



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 04:37 am BST

PDB ID : 5XJ2
Title : Structure of spRlmCD with U747 RNA
Authors : Jiang, Y.; Gong, Q.
Deposited on : 2017-04-28
Resolution : 2.84 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 : 2.11
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) : 2.11

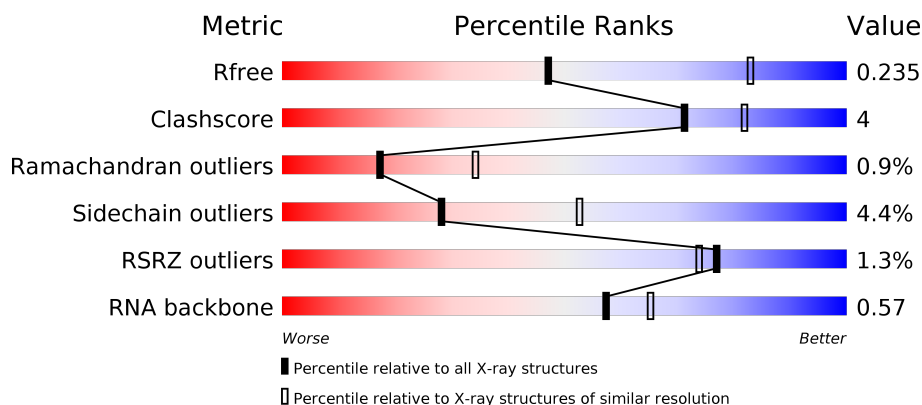
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION





The reported resolution of this entry is 2.84 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	1031 (2.86-2.82)
Clashscore	141614	1078 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)
RSRZ outliers	127900	1019 (2.86-2.82)
RNA backbone	3102	1077 (3.10-2.58)

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 on 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	454	
1	B	454	
1	C	454	
1	D	454	

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Mol	Chain	Length	Quality of chain
2	G	18	<p>17% 17% 33% 6% 44%</p>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 14555 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 Uncharacterized RNA methyltransferase SP_1029.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	454	Total	C	N	O	S	0	0	0
			3568	2283	612	661	12			
1	B	452	Total	C	N	O	S	0	0	0
			3524	2252	602	658	12			
1	C	451	Total	C	N	O	S	0	0	0
			3559	2275	611	662	11			
1	D	452	Total	C	N	O	S	0	0	0
			3570	2282	611	667	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	443	GLN	GLU	engineered mutation	UNP Q97R12
B	443	GLN	GLU	engineered mutation	UNP Q97R12
C	443	GLN	GLU	engineered mutation	UNP Q97R12
D	443	GLN	GLU	engineered mutation	UNP Q97R12

- Molecule 2 is a RNA chain called RNA (5'-R(*GP*GP*CP*AP*CP*GP*UP*GP*CP*U)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	10	Total	C	N	O	P	0	0	0
			211	95	38	69	9			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

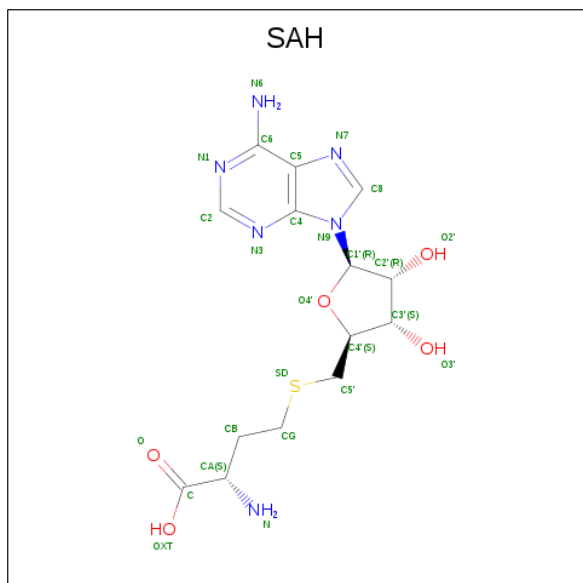
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	A	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		

- Molecule 4 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
4	B	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
4	C	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
4	D	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	8	Total	O	0	0
			8	8		
5	B	1	Total	O	0	0
			1	1		
5	C	3	Total	O	0	0
			3	3		

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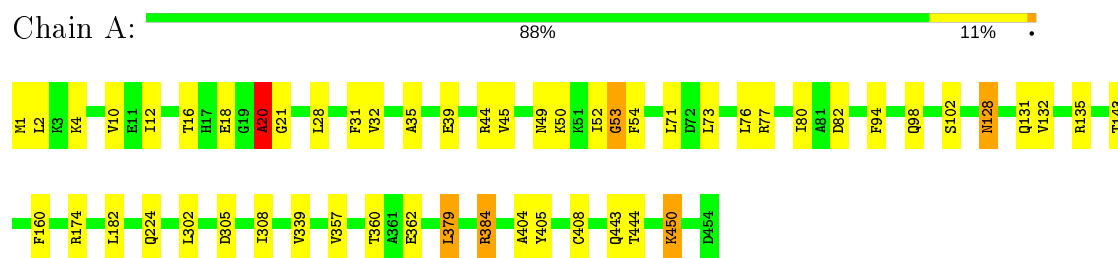
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	3	Total	O	0	0
			3	3		

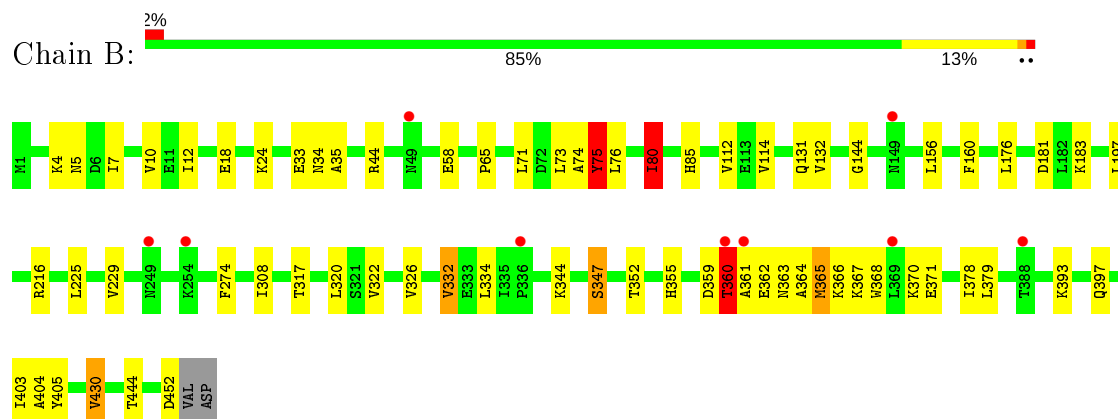
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

