N34	2.35	1.43	1.38
4	B	504	A1CG2	C21-N22	2.34	1.35	1.30
4	B	504	A1CG2	C35-C38	2.33	1.53	1.48
4	A	505	A1CG2	C29-C33	2.28	1.56	1.50
4	A	504	A1CG2	C03-N05	2.27	1.35	1.30
4	A	504	A1CG2	C43-N44	2.25	1.35	1.30
4	A	504	A1CG2	C68-C60	2.24	1.54	1.50
4	A	505	A1CG2	C33-N34	2.23	1.35	1.30
4	B	505	A1CG2	C29-C33	2.23	1.56	1.50
4	B	504	A1CG2	C45-N44	2.22	1.43	1.38
4	B	505	A1CG2	C61-C60	2.22	1.50	1.45
4	A	505	A1CG2	C69-C64	2.21	1.56	1.50
4	B	505	A1CG2	C68-C60	2.19	1.54	1.50
4	B	505	A1CG2	O42-C54	2.18	1.37	1.33
4	A	505	A1CG2	C43-N44	2.16	1.35	1.30
4	B	504	A1CG2	C20-C19	2.14	1.59	1.53
4	A	505	A1CG2	C03-N05	2.12	1.34	1.30
4	B	504	A1CG2	C13-C12	2.10	1.59	1.53
4	B	505	A1CG2	C43-N44	2.07	1.34	1.30
4	A	504	A1CG2	C61-C60	2.05	1.50	1.45
4	A	505	A1CG2	C45-N44	2.05	1.43	1.38
4	A	504	A1CG2	C20-C19	2.03	1.59	1.53
4	B	504	A1CG2	C40-C43	2.02	1.56	1.50
4	B	504	A1CG2	C35-N34	2.01	1.42	1.38

All (178) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	505	A1CG2	C19-C21-N22	10.50	137.57	123.81
4	B	504	A1CG2	C19-C21-N22	9.17	135.83	123.81
4	A	504	A1CG2	C02-C03-N05	8.75	137.86	123.61
4	B	504	A1CG2	C02-C03-N05	8.62	137.65	123.61
4	A	505	A1CG2	C02-C03-N05	7.95	136.56	123.61
4	B	505	A1CG2	C02-C03-N05	7.78	136.27	123.61
4	A	505	A1CG2	C29-C33-N34	7.77	136.26	123.61
4	A	504	A1CG2	C40-C43-N44	7.45	135.73	123.61
4	A	505	A1CG2	C40-C43-N44	7.41	135.66	123.61
4	A	505	A1CG2	C29-N28-C25	7.40	134.44	122.00
4	A	504	A1CG2	O42-C54-C56	7.37	122.96	112.39
4	B	504	A1CG2	C40-C43-N44	7.32	135.52	123.61
4	B	504	A1CG2	O42-C54-C56	7.12	122.59	112.39
4	B	504	A1CG2	C02-C03-S10	-7.11	112.32	121.79
4	A	504	A1CG2	C02-C03-S10	-7.04	112.41	121.79
4	B	505	A1CG2	C40-C43-N44	7.00	135.01	123.61
4	A	505	A1CG2	C40-C43-S47	-6.89	112.62	121.79
4	A	505	A1CG2	C29-C33-S37	-6.42	113.23	121.79
4	B	504	A1CG2	C06-C07-N08	6.35	124.25	115.22
4	A	505	A1CG2	C02-C03-S10	-6.23	113.49	121.79
4	B	505	A1CG2	C02-C03-S10	-6.19	113.54	121.79
4	B	505	A1CG2	C19-C21-S26	-6.15	111.32	121.87
4	A	504	A1CG2	C40-C43-S47	-6.14	113.62	121.79
4	B	505	A1CG2	C40-C43-S47	-6.08	113.70	121.79
4	A	505	A1CG2	O42-C54-C56	6.04	121.05	112.39
4	A	505	A1CG2	C19-C21-N22	5.85	131.48	123.81
4	B	504	A1CG2	C40-C43-S47	-5.73	114.16	121.79
4	B	504	A1CG2	C29-C33-N34	5.71	132.91	123.61
4	B	505	A1CG2	C29-C33-N34	5.51	132.57	123.61
4	B	505	A1CG2	O42-C54-C56	5.28	119.95	112.39
4	B	505	A1CG2	C12-N08-C07	5.23	132.21	121.57
4	B	505	A1CG2	C25-C23-N22	5.21	130.54	120.67
4	B	505	A1CG2	C23-C25-N28	5.19	122.60	115.22
4	A	504	A1CG2	C19-C21-N22	5.08	130.47	123.81
4	B	504	A1CG2	C21-C19-N17	4.85	115.75	108.66
4	A	504	A1CG2	C29-C33-N34	4.84	131.48	123.61
4	B	504	A1CG2	C19-C21-S26	-4.75	113.72	121.87
4	A	505	A1CG2	C23-N22-C21	4.68	115.48	110.65
4	A	505	A1CG2	C12-C16-N17	4.64	126.39	116.39
4	B	505	A1CG2	C06-C07-N08	4.61	121.78	115.22
4	A	504	A1CG2	O42-C54-O55	-4.60	115.11	123.37
4	B	504	A1CG2	O42-C54-O55	-4.53	115.23	123.37
4	B	505	A1CG2	C21-C19-N17	4.34	114.99	108.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	504	A1CG2	C07-C06-N05	4.27	128.76	120.67
4	A	505	A1CG2	C24-C23-C25	4.21	130.93	123.92
4	B	505	A1CG2	C35-N34-C33	4.18	114.97	110.65
4	B	504	A1CG2	O52-C32-C31	4.16	124.53	111.83
4	B	505	A1CG2	O52-C32-C31	4.14	124.46	111.83
4	A	505	A1CG2	C23-C25-N28	-4.06	109.46	115.22
4	B	504	A1CG2	C35-N34-C33	3.95	114.73	110.65
4	B	504	A1CG2	O49-C48-C45	-3.94	115.79	122.02
4	B	504	A1CG2	C12-C16-N17	3.94	124.89	116.39
4	B	505	A1CG2	O49-C48-C45	-3.93	115.81	122.02
4	A	504	A1CG2	C09-S10-C03	3.92	94.16	89.52
4	A	505	A1CG2	C33-C29-N28	-3.89	102.89	109.27
4	A	505	A1CG2	O49-C48-C45	-3.85	115.95	122.02
4	A	504	A1CG2	C35-N34-C33	3.82	114.59	110.65
4	A	504	A1CG2	C21-C19-N17	-3.80	103.11	108.66
4	A	505	A1CG2	O42-C54-O55	-3.76	116.60	123.37
4	B	505	A1CG2	C29-N28-C25	3.76	128.32	122.00
4	B	505	A1CG2	C12-C16-N17	3.72	124.40	116.39
4	A	505	A1CG2	C12-N08-C07	3.72	129.14	121.57
4	B	504	A1CG2	C29-C33-S37	-3.67	116.90	121.79
4	A	505	A1CG2	O52-C32-C31	3.66	123.00	111.83
4	A	504	A1CG2	O49-C48-C45	-3.66	116.24	122.02
4	A	504	A1CG2	O52-C32-C31	3.66	122.99	111.83
4	B	504	A1CG2	C45-N44-C43	3.58	114.35	110.65
4	B	504	A1CG2	O11-C07-N08	-3.57	116.80	123.09
4	A	504	A1CG2	C69-O52-C32	3.55	122.78	116.42
4	A	505	A1CG2	C09-S10-C03	3.54	93.72	89.52
4	A	505	A1CG2	C06-C07-N08	3.54	120.25	115.22
4	B	505	A1CG2	C40-N39-C38	3.53	127.94	122.00
4	B	505	A1CG2	O42-C54-O55	-3.47	117.13	123.37
4	B	505	A1CG2	S37-C33-N34	-3.46	109.67	114.19
4	B	504	A1CG2	C29-N28-C25	3.45	127.79	122.00
4	B	505	A1CG2	C31-C30-C29	3.43	119.48	113.16
4	A	505	A1CG2	O18-C16-N17	-3.43	116.82	122.96
4	A	504	A1CG2	C12-C16-N17	3.42	123.76	116.39
4	A	504	A1CG2	S10-C03-N05	-3.42	109.72	114.19
4	A	505	A1CG2	C40-N39-C38	3.41	127.73	122.00
4	B	505	A1CG2	C24-C23-C25	-3.39	118.28	123.92
4	A	504	A1CG2	C35-C38-N39	3.37	120.01	115.22
4	B	504	A1CG2	C09-C06-N05	-3.36	110.81	115.43
4	A	505	A1CG2	C21-C19-N17	3.33	113.53	108.66
4	B	505	A1CG2	O27-C25-N28	-3.29	117.29	123.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	505	A1CG2	C06-N05-C03	3.27	114.03	110.65
4	A	505	A1CG2	C36-S37-C33	3.27	93.39	89.52
4	B	504	A1CG2	C23-C25-N28	3.25	119.85	115.22
4	B	504	A1CG2	C09-S10-C03	3.25	93.37	89.52
4	B	504	A1CG2	O52-C32-O53	-3.25	115.51	123.63
4	B	505	A1CG2	C61-C60-C56	3.24	109.09	106.16
4	A	505	A1CG2	S10-C03-N05	-3.24	109.95	114.19
4	A	504	A1CG2	C23-N22-C21	3.24	113.99	110.65
4	B	505	A1CG2	C09-C06-N05	-3.20	111.03	115.43
4	B	504	A1CG2	S10-C03-N05	-3.18	110.03	114.19
4	B	505	A1CG2	C69-O52-C32	3.18	122.12	116.42
4	A	504	A1CG2	O18-C16-N17	-3.17	117.29	122.96
4	A	505	A1CG2	C41-O42-C54	3.16	121.26	116.45
4	B	505	A1CG2	C16-C12-N08	3.15	118.89	110.32
4	A	505	A1CG2	C30-C31-C32	-3.12	104.36	113.21
4	B	505	A1CG2	C07-C06-N05	3.12	126.57	120.67
4	B	505	A1CG2	C24-C23-N22	-3.09	111.18	115.43
4	A	505	A1CG2	C20-C19-C21	-3.08	103.24	110.69
4	A	504	A1CG2	C29-C33-S37	-3.07	117.69	121.79
4	B	504	A1CG2	S37-C33-N34	-3.06	110.19	114.19
4	B	505	A1CG2	S10-C03-N05	-3.06	110.19	114.19
4	B	505	A1CG2	C29-C33-S37	-3.06	117.72	121.79
4	A	504	A1CG2	C48-C45-N44	3.05	127.61	120.52
4	B	504	A1CG2	C61-C60-C56	3.05	108.92	106.16
4	A	504	A1CG2	C43-C40-N39	3.04	114.26	109.27
4	B	504	A1CG2	C12-N08-C07	3.02	127.72	121.57
4	B	504	A1CG2	C40-N39-C38	3.02	127.08	122.00
4	B	504	A1CG2	C41-O42-C54	3.00	121.01	116.45
4	A	504	A1CG2	C46-C45-C48	-2.99	118.50	124.28
4	A	505	A1CG2	S37-C33-N34	-2.99	110.28	114.19
4	B	504	A1CG2	S47-C43-N44	-2.97	110.31	114.19
4	A	505	A1CG2	S26-C21-N22	-2.96	110.32	114.19
4	A	504	A1CG2	C12-N08-C07	2.95	127.56	121.57
3	B	503	SAH	C4'-C5'-SD	-2.91	103.39	113.78
4	B	504	A1CG2	C06-N05-C03	2.91	113.65	110.65
4	B	504	A1CG2	C23-N22-C21	2.90	113.64	110.65
4	A	505	A1CG2	C35-N34-C33	2.89	113.64	110.65
3	A	502	SAH	C4'-C5'-SD	-2.88	103.52	113.78
4	B	505	A1CG2	C45-N44-C43	2.88	113.62	110.65
4	B	505	A1CG2	O52-C32-O53	-2.87	116.44	123.63
4	B	504	A1CG2	S26-C21-N22	-2.87	110.44	114.19
4	B	505	A1CG2	C09-S10-C03	2.84	92.89	89.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	504	A1CG2	C24-S26-C21	2.80	92.84	89.52
4	B	505	A1CG2	C24-S26-C21	2.74	92.77	89.52
4	A	504	A1CG2	S47-C43-N44	-2.71	110.65	114.19
4	A	505	A1CG2	C48-C45-N44	2.70	126.78	120.52
4	B	504	A1CG2	C24-C23-N22	-2.67	111.75	115.43
4	B	505	A1CG2	O18-C16-N17	-2.67	118.18	122.96
4	B	504	A1CG2	C69-O52-C32	2.67	121.20	116.42
4	B	505	A1CG2	C36-S37-C33	2.67	92.68	89.52
4	A	504	A1CG2	C33-C29-N28	2.64	113.61	109.27
4	A	504	A1CG2	C45-N44-C43	2.63	113.36	110.65
4	A	505	A1CG2	C13-C12-C16	-2.62	105.60	111.32
4	A	504	A1CG2	O52-C32-O53	-2.61	117.09	123.63
4	B	505	A1CG2	C41-O42-C54	2.60	120.40	116.45
4	A	504	A1CG2	S37-C33-N34	-2.59	110.80	114.19
4	A	505	A1CG2	C07-C06-N05	2.59	125.57	120.67
4	A	505	A1CG2	C06-N05-C03	2.58	113.31	110.65
4	B	505	A1CG2	C48-C45-N44	2.55	126.44	120.52
4	A	504	A1CG2	C06-N05-C03	2.54	113.27	110.65
4	B	505	A1CG2	C35-C38-N39	2.54	118.83	115.22
4	B	504	A1CG2	O27-C25-N28	-2.54	118.63	123.09
4	B	504	A1CG2	C48-C45-N44	2.53	126.39	120.52
4	A	505	A1CG2	C61-C60-C56	2.47	108.39	106.16
3	B	502	SAH	C5'-C4'-C3'	-2.45	108.93	115.06
4	A	505	A1CG2	C46-C45-C48	-2.45	119.55	124.28
4	B	504	A1CG2	C36-S37-C33	2.42	92.38	89.52
4	A	505	A1CG2	C45-N44-C43	2.42	113.14	110.65
4	A	504	A1CG2	C61-C60-C56	2.40	108.33	106.16
4	B	504	A1CG2	O18-C16-N17	-2.37	118.72	122.96
4	B	505	A1CG2	S26-C21-N22	-2.36	111.11	114.19
4	B	505	A1CG2	O11-C07-N08	-2.35	118.96	123.09
4	B	505	A1CG2	O50-C48-C45	2.34	117.15	113.40
4	A	505	A1CG2	O52-C32-O53	-2.30	117.87	123.63
4	B	504	A1CG2	C25-C23-N22	2.28	124.99	120.67
4	B	504	A1CG2	C35-C38-N39	2.27	118.45	115.22
4	A	504	A1CG2	C46-S47-C43	2.23	92.16	89.52
4	B	505	A1CG2	S47-C43-N44	-2.23	111.28	114.19
4	A	505	A1CG2	C43-C40-N39	2.22	112.92	109.27
4	B	504	A1CG2	C46-C45-C48	-2.22	119.99	124.28
4	A	505	A1CG2	C09-C06-N05	-2.21	112.39	115.43
4	A	505	A1CG2	C35-C38-N39	2.20	118.35	115.22
4	A	505	A1CG2	O11-C07-N08	-2.19	119.24	123.09
4	A	505	A1CG2	C24-C23-N22	-2.18	112.43	115.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	505	A1CG2	C46-C45-C48	-2.17	120.09	124.28
4	A	504	A1CG2	C19-C21-S26	-2.16	118.16	121.87
4	A	504	A1CG2	S26-C21-N22	-2.15	111.37	114.19
4	B	504	A1CG2	O50-C48-C45	2.15	116.86	113.40
4	A	505	A1CG2	C19-C21-S26	-2.15	118.19	121.87
4	A	504	A1CG2	O11-C07-N08	-2.15	119.31	123.09
4	B	504	A1CG2	O18-C16-C12	-2.14	116.40	120.75
4	A	505	A1CG2	C25-C23-N22	-2.13	116.64	120.67
4	B	504	A1CG2	C09-C06-C07	-2.11	120.41	123.92

