Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2024 – 01:05 PM EDT

PDB ID	:	7L4F
Title	:	Crystal structure of the DRM2-CAT DNA complex
Authors	:	Fang, J.; Song, J.
Deposited on	:	2020-12-19
Resolution	:	2.55 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:

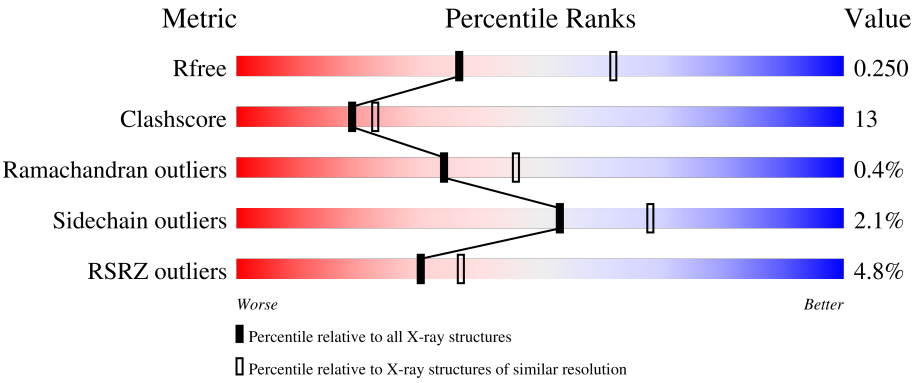
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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 <=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	357	10%, 63%, 34%, . .
1	B	357	79%, 18%, .
2	C	18	50%, 50%
2	E	18	44%, 56%
3	D	18	67%, 28%, 6%

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Mol	Chain	Length	Quality of chain
3	G	18	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7017 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 DNA (cytosine-5)-methyltransferase DRM2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	350	Total	C	N	O	S	0	0	0
			2770	1786	485	487	12			
1	A	350	Total	C	N	O	S	0	0	0
			2672	1717	465	478	12			

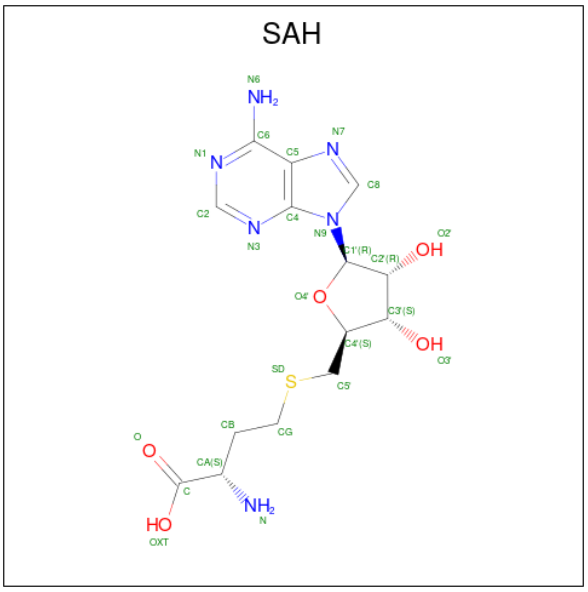
- Molecule 2 is a DNA chain called DNA (5'-D(*TP*AP*AP*AP*GP*GP*AP*TP*GP*AP*GP*GP*AP*GP*GP*AP*AP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	18	Total	C	N	O	P	0	0	0
			379	180	81	101	17			
2	E	18	Total	C	N	O	P	0	0	0
			378	180	81	100	17			

- Molecule 3 is a DNA chain called DNA (5'-D(*AP*TP*TP*CP*CP*TP*CP*CP*TP*(C49)P*AP*TP*CP*CP*TP*TP*TP*A)-3').

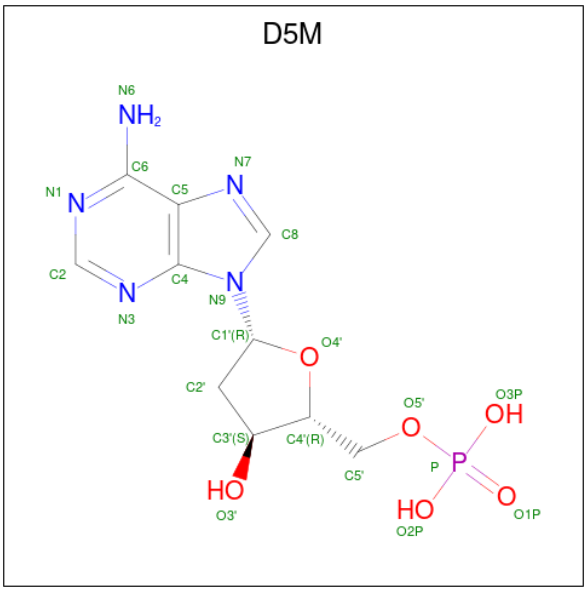
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	D	18	Total	C	F	N	O	P	0	0	0
			354	174	1	52	110	17			
3	G	17	Total	C	F	N	O	P	0	0	0
			337	164	1	47	108	17			

- 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	B	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
4	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

- Molecule 5 is 2'-DEOXYADENOSINE-5'-MONOPHOSPHATE (three-letter code: D5M) (formula: $C_{10}H_{14}N_5O_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	G	1	Total	C	N	O	P	0	0
			21	10	5	5	1		

- Molecule 6 is water.

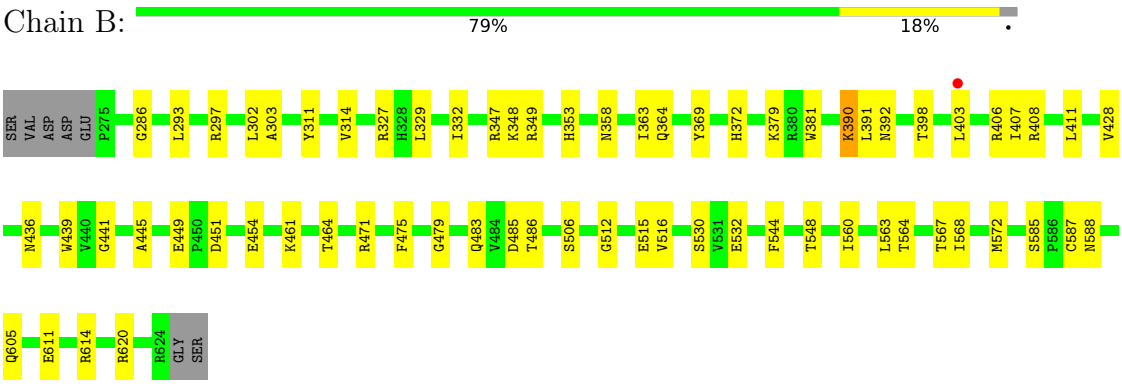
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	30	Total O 30 30	0	0
6	C	3	Total O 3 3	0	0
6	D	6	Total O 6 6	0	0
6	A	12	Total O 12 12	0	0
6	E	3	Total O 3 3	0	0

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.

