



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:06 PM UTC

PDB ID : 5E9W / pdb_00005e9w
Title : Crystal structure of mRNA cap guanine-N7 methyltransferase obtained by limited proteolysis
Authors : Petit, P.; Cowling, V.H.
Deposited on : 2015-10-15
Resolution : 2.28 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

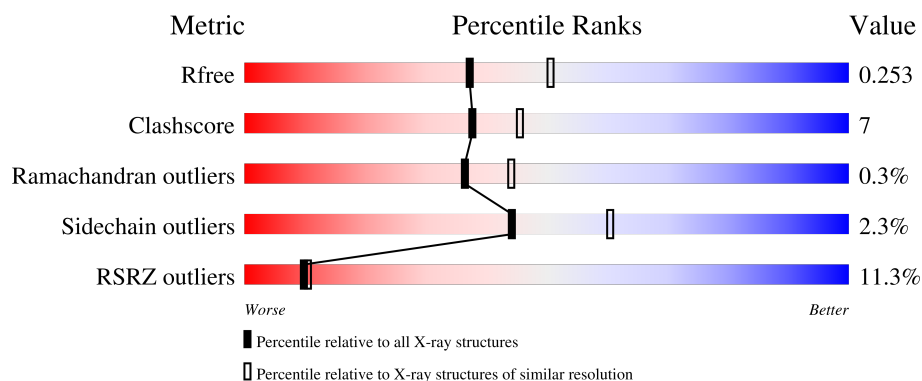
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.28 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	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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	312	12% 71% 15% • 13%
1	B	312	8% 71% 16% • 13%
1	C	312	11% 70% 16% • 13%
1	D	312	9% 75% 12% • 12%

2 Entry composition [i](#)

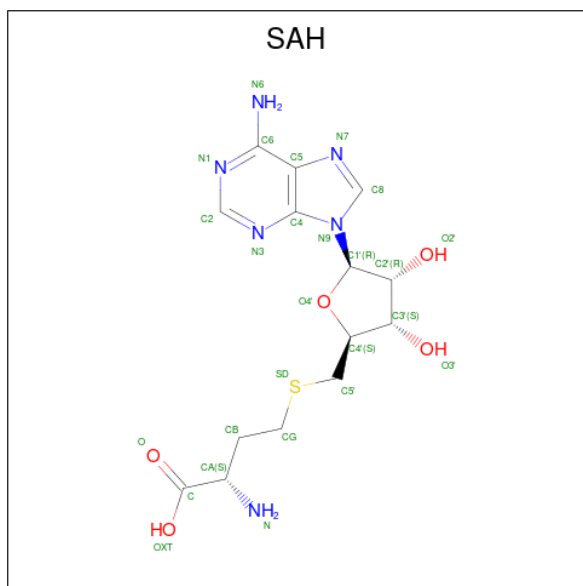
There are 3 unique types of molecules in this entry. The entry contains 9400 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 mRNA cap guanine-N7 methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	0	0
			2237	1441	364	414	18			
1	B	273	Total	C	N	O	S	0	0	0
			2252	1450	371	413	18			
1	C	273	Total	C	N	O	S	0	0	0
			2247	1447	368	414	18			
1	D	274	Total	C	N	O	S	0	0	0
			2253	1451	370	414	18			

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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		

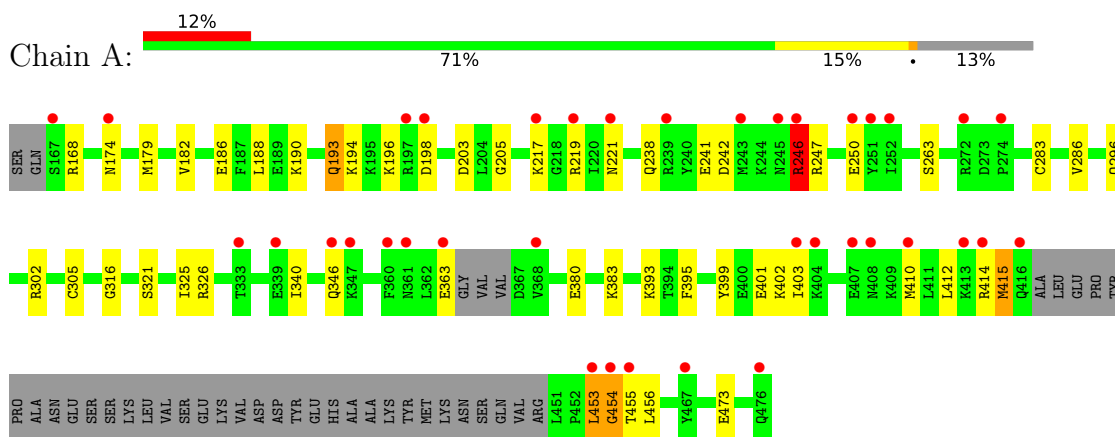
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	56	Total	O	0	0
			56	56		
3	B	94	Total	O	0	0
			94	94		
3	C	63	Total	O	0	0
			63	63		
3	D	94	Total	O	0	0
			94	94		

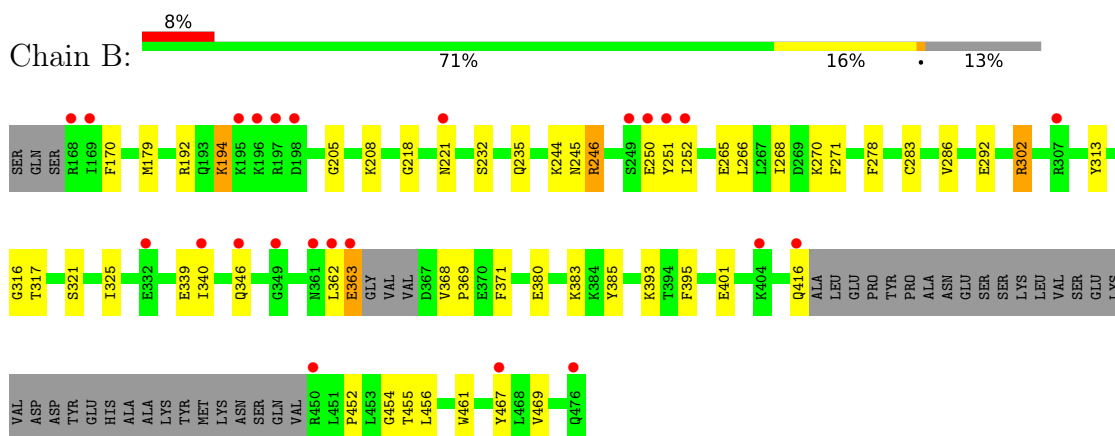
3 Residue-property plots [i](#)

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.

