



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:15 PM UTC

PDB ID : 2XBM / pdb_00002xbm
Title : Crystal structure of the dengue virus methyltransferase bound to a 5'- capped octameric RNA
Authors : Yap, L.J.; Luo, D.H.; Chung, K.Y.; Lim, S.P.; Bodenreider, C.; Noble, C.; Shi, P.Y.; Lescar, J.
Deposited on : 2010-04-13
Resolution : 2.90 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

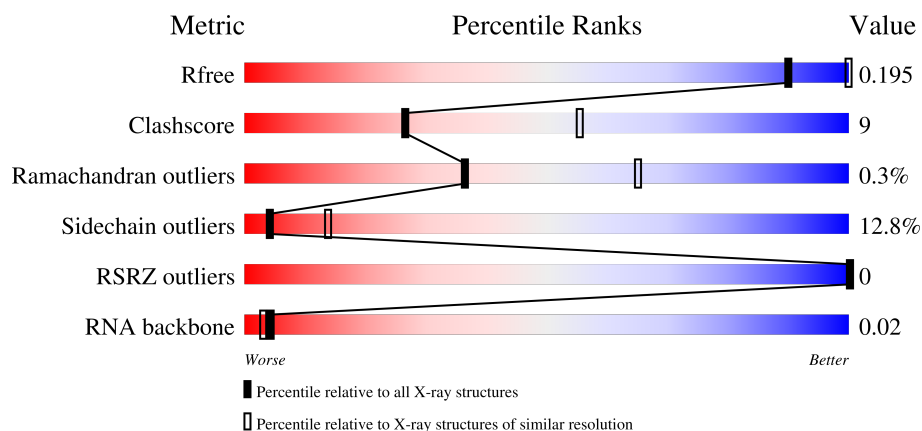
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)
RNA backbone	3983	1120 (3.10-2.70)

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	263	 79% 17% . .
1	B	263	 78% 16% . .
1	C	263	 77% 17% . .

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Mol	Chain	Length	Quality of chain
1	D	263	77% 17%
2	E	9	11% 11% 33% 44%
2	F	9	22% 11% 33% 33%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9297 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.

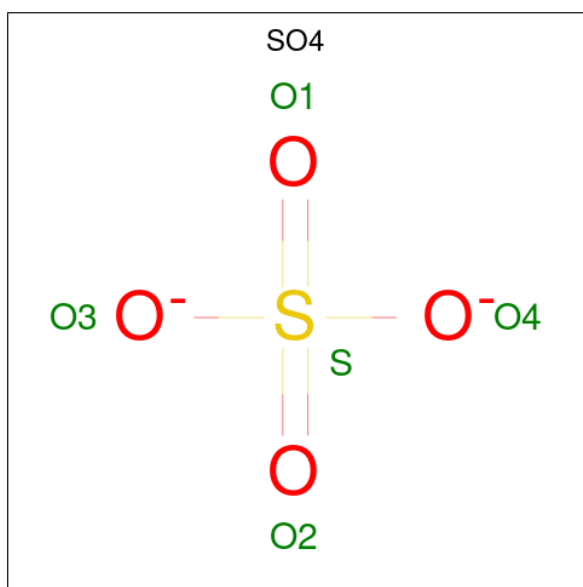
- Molecule 1 is a protein called NONSTRUCTURAL PROTEIN NS5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	261	Total	C	N	O	S	0	1	0
			2075	1304	376	380	15			
1	B	258	Total	C	N	O	S	0	1	0
			2056	1294	372	375	15			
1	C	259	Total	C	N	O	S	0	0	0
			2060	1295	374	377	14			
1	D	259	Total	C	N	O	S	0	0	0
			2060	1295	374	377	14			

- Molecule 2 is a RNA chain called 5'-(^{*}G3AP^{*}GP^{*}AP^{*}AP^{*}CP^{*}CP^{*}UP^{*}GP^{*}A)-3'.

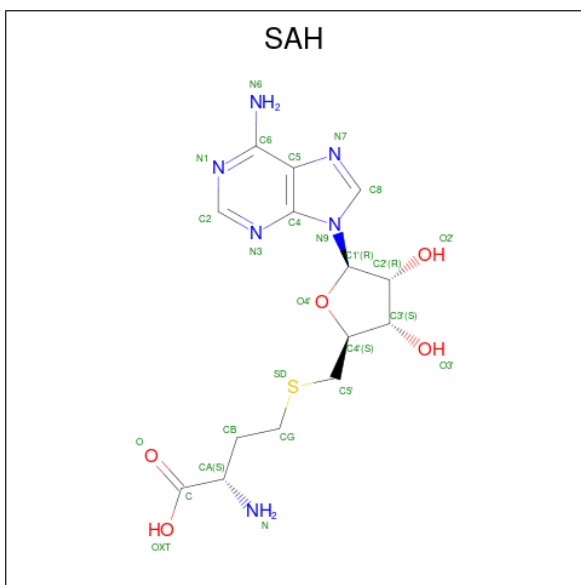
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	9	Total	C	N	O	P	0	0	0
			204	87	38	68	11			
2	F	9	Total	C	N	O	P	0	0	0
			204	87	38	68	11			

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



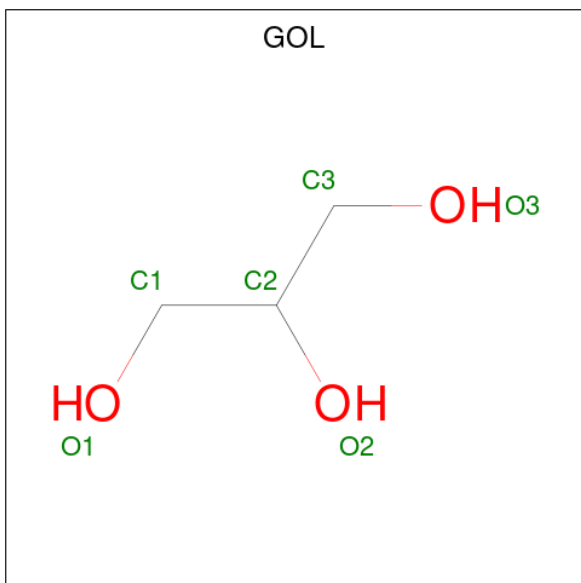
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

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



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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is water.

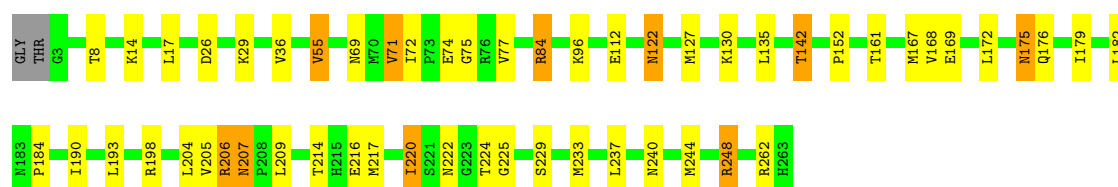
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	97	Total	O	0	0
			97	97		
6	B	119	Total	O	0	0
			119	119		
6	C	118	Total	O	0	0
			118	118		
6	D	103	Total	O	0	0
			103	103		
6	E	9	Total	O	0	0
			9	9		
6	F	16	Total	O	0	0
			16	16		

3 Residue-property plots

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.