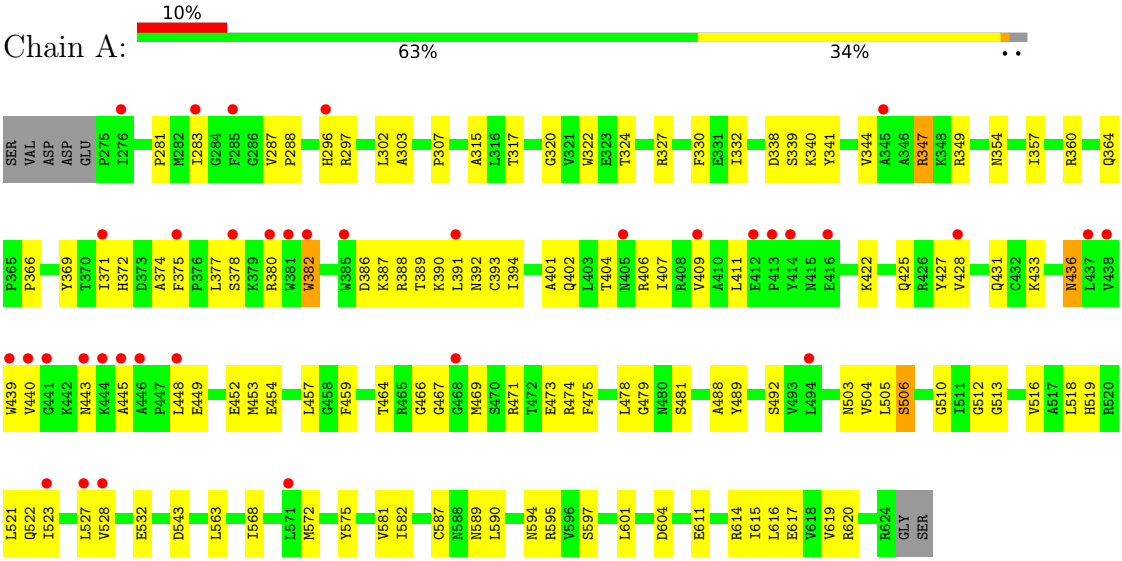
• Molecule 1: DNA (cytosine-5)-methyltransferase DRM2

Chain B:



• Molecule 1: DNA (cytosine-5)-methyltransferase DRM2

Chain A:

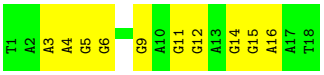


• Molecule 2: DNA (5'-D(*TP*AP*AP*AP*GP*GP*AP*TP*GP*AP*GP*GP*AP*GP*GP*AP *AP*T)-3')

Chain C:

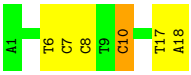
• Molecule 2: DNA (5'-D(*TP*AP*AP*AP*GP*GP*AP*TP*GP*AP*GP*GP*AP*GP*GP*AP *AP*T)-3')

Chain E:



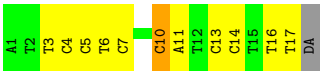
• Molecule 3: DNA (5'-D(*AP*TP*TP*CP*CP*TP*CP*CP*TP*(C49)P*AP*TP*CP*CP*TP* TP*TP*A)-3')

Chain D:



• Molecule 3: DNA (5'-D(*AP*TP*TP*CP*CP*TP*CP*CP*TP*(C49)P*AP*TP*CP*CP*TP* TP*TP*A)-3')

Chain G:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	172.22Å 70.83Å 103.73Å 90.00° 98.02° 90.00°	Depositor
Resolution (Å)	85.27 – 2.55 85.27 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.5 (85.27-2.55) 99.5 (85.27-2.55)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.22 (at 2.55Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.208 , 0.250 0.208 , 0.250	Depositor DCC
R_{free} test set	1999 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	78.8	Xtriage
Anisotropy	0.269	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 61.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7017	wwPDB-VP
Average B, all atoms (Å^2)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: SAH, D5M, C49

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	0.45	1/2749 (0.0%)	0.63	1/3757 (0.0%)
1	B	0.46	0/2848	0.61	0/3870
2	C	0.87	0/429	0.97	0/663
2	E	0.60	0/428	0.84	0/662
3	D	0.95	0/368	1.13	1/562 (0.2%)
3	G	0.76	0/348	1.19	0/530
All	All	0.55	1/7170 (0.0%)	0.74	2/10044 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	380	ARG	CZ-NH2	-5.03	1.26	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	543	ASP	CB-CG-OD2	7.00	124.60	118.30
3	D	6	DT	N3-C4-O4	5.37	123.12	119.90

There are no chirality outliers.

There are no planarity outliers.

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	2672	0	2524	96	0
1	B	2770	0	2738	43	0
2	C	379	0	203	8	0
2	E	378	0	200	14	0
3	D	354	0	205	7	0
3	G	337	0	196	11	0
4	A	26	0	19	2	0
4	B	26	0	17	1	0
5	G	21	0	12	0	0
6	A	12	0	0	4	0
6	B	30	0	0	1	0
6	C	3	0	0	0	0
6	D	6	0	0	0	0
6	E	3	0	0	0	0
All	All	7017	0	6114	166	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 13.