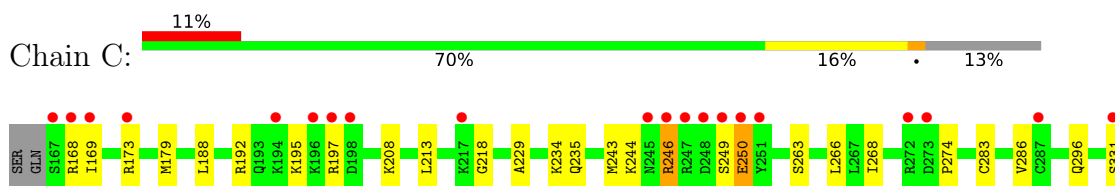
- Molecule 1: mRNA cap guanine-N7 methyltransferase

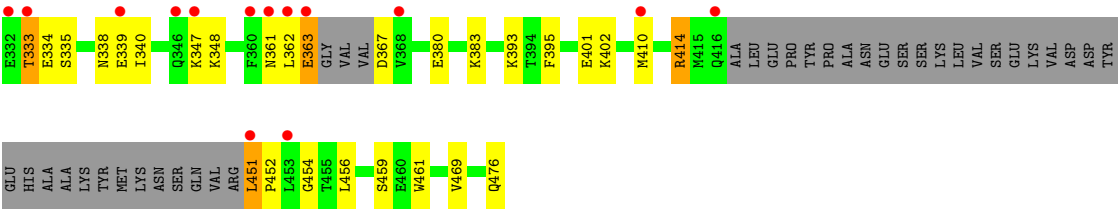


- Molecule 1: mRNA cap guanine-N7 methyltransferase

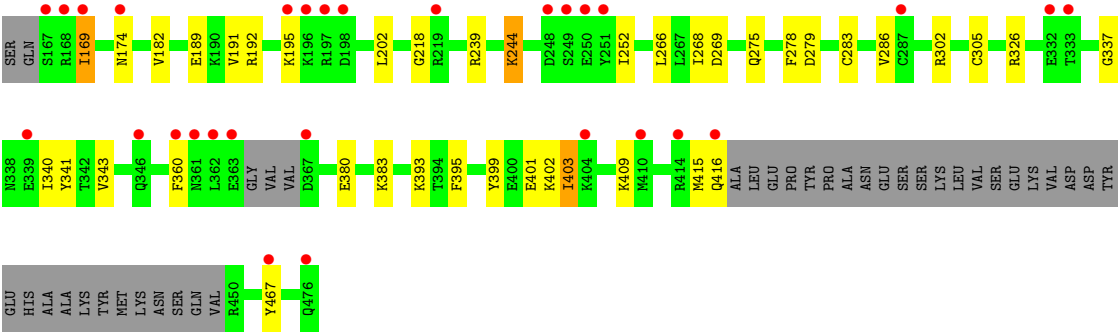


- Molecule 1: mRNA cap guanine-N7 methyltransferase





● Molecule 1: mRNA cap guanine-N7 methyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	77.46Å 99.16Å 167.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.58 – 2.28 29.58 – 2.28	Depositor EDS
% Data completeness (in resolution range)	96.3 (29.58-2.28) 96.4 (29.58-2.28)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.55 (at 2.29Å)	Xtriage
Refinement program	PHENIX dev_1702	Depositor
R, R_{free}	0.220 , 0.255 0.221 , 0.253	Depositor DCC
R_{free} test set	2891 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	21.9	Xtriage
Anisotropy	0.918	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9400	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.42 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5293e-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

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	0.62	2/2283 (0.1%)	0.91	6/3062 (0.2%)
1	B	0.61	1/2298 (0.0%)	0.87	3/3079 (0.1%)
1	C	0.62	1/2293 (0.0%)	0.88	3/3073 (0.1%)
1	D	0.56	0/2299	0.85	1/3081 (0.0%)
All	All	0.60	4/9173 (0.0%)	0.88	13/12295 (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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	247	ARG	CA-C	-5.51	1.46	1.52
1	B	245	ASN	C-O	-5.31	1.16	1.24
1	A	302	ARG	C-O	-5.08	1.18	1.24
1	C	244	LYS	C-O	-5.00	1.17	1.24

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	454	GLY	N-CA-C	8.76	133.93	113.18
1	A	246	ARG	N-CA-C	-8.54	98.57	110.35
1	C	246	ARG	N-CA-C	-7.25	100.35	110.35
1	B	194	LYS	N-CA-C	-7.19	100.16	110.59
1	C	218	GLY	N-CA-C	-5.68	107.88	115.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	305	CYS	N-CA-C	5.65	120.83	113.88
1	A	415	MET	N-CA-C	-5.65	106.23	113.01
1	A	453	LEU	N-CA-C	-5.51	105.19	111.14
1	A	305	CYS	N-CA-C	5.31	120.76	113.97
1	A	316	GLY	N-CA-C	5.23	118.21	110.42
1	B	316	GLY	N-CA-C	5.20	118.17	110.42
1	B	454	GLY	N-CA-C	5.13	117.36	111.36
1	C	454	GLY	N-CA-C	5.11	121.39	112.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	346	GLN	Peptide
1	A	453	LEU	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	2237	0	2192	31	5
1	B	2252	0	2222	30	5
1	C	2247	0	2214	44	3
1	D	2253	0	2220	22	3
2	A	26	0	19	0	0
2	B	26	0	19	0	0
2	C	26	0	19	0	0
2	D	26	0	19	0	0
3	A	56	0	0	3	0
3	B	94	0	0	2	0
3	C	63	0	0	4	0
3	D	94	0	0	3	0
All	All	9400	0	8924	126	8

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 7.