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	502	SAH	C-CA-CB-CG
3	A	503[A]	SAH	O4'-C4'-C5'-SD
3	A	503[A]	SAH	C3'-C4'-C5'-SD
3	A	503[B]	SAH	O4'-C4'-C5'-SD
3	A	503[B]	SAH	C3'-C4'-C5'-SD
4	B	504	A1CG2	C04-C02-C03-N05
4	B	504	A1CG2	C04-C02-C03-S10
4	B	505	A1CG2	C03-C02-C04-O59
4	B	505	A1CG2	N01-C02-C04-O59
4	B	505	A1CG2	C16-C12-N08-C07
4	B	505	A1CG2	C24-C23-C25-N28
4	B	505	A1CG2	C24-C23-C25-O27
4	B	505	A1CG2	N39-C40-C43-N44
4	B	505	A1CG2	N39-C40-C43-S47
4	B	505	A1CG2	C46-C45-C48-O49
4	B	505	A1CG2	C46-C45-C48-O50
4	B	505	A1CG2	N44-C45-C48-O49
4	B	505	A1CG2	N44-C45-C48-O50
4	A	505	A1CG2	C03-C02-C04-O59
4	A	505	A1CG2	N01-C02-C04-O59
4	A	505	A1CG2	N28-C29-C33-S37
4	A	505	A1CG2	C40-C41-O42-C54
4	A	505	A1CG2	C46-C45-C48-O49
4	A	505	A1CG2	C46-C45-C48-O50
4	A	505	A1CG2	N44-C45-C48-O49
4	A	505	A1CG2	N44-C45-C48-O50
4	A	505	A1CG2	C30-C29-N28-C25
4	B	505	A1CG2	C12-C16-N17-C19

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Mol	Chain	Res	Type	Atoms
4	B	505	A1CG2	O18-C16-N17-C19
4	B	505	A1CG2	N22-C23-C25-N28
4	B	505	A1CG2	C40-C41-O42-C54
3	A	503[A]	SAH	C-CA-CB-CG
4	B	505	A1CG2	N22-C23-C25-O27
4	A	504	A1CG2	C30-C31-C32-O52
4	A	505	A1CG2	N08-C12-C16-O18
4	A	504	A1CG2	C21-C19-N17-C16
4	A	505	A1CG2	N08-C12-C16-N17
4	B	504	A1CG2	C30-C31-C32-O52
4	B	504	A1CG2	C03-C02-C04-O59
4	A	505	A1CG2	N28-C29-C33-N34
4	A	505	A1CG2	C41-C40-C43-N44
4	A	505	A1CG2	N39-C40-C43-N44
4	A	505	A1CG2	N39-C40-C43-S47
4	A	505	A1CG2	C20-C19-C21-N22
4	A	505	A1CG2	O42-C54-C56-N63
3	B	503	SAH	O-C-CA-N
4	B	504	A1CG2	C21-C19-N17-C16
4	A	505	A1CG2	C20-C19-C21-S26
4	A	504	A1CG2	C30-C31-C32-O53
4	A	505	A1CG2	N17-C19-C21-S26
4	B	505	A1CG2	N17-C19-C20-O57
3	B	502	SAH	C3'-C4'-C5'-SD
4	A	504	A1CG2	N01-C02-C04-O59
4	B	504	A1CG2	C30-C31-C32-O53
4	B	505	A1CG2	C41-C40-C43-S47