All (166) 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:A:287:VAL:HG11	1:A:341:TYR:HB3	1.52	0.92
1:A:344:VAL:O	6:A:801:HOH:O	2.02	0.77
1:B:483:GLN:HE21	1:B:485:ASP:HB2	1.49	0.76
1:A:297:ARG:HD3	1:A:357:ILE:HG12	1.67	0.76
1:B:348:LYS:NZ	6:B:801:HOH:O	2.14	0.76
1:A:317:THR:HG22	1:A:590:LEU:HD13	1.69	0.74
1:A:611:GLU:OE2	1:A:614:ARG:NH2	2.17	0.74
1:A:407:ILE:HG21	1:A:445:ALA:HB3	1.70	0.72
1:A:324:THR:HG22	1:A:327:ARG:HH12	1.54	0.72
2:E:11:DG:H2"	2:E:12:DG:H5"	1.73	0.71
1:A:471:ARG:HB2	2:E:5:DG:OP2	1.91	0.70
1:A:392:ASN:ND2	1:A:433:LYS:O	2.24	0.69
1:B:563:LEU:O	1:B:614:ARG:NH1	2.26	0.68
1:A:302:LEU:O	1:A:620:ARG:NH2	2.27	0.68
1:B:302:LEU:O	1:B:620:ARG:NH2	2.27	0.67
1:A:339:SER:OG	1:A:347:ARG:HB3	1.94	0.67
1:B:587:CYS:CB	3:D:10:C49:F	2.33	0.67
1:B:532:GLU:OE1	4:B:701:SAH:O2'	2.13	0.66
1:A:532:GLU:OE2	6:A:802:HOH:O	2.14	0.66
1:B:314:VAL:HG21	3:D:10:C49:O2P	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:12:DG:H2"	2:C:13:DA:C8	2.31	0.65
1:B:403:LEU:HD23	1:B:406:ARG:HH11	1.61	0.65
1:B:451:ASP:HB2	1:B:461:LYS:HG2	1.77	0.65
1:B:303:ALA:HB1	1:B:332:ILE:HD11	1.79	0.64
2:E:6:DG:N2	3:G:14:DC:O2	2.31	0.64
1:B:611:GLU:OE2	1:B:614:ARG:NH2	2.31	0.64
1:A:478:LEU:O	1:A:481:SER:OG	2.15	0.64
1:A:307:PRO:HG3	1:A:619:VAL:HG23	1.80	0.62
1:A:375:PHE:O	1:A:378:SER:OG	2.11	0.62
2:E:5:DG:H2'	2:E:6:DG:C8	2.35	0.61
1:B:588:ASN:ND2	1:B:605:GLN:OE1	2.33	0.61
1:A:492:SER:HA	1:A:521:LEU:HD21	1.82	0.61
1:B:587:CYS:HB3	3:D:10:C49:F	1.90	0.60
1:A:360:ARG:HB3	1:A:489:TYR:CE1	2.37	0.60
1:B:286:GLY:HA3	1:B:293:LEU:HD12	1.83	0.59
1:A:347:ARG:HG3	1:A:393:CYS:SG	2.42	0.59
1:A:297:ARG:NH1	1:A:354:ASN:HA	2.18	0.59
1:A:521:LEU:HB3	1:A:523:ILE:HG13	1.85	0.58
1:A:481:SER:HA	4:A:701:SAH:HA	1.85	0.58
1:B:515:GLU:OE1	1:B:515:GLU:N	2.30	0.58
1:A:475:PHE:O	1:A:479:GLY:N	2.36	0.57
1:A:407:ILE:HD13	1:A:428:VAL:HB	1.88	0.56
1:B:311:TYR:OH	1:B:585:SER:HB2	2.06	0.55
1:B:587:CYS:SG	3:D:10:C49:H2'2	2.45	0.55
1:A:303:ALA:HB1	1:A:332:ILE:HD11	1.89	0.55
1:B:347:ARG:NH2	1:B:479:GLY:O	2.38	0.55
1:A:287:VAL:HG12	1:A:288:PRO:O	2.07	0.55
2:C:12:DG:H2"	2:C:13:DA:H8	1.70	0.54
1:A:568:ILE:O	1:A:572:MET:HG3	2.07	0.54
1:B:564:THR:HG23	1:B:567:THR:HG23	1.89	0.54
2:C:15:DG:H2'	2:C:16:DA:C8	2.43	0.54
1:A:510:GLY:N	6:A:802:HOH:O	2.40	0.54
1:B:349:ARG:NH2	3:D:10:C49:O2	2.36	0.54
1:A:404:THR:OG1	1:A:445:ALA:O	2.18	0.54
1:A:563:LEU:O	1:A:614:ARG:NH1	2.40	0.53
1:B:297:ARG:NH1	1:B:353:HIS:O	2.40	0.53
1:B:483:GLN:HG3	1:B:486:THR:H	1.74	0.53
3:G:13:DC:H2"	3:G:14:DC:O5'	2.09	0.53
1:A:411:LEU:HB3	1:A:443:ASN:HD22	1.74	0.53
1:B:568:ILE:O	1:B:572:MET:HG3	2.09	0.53
4:A:701:SAH:H4'	6:A:802:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:11:DG:H2"	2:C:12:DG:H5"	1.91	0.52
2:E:3:DA:H2'	2:E:4:DA:C8	2.44	0.52
1:A:614:ARG:O	1:A:617:GLU:HG2	2.10	0.52
1:A:302:LEU:HD12	1:A:330:PHE:HD1	1.75	0.52
1:A:340:LYS:O	1:A:390:LYS:NZ	2.42	0.52
1:A:587:CYS:CB	3:G:10:C49:F	2.48	0.51
1:A:302:LEU:CD1	1:A:330:PHE:CD1	2.94	0.51
2:E:14:DG:H1	3:G:5:DC:H42	1.59	0.51
1:B:454:GLU:OE2	1:B:464:THR:OG1	2.23	0.51
1:A:307:PRO:HG3	1:A:619:VAL:CG2	2.40	0.51
1:B:372:HIS:HA	1:B:379:LYS:HE3	1.92	0.51
2:E:15:DG:H2'	2:E:16:DA:C8	2.46	0.51
1:A:320:GLY:O	1:A:324:THR:HG23	2.11	0.50
1:A:372:HIS:HD1	1:A:382:TRP:HZ2	1.58	0.50
1:A:454:GLU:OE2	1:A:464:THR:OG1	2.23	0.50
1:A:297:ARG:HH12	1:A:354:ASN:HA	1.77	0.50
1:A:338:ASP:OD1	1:A:339:SER:N	2.44	0.50
1:B:392:ASN:HB2	1:B:436:ASN:HD21	1.77	0.50
2:C:18:DT:H5"	2:C:18:DT:H6	1.77	0.49
1:B:512:GLY:O	1:B:516:VAL:HG23	2.12	0.49
1:A:448:LEU:HB2	1:A:453:MET:HE2	1.93	0.49
1:B:544:PHE:O	1:B:548:THR:OG1	2.17	0.49
1:A:401:ALA:HA	1:A:404:THR:HG22	1.94	0.49
1:A:587:CYS:HB3	3:G:10:C49:F	2.02	0.49