All (126) 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:246:ARG:HH11	1:B:246:ARG:HG2	1.29	0.96
1:A:198:ASP:OD2	1:A:221:ASN:ND2	2.06	0.89
1:D:192:ARG:NH2	1:D:218:GLY:O	2.12	0.82
1:C:168:ARG:HB2	1:C:363:GLU:OE1	1.81	0.81
1:C:347:LYS:NZ	3:C:602:HOH:O	2.15	0.80
1:C:333:THR:HG22	1:C:335:SER:H	1.52	0.75
1:C:476:GLN:O	3:C:601:HOH:O	2.06	0.74
1:C:195:LYS:HE2	1:C:197:ARG:HE	1.55	0.72
1:A:380:GLU:OE2	1:A:383:LYS:NZ	2.26	0.69
1:D:380:GLU:OE2	1:D:383:LYS:NZ	2.25	0.69
1:B:302:ARG:NH2	3:B:603:HOH:O	2.24	0.69
1:B:208:LYS:HD3	1:B:232:SER:HA	1.73	0.69
1:D:415:MET:O	1:D:416:GLN:HG2	1.93	0.68
1:C:361:ASN:ND2	1:C:367:ASP:OD1	2.26	0.68
1:B:246:ARG:HG2	1:B:246:ARG:NH1	1.99	0.68
1:C:451:LEU:HD12	1:C:452:PRO:HD2	1.77	0.66
1:C:339:GLU:OE2	1:C:459:SER:OG	2.09	0.65
1:C:380:GLU:OE2	1:C:383:LYS:NZ	2.29	0.65
1:A:186:GLU:OE2	1:A:190:LYS:NZ	2.30	0.64
1:B:467:TYR:OH	3:B:601:HOH:O	2.07	0.64
1:B:244:LYS:HG3	1:B:252:ILE:HG21	1.80	0.63
1:A:414:ARG:HG3	1:A:414:ARG:HH21	1.63	0.63
1:C:410:MET:HE2	1:C:414:ARG:HH12	1.64	0.62
1:C:192:ARG:NH1	3:C:603:HOH:O	2.17	0.62
1:A:238:GLN:NE2	1:A:242:ASP:OD1	2.33	0.61
1:D:169:ILE:HD11	1:D:340:ILE:HG23	1.81	0.60
1:A:194:LYS:NZ	1:A:473:GLU:OE2	2.34	0.60
1:C:456:LEU:HB2	1:C:461:TRP:NE1	2.15	0.60
1:C:234:LYS:NZ	3:C:605:HOH:O	2.31	0.59
1:D:399:TYR:O	1:D:403:ILE:HG13	2.02	0.59
1:B:192:ARG:NH2	1:B:218:GLY:O	2.31	0.59
1:D:195:LYS:HE3	1:D:279:ASP:HB3	1.84	0.59
1:C:456:LEU:HB2	1:C:461:TRP:CD1	2.37	0.59
1:B:283:CYS:SG	1:B:286:VAL:HB	2.44	0.58
1:A:412:LEU:HD21	1:A:455:THR:HG21	1.86	0.57
1:B:244:LYS:CG	1:B:252:ILE:HG21	2.35	0.57
1:A:283:CYS:SG	1:A:286:VAL:HB	2.45	0.56
1:A:193:GLN:HG2	1:C:229:ALA:HB1	1.88	0.56
1:C:213:LEU:CD2	1:C:243:MET:HE3	2.36	0.56
1:C:451:LEU:CD1	1:C:452:PRO:HD2	2.36	0.56
1:D:393:LYS:HE2	1:D:401:GLU:OE1	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:380:GLU:OE2	1:B:383:LYS:NZ	2.39	0.56
1:B:170:PHE:HZ	1:B:416:GLN:HE21	1.55	0.55
1:B:221:ASN:ND2	1:B:251:TYR:OH	2.38	0.55
1:A:174:ASN:ND2	1:A:415:MET:O	2.40	0.54
1:B:339:GLU:HG3	1:B:340:ILE:HG13	1.89	0.54
1:C:451:LEU:HD12	1:C:452:PRO:CD	2.38	0.53
1:A:198:ASP:CB	1:A:221:ASN:HD22	2.21	0.52
1:C:169:ILE:HG23	1:C:363:GLU:CD	2.36	0.51
1:C:401:GLU:HG3	1:C:402:LYS:HD2	1.92	0.51
1:D:326:ARG:NH1	3:D:602:HOH:O	2.29	0.51
1:A:203:ASP:OD2	3:A:601:HOH:O	2.19	0.51
1:A:393:LYS:HE2	1:A:401:GLU:OE1	2.11	0.51
1:D:239:ARG:NH2	3:D:609:HOH:O	2.45	0.50
1:B:393:LYS:HE2	1:B:401:GLU:OE1	2.11	0.50
1:B:455:THR:HG22	1:B:456:LEU:HD12	1.93	0.50
1:D:191:VAL:HG13	1:D:195:LYS:HE2	1.94	0.50
1:A:340:ILE:O	1:A:363:GLU:HG2	2.12	0.50
1:B:455:THR:C	1:B:456:LEU:HD12	2.36	0.50
1:C:393:LYS:HE2	1:C:401:GLU:OE1	2.12	0.49
1:B:205:GLY:HA3	1:B:286:VAL:HG21	1.94	0.49
1:A:454:GLY:O	1:A:456:LEU:N	2.42	0.49
1:D:266:LEU:HD11	1:D:302:ARG:HD3	1.94	0.49
1:D:269:ASP:O	3:D:601:HOH:O	2.19	0.49
1:A:241:GLU:HA	1:A:241:GLU:OE1	2.13	0.48
1:D:182:VAL:HG12	1:D:402:LYS:HE3	1.96	0.48
1:B:362:LEU:O	1:B:363:GLU:HB2	2.13	0.47
1:B:302:ARG:HB2	1:B:385:TYR:CZ	2.48	0.47
1:B:321:SER:O	1:B:325:ILE:HG12	2.13	0.47
1:D:275:GLN:OE1	1:D:275:GLN:N	2.41	0.47
1:C:168:ARG:CB	1:C:363:GLU:OE1	2.58	0.47
1:C:179:MET:HE2	1:C:395:PHE:CG	2.50	0.47
1:D:337:GLY:HA2	1:D:341:TYR:CZ	2.50	0.47
1:B:452:PRO:HG2	1:B:461:TRP:CE2	2.51	0.46
1:C:283:CYS:SG	1:C:286:VAL:HB	2.55	0.46
1:D:283:CYS:SG	1:D:286:VAL:HB	2.55	0.46
1:A:198:ASP:CG	1:A:221:ASN:HD22	2.23	0.46
1:D:266:LEU:HG	1:D:268:ILE:HG12	1.98	0.46
1:D:244:LYS:HB2	1:D:252:ILE:HG21	1.97	0.46
1:B:266:LEU:HG	1:B:268:ILE:HG12	1.98	0.45
1:B:194:LYS:NZ	1:B:313:TYR:OH	2.50	0.45
1:C:333:THR:HG22	1:C:335:SER:N	2.26	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:410:MET:HE2	1:C:414:ARG:NH1	2.30	0.45
1:C:249:SER:O	1:C:250:GLU:O	2.33	0.45
1:A:174:ASN:HB3	3:A:605:HOH:O	2.17	0.45
1:A:198:ASP:CG	1:A:221:ASN:ND2	2.73	0.45
1:A:205:GLY:HA3	1:A:286:VAL:HG21	1.99	0.45
1:C:266:LEU:HG	1:C:268:ILE:HG22	1.99	0.45
1:D:202:LEU:HB2	1:D:278:PHE:CE1	2.52	0.45
1:B:265:GLU:OE2	1:B:270:LYS:NZ	2.42	0.44
1:A:217:LYS:HA	1:A:217:LYS:HE3	2.00	0.44
1:A:246:ARG:HA	1:A:246:ARG:HD2	1.71	0.44
1:A:182:VAL:HG11	1:A:402:LYS:HG3	1.98	0.44
1:C:213:LEU:HD23	1:C:243:MET:HE3	1.98	0.44
1:C:331:SER:O	1:C:348:LYS:NZ	2.51	0.44
1:B:271:PHE:CZ	1:B:278:PHE:HZ	2.36	0.43
1:B:292:GLU:HB2	1:B:371:PHE:CE2	2.53	0.43
1:A:198:ASP:HB3	1:A:221:ASN:HD22	1.83	0.43
1:A:263:SER:HB2	1:A:296:GLN:HB3	2.00	0.43
1:C:268:ILE:HD12	1:C:268:ILE:HA	1.81	0.43
1:C:208:LYS:HD3	1:C:235:GLN:OE1	2.19	0.43
1:D:395:PHE:CE1	1:D:467:TYR:HB3	2.53	0.43
1:C:263:SER:HB2	1:C:296:GLN:HB3	2.00	0.42
1:D:275:GLN:H	1:D:275:GLN:CD	2.26	0.42
1:A:399:TYR:O	1:A:403:ILE:HG12	2.19	0.42
1:C:456:LEU:HB2	1:C:461:TRP:CE2	2.55	0.42
1:C:452:PRO:HG2	1:C:461:TRP:CZ2	2.55	0.42
1:A:414:ARG:HG3	1:A:414:ARG:NH2	2.31	0.42
1:C:168:ARG:N	1:C:168:ARG:HD3	2.34	0.42
1:C:451:LEU:HD12	1:C:452:PRO:N	2.34	0.42
1:B:208:LYS:HE2	1:B:235:GLN:OE1	2.20	0.42
1:C:268:ILE:HD11	1:C:274:PRO:O	2.19	0.42
1:A:179:MET:HE2	1:A:395:PHE:CG	2.54	0.41
1:B:317:THR:HG22	1:B:469:VAL:HG12	2.01	0.41
1:A:188:LEU:HD23	1:A:188:LEU:HA	1.94	0.41
1:C:249:SER:O	1:C:250:GLU:C	2.61	0.41
1:C:338:ASN:HB2	1:C:339:GLU:OE1	2.20	0.41
1:C:362:LEU:HD12	1:C:362:LEU:HA	1.94	0.41
1:B:368:VAL:HA	1:B:369:PRO:HD3	1.92	0.41
1:C:188:LEU:HD23	1:C:188:LEU:HA	1.97	0.41
1:C:339:GLU:HG2	1:C:340:ILE:HG13	2.02	0.41
1:A:321:SER:O	1:A:325:ILE:HG12	2.20	0.41
1:B:179:MET:HE2	1:B:395:PHE:CG	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:343:VAL:HG22	1:D:360:PHE:HD1	1.86	0.41
1:A:326:ARG:NH2	3:A:602:HOH:O	2.29	0.40
1:C:361:ASN:HD22	1:C:367:ASP:CG	2.29	0.40