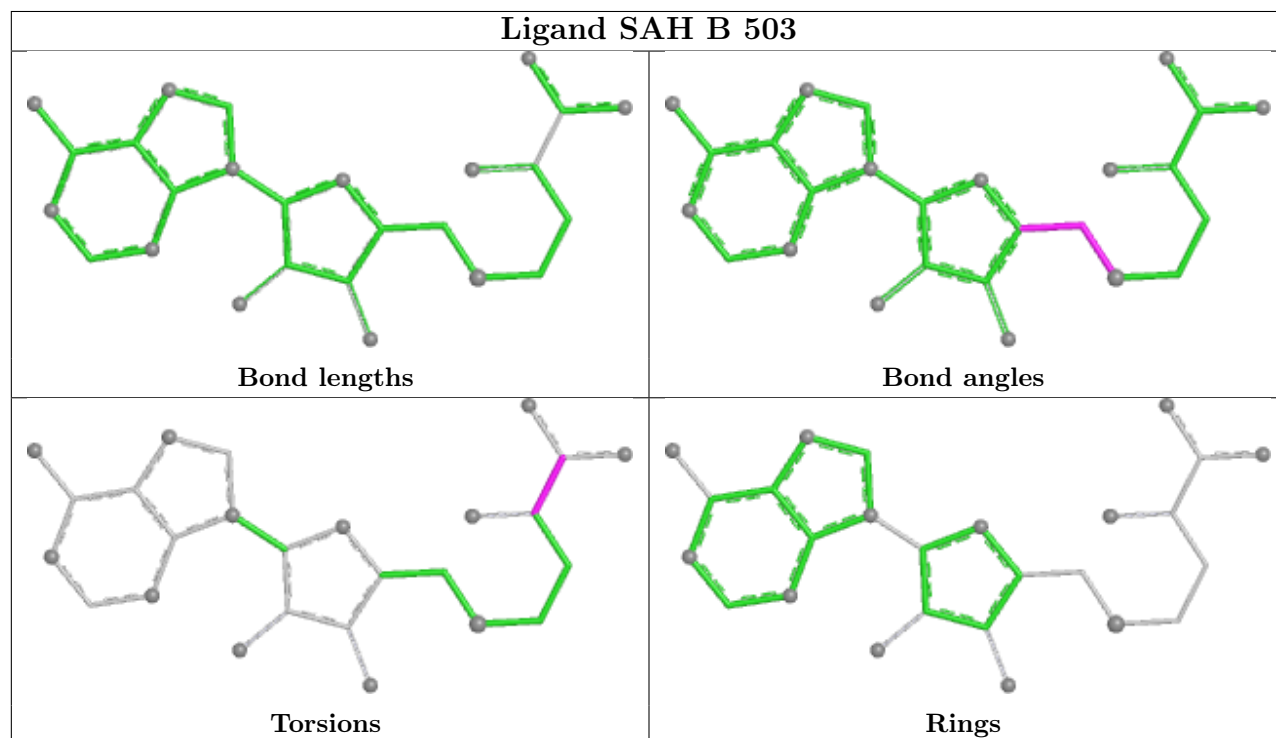
There are no ring outliers.

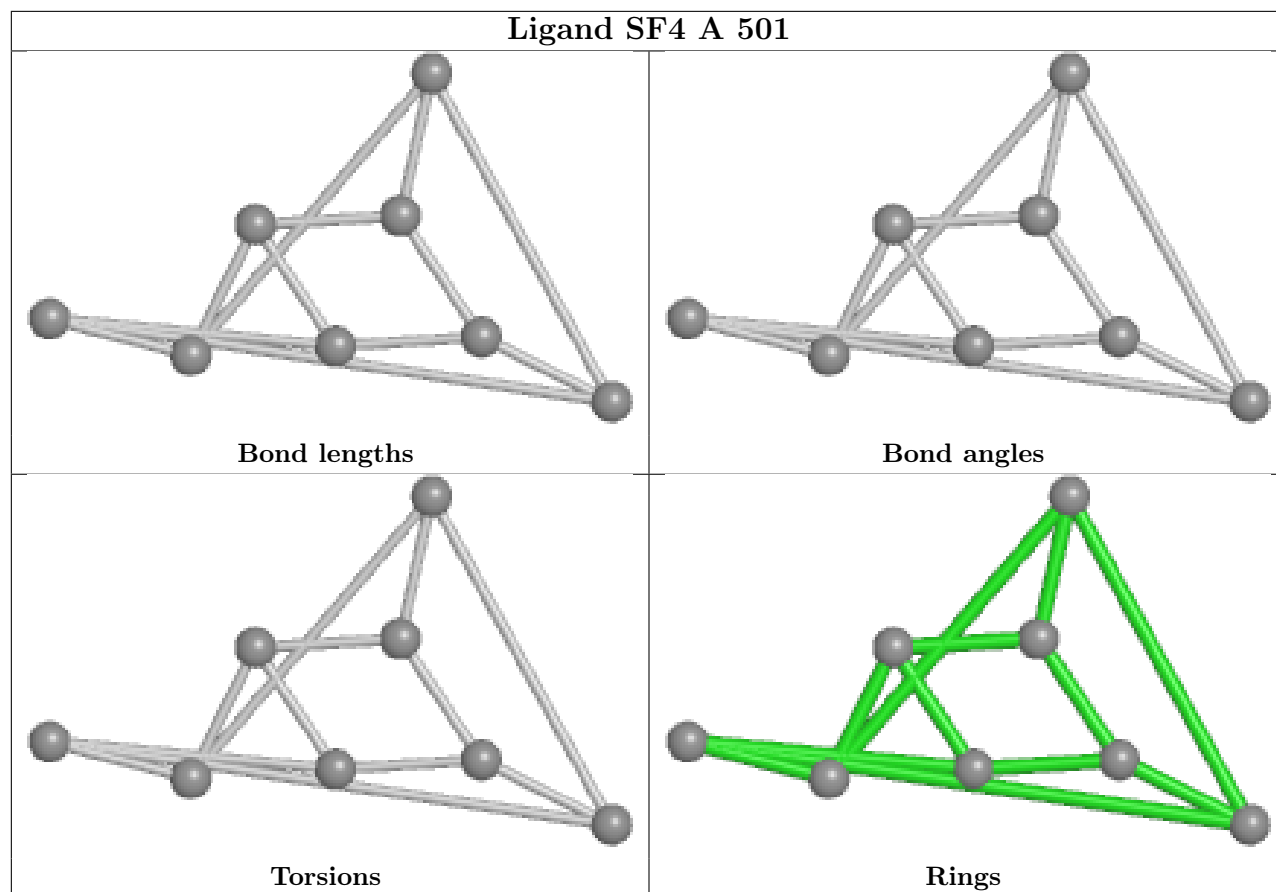
4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	505	A1CG2	2	0
4	B	504	A1CG2	2	0
4	A	504	A1CG2	1	0
4	B	505	A1CG2	2	0

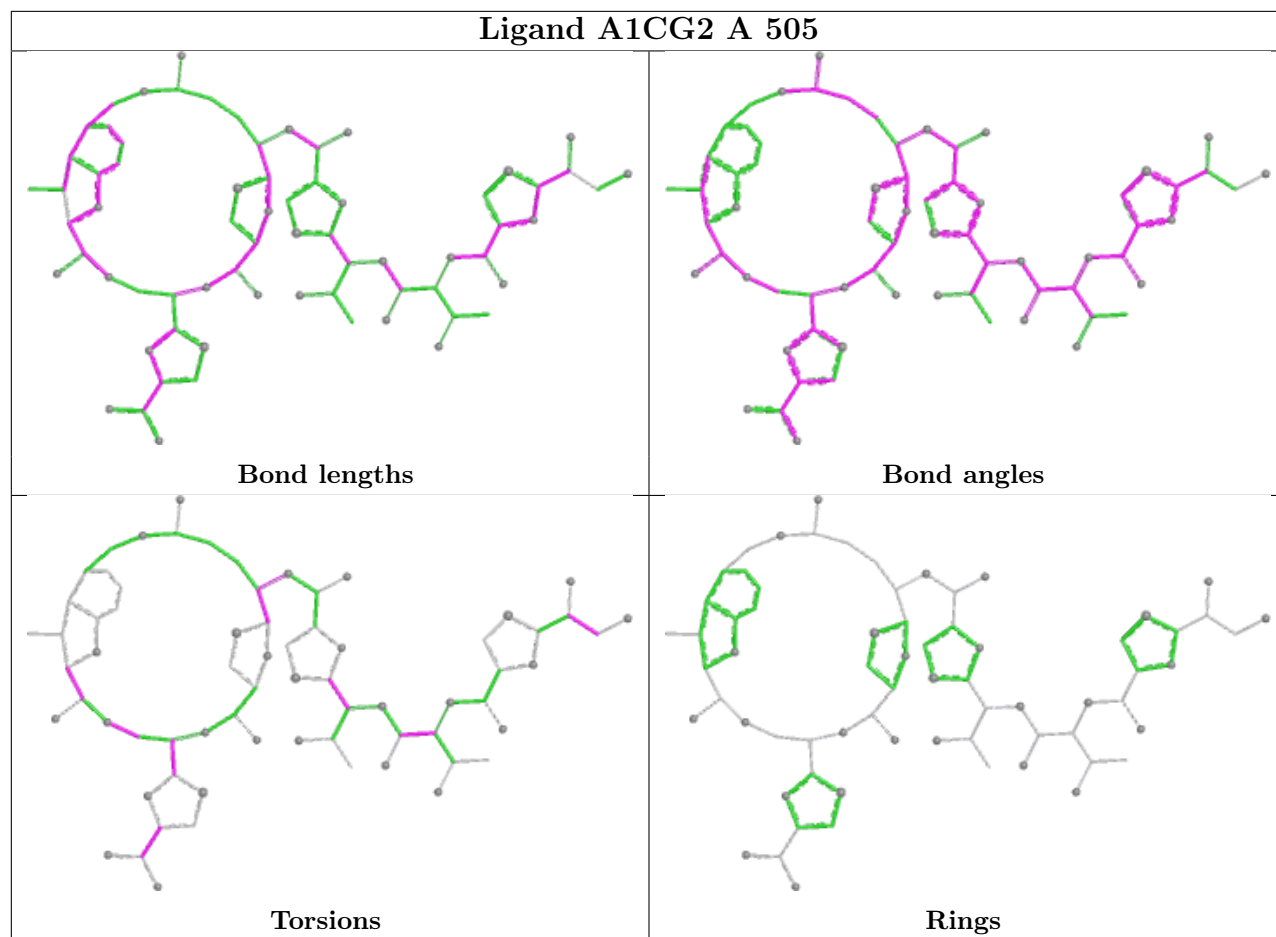
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