1:A:595:ARG:HG2	2:E:9:DG:C4	2.48	0.49
1:A:302:LEU:HD12	1:A:330:PHE:CD1	2.48	0.48
2:E:4:DA:H2'	2:E:5:DG:C8	2.48	0.48
1:A:302:LEU:CD1	1:A:330:PHE:HD1	2.26	0.48
1:A:519:HIS:O	1:A:522:GLN:N	2.46	0.48
1:A:406:ARG:HA	1:A:409:VAL:HG22	1.96	0.48
1:A:505:LEU:HD21	1:A:615:ILE:HG21	1.95	0.48
1:A:453:MET:HG3	1:A:478:LEU:HD13	1.95	0.48
1:A:563:LEU:HD21	1:A:568:ILE:HD11	1.95	0.48
1:B:372:HIS:ND1	1:B:379:LYS:HG3	2.29	0.47
1:A:369:TYR:O	1:A:390:LYS:HE2	2.15	0.47
1:A:504:VAL:HG12	1:A:527:LEU:O	2.14	0.47
1:B:363:ILE:HG22	1:B:364:GLN:O	2.14	0.47
1:A:469:MET:HG2	1:A:473:GLU:HB2	1.97	0.47
2:E:4:DA:H4'	2:E:5:DG:OP1	2.14	0.47
3:G:3:DT:H2"	3:G:4:DC:OP2	2.14	0.47
1:A:589:ASN:HA	1:A:597:SER:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:MET:HE3	1:A:474:ARG:HA	1.97	0.47
2:E:3:DA:H4'	2:E:4:DA:OP1	2.15	0.46
2:C:16:DA:H2"	2:C:17:DA:H8	1.80	0.46
1:A:428:VAL:O	1:A:431:GLN:N	2.49	0.46
1:B:327:ARG:HD2	1:A:611:GLU:OE2	2.15	0.46
1:B:449:GLU:CD	1:B:471:ARG:HH22	2.18	0.46
1:B:560:ILE:HG23	1:B:611:GLU:HG2	1.97	0.46
1:A:594:ASN:HD21	1:A:597:SER:HB2	1.81	0.46
1:A:402:GLN:N	1:A:402:GLN:OE1	2.48	0.45
1:A:512:GLY:O	1:A:516:VAL:HG23	2.17	0.45
2:E:3:DA:H2"	2:E:4:DA:O5'	2.16	0.45
1:A:504:VAL:CG1	1:A:528:VAL:HG22	2.46	0.45
1:A:347:ARG:NH2	1:A:479:GLY:O	2.42	0.45
1:A:503:ASN:ND2	1:A:575:TYR:O	2.50	0.44
1:A:505:LEU:O	1:A:581:VAL:HA	2.18	0.44
1:A:489:TYR:O	1:A:492:SER:OG	2.30	0.44
1:B:391:LEU:HB3	1:B:436:ASN:OD1	2.17	0.44
1:A:394:ILE:HD12	1:A:457:LEU:HD21	1.99	0.44
1:A:488:ALA:HB1	1:A:521:LEU:HD11	2.00	0.44
1:A:281:PRO:HB2	1:A:283:ILE:HD11	1.99	0.44
1:A:339:SER:HG	1:A:347:ARG:HB3	1.83	0.44
3:G:11:DA:OP2	3:G:11:DA:H8	2.01	0.44
1:B:407:ILE:HG22	1:B:411:LEU:HD22	1.99	0.44
1:B:411:LEU:HD11	1:B:428:VAL:HG11	1.99	0.44
1:A:347:ARG:NH1	1:A:349:ARG:HH11	2.15	0.44
3:D:17:DT:H2"	3:D:18:DA:C8	2.53	0.43
1:A:386:ASP:OD2	1:A:388:ARG:HB3	2.18	0.43
1:A:422:LYS:HA	1:A:425:GLN:HB3	1.99	0.43
1:A:324:THR:HG22	1:A:327:ARG:NH1	2.28	0.43
1:A:391:LEU:HB3	1:A:436:ASN:ND2	2.33	0.43
1:B:369:TYR:O	1:B:390:LYS:HE3	2.19	0.43
1:A:371:ILE:HG22	1:A:389:THR:O	2.19	0.43
1:A:616:LEU:O	1:A:619:VAL:HG22	2.18	0.43
3:G:6:DT:H4'	3:G:7:DC:OP1	2.18	0.43
2:C:16:DA:H2"	2:C:17:DA:C8	2.54	0.43
1:B:329:LEU:HD23	1:B:329:LEU:HA	1.83	0.43
2:C:1:DT:H2"	2:C:2:DA:C8	2.54	0.43
1:A:283:ILE:HD13	1:A:341:TYR:CE2	2.53	0.43
1:A:506:SER:HA	1:A:582:ILE:O	2.19	0.43
1:A:527:LEU:HD22	1:A:575:TYR:CG	2.54	0.43
1:A:407:ILE:CD1	1:A:428:VAL:HB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:439:TRP:CZ3	1:B:445:ALA:HB2	2.55	0.42
3:D:7:DC:H2'	3:D:8:DC:C6	2.53	0.42
1:B:564:THR:CG2	1:B:567:THR:HG23	2.49	0.42
1:A:349:ARG:NH1	3:G:10:C49:O4'	2.52	0.42
1:A:439:TRP:CZ3	1:A:445:ALA:HB2	2.54	0.42
1:B:358:ASN:ND2	1:B:358:ASN:H	2.17	0.42
1:A:448:LEU:HB2	1:A:453:MET:CE	2.50	0.42
3:G:16:DT:H2"	3:G:17:DT:H5"	2.01	0.42
1:B:398:THR:HG21	1:B:475:PHE:CE2	2.55	0.42
1:A:601:LEU:HD23	1:A:601:LEU:HA	1.80	0.42
1:A:344:VAL:HG21	1:A:374:ALA:HB2	2.01	0.41
1:A:459:PHE:CZ	1:A:513:GLY:HA2	2.55	0.41
2:E:4:DA:H2"	2:E:5:DG:O5'	2.20	0.41
1:B:381:TRP:CE2	1:B:441:GLY:HA2	2.55	0.41
1:A:315:ALA:HA	1:A:322:TRP:HE1	1.84	0.41
1:A:449:GLU:O	1:A:452:GLU:N	2.40	0.41
2:E:14:DG:H1	3:G:5:DC:N4	2.19	0.41
1:A:364:GLN:OE1	1:A:366:PRO:HD3	2.20	0.41
1:A:518:LEU:HD23	1:A:518:LEU:HA	1.83	0.41
1:A:440:VAL:O	1:A:440:VAL:HG22	2.21	0.41
1:A:302:LEU:O	1:A:302:LEU:HD13	2.21	0.40
1:A:518:LEU:HD22	1:A:523:ILE:HB	2.03	0.40
1:A:407:ILE:CD1	1:A:428:VAL:HG21	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	348/357 (98%)	312 (90%)	33 (10%)	3 (1%)	17 24
1	B	348/357 (98%)	340 (98%)	8 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	696/714 (98%)	652 (94%)	41 (6%)	3 (0%)	34 46