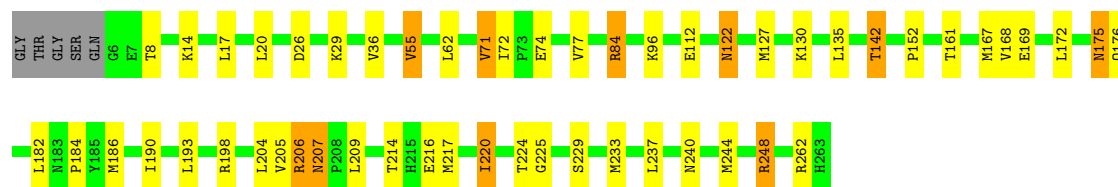
• Molecule 1: NONSTRUCTURAL PROTEIN NS5

Chain A: 



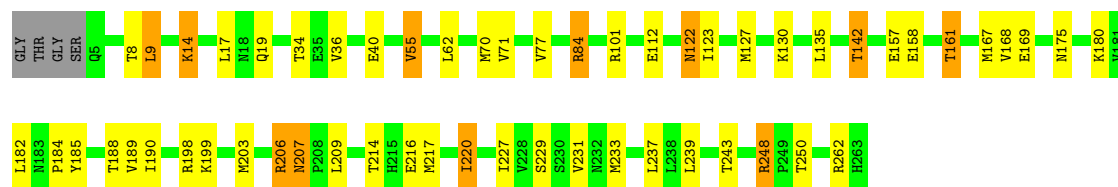
• Molecule 1: NONSTRUCTURAL PROTEIN NS5

Chain B: 



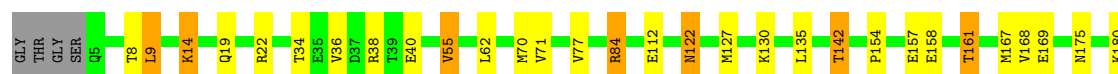
• Molecule 1: NONSTRUCTURAL PROTEIN NS5

Chain C: 



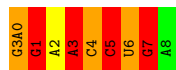
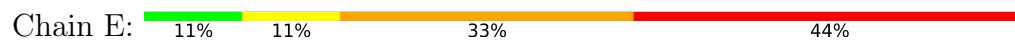
• Molecule 1: NONSTRUCTURAL PROTEIN NS5

Chain D: 

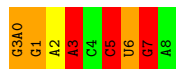




- Molecule 2: 5'-(^{*}G3AP*GP*AP*AP*CP*CP*UP*GP*A)-3'



- Molecule 2: 5'-(^{*}G3AP*GP*AP*AP*CP*CP*UP*GP*A)-3'



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	137.54Å 137.54Å 109.39Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.71 – 2.90 39.71 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.8 (39.71-2.90) 98.6 (39.71-2.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.204 , 0.231 (Not available) , 0.195	Depositor DCC
R_{free} test set	2567 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	54.2	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 29.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.020 for -h,-k,l 0.467 for h,-h-k,-l 0.021 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	9297	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SAH, GOL, SO4, G3A

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	0.44	0/2122	0.79	0/2859
1	B	0.44	0/2103	0.79	2/2834 (0.1%)
1	C	0.44	0/2104	0.79	0/2836
1	D	0.44	0/2104	0.79	0/2836
2	E	1.90	2/171 (1.2%)	1.67	5/265 (1.9%)
2	F	1.57	2/171 (1.2%)	1.59	5/265 (1.9%)
All	All	0.55	4/8775 (0.0%)	0.85	12/11895 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1	G	P-O5'	-15.21	1.36	1.59
2	F	1	G	P-OP2	-10.37	1.28	1.49
2	F	1	G	P-OP1	-5.62	1.37	1.49
2	E	1	G	O5'-C5'	-5.35	1.34	1.42

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	7	G	C4'-C3'-C2'	-8.46	94.14	102.60
2	E	1	G	O4'-C1'-C2'	-6.46	99.34	105.80
2	F	7	G	C4'-C3'-C2'	-6.42	96.18	102.60
2	F	3	A	O4'-C4'-C3'	-6.38	97.62	104.00
2	F	2	A	C1'-O4'-C4'	-6.12	103.78	109.90
2	E	1	G	P-O5'-C5'	5.79	129.58	120.90
2	F	3	A	C4'-C3'-C2'	-5.56	97.04	102.60
2	E	3	A	O4'-C4'-C3'	-5.42	98.58	104.00
2	E	5	C	O3'-P-O5'	-5.28	96.07	104.00
2	F	5	C	P-O5'-C5'	-5.18	113.12	120.90
1	B	186	MET	CA-C-N	5.01	124.45	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	186	MET	C-N-CA	5.01	124.45	119.24

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	2075	0	2096	30	0
1	B	2056	0	2080	27	0
1	C	2060	0	2079	29	0
1	D	2060	0	2079	35	0
2	E	204	0	100	23	0
2	F	204	0	99	23	0
3	A	20	0	0	0	0
3	B	20	0	0	0	0
3	C	10	0	0	0	0
3	D	10	0	0	1	0
4	A	26	0	19	0	0
4	B	26	0	19	0	0
4	C	26	0	18	0	0
4	D	26	0	16	0	0
5	A	6	0	8	0	0
5	B	6	0	8	0	0
6	A	97	0	0	4	0
6	B	119	0	0	0	0
6	C	118	0	0	2	0
6	D	103	0	0	7	0
6	E	9	0	0	0	0
6	F	16	0	0	2	0
All	All	9297	0	8621	162	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 9.