All (8) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:ARG:NH1	1:B:416:GLN:NE2[4_466]	0.40	1.80
1:C:246:ARG:NH1	1:D:416:GLN:NE2[4_366]	1.05	1.15
1:C:246:ARG:NH1	1:D:416:GLN:CD[4_366]	1.25	0.95
1:A:246:ARG:NH1	1:B:416:GLN:CD[4_466]	1.27	0.93
1:C:246:ARG:NH1	1:D:416:GLN:OE1[4_366]	1.51	0.69
1:A:246:ARG:CZ	1:B:416:GLN:NE2[4_466]	1.67	0.53
1:A:246:ARG:NH1	1:B:416:GLN:OE1[4_466]	2.08	0.12
1:A:246:ARG:CZ	1:B:416:GLN:CD[4_466]	2.16	0.04

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	267/312 (86%)	258 (97%)	8 (3%)	1 (0%)	30	36
1	B	267/312 (86%)	260 (97%)	6 (2%)	1 (0%)	30	36
1	C	267/312 (86%)	258 (97%)	8 (3%)	1 (0%)	30	36
1	D	268/312 (86%)	258 (96%)	10 (4%)	0	100	100
All	All	1069/1248 (86%)	1034 (97%)	32 (3%)	3 (0%)	36	44

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	250	GLU
1	A	250	GLU
1	B	250	GLU

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	244/285 (86%)	238 (98%)	6 (2%)	42	58
1	B	246/285 (86%)	242 (98%)	4 (2%)	55	71
1	C	246/285 (86%)	239 (97%)	7 (3%)	38	53
1	D	246/285 (86%)	240 (98%)	6 (2%)	43	59
All	All	982/1140 (86%)	959 (98%)	23 (2%)	44	60

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	168	ARG
1	A	193	GLN
1	A	196	LYS
1	A	219	ARG
1	A	246	ARG
1	A	410	MET
1	B	246	ARG
1	B	302	ARG
1	B	346	GLN
1	B	363	GLU
1	C	173	ARG
1	C	333	THR
1	C	334	GLU
1	C	363	GLU
1	C	414	ARG
1	C	451	LEU
1	C	469	VAL
1	D	169	ILE
1	D	174	ASN

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Mol	Chain	Res	Type
1	D	189	GLU
1	D	244	LYS
1	D	403	ILE
1	D	409	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	221	ASN
1	A	235	GLN
1	A	296	GLN
1	A	405	ASN
1	A	406	ASN
1	A	475	GLN
1	A	476	GLN
1	B	296	GLN
1	B	416	GLN
1	B	475	GLN
1	C	379	ASN
1	C	406	ASN
1	C	475	GLN
1	D	296	GLN
1	D	416	GLN
1	D	475	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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 oligosaccharides in this entry.

5.6 Ligand geometry

4 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	C	501	-	27,28,28	1.02	3 (11%)	36,40,40	2.05	11 (30%)
2	SAH	A	500	-	27,28,28	1.01	4 (14%)	36,40,40	2.00	11 (30%)
2	SAH	B	501	-	27,28,28	1.08	4 (14%)	36,40,40	1.98	11 (30%)
2	SAH	D	501	-	27,28,28	1.08	3 (11%)	36,40,40	2.11	11 (30%)

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	C	501	-	-	1/15/31/31	0/3/3/3
2	SAH	A	500	-	-	1/15/31/31	0/3/3/3
2	SAH	B	501	-	-	0/15/31/31	0/3/3/3
2	SAH	D	501	-	-	0/15/31/31	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	SAH	OXT-C	-2.56	1.22	1.30
2	B	501	SAH	C2-N1	2.44	1.38	1.33
2	B	501	SAH	C2-N3	2.39	1.38	1.33
2	D	501	SAH	C2-N1	2.33	1.38	1.33
2	D	501	SAH	C8-N7	2.32	1.36	1.31
2	B	501	SAH	OXT-C	-2.31	1.23	1.30
2	A	500	SAH	OXT-C	-2.30	1.23	1.30
2	A	500	SAH	C8-N7	2.24	1.36	1.31
2	A	500	SAH	C2-N3	2.24	1.37	1.33
2	A	500	SAH	C2-N1	2.21	1.37	1.33
2	D	501	SAH	OXT-C	-2.20	1.23	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	SAH	C2-N1	2.18	1.37	1.33
2	C	501	SAH	C2-N3	2.13	1.37	1.33
2	B	501	SAH	C5-N7	-2.07	1.35	1.39