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	466	GLY
1	A	387	LYS
1	A	467	GLY

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	274/315 (87%)	266 (97%)	8 (3%)	42 57
1	B	296/315 (94%)	292 (99%)	4 (1%)	67 79
All	All	570/630 (90%)	558 (98%)	12 (2%)	53 68

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	390	LYS
1	B	408	ARG
1	B	506	SER
1	B	530	SER
1	A	296	HIS
1	A	347	ARG
1	A	377	LEU
1	A	382	TRP
1	A	427	TYR
1	A	436	ASN
1	A	506	SER
1	A	604	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	358	ASN
1	B	483	GLN
1	B	539	ASN
1	B	588	ASN
1	B	605	GLN
1	A	296	HIS
1	A	405	ASN
1	A	443	ASN
1	A	547	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
3	C49	G	10	1,3	18,22,24	4.78	10 (55%)	19,33,38	1.15	2 (10%)
3	C49	D	10	1,3	18,22,24	4.56	11 (61%)	19,33,38	2.33	7 (36%)

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	C49	G	10	1,3	-	4/7/40/46	0/2/2/2
3	C49	D	10	1,3	-	4/7/40/46	0/2/2/2

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	10	C49	C2-N1	10.98	1.51	1.35
3	D	10	C49	C2-N1	9.57	1.49	1.35
3	G	10	C49	C3'-C4'	-8.31	1.30	1.53
3	D	10	C49	C3'-C4'	-7.82	1.31	1.53
3	G	10	C49	O4'-C4'	7.62	1.62	1.45
3	D	10	C49	O4'-C4'	7.02	1.60	1.45
3	G	10	C49	C2-N3	6.69	1.49	1.38
3	D	10	C49	C6-N1	-6.15	1.40	1.46
3	D	10	C49	CM5-C5	5.98	1.64	1.51
3	G	10	C49	CM5-C5	5.98	1.64	1.51
3	D	10	C49	C2-N3	5.79	1.48	1.38
3	G	10	C49	O4'-C1'	-5.22	1.30	1.42
3	D	10	C49	O4'-C1'	-4.80	1.31	1.42
3	G	10	C49	F-C5	-4.30	1.34	1.42
3	D	10	C49	F-C5	-4.24	1.34	1.42
3	G	10	C49	C6-N1	-4.15	1.42	1.46
3	G	10	C49	O3'-C3'	2.74	1.49	1.43
3	D	10	C49	O3'-C3'	2.22	1.48	1.43
3	D	10	C49	C4-N4	2.22	1.33	1.27
3	D	10	C49	C1'-N1	-2.19	1.42	1.45
3	G	10	C49	C4-N3	2.19	1.43	1.36

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	10	C49	CM5-C5-C4	6.62	119.59	109.22
3	D	10	C49	C2'-C1'-N1	-4.81	109.73	115.61
3	D	10	C49	N3-C2-N1	3.19	120.02	116.65
3	G	10	C49	C2'-C1'-N1	-2.88	112.09	115.61
3	D	10	C49	O2-C2-N1	-2.41	120.08	123.11
3	D	10	C49	C4'-O4'-C1'	-2.31	103.87	109.45
3	D	10	C49	O3'-C3'-C2'	-2.12	103.33	110.90
3	G	10	C49	C2'-C3'-C4'	2.03	107.00	102.76
3	D	10	C49	C2'-C3'-C4'	2.00	106.93	102.76

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	10	C49	O4'-C1'-N1-C6
3	G	10	C49	O4'-C1'-N1-C6
3	D	10	C49	C2'-C1'-N1-C6

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Mol	Chain	Res	Type	Atoms
3	G	10	C49	C2'-C1'-N1-C6
3	D	10	C49	C2'-C1'-N1-C2
3	G	10	C49	C2'-C1'-N1-C2
3	G	10	C49	O4'-C1'-N1-C2
3	D	10	C49	O4'-C1'-N1-C2

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	10	C49	3	0
3	D	10	C49	5	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

3 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	$\#\|Z\| > 2$
4	SAH	B	701	1	24,28,28	1.31	3 (12%)	25,40,40	1.73	4 (16%)
4	SAH	A	701	-	24,28,28	1.23	2 (8%)	25,40,40	1.80	8 (32%)
5	D5M	G	101	-	18,23,24	0.60	0	17,33,36	0.70	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SAH	B	701	1	-	6/11/31/31	0/3/3/3
4	SAH	A	701	-	-	7/11/31/31	0/3/3/3
5	D5M	G	101	-	-	3/3/21/22	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	701	SAH	C2-N3	4.47	1.39	1.32
4	A	701	SAH	C2-N3	4.40	1.39	1.32
4	A	701	SAH	C2-N1	2.33	1.38	1.33
4	B	701	SAH	OXT-C	-2.25	1.23	1.30
4	B	701	SAH	C2-N1	2.25	1.38	1.33