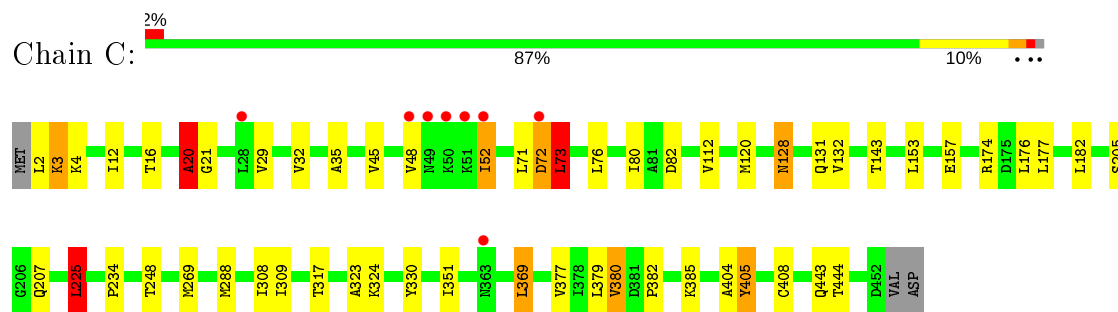
• Molecule 1: Uncharacterized RNA methyltransferase SP_1029



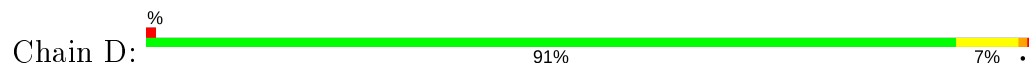
• Molecule 1: Uncharacterized RNA methyltransferase SP_1029

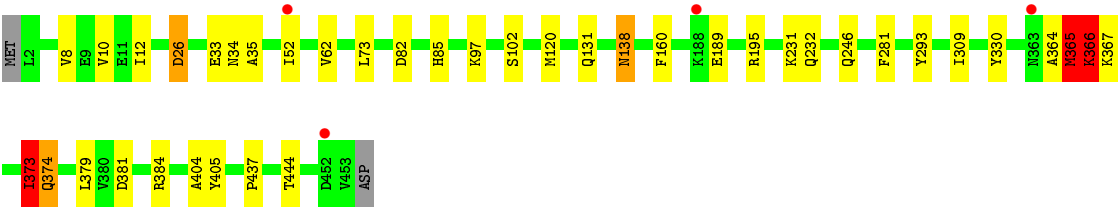


• Molecule 1: Uncharacterized RNA methyltransferase SP_1029



• Molecule 1: Uncharacterized RNA methyltransferase SP_1029





● Molecule 2: RNA (5'-R(*GP*GP*CP*AP*CP*GP*UP*GP*CP*U)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.38Å 94.92Å 164.16Å 90.00° 95.93° 90.00°	Depositor
Resolution (Å)	39.53 – 2.84 39.53 – 2.84	Depositor EDS
% Data completeness (in resolution range)	99.5 (39.53-2.84) 99.5 (39.53-2.84)	Depositor EDS
R_{merge}	0.37	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.195 , 0.236 0.197 , 0.235	Depositor DCC
R_{free} test set	1999 reflections (4.37%)	wwPDB-VP
Wilson B-factor (Å ²)	31.7	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 36.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	14555	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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	0.60	0/3632	0.85	13/4923 (0.3%)
1	B	0.57	0/3587	0.86	5/4868 (0.1%)
1	C	0.58	0/3623	0.82	5/4907 (0.1%)
1	D	0.60	0/3634	0.84	4/4924 (0.1%)
2	G	0.44	0/234	0.87	0/361
All	All	0.58	0/14710	0.84	27/19983 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	3
1	D	0	5
All	All	0	12

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	181	ASP	CB-CG-OD1	9.71	127.03	118.30
1	A	31	PHE	CB-CG-CD1	9.16	127.21	120.80
1	A	31	PHE	CB-CG-CD2	-8.70	114.71	120.80
1	A	305	ASP	CB-CG-OD1	8.33	125.80	118.30
1	B	80	ILE	N-CA-C	6.11	127.51	111.00
1	A	20	ALA	C-N-CA	6.01	134.93	122.30
1	D	26	ASP	CB-CG-OD2	6.00	123.70	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	225	LEU	CB-CG-CD1	5.96	121.14	111.00
1	A	305	ASP	CB-CG-OD2	-5.84	113.04	118.30
1	C	20	ALA	C-N-CA	5.83	134.54	122.30
1	B	75	TYR	N-CA-CB	5.72	120.90	110.60
1	D	373	ILE	C-N-CA	5.62	135.74	121.70
1	A	77	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	A	53	GLY	C-N-CA	5.45	135.34	121.70
1	B	181	ASP	CB-CG-OD2	-5.45	113.40	118.30
1	C	73	LEU	CA-CB-CG	5.41	127.75	115.30
1	A	50	LYS	N-CA-C	-5.29	96.72	111.00
1	D	138	ASN	O-C-N	-5.26	114.25	123.20
1	A	135	ARG	NE-CZ-NH2	-5.25	117.68	120.30
1	B	216	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	D	232	GLN	CA-CB-CG	5.13	124.68	113.40
1	A	450	LYS	CA-CB-CG	5.11	124.64	113.40
1	C	2	LEU	C-N-CA	5.10	134.46	121.70
1	A	20	ALA	CA-C-N	5.10	126.39	116.20
1	C	369	LEU	CB-CG-CD2	5.07	119.61	111.00
1	A	174	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	A	384	ARG	NE-CZ-NH1	5.01	122.81	120.30