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	SAH	N3-C2-N1	-6.13	119.31	128.58
2	A	500	SAH	N3-C2-N1	-5.81	119.79	128.58
2	B	501	SAH	N3-C2-N1	-5.71	119.93	128.58
2	C	501	SAH	N3-C2-N1	-5.60	120.10	128.58
2	D	501	SAH	N9-C8-N7	-4.64	107.36	113.94
2	B	501	SAH	N9-C8-N7	-4.44	107.63	113.94
2	C	501	SAH	N9-C8-N7	-4.30	107.84	113.94
2	A	500	SAH	N9-C8-N7	-4.01	108.24	113.94
2	D	501	SAH	C5-C4-N3	-3.99	121.22	126.72
2	D	501	SAH	C5-N7-C8	3.73	109.32	103.45
2	A	500	SAH	C5-C4-N3	-3.70	121.61	126.72
2	C	501	SAH	C5-C4-N3	-3.67	121.66	126.72
2	D	501	SAH	C2-N3-C4	3.66	120.76	111.83
2	B	501	SAH	C5-C4-N3	-3.61	121.75	126.72
2	B	501	SAH	C5-N7-C8	3.56	109.04	103.45
2	C	501	SAH	C5-N7-C8	3.47	108.90	103.45
2	A	500	SAH	C2-N3-C4	3.36	120.04	111.83
2	C	501	SAH	C5'-SD-CG	-3.32	92.42	102.26
2	D	501	SAH	O4'-C1'-N9	3.31	114.45	108.09
2	C	501	SAH	C2-N3-C4	3.21	119.68	111.83
2	C	501	SAH	OXT-C-O	-3.14	116.96	124.08
2	B	501	SAH	C2-N3-C4	3.11	119.42	111.83
2	A	500	SAH	C5'-SD-CG	-3.03	93.28	102.26
2	A	500	SAH	C5-N7-C8	2.99	108.16	103.45
2	A	500	SAH	OXT-C-O	-2.97	117.34	124.08
2	A	500	SAH	O4'-C1'-N9	2.88	113.63	108.09
2	D	501	SAH	C4-C5-N7	-2.84	107.33	110.58
2	B	501	SAH	O4'-C1'-N9	2.76	113.39	108.09
2	C	501	SAH	C4-N9-C8	2.52	108.38	105.74
2	C	501	SAH	N3-C4-N9	2.49	131.40	127.17
2	D	501	SAH	OXT-C-O	-2.47	118.48	124.08
2	B	501	SAH	OXT-C-O	-2.46	118.49	124.08
2	B	501	SAH	C4-N9-C8	2.46	108.32	105.74
2	B	501	SAH	C5'-SD-CG	-2.40	95.14	102.26
2	B	501	SAH	C4-C5-N7	-2.39	107.84	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	SAH	C4-N9-C8	2.37	108.23	105.74
2	D	501	SAH	C4-N9-C8	2.34	108.20	105.74
2	D	501	SAH	C5'-SD-CG	-2.33	95.36	102.26
2	C	501	SAH	C4-C5-N7	-2.31	107.94	110.58
2	B	501	SAH	N3-C4-N9	2.31	131.09	127.17
2	A	500	SAH	N3-C4-N9	2.29	131.06	127.17
2	D	501	SAH	N3-C4-N9	2.25	131.00	127.17
2	A	500	SAH	C4-C5-N7	-2.22	108.05	110.58
2	C	501	SAH	O4'-C1'-N9	2.13	112.18	108.09

There are no chirality outliers.

All (2) torsion outliers are listed below:

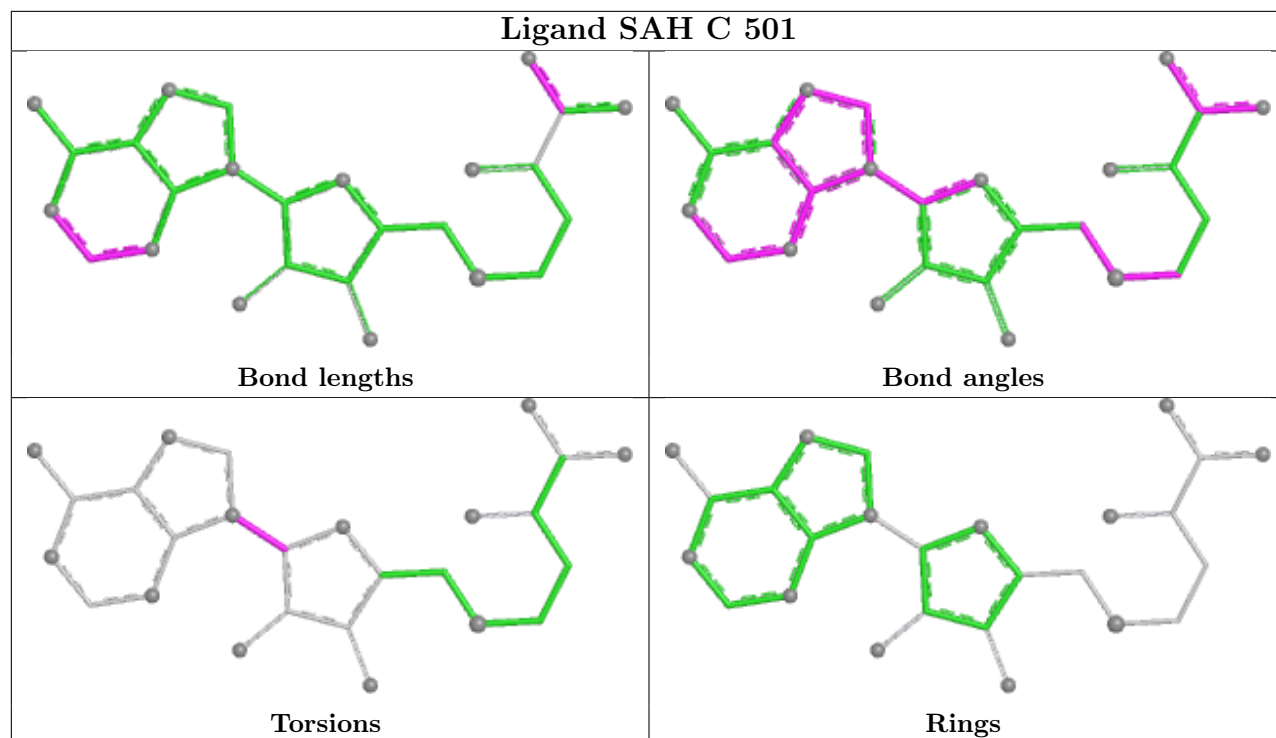
Mol	Chain	Res	Type	Atoms
2	A	500	SAH	CB-CG-SD-C5'
2	C	501	SAH	C2'-C1'-N9-C8

There are no ring outliers.