All (162) 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)
2:F:0:G3A:O23	2:F:1:G:P	1.15	1.53
2:E:0:G3A:O23	2:E:1:G:P	1.07	1.46
2:F:0:G3A:C23	2:F:1:G:P	2.44	1.04
1:A:184:PRO:HG2	1:A:217:MET:HE3	1.42	1.01
1:B:184:PRO:HG2	1:B:217:MET:HE3	1.43	1.01
2:E:0:G3A:HO23	2:E:1:G:P	1.19	0.97
2:E:0:G3A:C23	2:E:1:G:P	2.55	0.94
2:F:0:G3A:O23	2:F:1:G:O5'	1.88	0.91
1:C:184:PRO:HG2	1:C:217:MET:HE3	1.53	0.91
1:D:184:PRO:HG2	1:D:217:MET:HE3	1.50	0.91
2:E:0:G3A:O23	2:E:1:G:O5'	1.92	0.88
2:E:5:C:H2'	2:E:6:U:H5'	1.58	0.86
2:E:5:C:C2'	2:E:6:U:H5'	2.07	0.84
2:E:6:U:C6	2:E:6:U:H3'	2.13	0.83
1:C:248:ARG:CG	1:C:248:ARG:HH11	1.92	0.83
2:E:0:G3A:O23	2:E:1:G:OP1	1.96	0.82
1:A:72:ILE:HG13	6:A:2075:HOH:O	1.79	0.82
1:D:248:ARG:CG	1:D:248:ARG:HH11	1.93	0.81
2:F:5:C:H2'	2:F:6:U:H5'	1.61	0.81
2:E:6:U:C2'	2:E:7:G:O5'	2.30	0.79
2:E:6:U:C6	2:E:6:U:C3'	2.66	0.79
2:F:5:C:H5''	2:F:5:C:H6	1.48	0.79
2:E:6:U:H2'	2:E:7:G:O5'	1.84	0.77
2:F:5:C:C2'	2:F:6:U:H5'	2.15	0.76
1:D:157:GLU:O	1:D:161:THR:HG22	1.84	0.76
1:C:157:GLU:O	1:C:161:THR:HG22	1.87	0.74
1:A:55:VAL:CG1	1:A:84:ARG:HB3	2.18	0.73
1:B:55:VAL:CG1	1:B:84:ARG:HB3	2.19	0.72
1:B:207:ASN:HD22	1:B:209:LEU:H	1.37	0.72
2:F:0:G3A:O23	2:F:1:G:OP1	2.02	0.71
1:A:122:ASN:HD22	1:A:122:ASN:H	1.36	0.71
2:F:6:U:C2'	2:F:7:G:O5'	2.39	0.71
1:A:207:ASN:HD22	1:A:209:LEU:H	1.36	0.71
1:B:122:ASN:HD22	1:B:122:ASN:H	1.37	0.71
2:E:6:U:H3'	2:E:6:U:H6	1.53	0.70
1:A:179:ILE:HG13	6:A:2048:HOH:O	1.90	0.70
2:E:5:C:C3'	2:E:6:U:H5'	2.21	0.70
1:A:222:ASN:ND2	6:A:2075:HOH:O	2.10	0.69
1:C:122:ASN:H	1:C:122:ASN:HD22	1.38	0.69
1:C:207:ASN:HD22	1:C:209:LEU:H	1.41	0.68
1:D:122:ASN:HD22	1:D:122:ASN:H	1.39	0.68
1:D:207:ASN:HD22	1:D:209:LEU:H	1.42	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:154:PRO:O	6:D:2059:HOH:O	2.11	0.67
1:C:248:ARG:HH11	1:C:248:ARG:HG2	1.61	0.65
1:A:229:SER:O	1:A:233:MET:HG3	1.97	0.65
2:F:0:G3A:H24	6:F:2003:HOH:O	1.95	0.65
1:B:229:SER:O	1:B:233:MET:HG3	1.98	0.64
1:D:248:ARG:HH11	1:D:248:ARG:HG2	1.61	0.63
2:F:5:C:H6	2:F:5:C:C5'	2.11	0.63
1:D:122:ASN:HD21	1:D:262:ARG:H	1.45	0.63
1:A:193:LEU:HD13	1:A:204:LEU:HD11	1.80	0.62
1:B:248:ARG:HH11	1:B:248:ARG:CG	2.11	0.62
2:F:6:U:H2'	2:F:7:G:O5'	2.00	0.62
1:D:22:ARG:NH2	6:D:2005:HOH:O	2.33	0.61
2:E:6:U:C3'	2:E:6:U:H6	2.09	0.61
1:B:193:LEU:HD13	1:B:204:LEU:HD11	1.83	0.61
1:C:122:ASN:HD21	1:C:262:ARG:H	1.47	0.61
1:C:55:VAL:CG1	1:C:84:ARG:HB3	2.31	0.61
2:E:3:A:N3	2:E:3:A:O4'	2.30	0.61
1:C:248:ARG:HH11	1:C:248:ARG:HG3	1.65	0.60
1:D:248:ARG:HH11	1:D:248:ARG:HG3	1.66	0.60
1:A:248:ARG:HH11	1:A:248:ARG:CG	2.14	0.60
1:D:55:VAL:CG1	1:D:84:ARG:HB3	2.32	0.59
1:A:206:ARG:NH2	1:A:214:THR:O	2.34	0.59
1:B:206:ARG:NH2	1:B:214:THR:O	2.35	0.58
2:F:6:U:C6	2:F:6:U:C3'	2.86	0.58
1:B:248:ARG:HH11	1:B:248:ARG:HG2	1.68	0.58
1:C:248:ARG:CG	1:C:248:ARG:NH1	2.59	0.58
2:F:0:G3A:O23	2:F:1:G:C5'	2.51	0.57
2:F:0:G3A:H18	6:F:2001:HOH:O	2.05	0.57
1:D:248:ARG:CG	1:D:248:ARG:NH1	2.60	0.57
1:C:248:ARG:HG3	1:C:248:ARG:NH1	2.21	0.56
1:A:248:ARG:HH11	1:A:248:ARG:HG2	1.70	0.55
2:E:5:C:C3'	2:E:6:U:C5'	2.83	0.55
1:A:172:LEU:HA	1:A:175:ASN:HD21	1.71	0.55
1:B:172:LEU:HA	1:B:175:ASN:HD21	1.72	0.55
1:D:34:THR:HG22	1:D:250:THR:HB	1.88	0.55
1:D:248:ARG:HG3	1:D:248:ARG:NH1	2.22	0.54
1:C:34:THR:HG22	1:C:250:THR:HB	1.89	0.54
2:F:5:C:C5'	2:F:5:C:C6	2.90	0.53
2:E:5:C:C2'	2:E:6:U:C5'	2.85	0.53
1:B:122:ASN:HD21	1:B:262:ARG:H	1.57	0.53
2:F:6:U:C6	2:F:6:U:H3'	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:ASN:HD21	1:A:262:ARG:H	1.57	0.52
1:D:70:MET:HB3	1:D:220:ILE:HG12	1.91	0.52
1:C:70:MET:HB3	1:C:220:ILE:HG12	1.91	0.52
1:B:248:ARG:CG	1:B:248:ARG:NH1	2.73	0.52
1:C:122:ASN:H	1:C:122:ASN:ND2	2.06	0.51
1:A:122:ASN:H	1:A:122:ASN:ND2	2.07	0.51
1:C:206:ARG:NH2	1:C:214:THR:O	2.43	0.51
1:D:180:LYS:HD2	1:D:216:GLU:HG2	1.92	0.51
1:A:55:VAL:HG11	1:A:84:ARG:HB3	1.93	0.51
1:C:217:MET:HE1	1:C:231:VAL:HA	1.92	0.51
1:B:122:ASN:H	1:B:122:ASN:ND2	2.08	0.50
1:D:183:ASN:ND2	6:D:2059:HOH:O	2.43	0.50
1:A:225:GLY:HA2	1:C:19:GLN:HE21	1.76	0.50
1:C:123:ILE:HG13	6:C:2060:HOH:O	2.11	0.50
2:F:6:U:O2'	2:F:7:G:O5'	2.30	0.50
2:F:5:C:C3'	2:F:6:U:H5'	2.41	0.50
2:E:0:G3A:O45	2:E:0:G3A:O3B	2.29	0.50
2:E:6:U:O2'	2:E:7:G:O5'	2.30	0.49
1:C:77:VAL:HG22	1:C:142:THR:HG23	1.94	0.49
1:D:217:MET:HE1	1:D:231:VAL:HA	1.93	0.49
1:D:9:LEU:HD23	1:D:239:LEU:HD12	1.94	0.49
1:D:206:ARG:NH2	1:D:214:THR:O	2.42	0.49
1:C:180:LYS:HD2	1:C:216:GLU:HG2	1.94	0.49
1:D:77:VAL:HG22	1:D:142:THR:HG23	1.93	0.49
1:D:229:SER:O	1:D:233:MET:HG3	2.11	0.49
1:C:9:LEU:HD23	1:C:239:LEU:HD12	1.94	0.49
1:B:225:GLY:HA2	1:D:19:GLN:HE21	1.76	0.48
1:D:122:ASN:H	1:D:122:ASN:ND2	2.07	0.48
1:C:229:SER:O	1:C:233:MET:HG3	2.13	0.48
1:B:77:VAL:HG22	1:B:142:THR:HG23	1.94	0.48
1:B:152:PRO:HG3	2:E:0:G3A:H21	1.95	0.48
2:E:0:G3A:O3B	2:E:0:G3A:O25	2.32	0.48
1:A:77:VAL:HG22	1:A:142:THR:HG23	1.95	0.47
1:D:14:LYS:HG3	1:D:185:TYR:OH	2.14	0.47
1:A:71:VAL:HG22	1:A:220:ILE:CG2	2.44	0.47
1:A:26:ASP:HA	1:A:29:LYS:HE2	1.97	0.47
1:A:240:ASN:HB3	1:A:244:MET:HE2	1.95	0.47
1:B:205:VAL:HB	1:B:220:ILE:HD11	1.97	0.47
1:A:74:GLU:H	1:A:142:THR:HG21	1.80	0.47
1:B:71:VAL:HG22	1:B:220:ILE:CG2	2.45	0.47
1:A:248:ARG:CG	1:A:248:ARG:NH1	2.75	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:122:ASN:HD21	1:D:262:ARG:N	2.13	0.46
1:C:14:LYS:HG3	1:C:185:TYR:OH	2.16	0.46
1:B:240:ASN:HB3	1:B:244:MET:HE2	1.97	0.46
1:B:26:ASP:HA	1:B:29:LYS:HE2	1.97	0.45
1:B:55:VAL:HG11	1:B:84:ARG:HB3	1.95	0.45
1:B:74:GLU:H	1:B:142:THR:HG21	1.81	0.45
1:A:152:PRO:HG3	2:F:0:G3A:H21	1.98	0.45
1:C:122:ASN:HD21	1:C:262:ARG:N	2.14	0.45
1:D:130:LYS:HB2	6:D:2049:HOH:O	2.17	0.44
1:B:74:GLU:HG2	1:B:96:LYS:HE3	1.99	0.44
1:A:205:VAL:HB	1:A:220:ILE:HD11	1.98	0.44
2:E:6:U:C6	2:E:6:U:C4'	3.01	0.44
1:D:158:GLU:HG3	1:D:189:VAL:HG23	2.00	0.43
2:F:6:U:O2'	2:F:7:G:C5'	2.67	0.43
1:A:142:THR:HB	1:A:176:GLN:HB2	1.99	0.43
1:C:175:ASN:N	1:C:175:ASN:OD1	2.51	0.43
1:C:130:LYS:HB2	6:C:2062:HOH:O	2.17	0.43
1:D:227:ILE:O	1:D:231:VAL:HG23	2.18	0.43
1:B:77:VAL:HG22	1:B:142:THR:CG2	2.49	0.43
1:D:175:ASN:N	1:D:175:ASN:OD1	2.51	0.43
1:B:142:THR:HB	1:B:176:GLN:HB2	2.01	0.42
1:D:77:VAL:HG22	1:D:142:THR:CG2	2.48	0.42
1:D:38:ARG:NE	3:D:265:SO4:O4	2.52	0.42
2:E:4:C:O2	2:F:5:C:N3	2.52	0.42
2:F:3:A:O4'	2:F:3:A:N3	2.53	0.42
1:C:77:VAL:HG22	1:C:142:THR:CG2	2.49	0.42
1:B:72:ILE:O	1:B:176:GLN:HG3	2.20	0.42
1:A:74:GLU:HG2	1:A:96:LYS:HE3	2.01	0.42
1:B:55:VAL:HG13	1:B:84:ARG:HB3	2.00	0.41
1:C:158:GLU:HG3	1:C:189:VAL:HG23	2.02	0.41
2:F:6:U:C6	2:F:6:U:C4'	3.03	0.41
1:C:227:ILE:O	1:C:231:VAL:HG23	2.20	0.41
1:D:186:MET:HG3	6:D:2059:HOH:O	2.20	0.41
1:D:183:ASN:CG	6:D:2059:HOH:O	2.63	0.40
1:A:122:ASN:HD21	1:A:262:ARG:N	2.19	0.40
1:D:158:GLU:N	6:D:2059:HOH:O	2.53	0.40
1:A:72:ILE:O	1:A:176:GLN:HG3	2.21	0.40
1:A:69:ASN:C	6:A:2075:HOH:O	2.63	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	260/263 (99%)	253 (97%)	5 (2%)	2 (1%)	16	44
1	B	257/263 (98%)	250 (97%)	6 (2%)	1 (0%)	30	59
1	C	257/263 (98%)	247 (96%)	10 (4%)	0	100	100
1	D	257/263 (98%)	247 (96%)	10 (4%)	0	100	100
All	All	1031/1052 (98%)	997 (97%)	31 (3%)	3 (0%)	36	65