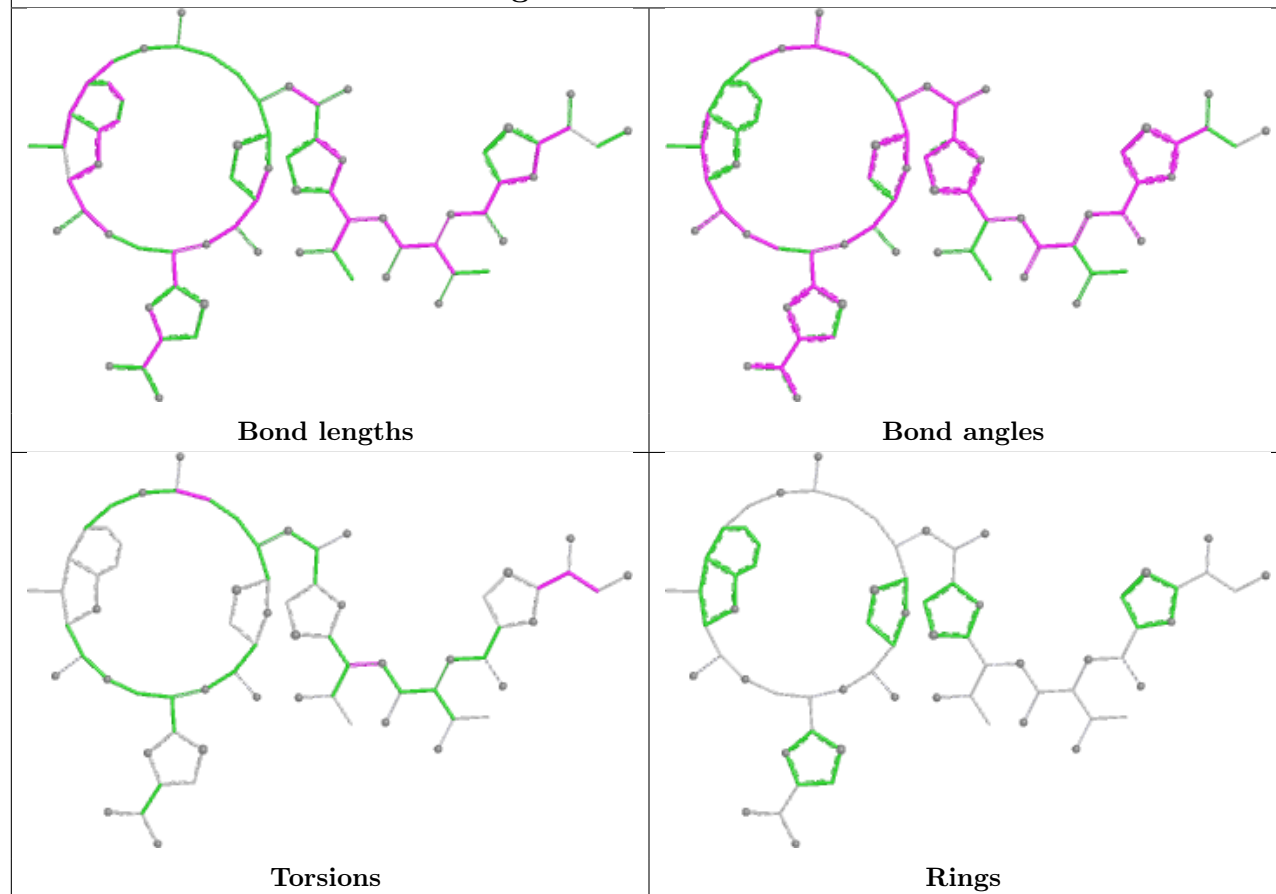




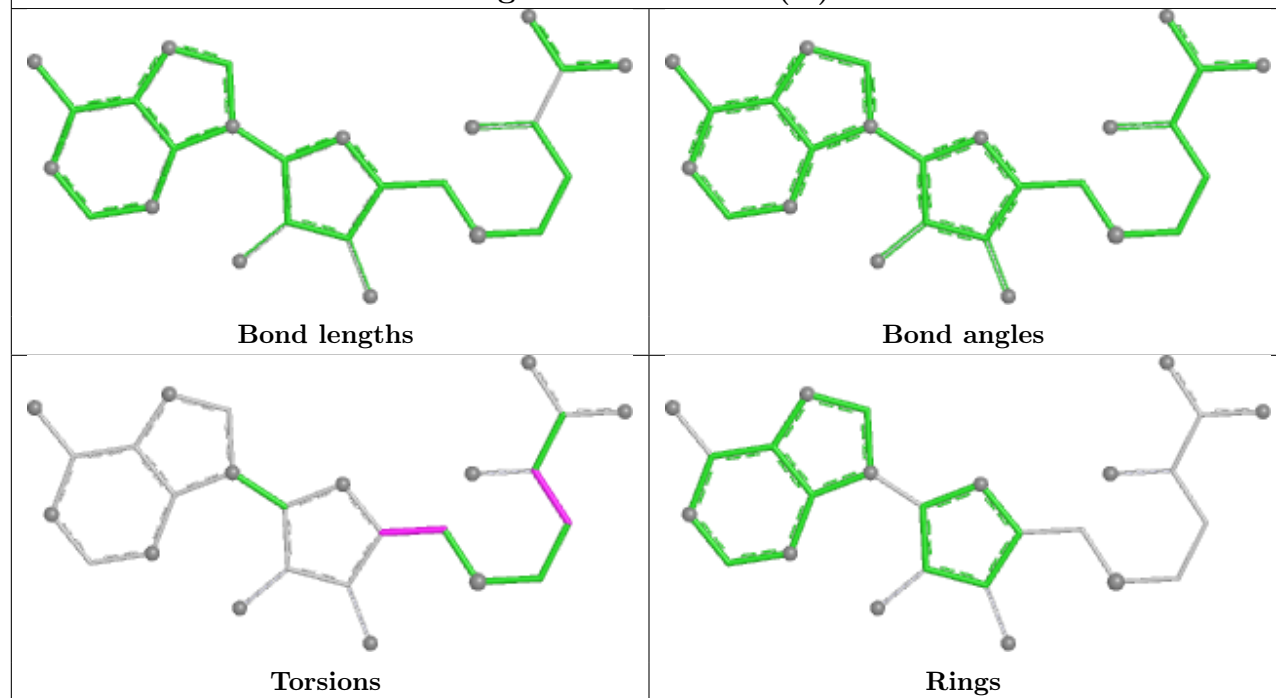
Ligand A1CG2 A 505



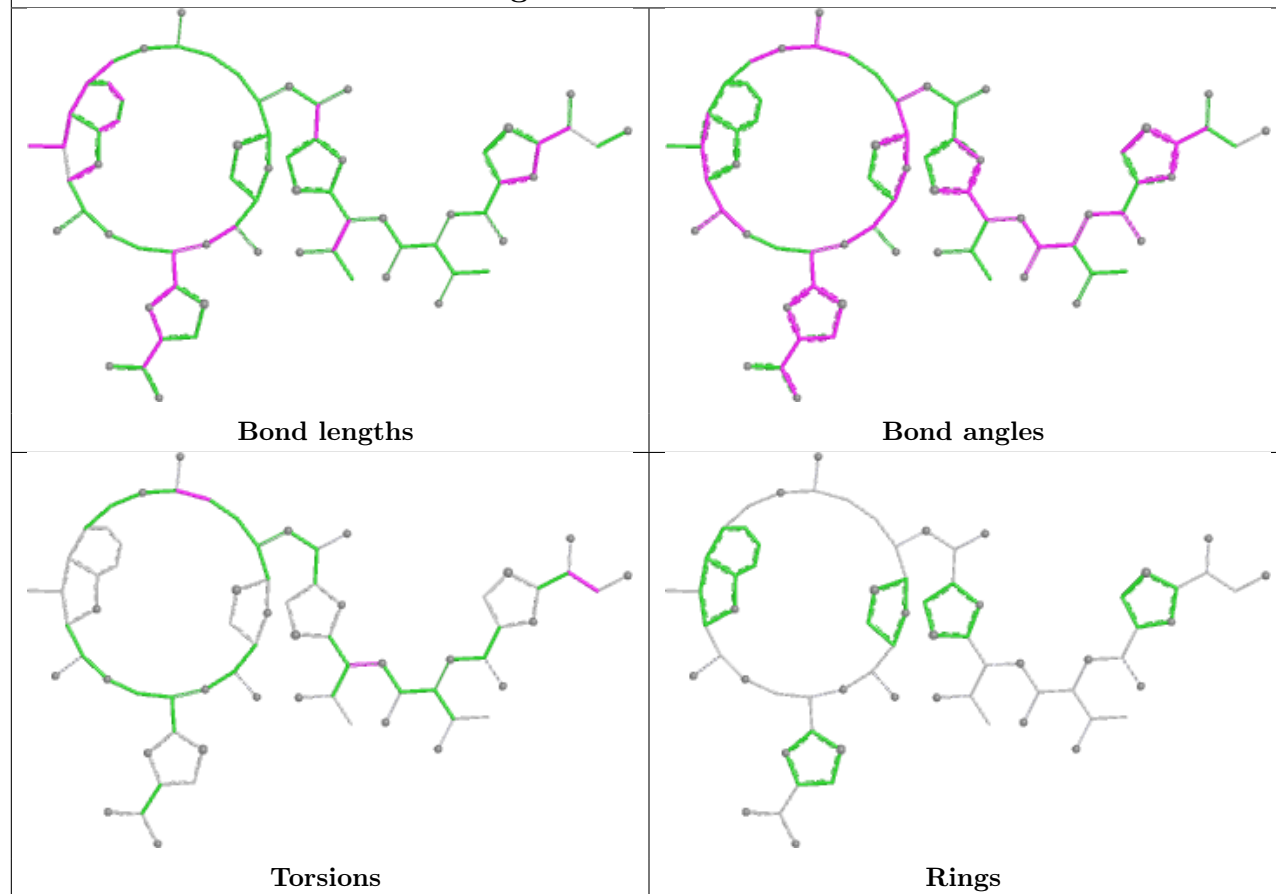
Ligand A1CG2 B 504



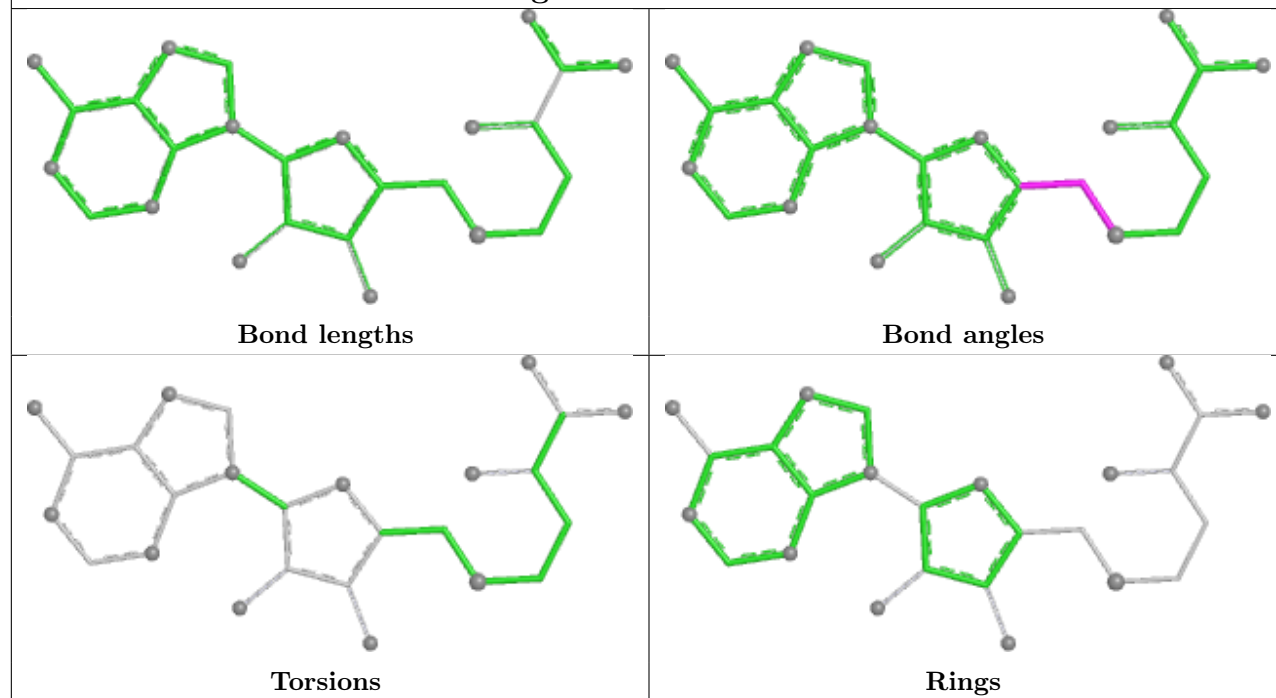