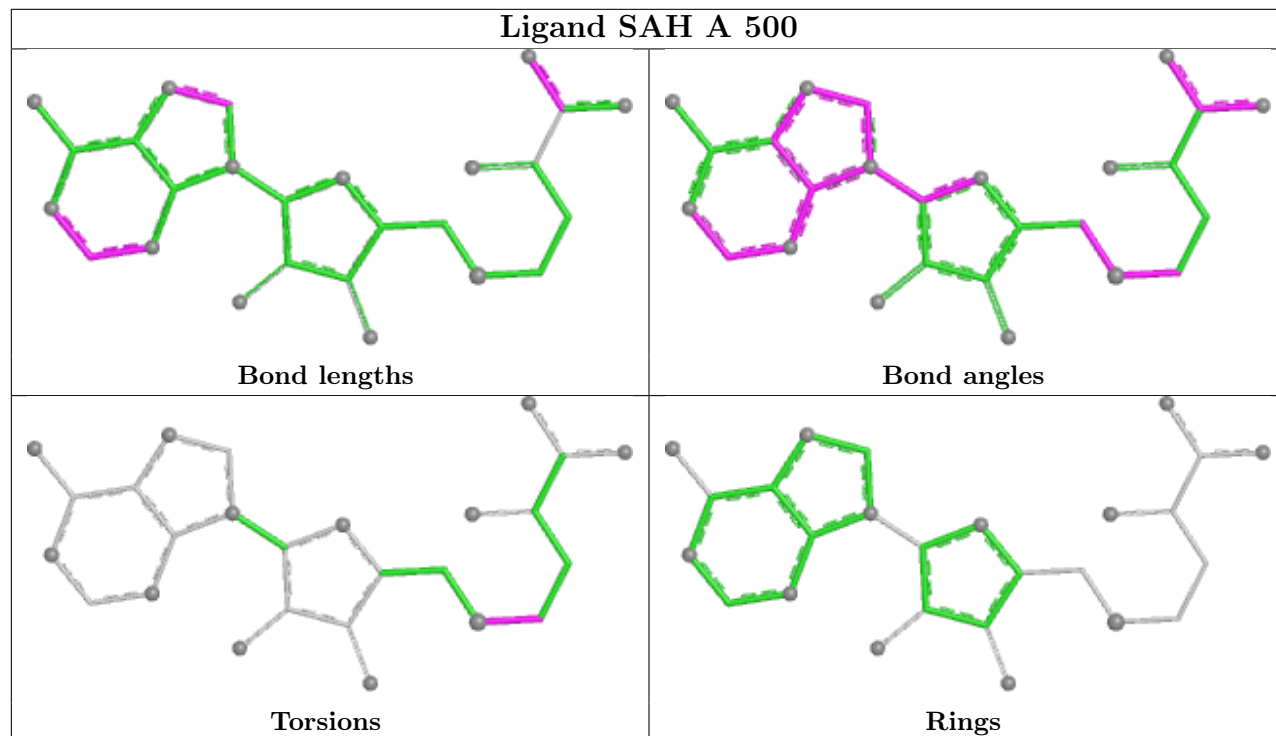
No monomer is involved in short contacts.

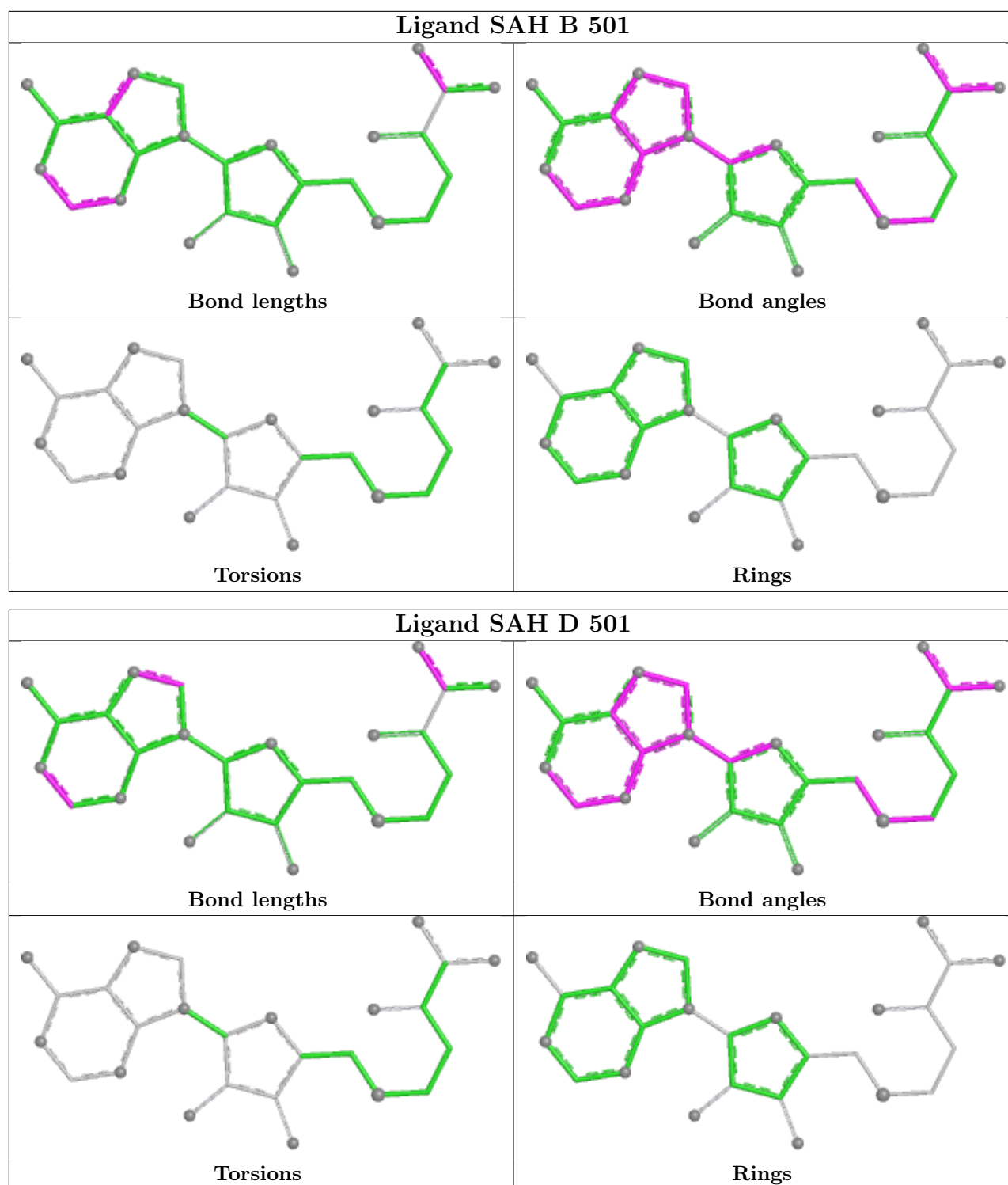
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 501



Ligand SAH A 500





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	273/312 (87%)	0.63	37 (13%) 7 7	13, 30, 65, 93	0
1	B	273/312 (87%)	0.40	24 (8%) 15 16	10, 24, 54, 82	0
1	C	273/312 (87%)	0.57	34 (12%) 8 8	13, 28, 66, 84	0
1	D	274/312 (87%)	0.45	29 (10%) 11 12	10, 24, 60, 104	0
All	All	1093/1248 (87%)	0.51	124 (11%) 10 10	10, 26, 63, 104	0