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	701	SAH	N3-C2-N1	-5.06	120.76	128.68
4	A	701	SAH	N3-C2-N1	-4.72	121.29	128.68
4	B	701	SAH	C5'-C4'-C3'	-3.55	106.18	115.06
4	B	701	SAH	CB-CG-SD	-3.19	106.15	113.31
4	A	701	SAH	C5'-C4'-C3'	-3.19	107.09	115.06
4	A	701	SAH	C5'-SD-CG	-3.17	92.76	102.27
4	B	701	SAH	O3'-C3'-C4'	-2.79	102.99	111.05
4	A	701	SAH	CB-CG-SD	-2.46	107.78	113.31
4	A	701	SAH	OXT-C-CA	2.44	121.68	113.38
4	A	701	SAH	C3'-C2'-C1'	2.23	104.34	100.98
4	A	701	SAH	O4'-C4'-C5'	2.11	114.26	108.83
4	A	701	SAH	C4-C5-N7	-2.03	107.28	109.40

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	701	SAH	N-CA-CB-CG
4	B	701	SAH	O4'-C4'-C5'-SD
4	B	701	SAH	C3'-C4'-C5'-SD
5	G	101	D5M	O4'-C4'-C5'-O5'
4	A	701	SAH	OXT-C-CA-CB
4	B	701	SAH	CA-CB-CG-SD
4	A	701	SAH	O-C-CA-CB
4	A	701	SAH	OXT-C-CA-N

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Mol	Chain	Res	Type	Atoms
4	A	701	SAH	O-C-CA-N
4	A	701	SAH	C-CA-CB-CG
4	B	701	SAH	C4'-C5'-SD-CG
4	A	701	SAH	CB-CG-SD-C5'
5	G	101	D5M	C4'-C5'-O5'-P
4	B	701	SAH	C-CA-CB-CG
4	A	701	SAH	N-CA-CB-CG
5	G	101	D5M	C3'-C4'-C5'-O5'

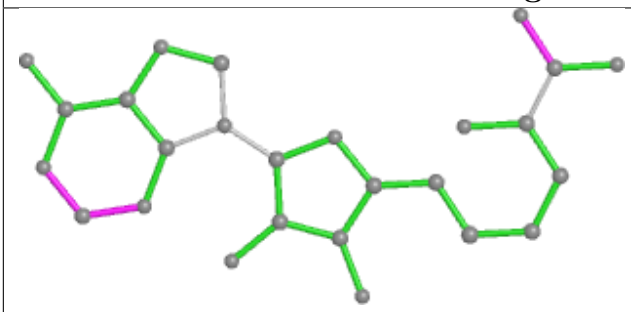
There are no ring outliers.

2 monomers are involved in 3 short contacts:

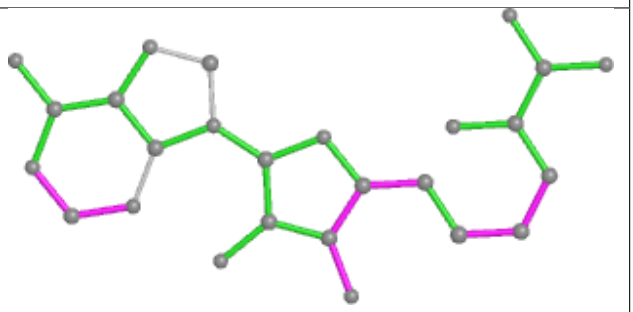
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	701	SAH	1	0
4	A	701	SAH	2	0

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 then 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.