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	20	ALA	Peptide
1	A	52	ILE	Peptide
1	B	33	GLU	Peptide
1	B	360	THR	Peptide
1	C	20	ALA	Peptide
1	C	72	ASP	Peptide
1	C	73	LEU	Peptide
1	D	138	ASN	Peptide
1	D	33	GLU	Peptide
1	D	365	MET	Peptide
1	D	366	LYS	Peptide
1	D	373	ILE	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3568	0	3606	19	0
1	B	3524	0	3524	38	0
1	C	3559	0	3597	32	0
1	D	3570	0	3605	17	0
2	G	211	0	111	4	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	26	0	19	1	0
4	B	26	0	19	0	0
4	C	26	0	19	0	0
4	D	26	0	19	4	0
5	A	8	0	0	0	0
5	B	1	0	0	0	0
5	C	3	0	0	0	0
5	D	3	0	0	0	0
All	All	14555	0	14519	103	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 4.

All (103) 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:D:120:MET:HE2	1:D:437:PRO:HG2	1.59	0.85
1:B:176:LEU:HD13	1:B:229:VAL:HG22	1.59	0.84
1:A:2:LEU:HD11	1:A:45:VAL:HG21	1.61	0.82
1:D:73:LEU:HD21	1:D:160:PHE:CE2	2.18	0.78
1:B:332:VAL:HG22	1:B:368:TRP:CH2	2.21	0.75
1:C:379:LEU:HD23	1:C:404:ALA:HB3	1.70	0.73
1:D:379:LEU:HD23	1:D:404:ALA:HB3	1.70	0.72
1:C:73:LEU:HB2	1:C:76:LEU:HG	1.73	0.71
1:B:379:LEU:HD23	1:B:404:ALA:HB3	1.72	0.70
1:D:120:MET:CE	1:D:437:PRO:HG2	2.22	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:72:ASP:HA	1:C:73:LEU:HG	1.76	0.67
1:B:114:VAL:HA	1:B:430:VAL:HG23	1.76	0.67
1:C:269:MET:CE	1:C:317:THR:HG21	2.26	0.66
1:D:364:ALA:HB3	1:D:367:LYS:HG3	1.78	0.66
1:B:332:VAL:HG22	1:B:368:TRP:HH2	1.57	0.65
1:B:7:ILE:HD12	1:B:58:GLU:HG3	1.79	0.64
1:C:157:GLU:OE2	1:C:174:ARG:NH2	2.29	0.64
1:A:128:ASN:C	1:A:128:ASN:HD22	2.02	0.63
1:C:128:ASN:HD22	1:C:128:ASN:C	2.02	0.62
1:B:347:SER:HB2	1:C:234:PRO:HB2	1.82	0.60
1:C:73:LEU:HD13	1:C:76:LEU:HD11	1.84	0.60
1:B:114:VAL:HG22	1:B:430:VAL:HG21	1.85	0.59
1:D:12:ILE:HG13	1:D:35:ALA:HB1	1.84	0.59
1:C:73:LEU:CB	1:C:76:LEU:HG	2.34	0.58
1:B:12:ILE:HG13	1:B:35:ALA:HB1	1.85	0.57
1:C:12:ILE:HG13	1:C:35:ALA:HB1	1.85	0.57
1:A:224:GLN:HE22	1:B:65:PRO:HB3	1.70	0.57
1:D:365:MET:O	1:D:366:LYS:HG2	2.05	0.56
1:B:73:LEU:HD21	1:B:160:PHE:CZ	2.41	0.55
1:C:380:VAL:HG12	1:C:405:TYR:HA	1.88	0.55
1:C:72:ASP:CA	1:C:73:LEU:HG	2.36	0.55
1:A:408:CYS:HB3	1:A:443:GLN:NE2	2.22	0.53
1:C:76:LEU:HD22	1:C:80:ILE:HD12	1.91	0.52
1:A:12:ILE:HD13	1:A:39:GLU:HB2	1.90	0.52
1:C:408:CYS:HB3	1:C:443:GLN:NE2	2.25	0.52
1:B:352:THR:HB	1:C:207:GLN:NE2	2.26	0.50
1:C:324:LYS:HG2	1:C:351:ILE:HD13	1.95	0.49
1:D:364:ALA:HB1	1:D:367:LYS:N	2.27	0.49
1:A:302:LEU:HD22	1:A:308:ILE:HD11	1.95	0.49
1:C:380:VAL:HG13	1:C:382:PRO:HD3	1.95	0.49
1:D:365:MET:O	1:D:366:LYS:CG	2.60	0.49
1:B:34:ASN:HB2	1:B:85:HIS:CD2	2.47	0.49
1:A:76:LEU:HD22	1:A:80:ILE:HD12	1.95	0.49
1:B:274:PHE:CE2	1:B:317:THR:HA	2.48	0.49
1:D:34:ASN:HB2	1:D:85:HIS:CD2	2.48	0.49
1:C:71:LEU:O	1:C:73:LEU:HA	2.13	0.48
1:B:363:ASN:HA	1:B:366:LYS:HG3	1.95	0.48
1:B:359:ASP:C	1:B:361:ALA:HA	2.34	0.48
1:B:359:ASP:O	1:B:360:THR:OG1	2.28	0.47
1:D:309:ILE:HD13	1:D:330:TYR:HB2	1.96	0.47
1:C:120:MET:HG3	1:C:288:MET:HE3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:364:ALA:O	1:B:365:MET:HB2	2.14	0.47
1:C:21:GLY:HA3	1:C:32:VAL:O	2.15	0.47
1:B:132:VAL:HG13	1:B:197:LEU:HB2	1.96	0.47
1:B:393:LYS:O	1:B:397:GLN:HG3	2.14	0.47
1:B:308:ILE:HD12	1:B:326:VAL:HG21	1.96	0.47
1:A:18:GLU:OE2	2:G:757:U:O2'	2.31	0.47
1:C:308:ILE:HG13	1:C:377:VAL:CG2	2.45	0.47
1:C:132:VAL:HG11	1:C:143:THR:HB	1.97	0.46
1:D:281:PHE:CD1	4:D:502:SAH:HG2	2.50	0.46
1:A:21:GLY:HA3	1:A:32:VAL:O	2.15	0.46
1:B:378:ILE:HB	1:B:403:ILE:HD13	1.97	0.46
1:B:44:ARG:HB2	1:B:58:GLU:HG2	1.98	0.46
1:C:308:ILE:HD12	1:C:377:VAL:HG22	1.97	0.46
1:A:73:LEU:HD21	1:A:160:PHE:CZ	2.50	0.46
1:B:71:LEU:O	1:B:74:ALA:O	2.34	0.46
1:A:379:LEU:HG	1:A:404:ALA:HB3	1.98	0.45
1:C:309:ILE:HD13	1:C:330:TYR:HB2	1.98	0.45
1:A:132:VAL:HG11	1:A:143:THR:HB	2.00	0.44
1:B:378:ILE:HB	1:B:403:ILE:CD1	2.47	0.44
1:C:176:LEU:HB3	1:C:225:LEU:CD2	2.47	0.44
1:C:323:ALA:HB3	1:C:351:ILE:HD12	2.00	0.44
1:A:384:ARG:NH1	2:G:742:C:H4'	2.33	0.44
1:A:53:GLY:HA3	1:A:54:PHE:CD1	2.53	0.44
1:D:281:PHE:CE1	4:D:502:SAH:HG2	2.52	0.44
1:A:224:GLN:NE2	1:B:65:PRO:HB3	2.32	0.44
1:B:74:ALA:O	1:B:75:TYR:CB	2.66	0.44
1:B:355:HIS:CE1	1:C:205:SER:HA	2.53	0.44
1:D:381:ASP:OD2	4:D:502:SAH:HB1	2.18	0.44
1:B:360:THR:N	1:B:361:ALA:HA	2.33	0.44
1:B:76:LEU:HD22	1:B:80:ILE:HD12	2.00	0.43
1:C:177:LEU:HD23	1:C:182:LEU:HD12	1.99	0.43
1:B:308:ILE:HD13	1:B:322:VAL:HG21	2.01	0.43
1:B:132:VAL:HG23	1:B:144:GLY:O	2.19	0.43
1:D:364:ALA:CB	1:D:367:LYS:HG3	2.47	0.43
1:A:16:THR:N	1:A:20:ALA:O	2.41	0.43
1:C:16:THR:N	1:C:20:ALA:O	2.39	0.43
1:C:128:ASN:ND2	1:C:128:ASN:C	2.71	0.42
1:B:225:LEU:O	1:B:229:VAL:HG23	2.19	0.42
1:C:269:MET:CE	1:C:317:THR:CG2	2.96	0.42
1:D:373:ILE:HA	1:D:374:GLN:HB2	2.01	0.42
1:A:384:ARG:HH12	2:G:742:C:H4'	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:755:G:H2'	2:G:756:C:C6	2.55	0.42
1:C:3:LYS:HE2	1:C:45:VAL:HG21	2.01	0.42
1:B:367:LYS:O	1:B:371:GLU:HG3	2.20	0.41
4:A:502:SAH:H4'	4:A:502:SAH:HB1	2.02	0.41
1:B:334:LEU:HA	1:B:359:ASP:CB	2.50	0.41
1:A:12:ILE:HG12	1:A:35:ALA:HB1	2.02	0.41
1:B:360:THR:HB	1:B:363:ASN:HB2	2.03	0.41
1:B:44:ARG:HD3	1:B:58:GLU:OE2	2.20	0.41
1:A:94:PHE:O	1:A:98:GLN:HG3	2.19	0.41
1:D:293:TYR:OH	4:D:502:SAH:O	2.34	0.41
1:B:332:VAL:HG11	1:B:364:ALA:HB3	2.02	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	452/454 (100%)	433 (96%)	18 (4%)	1 (0%)	47	69
1	B	450/454 (99%)	428 (95%)	16 (4%)	6 (1%)	12	26
1	C	449/454 (99%)	423 (94%)	23 (5%)	3 (1%)	22	42
1	D	450/454 (99%)	420 (93%)	24 (5%)	6 (1%)	12	26
All	All	1801/1816 (99%)	1704 (95%)	81 (4%)	16 (1%)	17	34