All (124) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	451	LEU	6.5
1	B	250	GLU	5.9
1	B	416	GLN	5.1
1	D	195	LYS	5.1
1	D	196	LYS	4.9
1	C	368	VAL	4.9
1	B	197	ARG	4.8
1	C	416	GLN	4.7
1	D	197	ARG	4.7
1	A	251	TYR	4.7
1	D	416	GLN	4.5
1	C	198	ASP	4.4
1	A	416	GLN	4.4
1	A	167	SER	4.2
1	B	168	ARG	4.2
1	C	363	GLU	4.2
1	C	167	SER	4.1
1	B	251	TYR	4.1
1	D	250	GLU	4.1
1	D	251	TYR	4.0
1	A	245	ASN	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	168	ARG	3.9
1	B	363	GLU	3.8
1	D	169	ILE	3.8
1	A	403	ILE	3.8
1	A	454	GLY	3.7
1	A	250	GLU	3.7
1	A	197	ARG	3.6
1	D	346	GLN	3.5
1	D	360	PHE	3.5
1	D	476	GLN	3.5
1	D	198	ASP	3.5
1	A	404	LYS	3.3
1	A	413	LYS	3.3
1	B	196	LYS	3.2
1	C	169	ILE	3.2
1	A	243	MET	3.2
1	B	346	GLN	3.2
1	A	368	VAL	3.2
1	D	174	ASN	3.2
1	A	476	GLN	3.2
1	B	169	ILE	3.2
1	D	362	LEU	3.1
1	B	249	SER	3.1
1	D	361	ASN	3.1
1	C	194	LYS	3.0
1	D	414	ARG	3.0
1	C	339	GLU	3.0
1	C	361	ASN	3.0
1	A	347	LYS	3.0
1	C	217	LYS	2.9
1	A	174	ASN	2.9
1	C	196	LYS	2.9
1	C	197	ARG	2.9
1	A	408	ASN	2.9
1	B	467	TYR	2.9
1	A	346	GLN	2.9
1	A	198	ASP	2.8
1	A	414	ARG	2.8
1	C	347	LYS	2.8
1	A	252	ILE	2.8
1	B	361	ASN	2.8
1	A	217	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	167	SER	2.8
1	D	249	SER	2.8
1	C	272	ARG	2.8
1	D	219	ARG	2.8
1	C	362	LEU	2.7
1	C	360	PHE	2.7
1	C	346	GLN	2.7
1	D	363	GLU	2.7
1	B	195	LYS	2.6
1	A	360	PHE	2.6
1	A	333	THR	2.6
1	A	363	GLU	2.6
1	B	450	ARG	2.6
1	C	332	GLU	2.5
1	D	339	GLU	2.5
1	D	248	ASP	2.5
1	D	332	GLU	2.5
1	A	453	LEU	2.5
1	B	476	GLN	2.5
1	A	246	ARG	2.4
1	C	173	ARG	2.4
1	C	331	SER	2.4
1	A	455	THR	2.4
1	C	333	THR	2.4
1	A	467	TYR	2.4
1	C	248	ASP	2.4
1	B	307	ARG	2.4
1	C	247	ARG	2.4
1	A	221	ASN	2.3
1	D	287	CYS	2.3
1	B	349	GLY	2.3
1	B	198	ASP	2.3
1	B	404	LYS	2.3
1	C	246	ARG	2.3
1	C	249	SER	2.3
1	A	407	GLU	2.3
1	C	453	LEU	2.3
1	A	219	ARG	2.3
1	B	252	ILE	2.3
1	A	272	ARG	2.2
1	A	410	MET	2.2
1	B	340	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	333	THR	2.2
1	B	221	ASN	2.2
1	D	410	MET	2.2
1	B	332	GLU	2.2
1	C	251	TYR	2.2
1	D	467	TYR	2.2
1	C	245	ASN	2.1
1	C	273	ASP	2.1
1	A	239	ARG	2.1
1	C	168	ARG	2.1
1	C	250	GLU	2.1
1	A	361	ASN	2.1
1	C	410	MET	2.0
1	A	339	GLU	2.0
1	C	287	CYS	2.0
1	A	274	PRO	2.0
1	D	404	LYS	2.0
1	B	362	LEU	2.0
1	D	367	ASP	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](#)

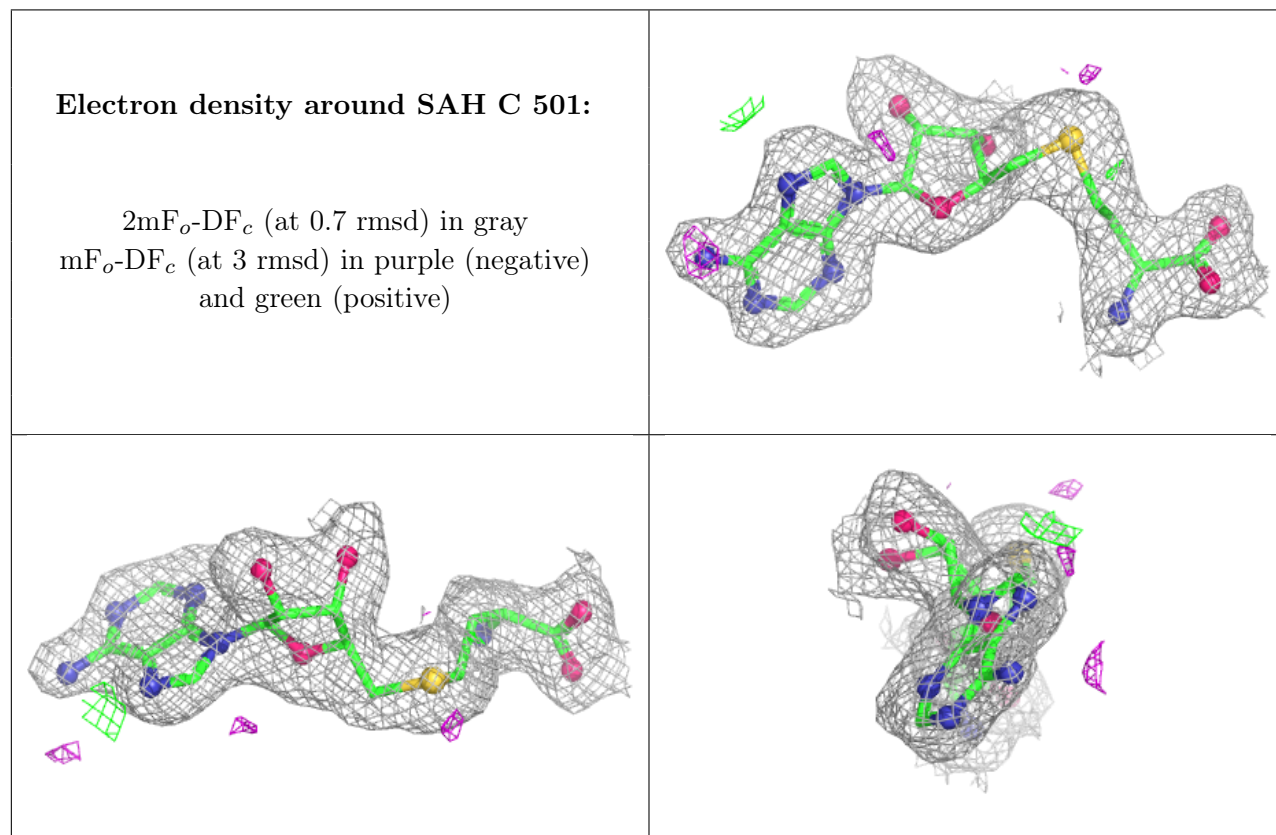
There are no oligosaccharides in this entry.

