



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2026 – 12:46 AM EDT

PDB ID : 7L4F / pdb_0000714f
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 : 4-5-2 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

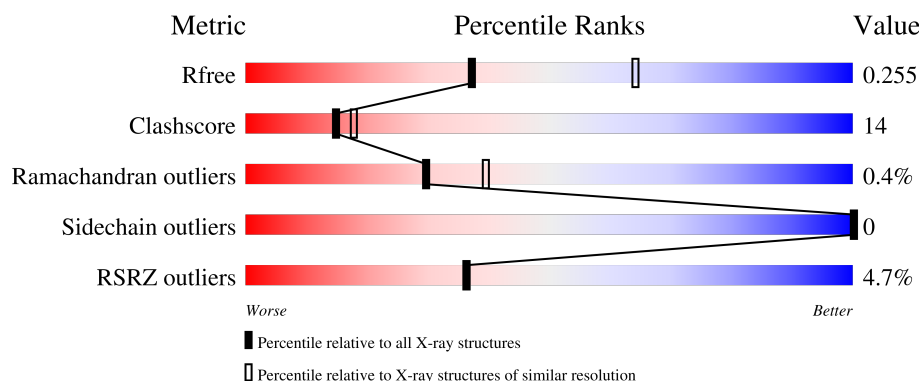
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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}	180053	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	357	10% 64% 34% .
1	B	357	78% 20% .
2	C	18	50% 50%
2	E	18	44% 56%
3	D	18	72% 22% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	G	18	33% 56% 6% 6%

2 Entry composition

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			

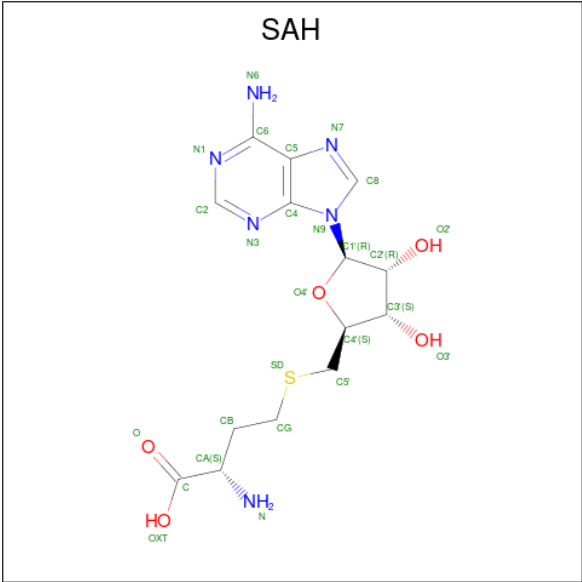
- Molecule 2 is a DNA chain called DNA (5'-D(*TP*AP*AP*AP*GP*GP*AP*TP*GP*AP*GP*GP*AP*GP*AP*AP*T)-3').

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').

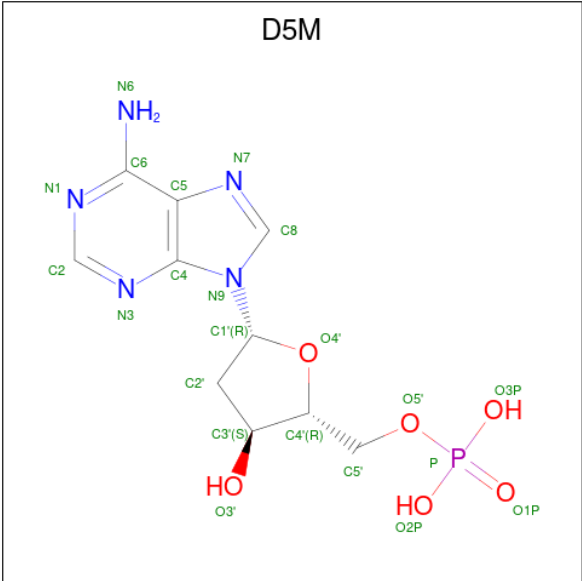
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	18	Total	C	F	N	O	P	0	0
			354	174	1	52	110	17		
3	G	17	Total	C	F	N	O	P	0	0
			337	164	1	47	108	17		

- Molecule 4 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: C₁₄H₂₀N₆O₅S).



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 (CCD ID: D5M) (formula: C₁₀H₁₄N₅O₆P).