Ligand SAH A 503 (A)



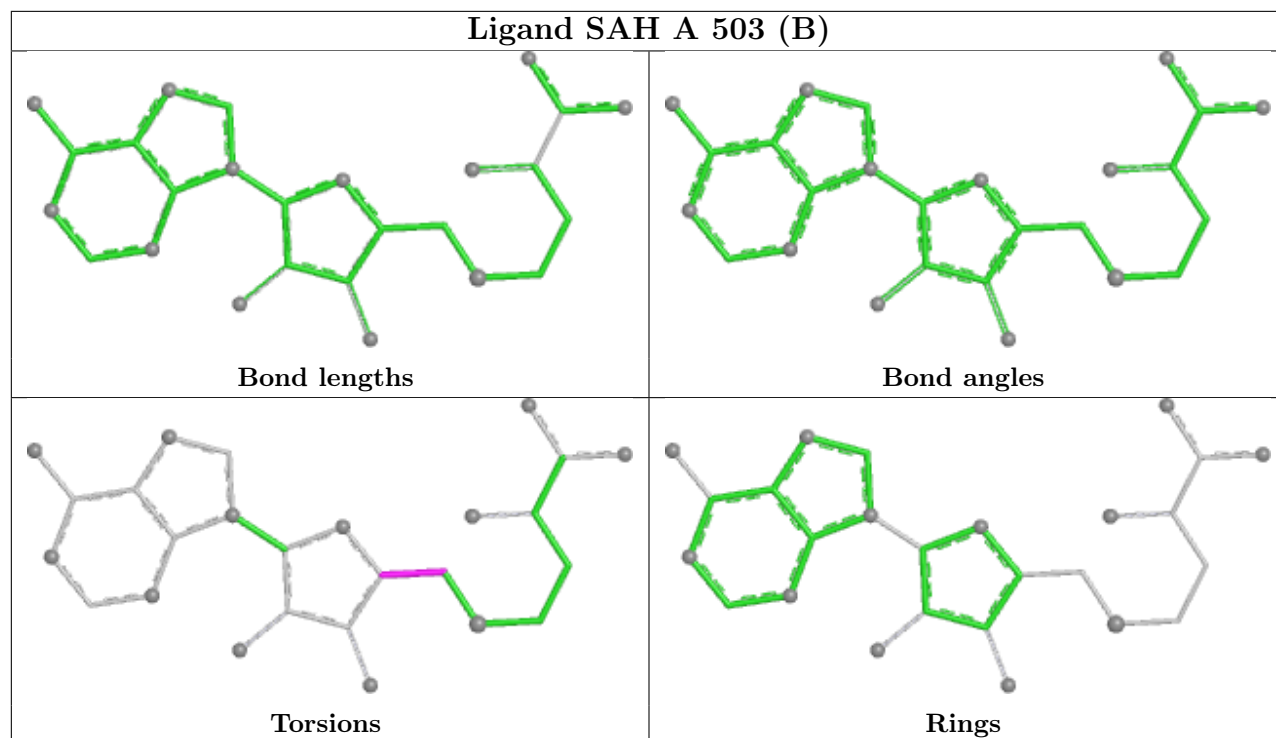
Ligand A1CG2 A 504



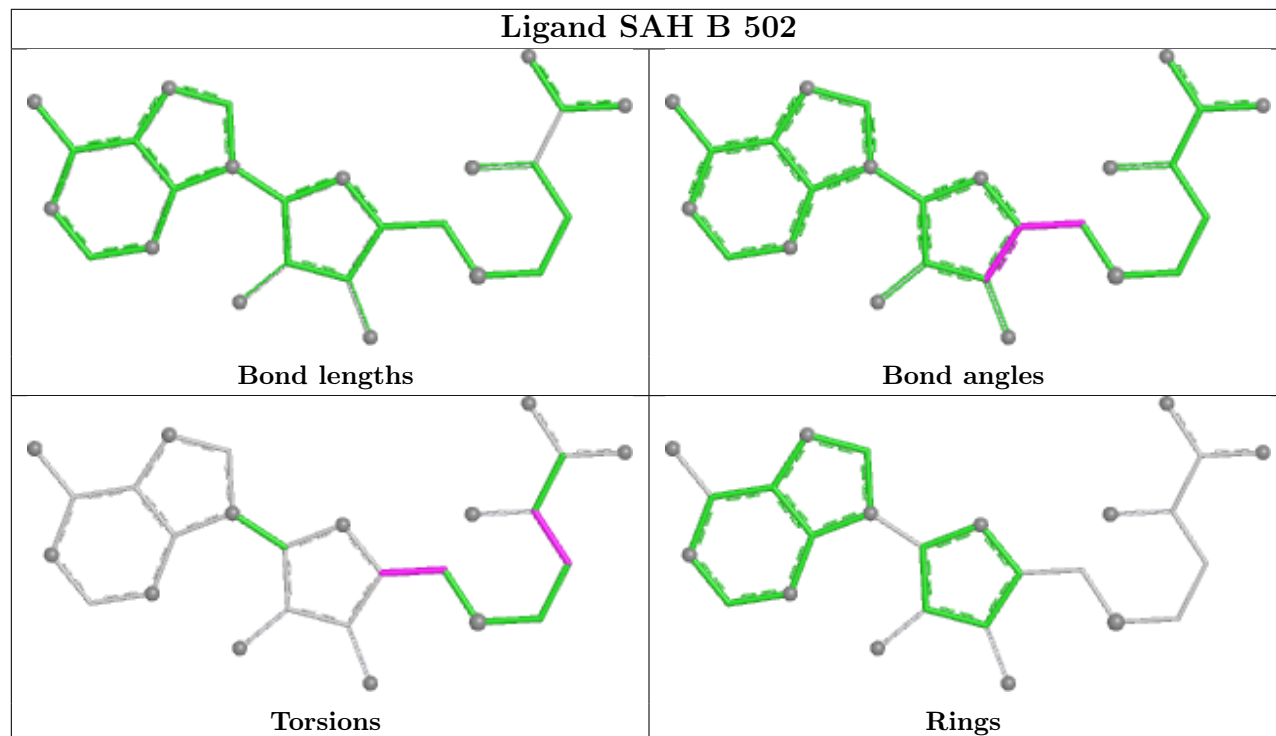
Ligand SAH A 502



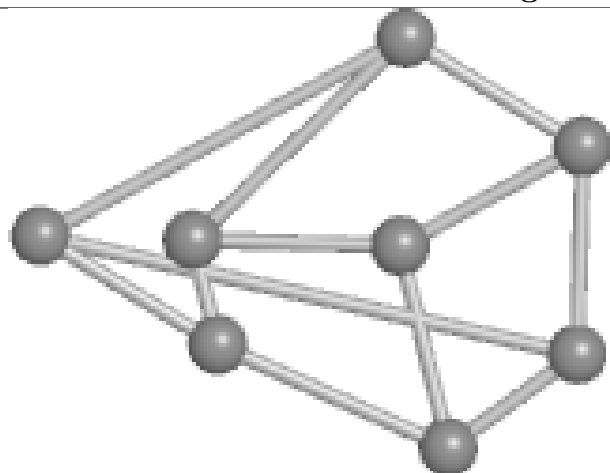
Ligand SAH A 503 (B)