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	216	GLU
1	B	216	GLU
1	A	75	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	230/231 (100%)	203 (88%)	27 (12%)	5	17
1	B	228/231 (99%)	199 (87%)	29 (13%)	4	14
1	C	228/231 (99%)	196 (86%)	32 (14%)	3	11
1	D	228/231 (99%)	199 (87%)	29 (13%)	4	14
All	All	914/924 (99%)	797 (87%)	117 (13%)	4	14

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	THR
1	A	14	LYS
1	A	17	LEU
1	A	36	VAL
1	A	55	VAL
1	A	71	VAL
1	A	84	ARG
1	A	112	GLU
1	A	122	ASN
1	A	127	MET
1	A	130	LYS
1	A	135	LEU
1	A	142	THR
1	A	161	THR
1	A	167	MET
1	A	168	VAL
1	A	169	GLU
1	A	175	ASN
1	A	182	LEU
1	A	190	ILE
1	A	198	ARG
1	A	206	ARG
1	A	207	ASN
1	A	220	ILE
1	A	224	THR
1	A	237	LEU
1	A	248	ARG
1	B	8	THR
1	B	14	LYS
1	B	17	LEU
1	B	20	LEU
1	B	36	VAL
1	B	55	VAL
1	B	62	LEU
1	B	71	VAL
1	B	84	ARG
1	B	112	GLU
1	B	122	ASN
1	B	127	MET
1	B	130	LYS
1	B	135	LEU
1	B	142	THR
1	B	161	THR