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

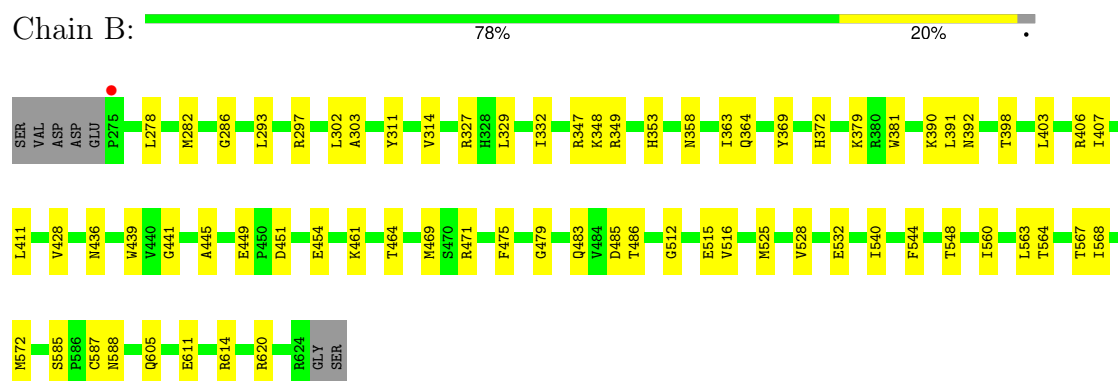
- Molecule 6 is water.

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

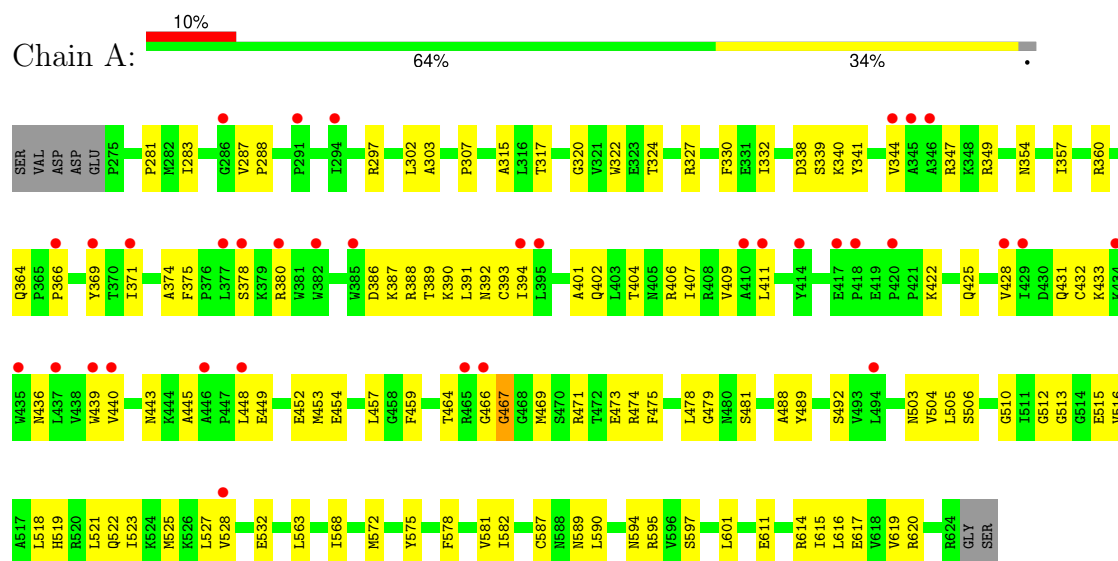
3 Residue-property plots [i](#)

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

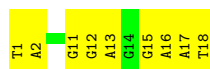


- Molecule 1: DNA (cytosine-5)-methyltransferase DRM2

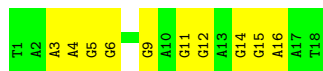


- Molecule 2: DNA (5'-D(*TP*AP*AP*AP*GP*GP*AP*TP*GP*AP*GP*GP*AP*GP*GP*AP*AP*T)-3')





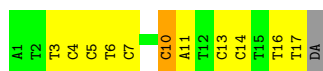
- Molecule 2: DNA (5'-D(*TP*AP*AP*AP*GP*GP*AP*TP*GP*AP*GP*GP*AP*GP*GP*AP*AP*T)-3')



- 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')



- 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')



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 2.55Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.208 , 0.250 0.215 , 0.255	Depositor DCC
R_{free} test set	2000 reflections (4.92%)	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)	0.31 , 63.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	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.*