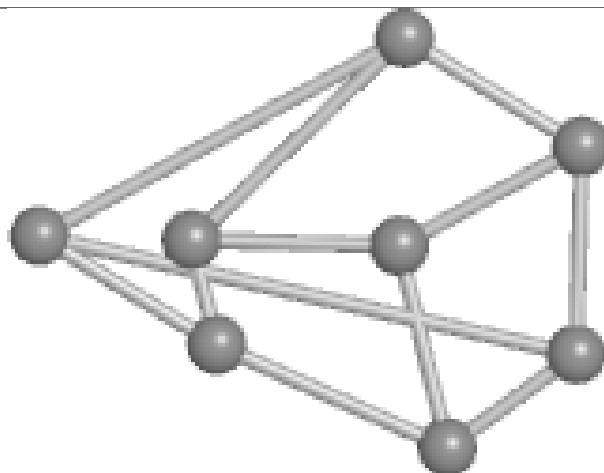
Ligand SAH B 502



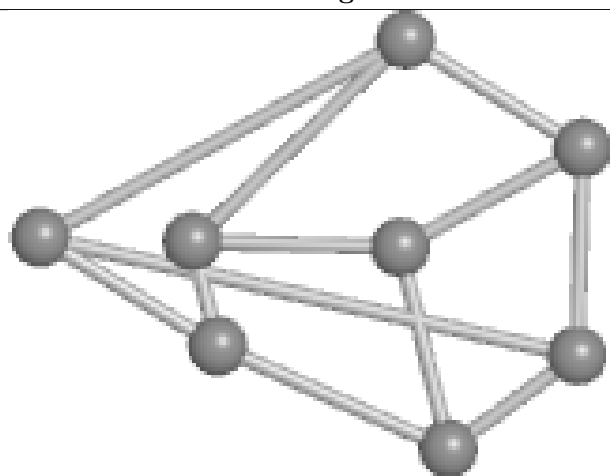
Ligand SF4 B 501



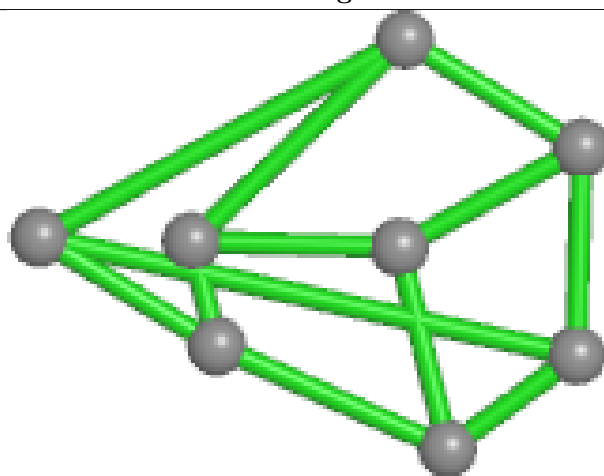
Bond lengths



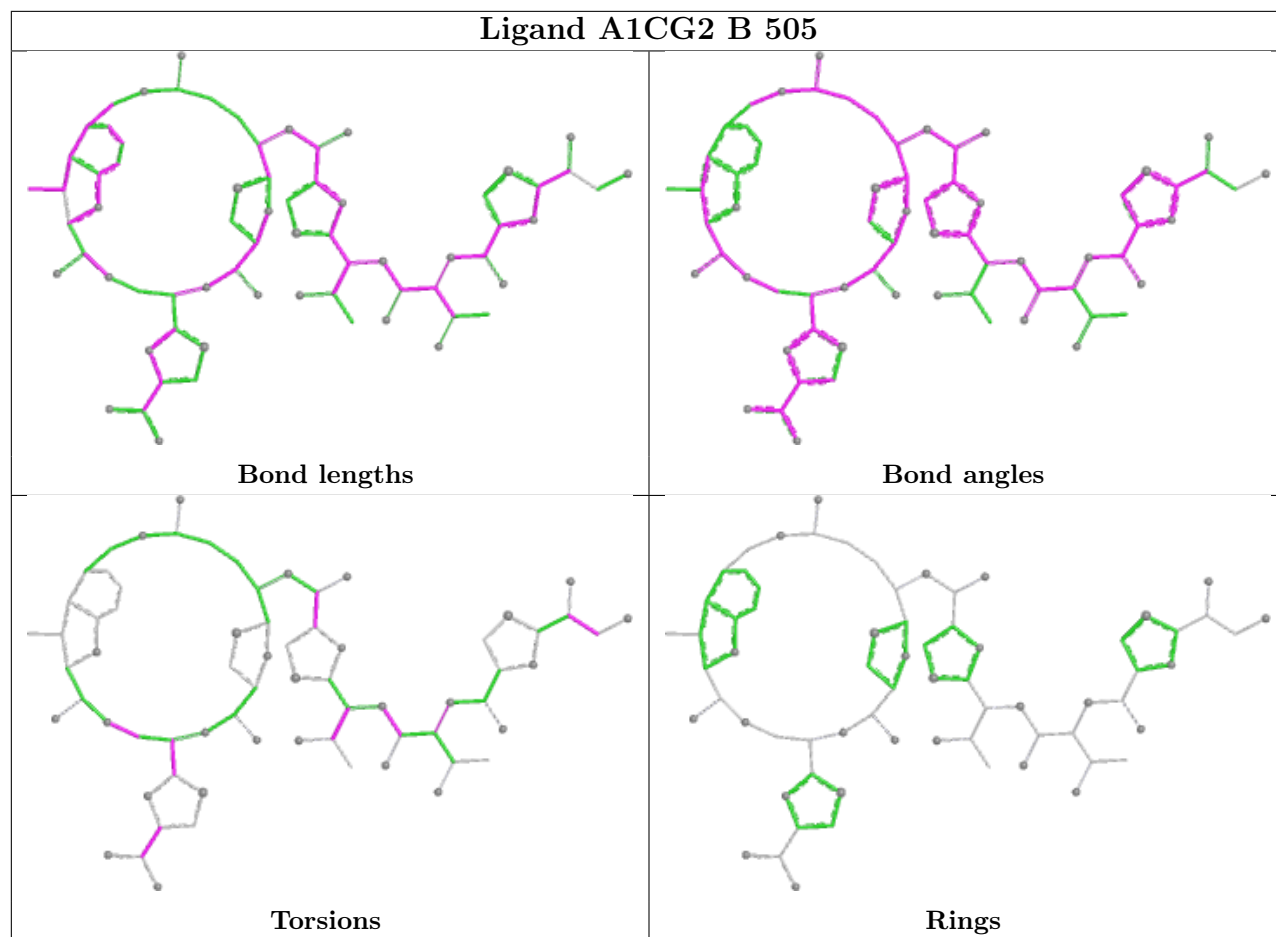
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	397/420 (94%)	-0.13	12 (3%)	52	60	9, 22, 45, 71	6 (1%)
1	B	386/420 (91%)	-0.17	11 (2%)	55	62	9, 23, 45, 76	5 (1%)
All	All	783/840 (93%)	-0.15	23 (2%)	53	61	9, 22, 45, 76	11 (1%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	413	ALA	4.8
1	A	399	ARG	3.3
1	A	232	THR	3.2
1	B	232	THR	2.9
1	A	242	ALA	2.7
1	B	233	PRO	2.7
1	A	416	GLN	2.6
1	B	244	THR	2.5
1	B	203	ASP	2.4
1	A	236	PHE	2.4
1	A	414	MET	2.4
1	B	243	GLY	2.4
1	B	45	THR	2.4
1	A	400	LEU	2.3
1	B	413	ALA	2.3
1	A	412[A]	MET	2.3
1	B	409	ALA	2.2
1	B	266	ASP	2.1
1	A	28	GLN	2.1
1	B	201	PHE	2.1
1	B	172	ARG	2.0
1	A	415	SER	2.0
1	A	411	GLU	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](#)

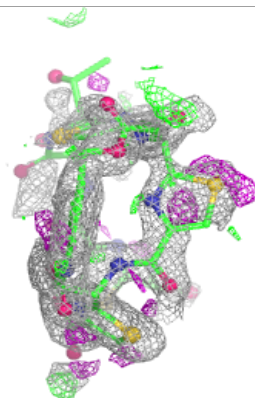
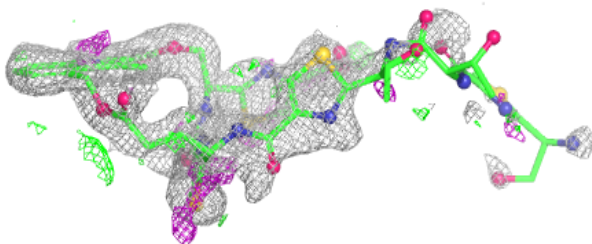
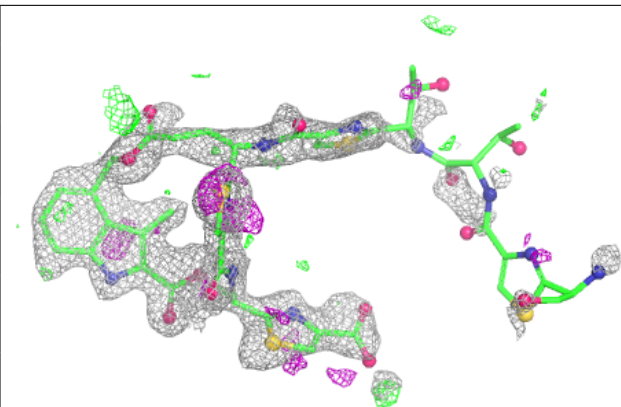
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	A1CG2	B	505	69/69	0.77	0.16	21,56,118,128	0
4	A1CG2	B	504	69/69	0.83	0.13	24,50,87,104	0
4	A1CG2	A	505	69/69	0.85	0.13	14,46,61,68	0
3	SAH	B	502	26/26	0.90	0.10	21,27,40,43	0
4	A1CG2	A	504	69/69	0.95	0.09	13,23,54,63	0
3	SAH	A	503[A]	26/26	0.96	0.06	10,13,16,18	26
3	SAH	A	503[B]	26/26	0.96	0.06	10,14,17,28	26
3	SAH	A	502	26/26	0.96	0.06	12,16,19,20	0
3	SAH	B	503	26/26	0.97	0.05	12,17,23,26	0
5	CA	A	506	1/1	0.97	0.09	40,40,40,40	0
5	CA	B	506	1/1	0.98	0.08	32,32,32,32	0
2	SF4	B	501	8/8	0.98	0.04	18,21,21,22	0
6	NI	A	507	1/1	0.98	0.03	13,13,13,13	1
2	SF4	A	501	8/8	0.99	0.03	12,13,14,14	0