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Mol	Chain	Res	Type
1	B	167	MET
1	B	168	VAL
1	B	169	GLU
1	B	175	ASN
1	B	182	LEU
1	B	190	ILE
1	B	198	ARG
1	B	206	ARG
1	B	207	ASN
1	B	220	ILE
1	B	224	THR
1	B	237	LEU
1	B	248	ARG
1	C	8	THR
1	C	9	LEU
1	C	14	LYS
1	C	17	LEU
1	C	36	VAL
1	C	40	GLU
1	C	55	VAL
1	C	62	LEU
1	C	71	VAL
1	C	84	ARG
1	C	101	ARG
1	C	112	GLU
1	C	122	ASN
1	C	127	MET
1	C	135	LEU
1	C	142	THR
1	C	161	THR
1	C	167	MET
1	C	168	VAL
1	C	169	GLU
1	C	182	LEU
1	C	188	THR
1	C	190	ILE
1	C	198	ARG
1	C	199	LYS
1	C	203	MET
1	C	206	ARG
1	C	207	ASN
1	C	220	ILE

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Mol	Chain	Res	Type
1	C	237	LEU
1	C	243	THR
1	C	248	ARG
1	D	8	THR
1	D	9	LEU
1	D	14	LYS
1	D	36	VAL
1	D	40	GLU
1	D	55	VAL
1	D	62	LEU
1	D	71	VAL
1	D	84	ARG
1	D	112	GLU
1	D	122	ASN
1	D	127	MET
1	D	135	LEU
1	D	142	THR
1	D	161	THR
1	D	167	MET
1	D	168	VAL
1	D	169	GLU
1	D	182	LEU
1	D	188	THR
1	D	190	ILE
1	D	198	ARG
1	D	203	MET
1	D	206	ARG
1	D	207	ASN
1	D	220	ILE
1	D	237	LEU
1	D	243	THR
1	D	248	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	19	GLN
1	A	63	GLN
1	A	122	ASN
1	A	197	GLN
1	A	200	HIS

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Mol	Chain	Res	Type
1	A	207	ASN
1	A	226	ASN
1	B	19	GLN
1	B	63	GLN
1	B	122	ASN
1	B	197	GLN
1	B	207	ASN
1	B	226	ASN
1	C	19	GLN
1	C	52	HIS
1	C	63	GLN
1	C	122	ASN
1	C	197	GLN
1	C	207	ASN
1	D	19	GLN
1	D	52	HIS
1	D	63	GLN
1	D	122	ASN
1	D	197	GLN
1	D	207	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	E	7/9 (77%)	6 (85%)	2 (28%)
2	F	6/9 (66%)	4 (66%)	1 (16%)
All	All	13/18 (72%)	10 (76%)	3 (23%)

All (10) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	E	2	A
2	E	3	A
2	E	4	C
2	E	5	C
2	E	6	U
2	E	7	G
2	F	3	A
2	F	5	C
2	F	6	U
2	F	7	G

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	E	1	G
2	E	6	U
2	F	5	C

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	$\# Z > 2$
2	G3A	F	0	-	55,55,55	3.13	16 (29%)	81,86,86	2.25	28 (34%)
2	G3A	E	0	-	55,55,55	2.74	20 (36%)	81,86,86	2.34	26 (32%)

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	G3A	F	0	-	-	6/32/64/64	0/6/6/6
2	G3A	E	0	-	-	8/32/64/64	0/6/6/6

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	0	G3A	PA-O1	-17.82	1.40	1.59
2	E	0	G3A	PA-O1	-9.81	1.48	1.59
2	E	0	G3A	PB-O1	-8.48	1.50	1.59
2	F	0	G3A	PB-O1	-6.48	1.52	1.59
2	E	0	G3A	PA-O2A	-6.22	1.29	1.50
2	E	0	G3A	PA-O1A	-5.17	1.31	1.55
2	E	0	G3A	C15-N17	-4.57	1.30	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	0	G3A	C15-N17	-4.22	1.31	1.39
2	F	0	G3A	O44-C44	-4.19	1.35	1.45
2	E	0	G3A	C35-N37	-3.81	1.31	1.39
2	E	0	G3A	O44-C44	-3.80	1.36	1.45
2	F	0	G3A	C35-N37	-3.75	1.31	1.39
2	E	0	G3A	O23-C23	3.70	1.52	1.43
2	E	0	G3A	C18-N19	-3.50	1.31	1.37
2	F	0	G3A	C18-N19	-3.28	1.32	1.37
2	E	0	G3A	PA-O45	-2.99	1.47	1.59
2	E	0	G3A	C34-N39	-2.78	1.31	1.38
2	F	0	G3A	PA-O1A	-2.75	1.42	1.55
2	F	0	G3A	C14-N19	-2.58	1.32	1.37
2	F	0	G3A	C38-N39	-2.56	1.31	1.37
2	F	0	G3A	C34-N39	-2.56	1.31	1.38
2	E	0	G3A	C38-N39	-2.40	1.32	1.37
2	E	0	G3A	C43-C42	-2.25	1.47	1.53
2	F	0	G3A	PB-O2B	-2.25	1.44	1.55
2	F	0	G3A	C43-C42	-2.24	1.47	1.53
2	F	0	G3A	C43-C44	-2.19	1.47	1.53
2	E	0	G3A	C43-C44	-2.16	1.47	1.53
2	E	0	G3A	C35-C36	-2.16	1.36	1.44
2	E	0	G3A	PB-O2B	-2.16	1.45	1.55
2	E	0	G3A	O24-C24	-2.13	1.40	1.45
2	E	0	G3A	C12-N11	-2.11	1.30	1.33
2	F	0	G3A	PG-O2G	-2.11	1.45	1.55
2	F	0	G3A	C12-N11	-2.08	1.30	1.33
2	E	0	G3A	PG-O2G	-2.07	1.45	1.55
2	F	0	G3A	C35-C36	-2.03	1.37	1.44
2	E	0	G3A	C14-N19	-2.02	1.33	1.37