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: D5M, C49, 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	0.43	1/2749 (0.0%)	0.62	0/3757
1	B	0.42	0/2848	0.60	0/3870
2	C	0.41	0/429	0.60	0/663
2	E	0.27	0/428	0.44	0/662
3	D	0.45	0/368	0.64	0/562
3	G	0.38	0/348	0.64	0/530
All	All	0.42	1/7170 (0.0%)	0.60	0/10044

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	380	ARG	CZ-NH2	-5.34	1.26	1.33

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2672	0	2524	101	0
1	B	2770	0	2738	48	0
2	C	379	0	203	8	0
2	E	378	0	200	14	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	354	0	205	8	0
3	G	337	0	196	11	0
4	A	26	0	19	2	0
4	B	26	0	17	2	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	176	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 14.

All (176) 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:B:348:LYS:NZ	6:B:801:HOH:O	2.14	0.81
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: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:B:469:MET:HE2	1:B:540:ILE:HD11	1.68	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
4:B:701:SAH:SD	3:D:10:C49:HM51	2.36	0.66
1:B:314:VAL:HG21	3:D:10:C49:OP2	1.96	0.65
1:A:572:MET:HE3	1:A:578:PHE:HD2	1.60	0.65

Continued on next page...

Continued from previous page...

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:544:PHE:O	1:B:548:THR:OG1	2.17	0.61
1:B:587:CYS:HB3	3:D:10:C49:F	1.90	0.60
1:A:448:LEU:HB2	1:A:453:MET:HE2	1.83	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:469:MET:HE3	1:A:474:ARG:HA	1.85	0.57
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:B:449:GLU:CD	1:B:471:ARG:HH22	2.18	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: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:572:MET:HE1	1:A:619:VAL:HB	1.94	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:B:525:MET:HE2	1:B:528:VAL:HG21	1.97	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:278:LEU:HD22	1:B:282:MET:HE2	1.97	0.46
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: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:B:525:MET:HE2	1:B:528:VAL:CG2	2.47	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:515:GLU:HB3	1:A:525:MET:HE1	1.98	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
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:A:467:GLY:C	1:A:469:MET:N	2.75	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:327:ARG:HH21	1:A:611:GLU:CD	2.27	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
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:A:388:ARG:HH22	1:A:432:CYS:C	2.29	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:448:LEU:HB2	1:A:453:MET:CE	2.50	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:B:358:ASN:ND2	1:B:358:ASN:H	2.17	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:386:ASP:C	1:A:388:ARG:H	2.30	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 ⓘ

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	348/357 (98%)	312 (90%)	33 (10%)	3 (1%)	14	20
1	B	348/357 (98%)	340 (98%)	8 (2%)	0	100	100
All	All	696/714 (98%)	652 (94%)	41 (6%)	3 (0%)	30	39

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%)	274 (100%)	0	100	100
1	B	296/315 (94%)	296 (100%)	0	100	100
All	All	570/630 (90%)	570 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	358	ASN
1	B	443	ASN
1	B	539	ASN
1	B	588	ASN
1	B	605	GLN
1	A	296	HIS
1	A	392	ASN
1	A	431	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	443	ASN
1	A	463	HIS
1	A	547	GLN
1	A	550	GLN
1	A	561	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	D	10	1,3	17,22,24	4.78	10 (58%)	17,33,38	2.72	8 (47%)
3	C49	G	10	1,3	17,22,24	5.02	10 (58%)	17,33,38	2.08	3 (17%)

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

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	10	C49	C2-N1	11.31	1.51	1.35
3	D	10	C49	C2-N1	9.87	1.49	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	10	C49	C3'-C4'	-8.69	1.30	1.53
3	D	10	C49	C3'-C4'	-8.17	1.31	1.53
3	G	10	C49	O4'-C4'	7.66	1.62	1.45
3	D	10	C49	O4'-C4'	7.06	1.60	1.45
3	G	10	C49	C2-N3	6.85	1.49	1.38
3	D	10	C49	C6-N1	-6.23	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	5.93	1.48	1.38
3	G	10	C49	O4'-C1'	-5.26	1.30	1.42
3	D	10	C49	O4'-C1'	-4.84	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	-4.19	1.42	1.46
3	D	10	C49	C4-N4	2.82	1.33	1.27
3	G	10	C49	O3'-C3'	2.78	1.49	1.43
3	G	10	C49	C4-N3	2.30	1.43	1.36
3	D	10	C49	O3'-C3'	2.25	1.48	1.43