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	75	TYR
1	B	365	MET
1	D	373	ILE
1	D	374	GLN

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Mol	Chain	Res	Type
1	A	4	LYS
1	B	4	LYS
1	B	80	ILE
1	C	3	LYS
1	C	52	ILE
1	D	26	ASP
1	D	189	GLU
1	D	366	LYS
1	B	360	THR
1	C	29	VAL
1	D	365	MET
1	B	370	LYS

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	386/398 (97%)	367 (95%)	19 (5%)	25	47
1	B	377/398 (95%)	358 (95%)	19 (5%)	24	46
1	C	386/398 (97%)	371 (96%)	15 (4%)	32	58
1	D	388/398 (98%)	374 (96%)	14 (4%)	35	60
All	All	1537/1592 (96%)	1470 (96%)	67 (4%)	28	53

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	10	VAL
1	A	28	LEU
1	A	44	ARG
1	A	49	ASN
1	A	71	LEU
1	A	82	ASP
1	A	102	SER
1	A	128	ASN

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Mol	Chain	Res	Type
1	A	131	GLN
1	A	182	LEU
1	A	339	VAL
1	A	357	VAL
1	A	360	THR
1	A	362	GLU
1	A	379	LEU
1	A	405	TYR
1	A	444	THR
1	A	450	LYS
1	B	5	ASN
1	B	10	VAL
1	B	18	GLU
1	B	24	LYS
1	B	80	ILE
1	B	112	VAL
1	B	131	GLN
1	B	156	LEU
1	B	183	LYS
1	B	320	LEU
1	B	332	VAL
1	B	344	LYS
1	B	347	SER
1	B	360	THR
1	B	362	GLU
1	B	405	TYR
1	B	430	VAL
1	B	444	THR
1	B	452	ASP
1	C	4	LYS
1	C	48	VAL
1	C	52	ILE
1	C	82	ASP
1	C	112	VAL
1	C	128	ASN
1	C	131	GLN
1	C	153	LEU
1	C	225	LEU
1	C	248	THR
1	C	369	LEU
1	C	380	VAL
1	C	385	LYS