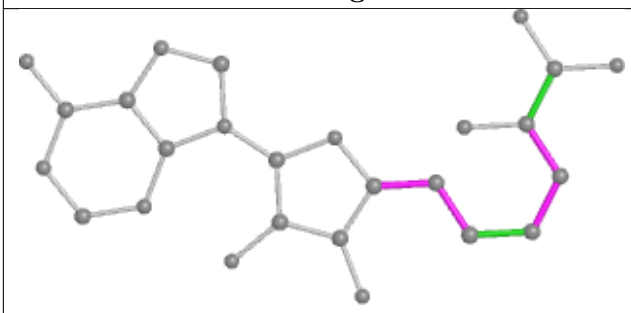
Ligand SAH B 701



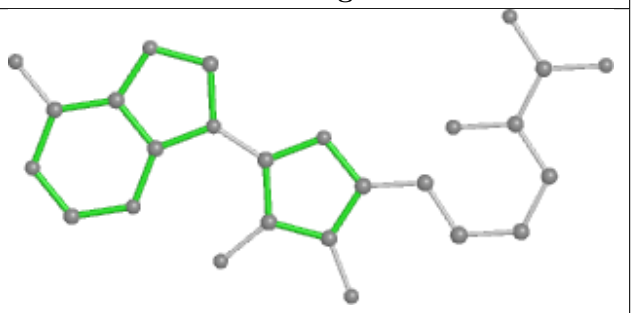
Bond lengths



Bond angles

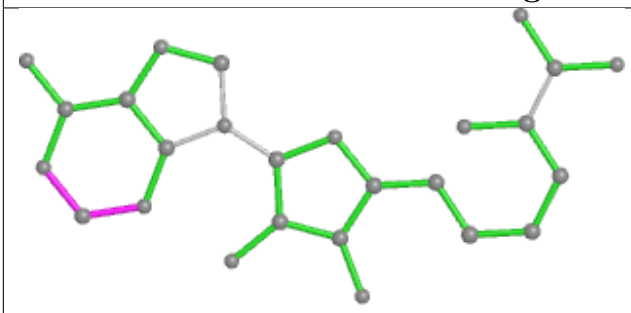


Torsions

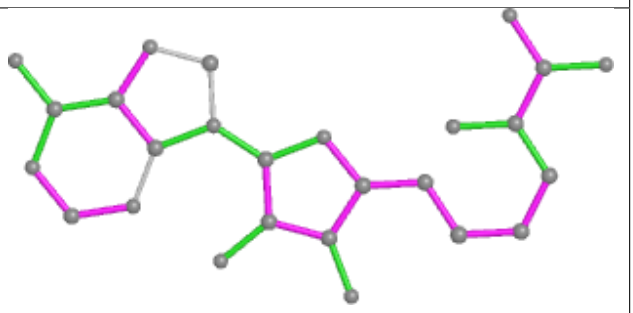


Rings

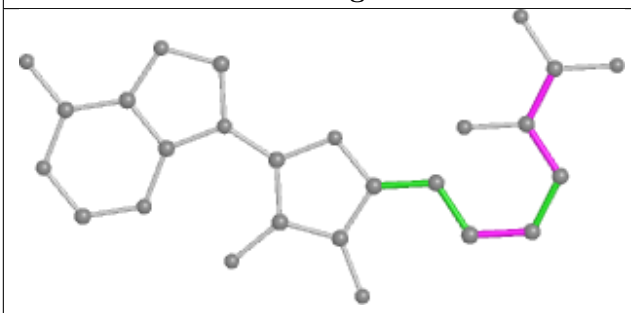
Ligand SAH A 701



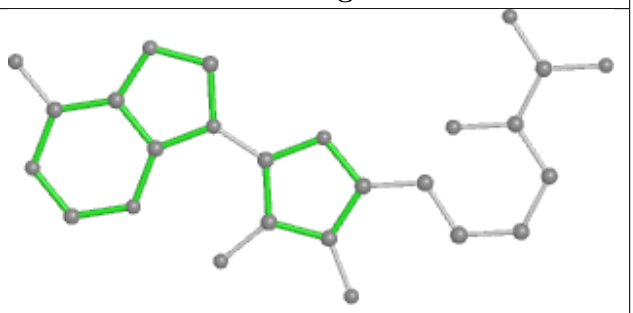
Bond lengths



Bond angles

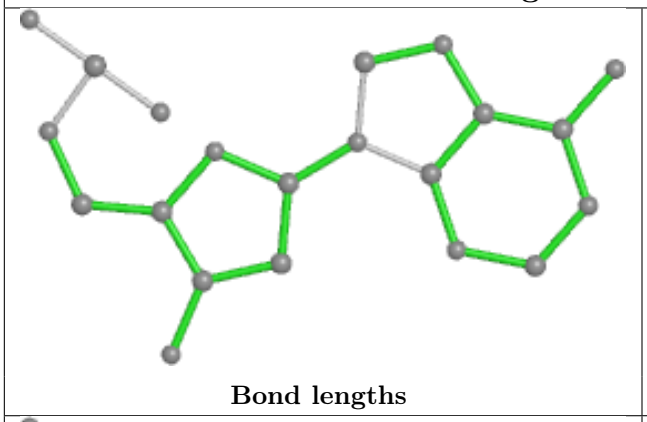


Torsions

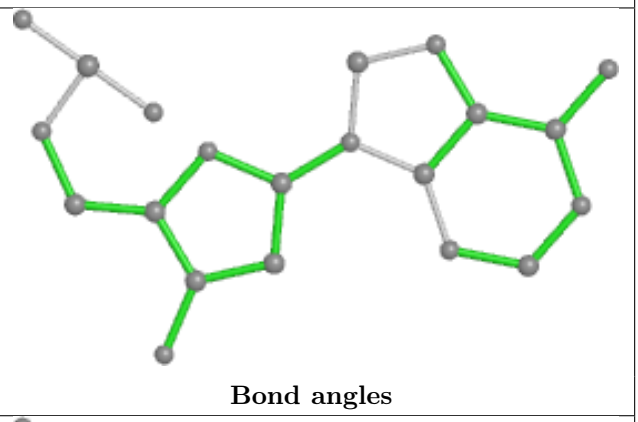


Rings

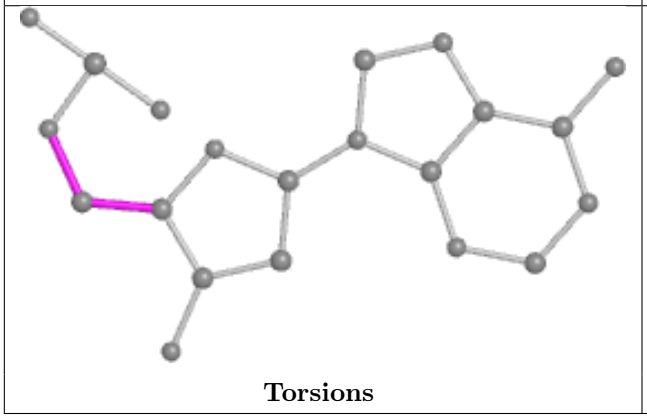
Ligand D5M G 101



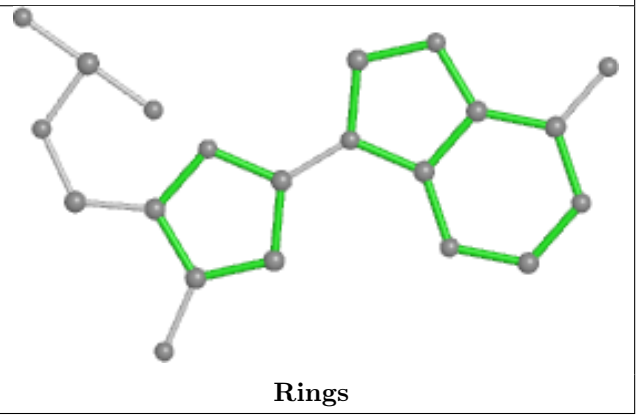
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

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, 95^{th} 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	350/357 (98%)	0.73	36 (10%) 6 8	69, 116, 163, 185	0
1	B	350/357 (98%)	0.33	1 (0%) 94 96	56, 71, 93, 114	0
2	C	18/18 (100%)	-0.21	0 100 100	80, 88, 136, 149	0
2	E	18/18 (100%)	-0.56	0 100 100	144, 157, 187, 192	0
3	D	17/18 (94%)	-0.21	0 100 100	66, 85, 119, 120	0
3	G	16/18 (88%)	-0.12	0 100 100	118, 163, 183, 184	0
All	All	769/786 (97%)	0.46	37 (4%) 30 37	56, 87, 161, 192	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	440	VAL	8.7
1	A	437	LEU	7.6
1	A	441	GLY	6.0
1	A	448	LEU	5.5
1	A	439	TRP	4.7
1	A	385	TRP	4.1
1	A	412	GLU	3.8
1	A	371	ILE	3.8
1	A	444	LYS	3.8
1	A	443	ASN	3.6
1	A	438	VAL	3.5
1	A	382	TRP	3.5
1	A	375	PHE	3.4
1	A	468	GLY	3.4
1	A	378	SER	3.4
1	A	428	VAL	3.3
1	A	494	LEU	3.3
1	A	445	ALA	3.2
1	A	380	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	528	VAL	3.0
1	A	409	VAL	3.0
1	A	381	TRP	2.9
1	A	276	ILE	2.8
1	A	446	ALA	2.8
1	A	523	ILE	2.8
1	A	413	PRO	2.7
1	A	283	ILE	2.6
1	A	416	GLU	2.6
1	A	527	LEU	2.5
1	A	405	ASN	2.3
1	A	296	HIS	2.3
1	A	391	LEU	2.2
1	B	403	LEU	2.1
1	A	345	ALA	2.1
1	A	414	TYR	2.0
1	A	571	LEU	2.0
1	A	285	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	C49	G	10	21/23	0.95	0.18	89,106,118,125	0
3	C49	D	10	21/23	0.98	0.16	53,61,78,105	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