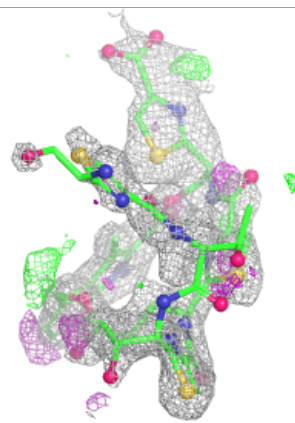
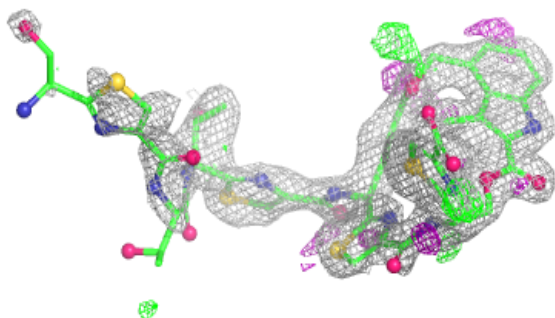
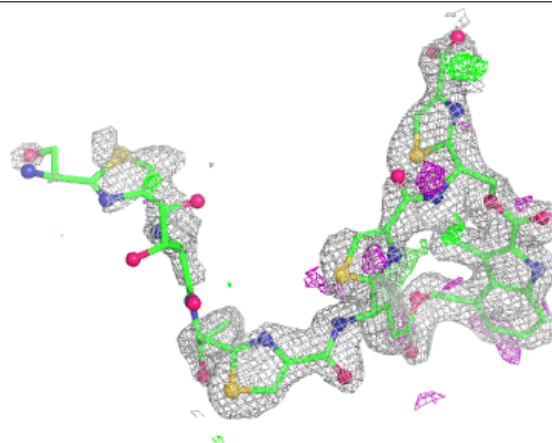
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1CG2 B 505:

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

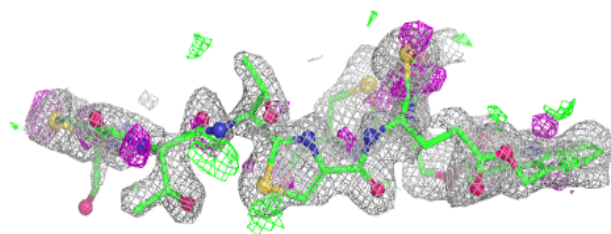
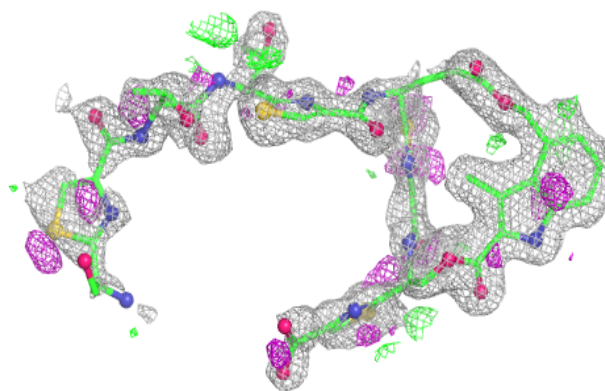
**Electron density around A1CG2 B 504:**

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

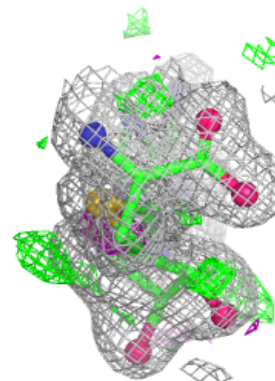
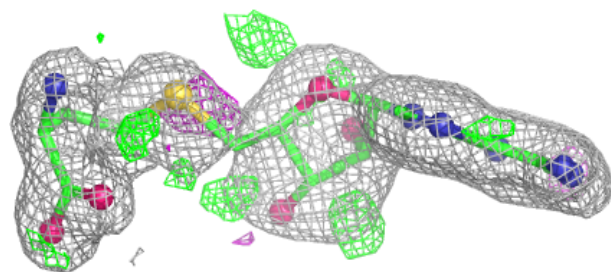
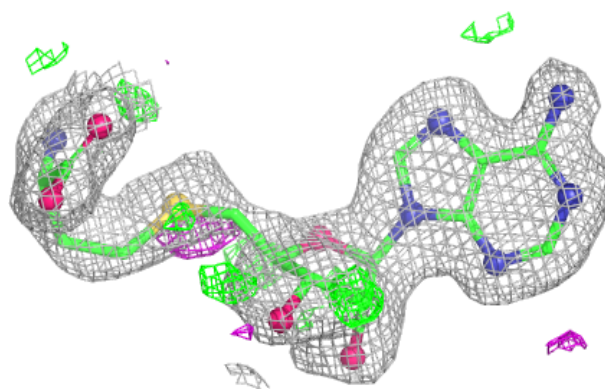


Electron density around A1CG2 A 505:

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

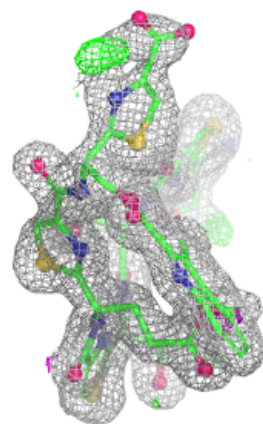
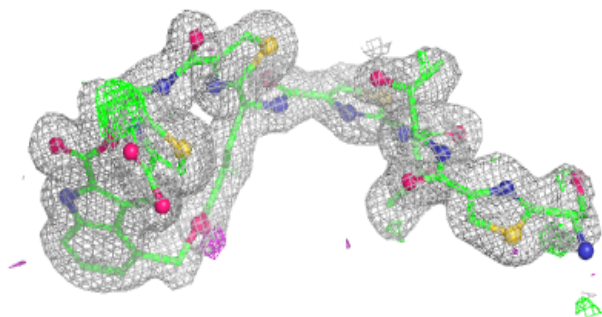
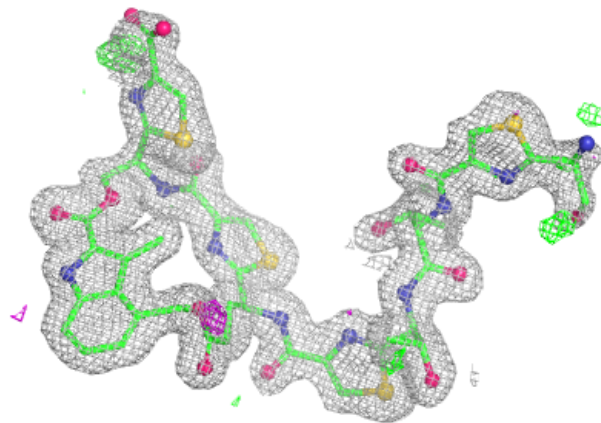
**Electron density around SAH B 502:**

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



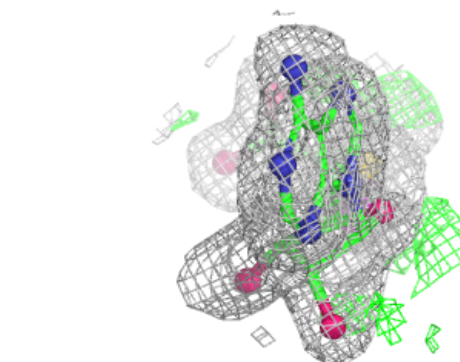
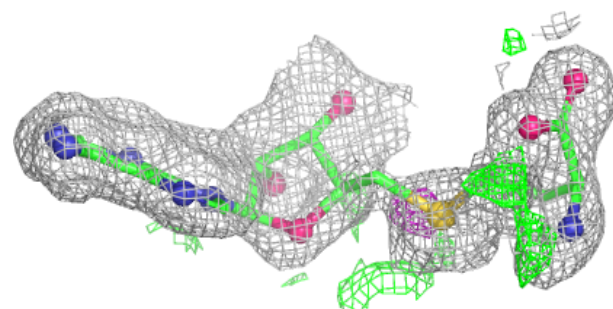
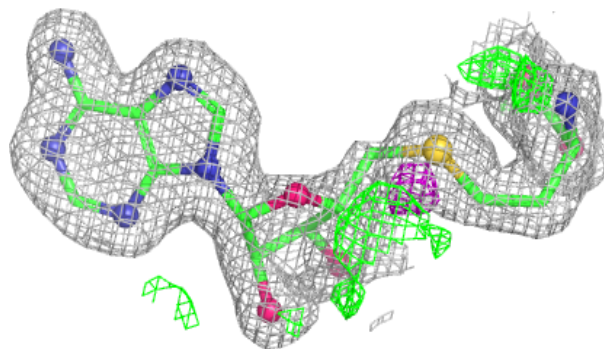
Electron density around A1CG2 A 504:

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

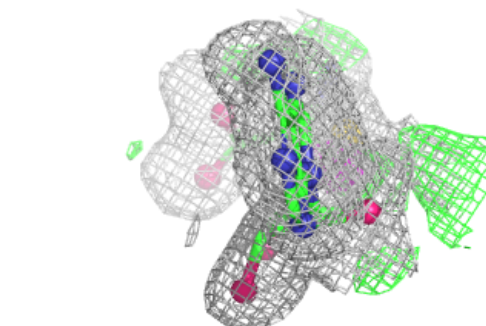
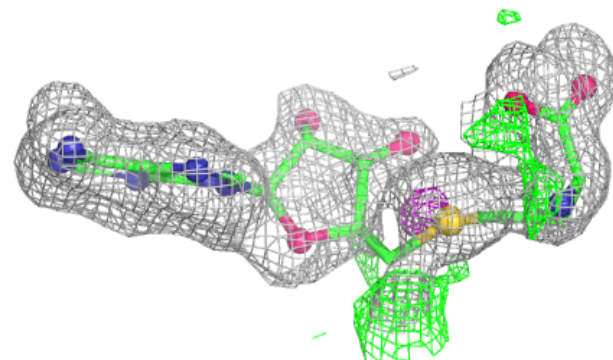
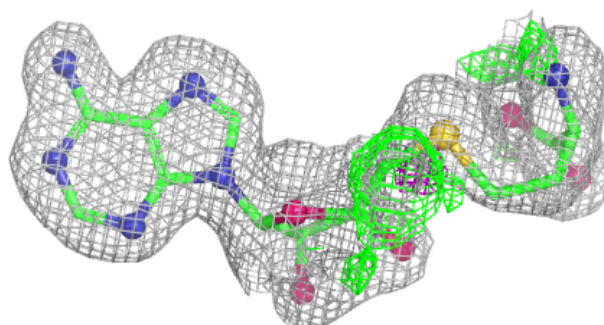