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.

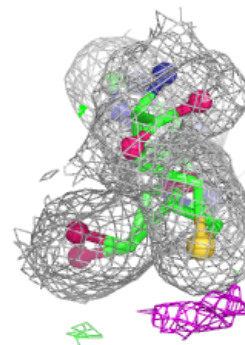
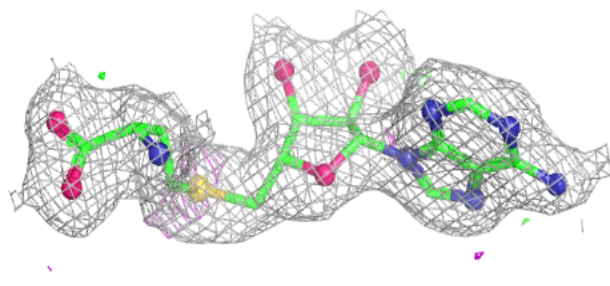
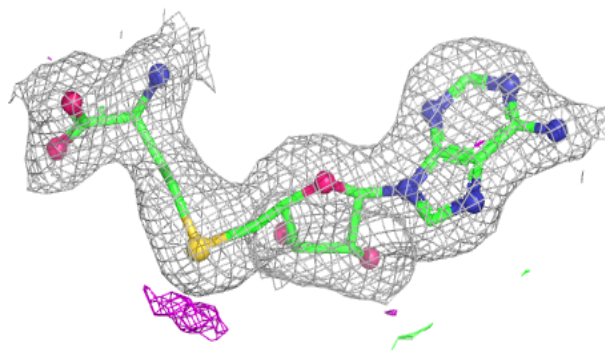
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SAH	C	501	26/26	0.96	0.07	12,16,22,25	0
2	SAH	D	501	26/26	0.96	0.06	10,12,14,24	0
2	SAH	A	500	26/26	0.97	0.06	16,19,26,26	0
2	SAH	B	501	26/26	0.97	0.06	9,14,15,15	0

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.

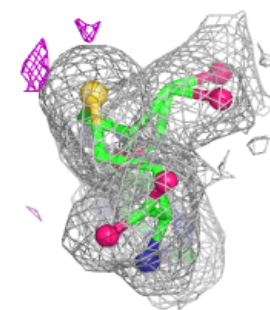
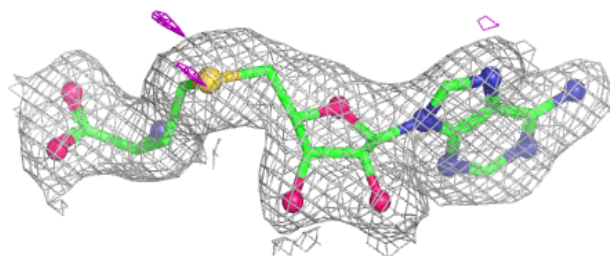
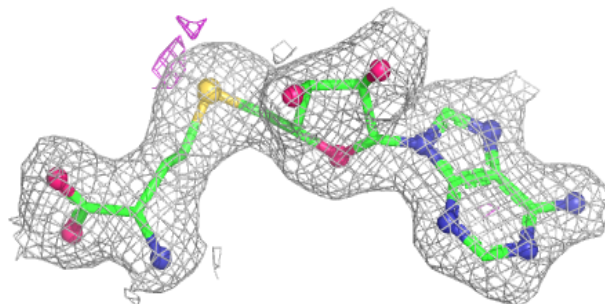


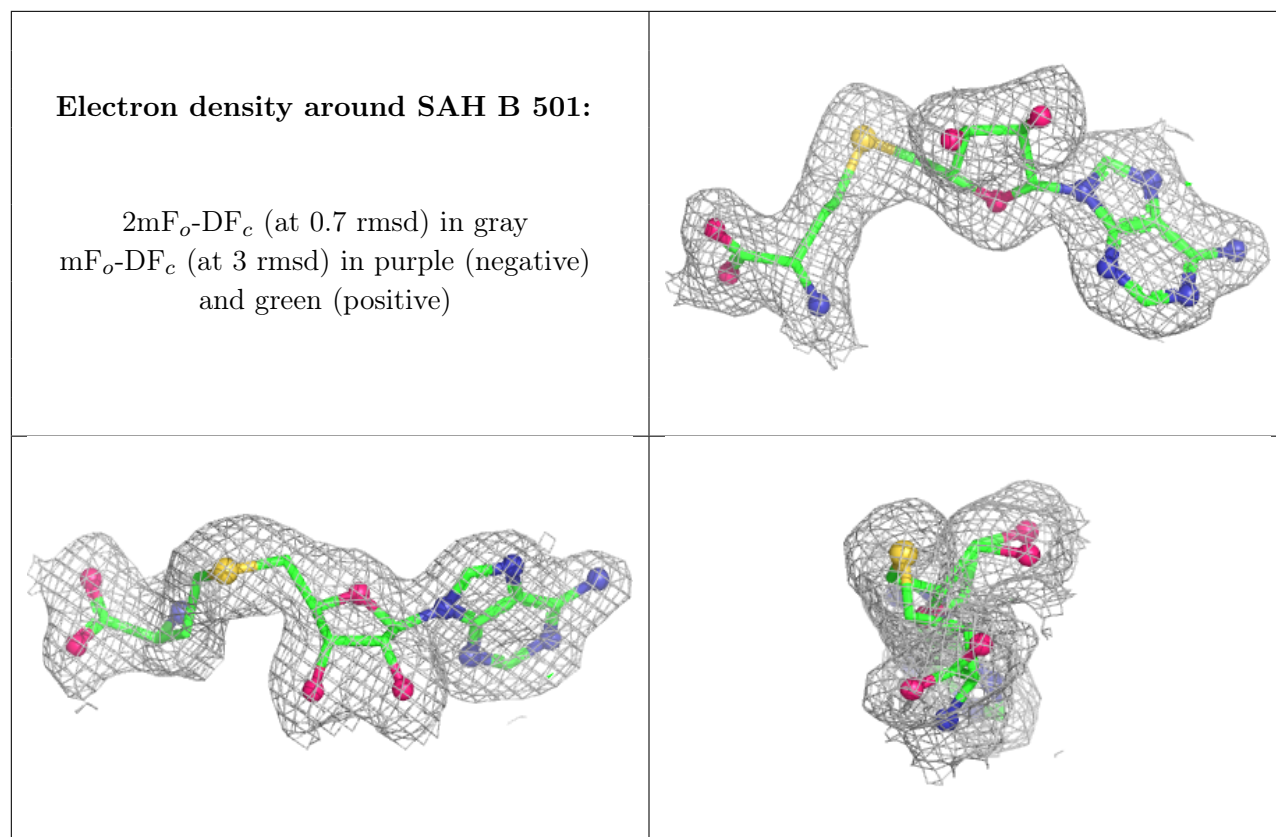
Electron density around SAH D 501:

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

**Electron density around SAH A 500:**

$2mF_o-DF_c$ (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.