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	10	C49	F-C5-CM5	-7.06	96.81	106.49
3	D	10	C49	CM5-C5-C4	6.77	119.59	109.11
3	D	10	C49	C2'-C1'-N1	-4.93	109.73	115.59
3	D	10	C49	F-C5-CM5	-4.28	100.62	106.49
3	D	10	C49	N3-C2-N1	3.36	120.02	116.65
3	G	10	C49	C2'-C1'-N1	-2.94	112.09	115.59
3	D	10	C49	O2-C2-N1	-2.51	120.08	123.10
3	D	10	C49	C4'-O4'-C1'	-2.38	103.87	109.51
3	D	10	C49	O3'-C3'-C2'	-2.17	103.33	110.88
3	G	10	C49	C2'-C3'-C4'	2.07	107.00	102.80
3	D	10	C49	C2'-C3'-C4'	2.04	106.93	102.80

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
3	G	10	C49	C2'-C1'-N1-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
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 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	10	C49	6	0
3	G	10	C49	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	A	701	-	27,28,28	1.10	3 (11%)	36,40,40	2.22	13 (36%)
5	D5M	G	101	-	20,23,24	0.26	0	28,33,36	0.24	0
4	SAH	B	701	-	27,28,28	1.18	3 (11%)	36,40,40	2.06	10 (27%)

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	A	701	-	-	6/15/31/31	0/3/3/3
5	D5M	G	101	-	-	3/7/21/22	0/3/3/3
4	SAH	B	701	-	-	6/15/31/31	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	701	SAH	C2-N3	3.02	1.39	1.33
4	A	701	SAH	C2-N3	2.96	1.39	1.33
4	A	701	SAH	C2-N1	2.43	1.38	1.33
4	B	701	SAH	OXT-C	-2.34	1.23	1.30
4	B	701	SAH	C2-N1	2.34	1.38	1.33
4	A	701	SAH	C8-N7	2.20	1.35	1.31

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	701	SAH	N3-C2-N1	-5.16	120.76	128.58
4	A	701	SAH	C5-C4-N3	-4.83	120.07	126.72
4	A	701	SAH	N3-C2-N1	-4.81	121.29	128.58
4	B	701	SAH	C5-C4-N3	-4.47	120.56	126.72
4	A	701	SAH	N9-C8-N7	-3.86	108.45	113.94
4	A	701	SAH	O4'-C1'-N9	3.65	115.10	108.09
4	B	701	SAH	N9-C8-N7	-3.63	108.79	113.94
4	A	701	SAH	C5-N7-C8	3.60	109.11	103.45
4	B	701	SAH	C5'-C4'-C3'	-3.55	106.18	115.06
4	A	701	SAH	C2-N3-C4	3.33	119.97	111.83
4	B	701	SAH	C2-N3-C4	3.28	119.85	111.83
4	B	701	SAH	CB-CG-SD	-3.27	106.15	113.45
4	B	701	SAH	C5-N7-C8	3.25	108.56	103.45
4	A	701	SAH	C5'-SD-CG	-3.20	92.76	102.26
4	A	701	SAH	C5'-C4'-C3'	-3.19	107.09	115.06
4	A	701	SAH	N3-C4-N9	3.12	132.47	127.17
4	A	701	SAH	C4-C5-N7	-2.89	107.28	110.58
4	B	701	SAH	N3-C4-N9	2.87	132.04	127.17
4	B	701	SAH	O3'-C3'-C4'	-2.82	102.99	111.08
4	A	701	SAH	CB-CG-SD	-2.54	107.78	113.45
4	B	701	SAH	C4-C5-N7	-2.54	107.68	110.58
4	A	701	SAH	C2'-C1'-N9	-2.15	107.95	113.30
4	A	701	SAH	O4'-C4'-C5'	2.11	114.26	108.83

There are no chirality outliers.