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Mol	Chain	Res	Type
1	C	405	TYR
1	C	444	THR
1	D	8	VAL
1	D	10	VAL
1	D	52	ILE
1	D	62	VAL
1	D	82	ASP
1	D	97	LYS
1	D	102	SER
1	D	131	GLN
1	D	195	ARG
1	D	231	LYS
1	D	246	GLN
1	D	384	ARG
1	D	405	TYR
1	D	444	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	GLN
1	A	128	ASN
1	A	224	GLN
1	B	98	GLN
1	B	190	GLN
1	B	275	GLN
1	B	441	HIS
1	C	128	ASN
1	D	98	GLN
1	D	190	GLN
1	D	247	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	G	9/18 (50%)	3 (33%)	1 (11%)

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	G	744	C
2	G	754	U
2	G	755	G

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	G	753	G

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	$\# Z > 2$
4	SAH	C	502	-	21,28,28	1.14	2 (9%)	20,40,40	1.68	4 (20%)
4	SAH	D	502	-	21,28,28	1.11	2 (9%)	20,40,40	1.55	4 (20%)
4	SAH	A	502	-	21,28,28	1.12	1 (4%)	20,40,40	2.00	7 (35%)
4	SAH	B	502	-	21,28,28	1.22	2 (9%)	20,40,40	1.65	5 (25%)

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
4	SAH	C	502	-	-	2/7/31/31	0/3/3/3
4	SAH	D	502	-	-	3/7/31/31	0/3/3/3
4	SAH	A	502	-	-	1/7/31/31	0/3/3/3
4	SAH	B	502	-	-	4/7/31/31	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	502	SAH	C5-C4	2.75	1.48	1.40
4	A	502	SAH	C2-N3	2.59	1.36	1.32
4	B	502	SAH	C2-N3	2.56	1.36	1.32
4	C	502	SAH	C5-C4	2.55	1.47	1.40
4	D	502	SAH	C5-C4	2.48	1.47	1.40
4	C	502	SAH	O4'-C1'	2.33	1.44	1.41
4	D	502	SAH	O4'-C1'	2.22	1.44	1.41

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	502	SAH	N3-C2-N1	-5.52	120.05	128.68
4	C	502	SAH	C1'-N9-C4	-4.31	119.06	126.64
4	C	502	SAH	N3-C2-N1	-4.09	122.29	128.68
4	D	502	SAH	N3-C2-N1	-4.06	122.33	128.68
4	B	502	SAH	N3-C2-N1	-3.63	123.00	128.68
4	A	502	SAH	C1'-N9-C4	-3.45	120.58	126.64
4	B	502	SAH	C5'-SD-CG	2.81	110.69	102.27
4	A	502	SAH	C5-C6-N6	-2.77	116.14	120.35
4	B	502	SAH	C4-C5-N7	-2.73	106.56	109.40
4	A	502	SAH	O3'-C3'-C4'	-2.54	103.69	111.05
4	D	502	SAH	C4-C5-N7	-2.52	106.77	109.40
4	C	502	SAH	C2-N1-C6	2.48	122.99	118.75
4	A	502	SAH	N6-C6-N1	2.46	123.69	118.57
4	B	502	SAH	C3'-C2'-C1'	2.42	104.63	100.98
4	D	502	SAH	C5'-SD-CG	2.33	109.25	102.27
4	D	502	SAH	O4'-C1'-C2'	-2.33	103.52	106.93
4	A	502	SAH	C2-N1-C6	2.23	122.57	118.75
4	C	502	SAH	C4-C5-N7	-2.22	107.09	109.40
4	A	502	SAH	O4'-C1'-C2'	-2.13	103.81	106.93
4	B	502	SAH	CB-CG-SD	2.10	118.01	113.31

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	502	SAH	CA-CB-CG-SD
4	B	502	SAH	C4'-C5'-SD-CG
4	B	502	SAH	O4'-C4'-C5'-SD
4	B	502	SAH	C3'-C4'-C5'-SD
4	D	502	SAH	C4'-C5'-SD-CG
4	D	502	SAH	O4'-C4'-C5'-SD
4	D	502	SAH	C3'-C4'-C5'-SD
4	C	502	SAH	N-CA-CB-CG
4	C	502	SAH	C-CA-CB-CG
4	A	502	SAH	N-CA-CB-CG