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	0	G3A	C15-C14-N13	-7.44	116.47	126.72
2	F	0	G3A	C15-C14-N13	-6.61	117.62	126.72
2	E	0	G3A	O1A-PA-O1	-6.40	89.98	107.27
2	E	0	G3A	C35-C34-N33	-5.32	119.92	128.39
2	F	0	G3A	O1A-PA-O2A	5.19	136.58	112.44
2	F	0	G3A	C35-C34-N33	-5.09	120.29	128.39
2	E	0	G3A	N13-C14-N19	5.04	135.73	127.17
2	E	0	G3A	C32-N33-C34	5.01	120.93	112.30
2	F	0	G3A	C32-N33-C34	4.86	120.68	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	0	G3A	O1-PA-O2A	4.76	125.02	110.70
2	E	0	G3A	N11-C12-N13	-4.53	121.72	128.58
2	E	0	G3A	C12-N13-C14	4.48	122.78	111.83
2	F	0	G3A	C25-C24-C23	-4.43	99.28	115.21
2	F	0	G3A	N11-C12-N13	-4.30	122.08	128.58
2	F	0	G3A	C12-N13-C14	4.15	121.95	111.83
2	F	0	G3A	N13-C14-N19	3.92	133.84	127.17
2	E	0	G3A	C32-N31-C36	-3.90	118.04	125.11
2	F	0	G3A	O1A-PA-O1	-3.80	97.01	107.27
2	F	0	G3A	C32-N31-C36	-3.66	118.48	125.11
2	F	0	G3A	C45-C44-C43	-3.61	102.23	115.21
2	E	0	G3A	O24-C21-C22	-3.42	99.30	106.62
2	F	0	G3A	C14-C15-N17	-3.36	106.74	110.58
2	F	0	G3A	N19-C18-N17	-3.25	109.33	113.94
2	E	0	G3A	O23-C23-C22	3.23	122.18	111.82
2	F	0	G3A	C15-N17-C18	3.13	108.37	103.45
2	F	0	G3A	O24-C24-C25	-3.13	99.32	109.33
2	F	0	G3A	O24-C21-C22	-3.11	99.95	106.62
2	E	0	G3A	C15-N17-C18	3.01	108.18	103.45
2	E	0	G3A	N39-C34-N33	2.97	131.90	125.95
2	F	0	G3A	N39-C34-N33	2.96	131.88	125.95
2	F	0	G3A	C22-C21-N19	-2.93	106.03	113.30
2	E	0	G3A	N19-C18-N17	-2.92	109.79	113.94
2	E	0	G3A	C35-C36-N31	2.77	120.29	113.25
2	E	0	G3A	O1A-PA-O2A	2.76	125.30	112.44
2	E	0	G3A	C14-C15-N17	-2.76	107.43	110.58
2	F	0	G3A	O2B-PB-O1	2.75	114.72	107.27
2	E	0	G3A	O1-PB-O3B	-2.68	102.65	110.70
2	E	0	G3A	C25-C24-C23	-2.56	106.00	115.21
2	F	0	G3A	C35-C36-N31	2.52	119.67	113.25
2	F	0	G3A	C15-C14-N19	2.50	108.54	105.81
2	F	0	G3A	C22-C23-C24	-2.44	97.90	102.61
2	E	0	G3A	C45-C44-C43	-2.38	106.63	115.21
2	F	0	G3A	O1-PB-O3B	-2.34	103.66	110.70
2	E	0	G3A	O36-C36-C35	-2.23	120.63	126.53
2	E	0	G3A	C42-C43-C44	-2.22	98.32	102.61
2	E	0	G3A	O24-C24-C25	-2.21	102.26	109.33
2	E	0	G3A	C22-C21-N19	-2.20	107.83	113.30
2	F	0	G3A	C34-C35-N37	-2.15	107.27	110.67
2	F	0	G3A	O44-C44-C43	-2.13	100.92	105.15
2	F	0	G3A	O44-C41-N39	-2.12	103.56	108.36
2	F	0	G3A	O36-C36-C35	-2.08	121.05	126.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	0	G3A	O2G-PG-O3A	2.07	112.86	107.27
2	E	0	G3A	O42-C42-C43	-2.03	105.32	111.82
2	E	0	G3A	C34-C35-N37	-2.01	107.48	110.67

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	0	G3A	C45-O45-PA-O2A
2	E	0	G3A	C45-O45-PA-O1
2	F	0	G3A	O44-C44-C45-O45
2	F	0	G3A	C45-O45-PA-O1A
2	F	0	G3A	C25-O25-PG-O3A
2	F	0	G3A	C43-C44-C45-O45
2	E	0	G3A	C23-C24-C25-O25
2	E	0	G3A	O24-C24-C25-O25
2	E	0	G3A	PB-O3A-PG-O25
2	E	0	G3A	PG-O3A-PB-O3B
2	E	0	G3A	C44-C45-O45-PA
2	F	0	G3A	C22-C21-N19-C18
2	E	0	G3A	PG-O3A-PB-O2B
2	F	0	G3A	PG-O3A-PB-O2B

There are no ring outliers.

2 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	0	G3A	8	0
2	E	0	G3A	8	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

18 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
3	SO4	A	265	-	4,4,4	0.23	0	6,6,6	0.14	0
3	SO4	B	267	-	4,4,4	0.22	0	6,6,6	0.13	0
4	SAH	C	266	-	27,28,28	3.29	11 (40%)	36,40,40	2.82	13 (36%)
5	GOL	B	269	-	5,5,5	0.32	0	5,5,5	0.28	0
3	SO4	A	267	-	4,4,4	0.23	0	6,6,6	0.10	0
4	SAH	A	268	-	27,28,28	2.48	16 (59%)	36,40,40	2.58	15 (41%)
3	SO4	C	265	-	4,4,4	0.24	0	6,6,6	0.07	0
5	GOL	A	269	-	5,5,5	0.43	0	5,5,5	0.19	0
3	SO4	B	266	-	4,4,4	0.24	0	6,6,6	0.08	0
3	SO4	C	264	-	4,4,4	0.24	0	6,6,6	0.06	0
4	SAH	D	266	-	27,28,28	5.17	16 (59%)	36,40,40	3.14	15 (41%)
4	SAH	B	268	-	27,28,28	2.73	16 (59%)	36,40,40	2.35	13 (36%)
3	SO4	B	265	-	4,4,4	0.23	0	6,6,6	0.11	0
3	SO4	D	264	-	4,4,4	0.23	0	6,6,6	0.14	0
3	SO4	B	264	-	4,4,4	0.23	0	6,6,6	0.05	0
3	SO4	A	266	-	4,4,4	0.26	0	6,6,6	0.09	0
3	SO4	D	265	-	4,4,4	0.25	0	6,6,6	0.13	0
3	SO4	A	264	-	4,4,4	0.25	0	6,6,6	0.11	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	C	266	-	-	2/15/31/31	0/3/3/3
5	GOL	B	269	-	-	2/4/4/4	-
4	SAH	A	268	-	-	2/15/31/31	0/3/3/3
5	GOL	A	269	-	-	2/4/4/4	-
4	SAH	D	266	-	-	3/15/31/31	0/3/3/3
4	SAH	B	268	-	-	2/15/31/31	0/3/3/3