All (15) 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
4	A	701	SAH	OXT-C-CA-CB
4	B	701	SAH	CA-CB-CG-SD
5	G	101	D5M	O4'-C4'-C5'-O5'
4	A	701	SAH	O-C-CA-CB
4	A	701	SAH	OXT-C-CA-N
4	A	701	SAH	O-C-CA-N
4	B	701	SAH	C4'-C5'-SD-CG
4	A	701	SAH	CB-CG-SD-C5'
4	B	701	SAH	C-CA-CB-CG
4	A	701	SAH	C-CA-CB-CG
5	G	101	D5M	C4'-C5'-O5'-P
5	G	101	D5M	C3'-C4'-C5'-O5'

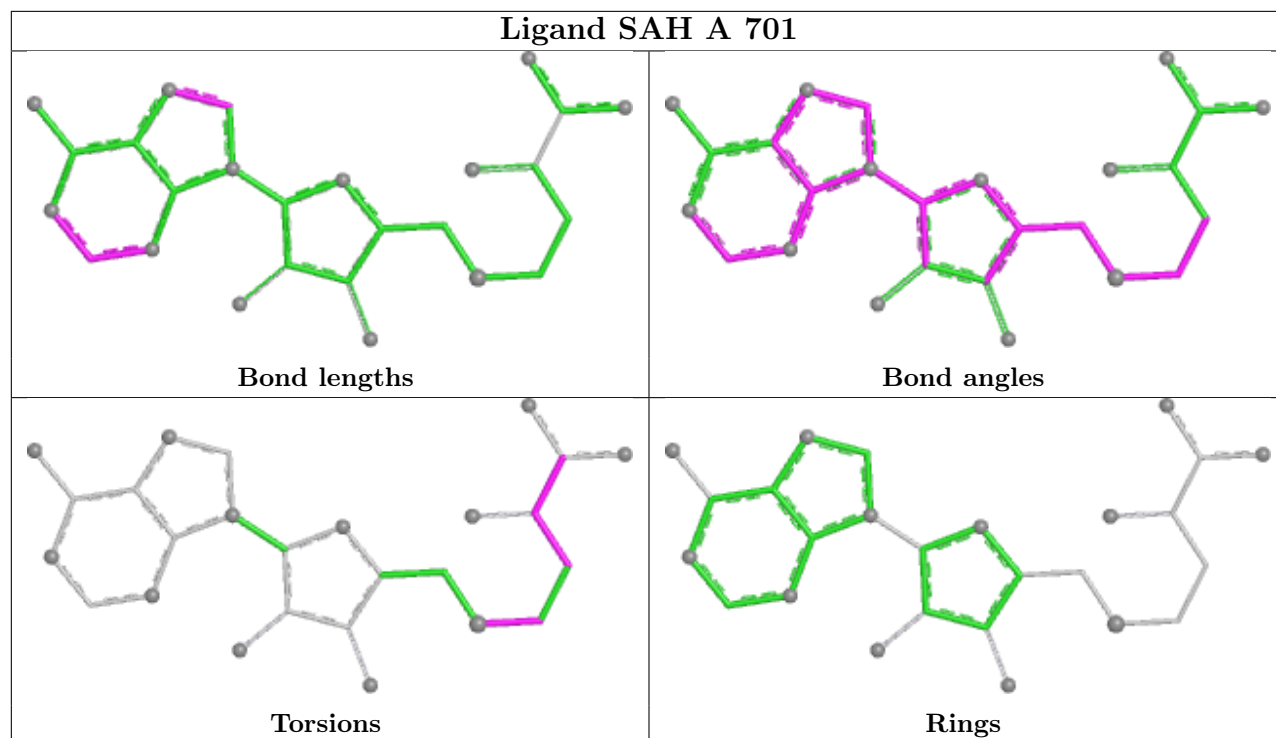
There are no ring outliers.

2 monomers are involved in 4 short contacts:

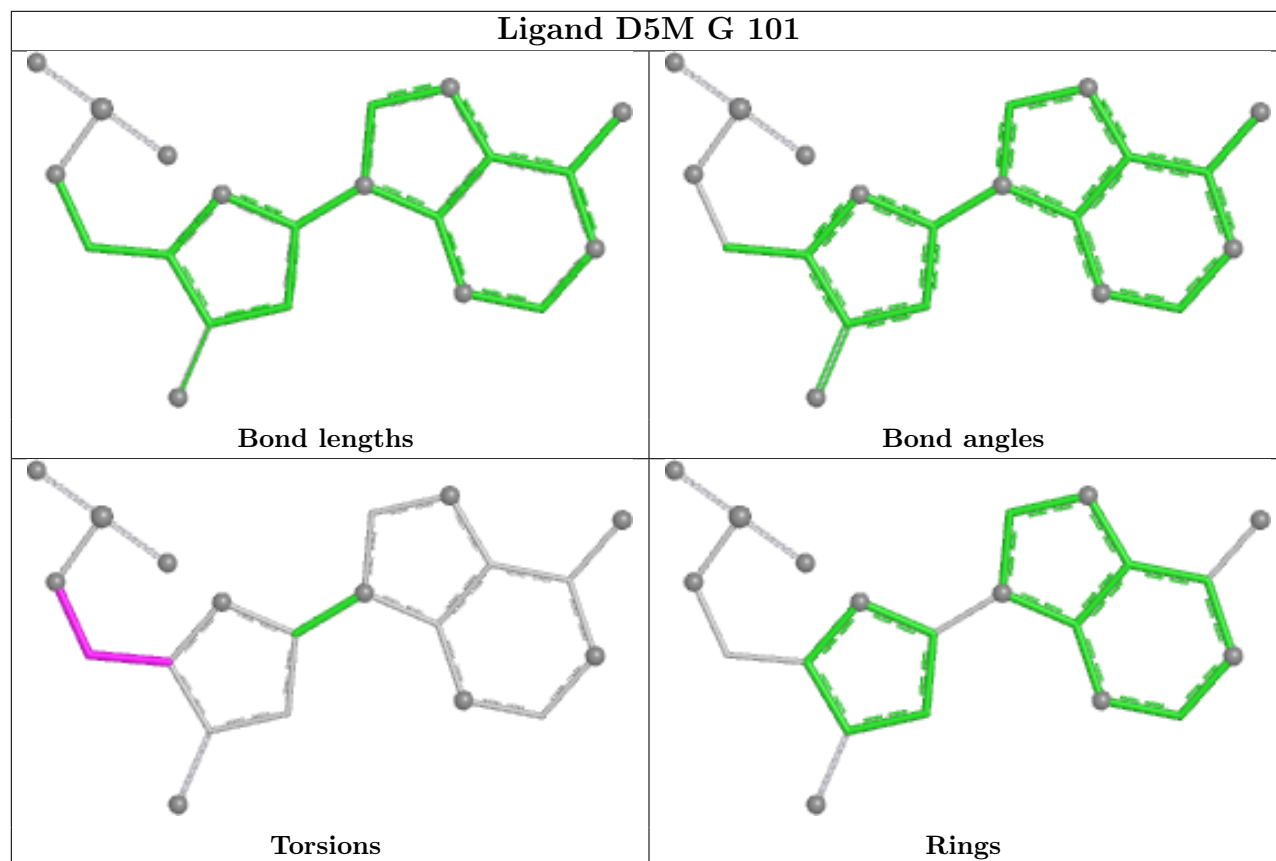
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	701	SAH	2	0
4	B	701	SAH	2	0

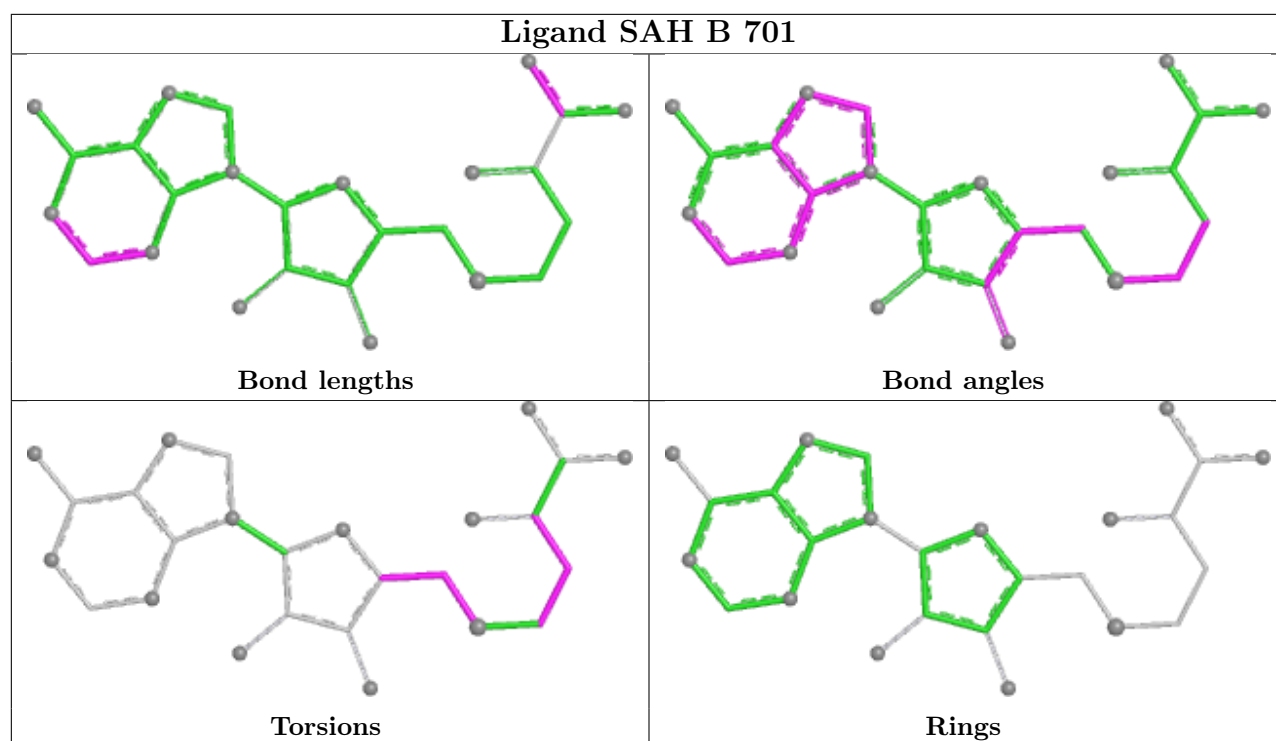
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 A 701