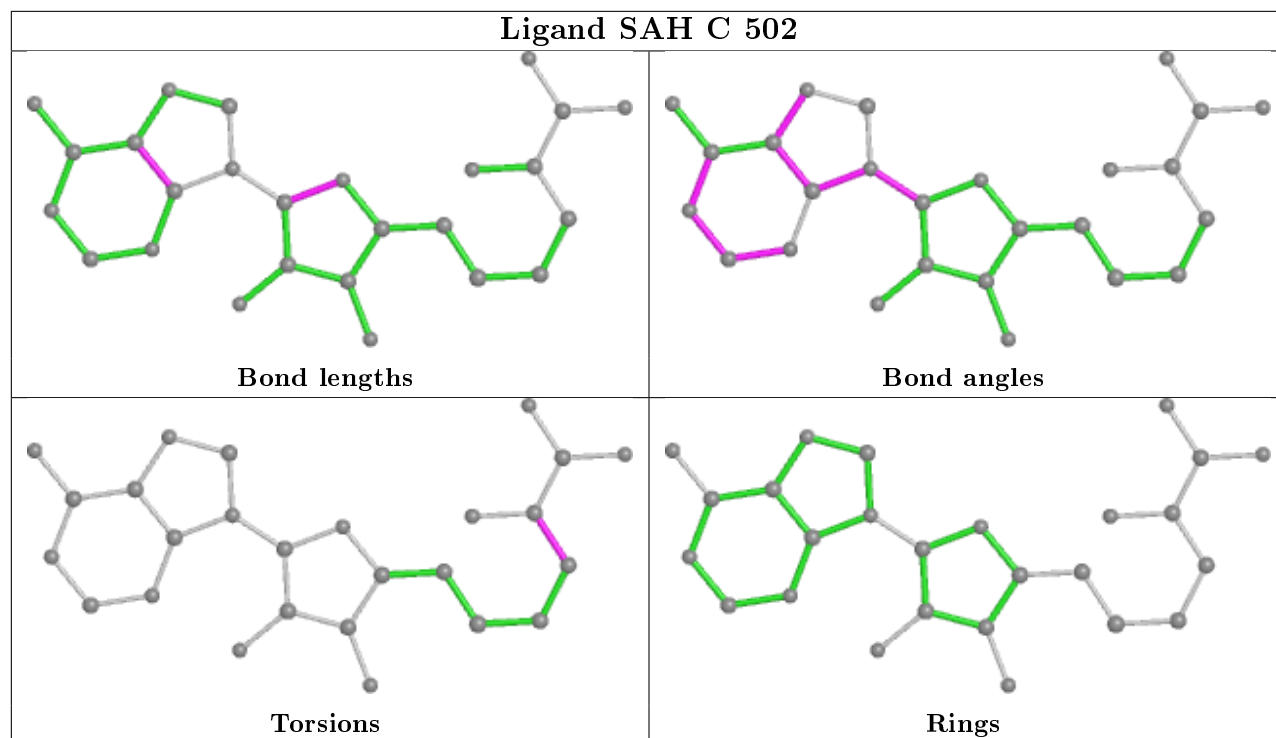
There are no ring outliers.

2 monomers are involved in 5 short contacts:

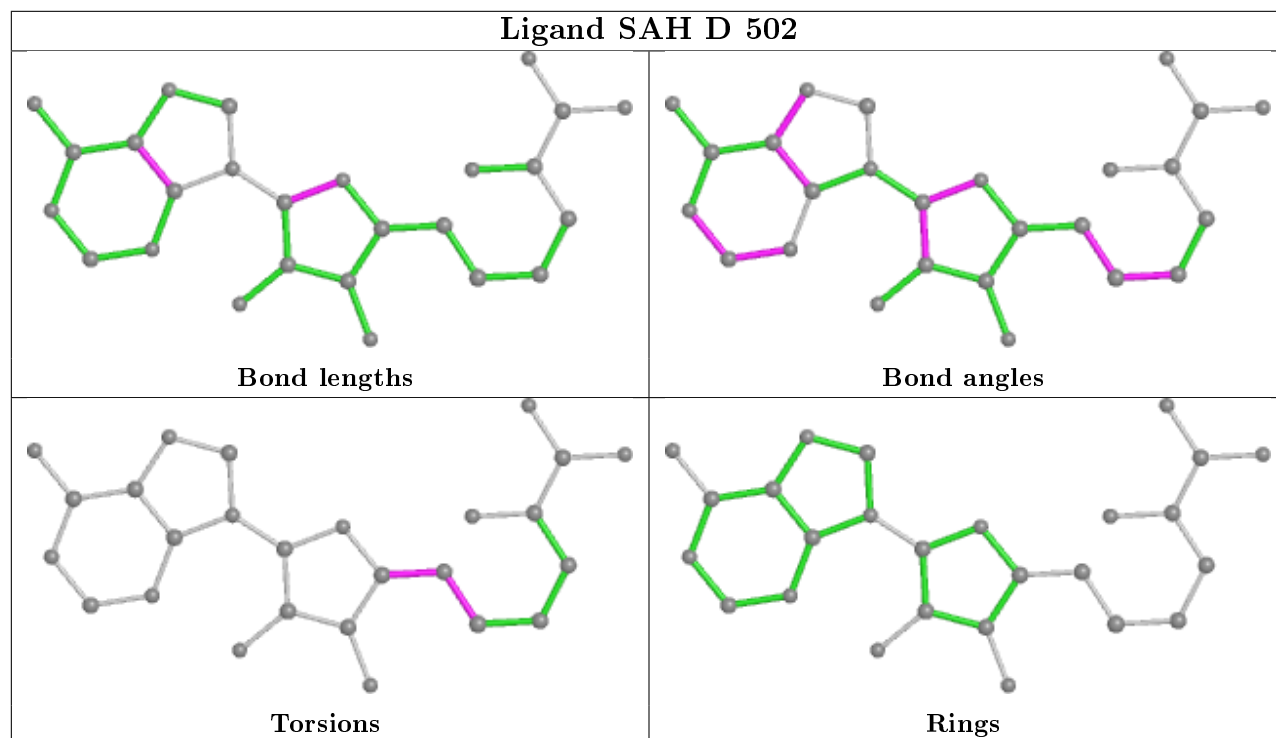
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	502	SAH	4	0
4	A	502	SAH	1	0