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	266	SAH	CB-CA	-23.30	1.03	1.53
4	C	266	SAH	CB-CA	-11.94	1.27	1.53
4	B	268	SAH	C5-N7	-5.44	1.29	1.39
4	D	266	SAH	C5-N7	-5.16	1.29	1.39
4	B	268	SAH	C5'-SD	5.12	2.00	1.81
4	A	268	SAH	C5-N7	-5.03	1.29	1.39
4	C	266	SAH	C5-N7	-4.97	1.30	1.39
4	C	266	SAH	CB-CG	-4.69	1.33	1.51
4	B	268	SAH	OXT-C	-4.45	1.16	1.30
4	D	266	SAH	C4-N9	-4.40	1.28	1.37
4	D	266	SAH	OXT-C	-4.40	1.16	1.30
4	D	266	SAH	C8-N9	-4.25	1.30	1.37
4	B	268	SAH	C8-N9	-4.19	1.30	1.37
4	D	266	SAH	O4'-C4'	-4.19	1.35	1.45
4	A	268	SAH	C8-N9	-4.18	1.30	1.37
4	C	266	SAH	C8-N9	-4.18	1.30	1.37
4	A	268	SAH	O4'-C4'	-4.08	1.35	1.45
4	B	268	SAH	C4-N9	-4.00	1.29	1.37
4	A	268	SAH	C4-N9	-3.89	1.29	1.37
4	C	266	SAH	O4'-C4'	-3.75	1.36	1.45
4	C	266	SAH	C4-N9	-3.68	1.30	1.37
4	B	268	SAH	O4'-C4'	-3.58	1.37	1.45
4	C	266	SAH	C2-N1	-3.04	1.28	1.33
4	D	266	SAH	CB-CG	-3.02	1.39	1.51
4	B	268	SAH	C5-C4	-3.01	1.33	1.39
4	A	268	SAH	CB-CG	3.00	1.63	1.51
4	A	268	SAH	O-C	2.96	1.30	1.22
4	B	268	SAH	CB-CA	-2.88	1.47	1.53
4	D	266	SAH	C5-C4	-2.87	1.34	1.39
4	A	268	SAH	C5-C4	-2.87	1.34	1.39
4	B	268	SAH	O4'-C1'	-2.87	1.35	1.42
4	A	268	SAH	O4'-C1'	-2.86	1.35	1.42
4	A	268	SAH	C2-N1	-2.77	1.29	1.33
4	A	268	SAH	C2-N3	-2.72	1.29	1.33
4	D	266	SAH	C2-N1	-2.70	1.29	1.33
4	D	266	SAH	CG-SD	-2.65	1.71	1.81
4	D	266	SAH	O4'-C1'	-2.62	1.36	1.42
4	B	268	SAH	C2-N3	-2.59	1.29	1.33
4	C	266	SAH	C2-N3	-2.53	1.29	1.33
4	A	268	SAH	C4-N3	-2.46	1.29	1.34
4	B	268	SAH	C2-N1	-2.44	1.29	1.33
4	C	266	SAH	OXT-C	-2.42	1.22	1.30
4	D	266	SAH	C4-N3	-2.39	1.30	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	266	SAH	C6-N1	-2.34	1.29	1.35
4	B	268	SAH	C5-C6	-2.33	1.34	1.41
4	D	266	SAH	C2-N3	-2.31	1.29	1.33
4	B	268	SAH	O3'-C3'	-2.24	1.37	1.43
4	D	266	SAH	C6-N6	-2.22	1.28	1.34
4	D	266	SAH	C6-N1	-2.18	1.29	1.35
4	B	268	SAH	C2'-C3'	-2.13	1.47	1.53
4	B	268	SAH	C4-N3	-2.11	1.30	1.34
4	A	268	SAH	C6-N6	-2.10	1.28	1.34
4	A	268	SAH	C5-C6	-2.06	1.35	1.41
4	C	266	SAH	C5-C4	-2.05	1.35	1.39
4	A	268	SAH	C6-N1	-2.03	1.30	1.35
4	B	268	SAH	C6-N1	-2.03	1.30	1.35
4	A	268	SAH	CB-CA	-2.03	1.48	1.53
4	D	266	SAH	C5-C6	-2.02	1.35	1.41
4	A	268	SAH	C3'-C4'	-2.02	1.47	1.53

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	266	SAH	CB-CG-SD	9.39	134.42	113.45
4	D	266	SAH	OXT-C-O	-7.88	106.21	124.08
4	C	266	SAH	CB-CG-SD	-7.61	96.46	113.45
4	A	268	SAH	O4'-C1'-N9	-7.22	94.21	108.09
4	C	266	SAH	CB-CA-N	-6.28	93.76	110.12
4	C	266	SAH	CB-CA-C	6.12	126.66	110.45
4	A	268	SAH	C5-C4-N3	-5.82	118.70	126.72
4	D	266	SAH	CB-CA-C	5.74	125.64	110.45
4	C	266	SAH	C5-C4-N3	-5.63	118.97	126.72
4	D	266	SAH	C5-C4-N3	-5.52	119.12	126.72
4	B	268	SAH	C5-C4-N3	-5.21	119.54	126.72
4	B	268	SAH	O4'-C1'-N9	-5.10	98.30	108.09
4	D	266	SAH	N3-C2-N1	-4.88	121.19	128.58
4	B	268	SAH	N3-C2-N1	-4.84	121.25	128.58
4	A	268	SAH	N3-C2-N1	-4.84	121.26	128.58
4	C	266	SAH	N3-C2-N1	-4.20	122.23	128.58
4	A	268	SAH	C5'-C4'-C3'	-4.15	104.68	115.06
4	A	268	SAH	C2-N3-C4	4.05	121.73	111.83
4	C	266	SAH	O4'-C1'-C2'	-3.81	98.46	106.62
4	D	266	SAH	C2-N3-C4	3.80	121.10	111.83
4	B	268	SAH	N3-C4-N9	3.72	133.50	127.17
4	B	268	SAH	C2-N3-C4	3.53	120.45	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	268	SAH	N9-C8-N7	-3.52	108.94	113.94
4	D	266	SAH	N9-C8-N7	-3.50	108.97	113.94
4	A	268	SAH	N9-C8-N7	-3.50	108.97	113.94
4	C	266	SAH	N3-C4-N9	3.48	133.09	127.17
4	C	266	SAH	C2-N3-C4	3.47	120.31	111.83
4	A	268	SAH	N3-C4-N9	3.45	133.04	127.17
4	D	266	SAH	O4'-C4'-C5'	-3.26	100.45	108.83
4	D	266	SAH	C4-C5-N7	-3.16	106.97	110.58
4	C	266	SAH	C5'-C4'-C3'	-3.14	107.22	115.06
4	D	266	SAH	N3-C4-N9	2.97	132.22	127.17
4	B	268	SAH	O3'-C3'-C2'	-2.97	102.31	111.82
4	B	268	SAH	O2'-C2'-C3'	-2.93	102.43	111.82
4	B	268	SAH	O4'-C1'-C2'	-2.92	100.37	106.62
4	A	268	SAH	O4'-C1'-C2'	-2.88	100.45	106.62
4	A	268	SAH	C4-C5-N7	-2.86	107.31	110.58
4	C	266	SAH	C4-C5-N7	-2.86	107.31	110.58
4	B	268	SAH	C5'-SD-CG	-2.80	93.96	102.26
4	A	268	SAH	C5-N7-C8	2.76	107.79	103.45
4	D	266	SAH	C5-N7-C8	2.76	107.78	103.45
4	C	266	SAH	N9-C8-N7	-2.72	110.08	113.94
4	B	268	SAH	OXT-C-O	-2.69	117.97	124.08
4	D	266	SAH	C5-C4-N9	2.62	108.67	105.81
4	C	266	SAH	C5-N7-C8	2.55	107.47	103.45
4	A	268	SAH	O2'-C2'-C3'	-2.51	103.77	111.82
4	D	266	SAH	O4'-C1'-C2'	-2.47	101.32	106.62
4	B	268	SAH	C5-N7-C8	2.44	107.28	103.45
4	B	268	SAH	C4-N9-C8	2.41	108.27	105.74
4	C	266	SAH	C4'-O4'-C1'	-2.38	104.21	109.47
4	A	268	SAH	O4'-C4'-C5'	-2.24	103.05	108.83
4	A	268	SAH	C5-C4-N9	2.24	108.25	105.81
4	A	268	SAH	O3'-C3'-C4'	-2.24	104.66	111.08
4	D	266	SAH	C4'-O4'-C1'	-2.20	104.61	109.47
4	A	268	SAH	CB-CA-C	2.20	116.26	110.45
4	D	266	SAH	O2'-C2'-C3'	-2.18	104.82	111.82