Ligand D5M G 101





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	350/357 (98%)	0.99	35 (10%) 12 12	69, 116, 163, 185	0
1	B	350/357 (98%)	0.06	1 (0%) 90 92	56, 71, 93, 114	0
2	C	18/18 (100%)	-0.30	0 100 100	80, 88, 136, 149	0
2	E	18/18 (100%)	0.47	0 100 100	144, 157, 187, 192	0
3	D	17/18 (94%)	-0.53	0 100 100	66, 85, 119, 120	0
3	G	16/18 (88%)	0.54	0 100 100	118, 163, 183, 184	0
All	All	769/786 (97%)	0.49	36 (4%) 36 36	56, 87, 161, 192	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	466	GLY	5.0
1	A	440	VAL	4.6
1	A	414	TYR	4.0
1	A	437	LEU	3.8
1	A	418	PRO	3.6
1	A	429	ILE	3.5
1	A	434	LYS	3.5
1	A	377	LEU	3.2
1	A	528	VAL	3.2
1	A	411	LEU	3.1
1	A	345	ALA	3.0
1	A	378	SER	2.8
1	A	382	TRP	2.7
1	B	275	PRO	2.7
1	A	446	ALA	2.7
1	A	385	TRP	2.7
1	A	344	VAL	2.6
1	A	291	PRO	2.6
1	A	346	ALA	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	494	LEU	2.5
1	A	366	PRO	2.4
1	A	439	TRP	2.4
1	A	410	ALA	2.4
1	A	380	ARG	2.4
1	A	417	GLU	2.4
1	A	294	ILE	2.4
1	A	369	TYR	2.3
1	A	465	ARG	2.3
1	A	395	LEU	2.3
1	A	371	ILE	2.3
1	A	448	LEU	2.3
1	A	394	ILE	2.2
1	A	286	GLY	2.2
1	A	420	PRO	2.1
1	A	435	TRP	2.0
1	A	428	VAL	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	C49	G	10	21/23	0.95	0.11	89,106,118,125	0
3	C49	D	10	21/23	0.97	0.07	53,61,78,105	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