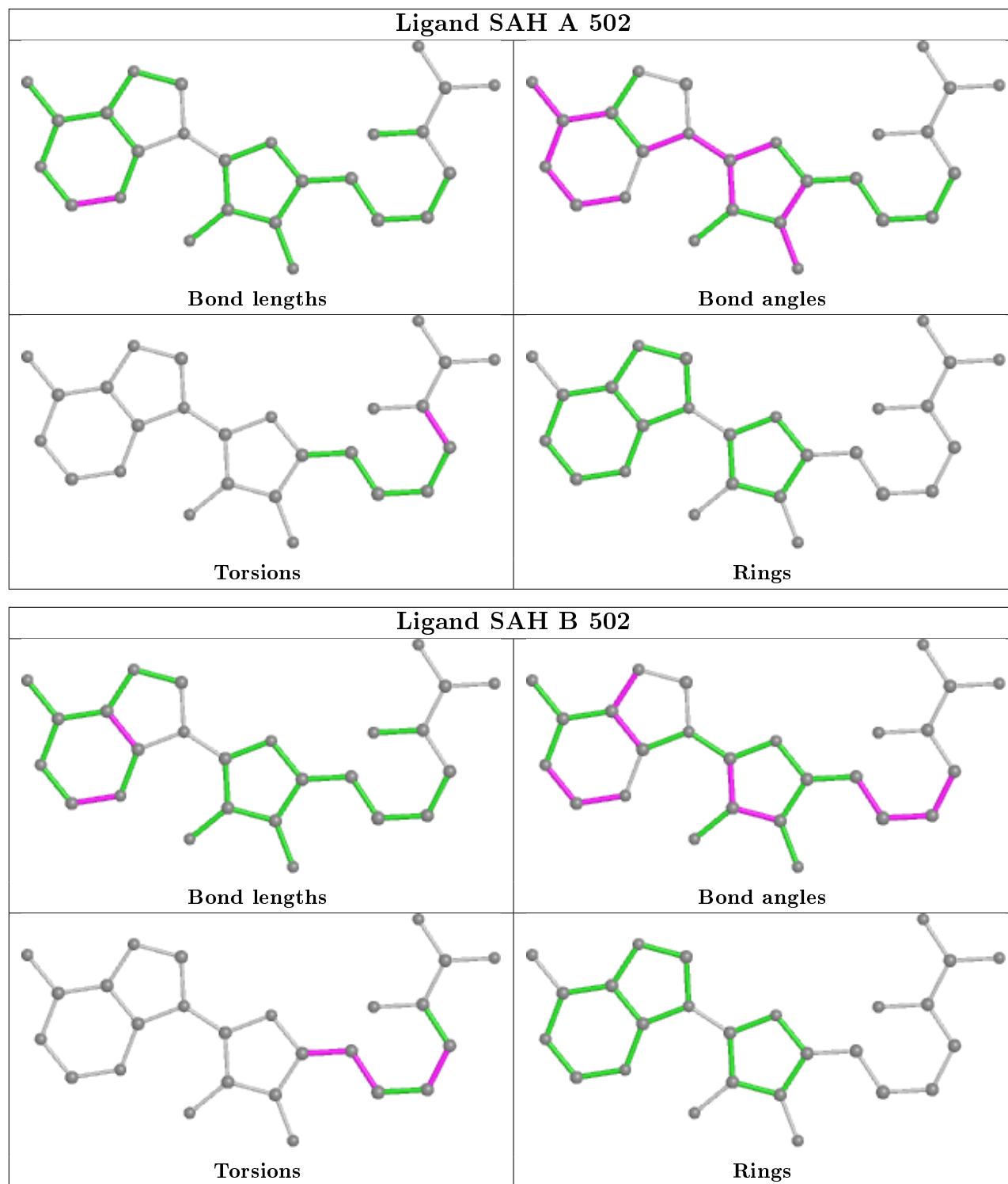
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand SAH C 502



Ligand SAH D 502





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	454/454 (100%)	-0.42	0 100 100	12, 20, 39, 63	0
1	B	452/454 (99%)	-0.09	9 (1%) 65 60	16, 34, 57, 87	0
1	C	451/454 (99%)	-0.25	8 (1%) 68 63	17, 29, 50, 75	0
1	D	452/454 (99%)	-0.30	4 (0%) 84 83	16, 29, 50, 75	0
2	G	10/18 (55%)	1.71	3 (30%) 0 0	53, 56, 106, 127	0
All	All	1819/1834 (99%)	-0.25	24 (1%) 77 74	12, 28, 52, 127	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	753	G	6.3
1	B	360	THR	5.4
1	C	49	ASN	4.0
1	C	50	LYS	4.0
1	D	363	ASN	3.2
2	G	755	G	3.0
1	B	49	ASN	2.9
1	C	48	VAL	2.8
1	C	51	LYS	2.8
1	D	452	ASP	2.5
1	B	254	LYS	2.5
1	B	149	ASN	2.5
1	D	188	LYS	2.5
2	G	754	U	2.5
1	B	336	PRO	2.4
1	B	361	ALA	2.4
1	B	369	LEU	2.3
1	D	52	ILE	2.2
1	C	28	LEU	2.2
1	B	249	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	388	THR	2.1
1	C	72	ASP	2.0
1	C	52	ILE	2.0
1	C	363	ASN	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 carbohydrates in this entry.

6.4 Ligands [i](#)

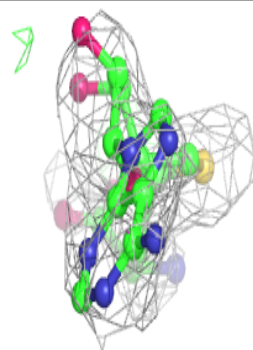
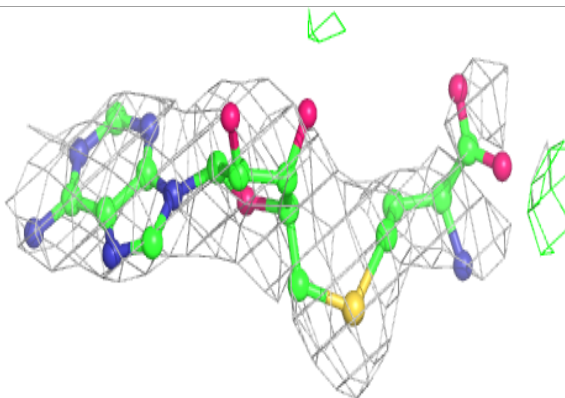
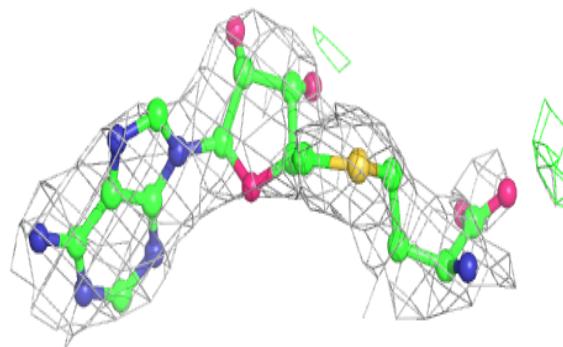
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	SAH	B	502	26/26	0.85	0.24	58,65,76,78	0
4	SAH	C	502	26/26	0.92	0.19	28,36,56,62	0
4	SAH	D	502	26/26	0.93	0.19	38,46,73,83	0
4	SAH	A	502	26/26	0.96	0.14	22,25,34,38	0
3	ZN	D	501	1/1	0.96	0.06	42,42,42,42	0
3	ZN	A	501	1/1	0.98	0.10	33,33,33,33	0
3	ZN	B	501	1/1	0.98	0.07	45,45,45,45	0
3	ZN	C	501	1/1	0.99	0.08	43,43,43,43	0