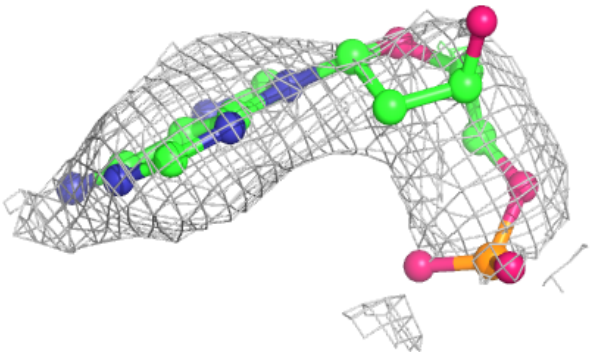
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

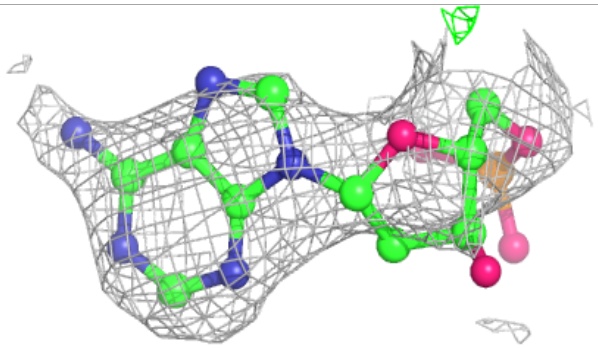
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	D5M	G	101	21/22	0.73	0.26	144,164,223,227	0
4	SAH	A	701	26/26	0.91	0.19	70,91,108,110	0
4	SAH	B	701	26/26	0.93	0.19	63,63,76,95	0

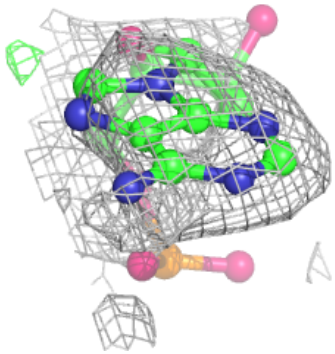
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around D5M G 101:

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

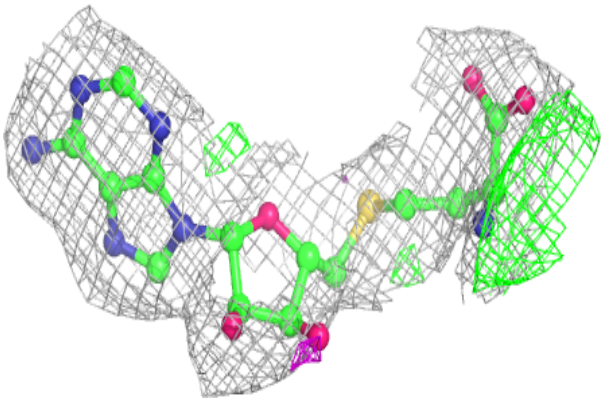


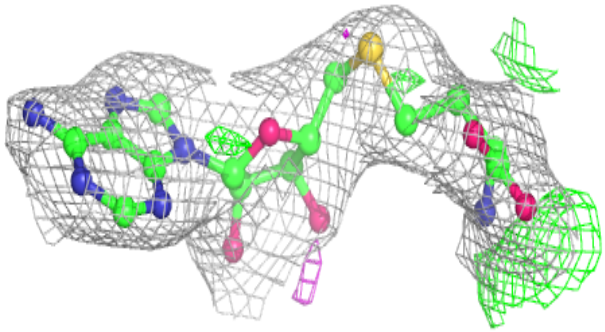


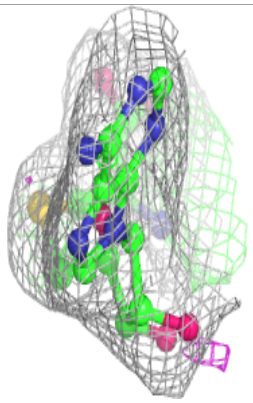


Electron density around SAH A 701:

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

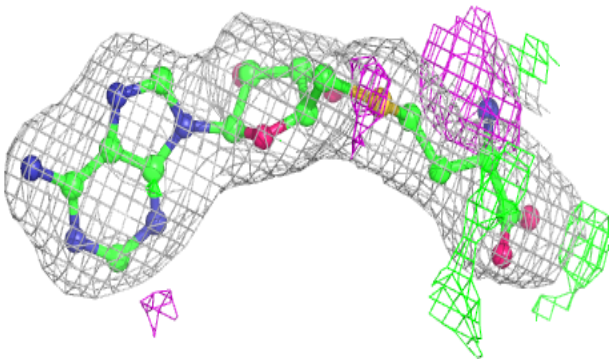


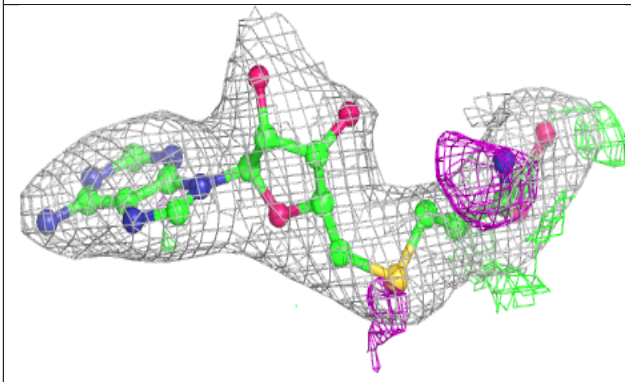


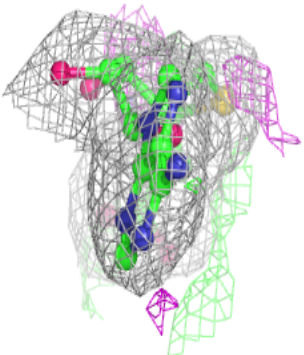


Electron density around SAH B 701:

$2mF_o$-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.