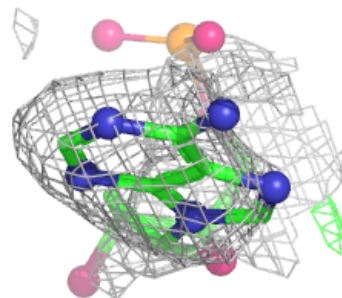
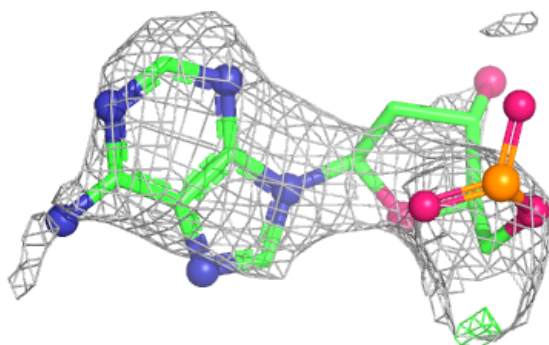
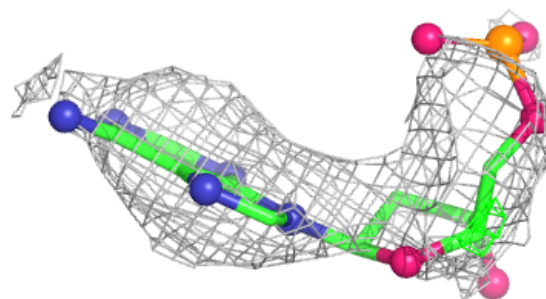
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
5	D5M	G	101	21/22	0.46	0.13	144,164,223,227	0
4	SAH	A	701	26/26	0.86	0.14	70,91,108,110	0
4	SAH	B	701	26/26	0.93	0.11	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.

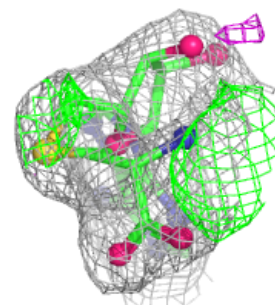
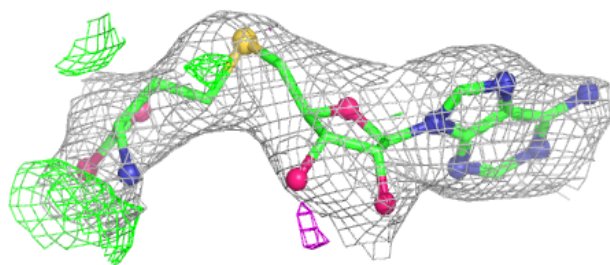
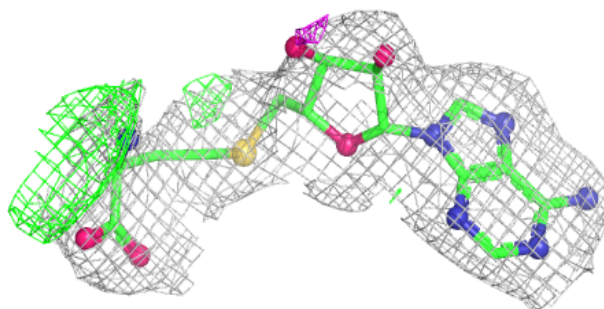
Electron density around D5M G 101:

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

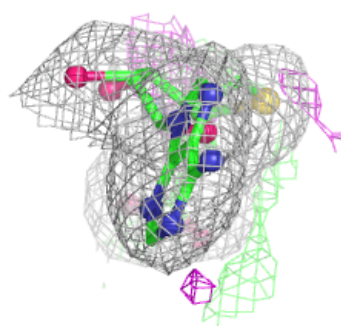
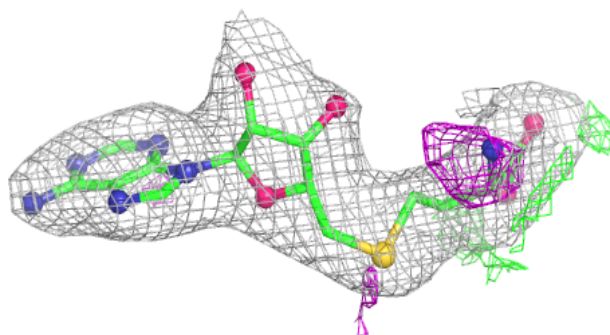
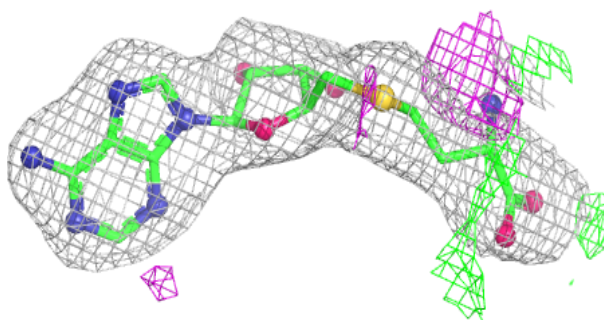


Electron density around SAH A 701:

$2mF_o-DF_c$ (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.