Electron density around SAH A 503 (A):

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

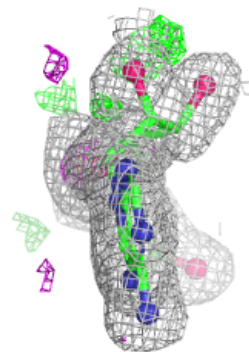
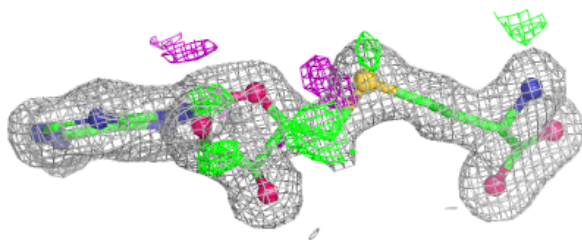
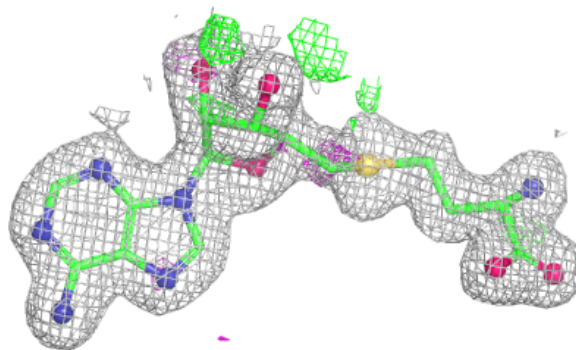
**Electron density around SAH A 503 (B):**

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and green (positive)

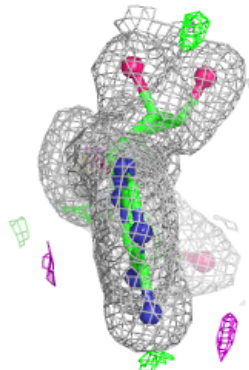
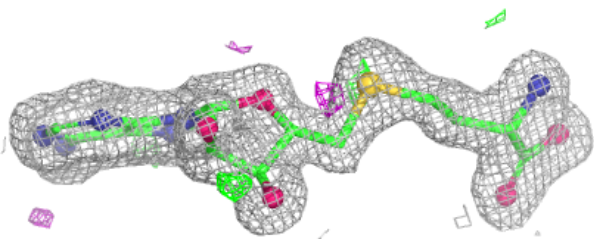
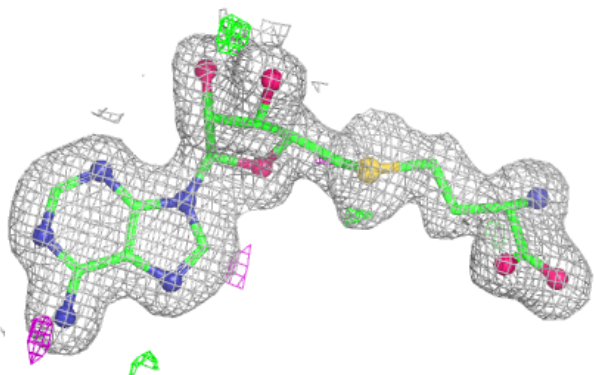


Electron density around SAH A 502:

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

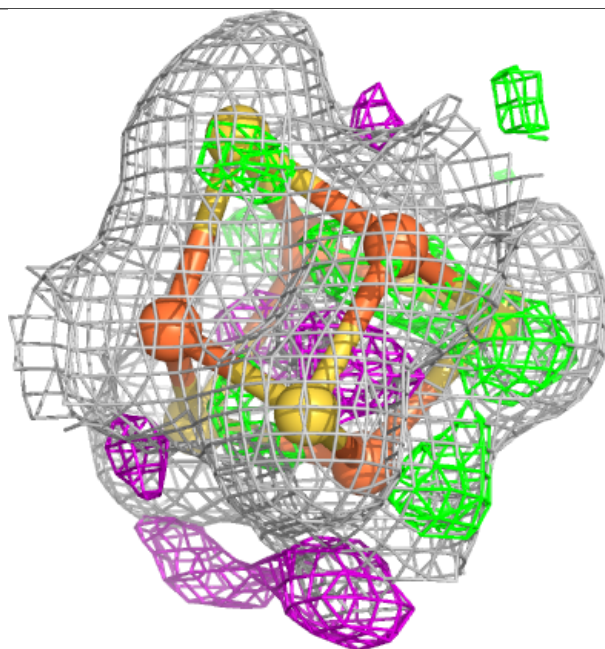
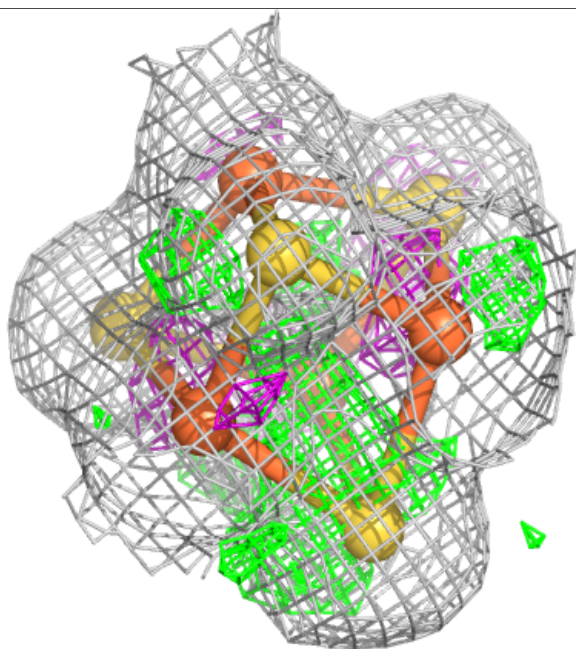
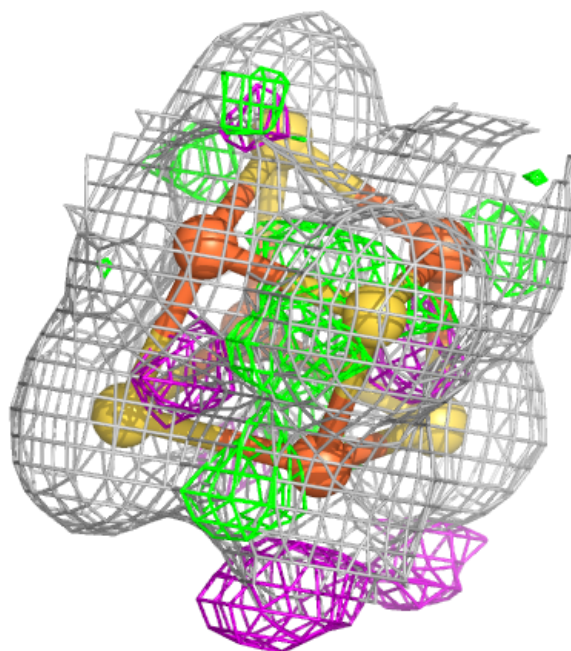
**Electron density around SAH B 503:**

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



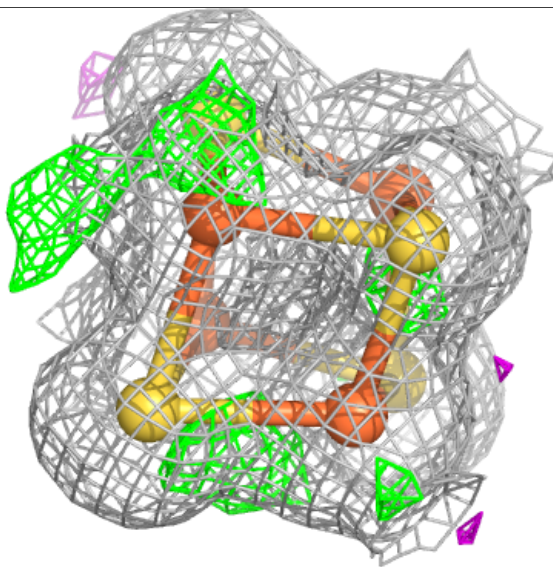
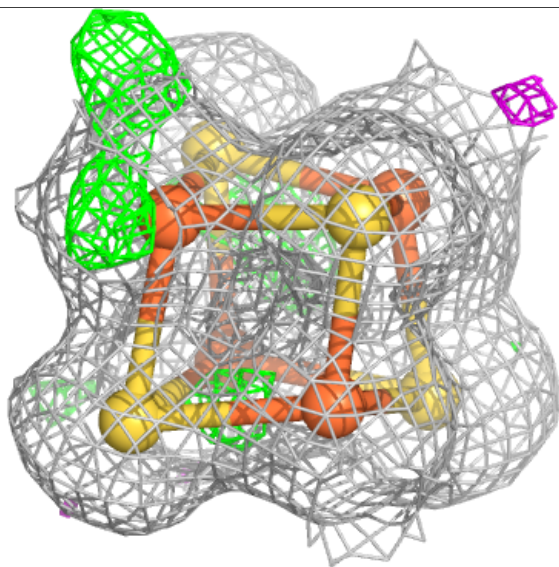
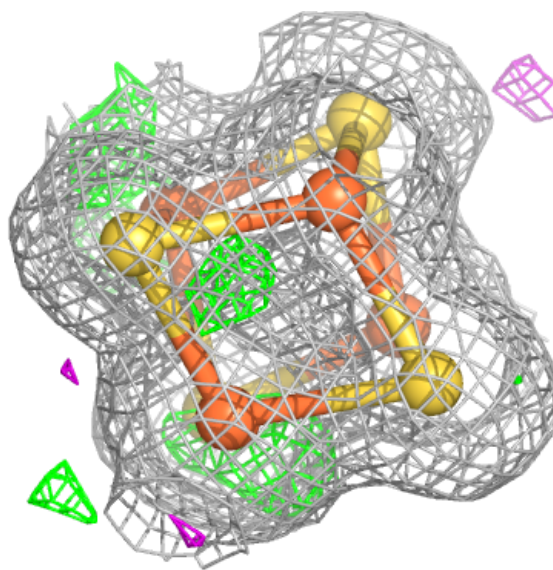
Electron density around SF4 B 501:

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



Electron density around SF4 A 501:

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.