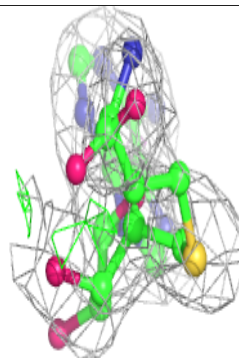
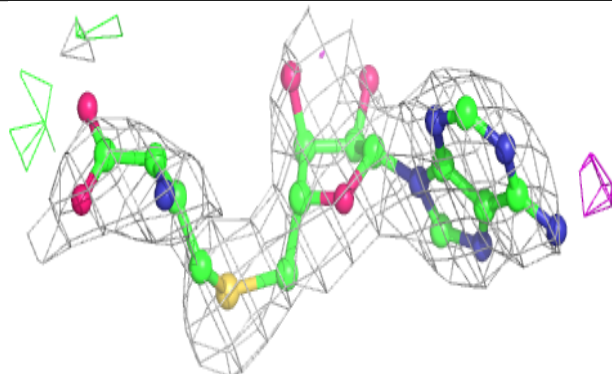
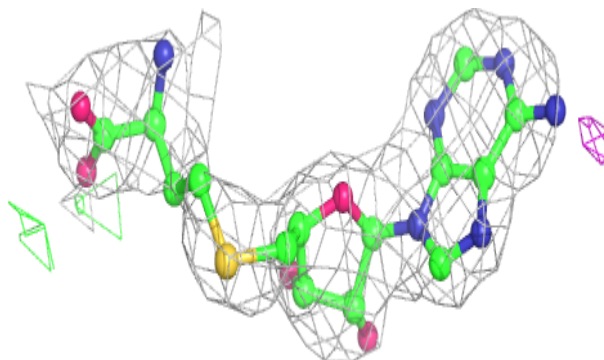
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

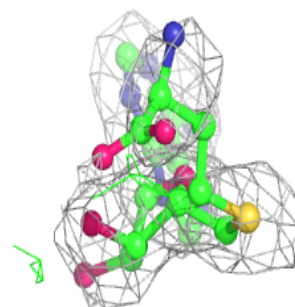
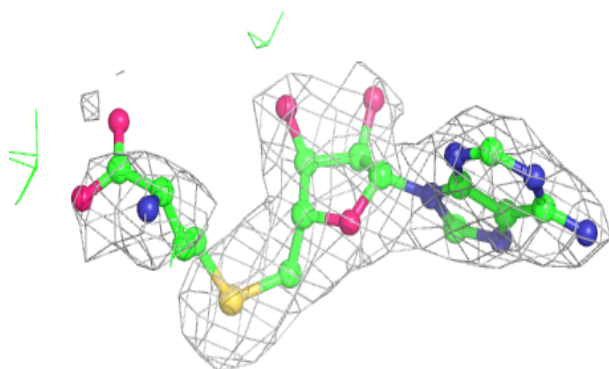
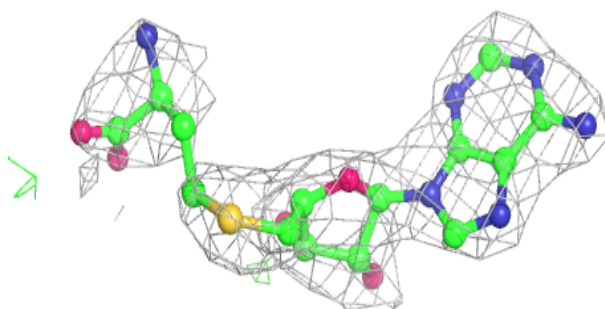
**Electron density around SAH C 502:**

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

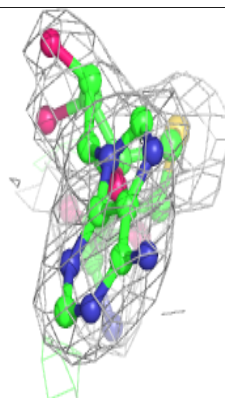
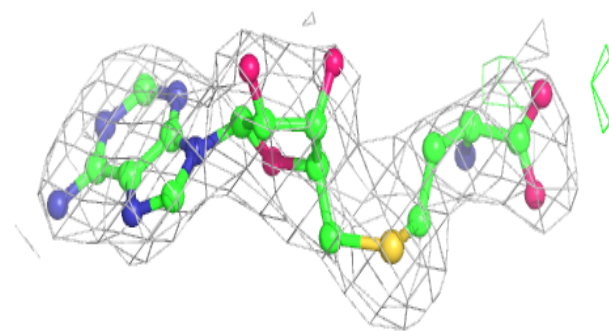
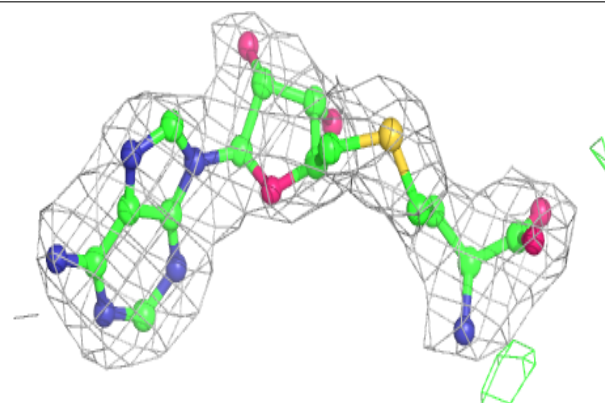


Electron density around SAH D 502:

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

**Electron density around SAH 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.