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	269	GOL	C1-C2-C3-O3
4	B	268	SAH	C-CA-CB-CG
4	D	266	SAH	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
4	A	268	SAH	C-CA-CB-CG
4	B	268	SAH	C2'-C1'-N9-C8
5	B	269	GOL	O2-C2-C3-O3
4	C	266	SAH	C-CA-CB-CG
5	B	269	GOL	C1-C2-C3-O3
4	A	268	SAH	C2'-C1'-N9-C8
4	C	266	SAH	C2'-C1'-N9-C8
4	D	266	SAH	C2'-C1'-N9-C8
5	A	269	GOL	O2-C2-C3-O3
4	D	266	SAH	CB-CG-SD-C5'

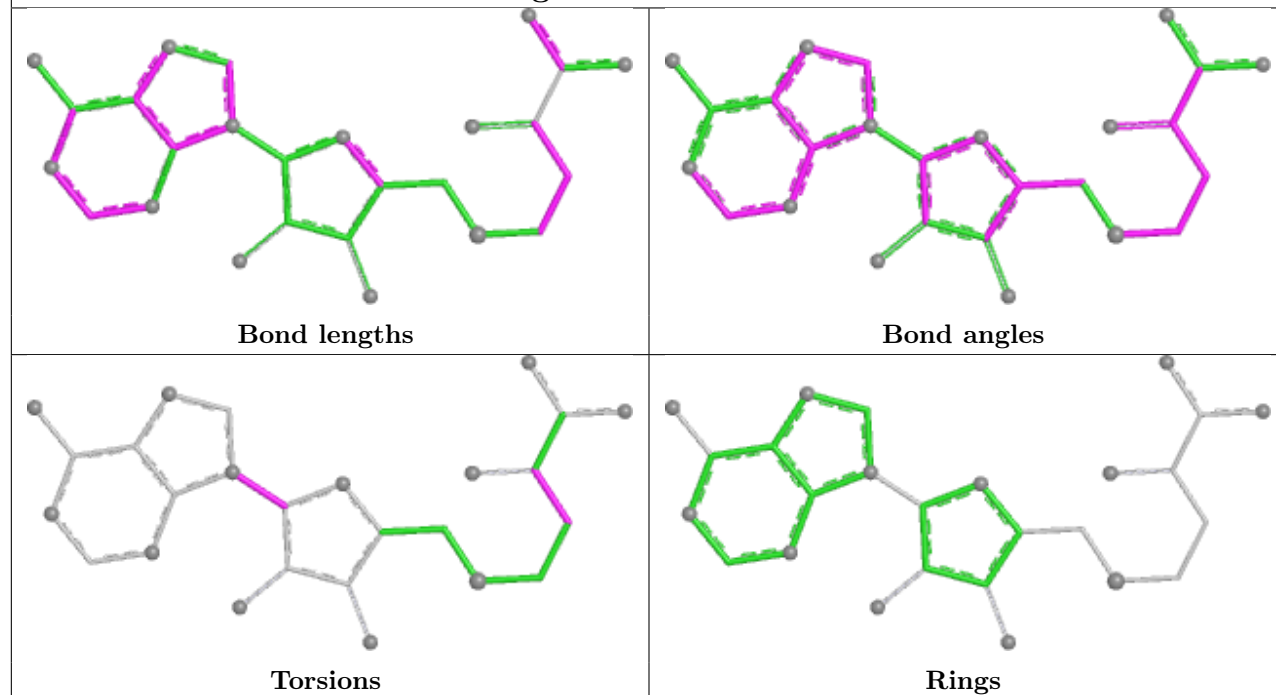
There are no ring outliers.

1 monomer is involved in 1 short contact:

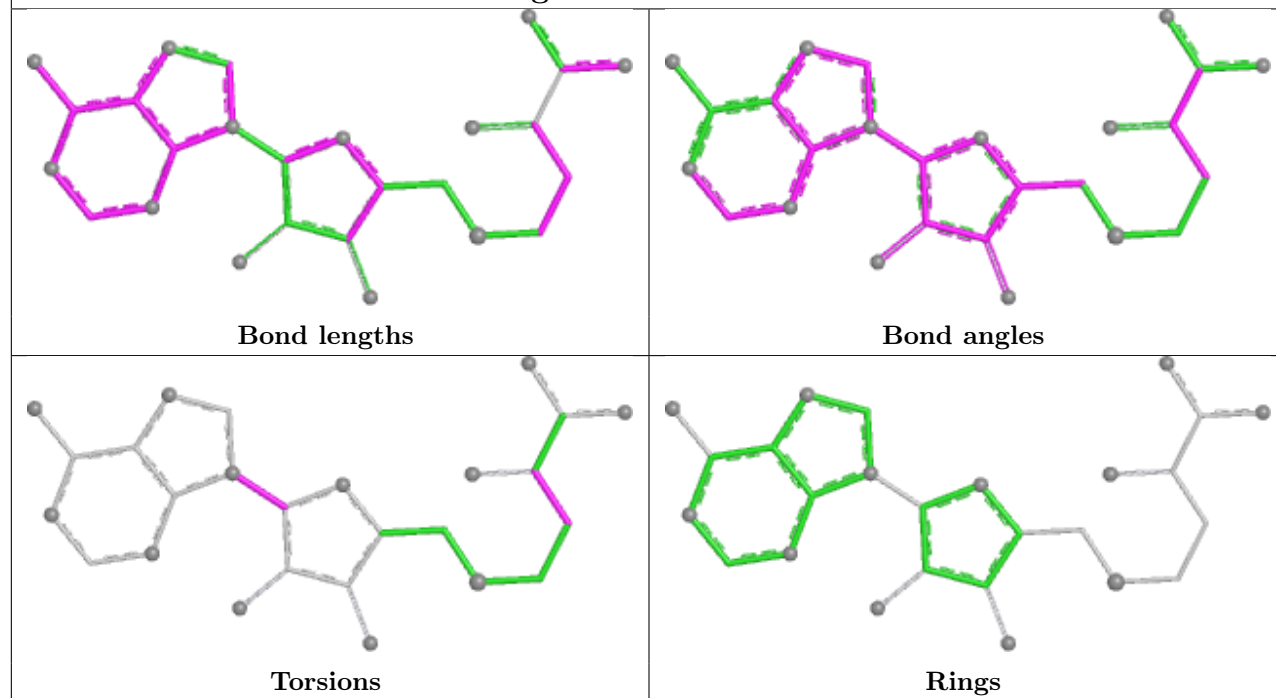
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	265	SO4	1	0

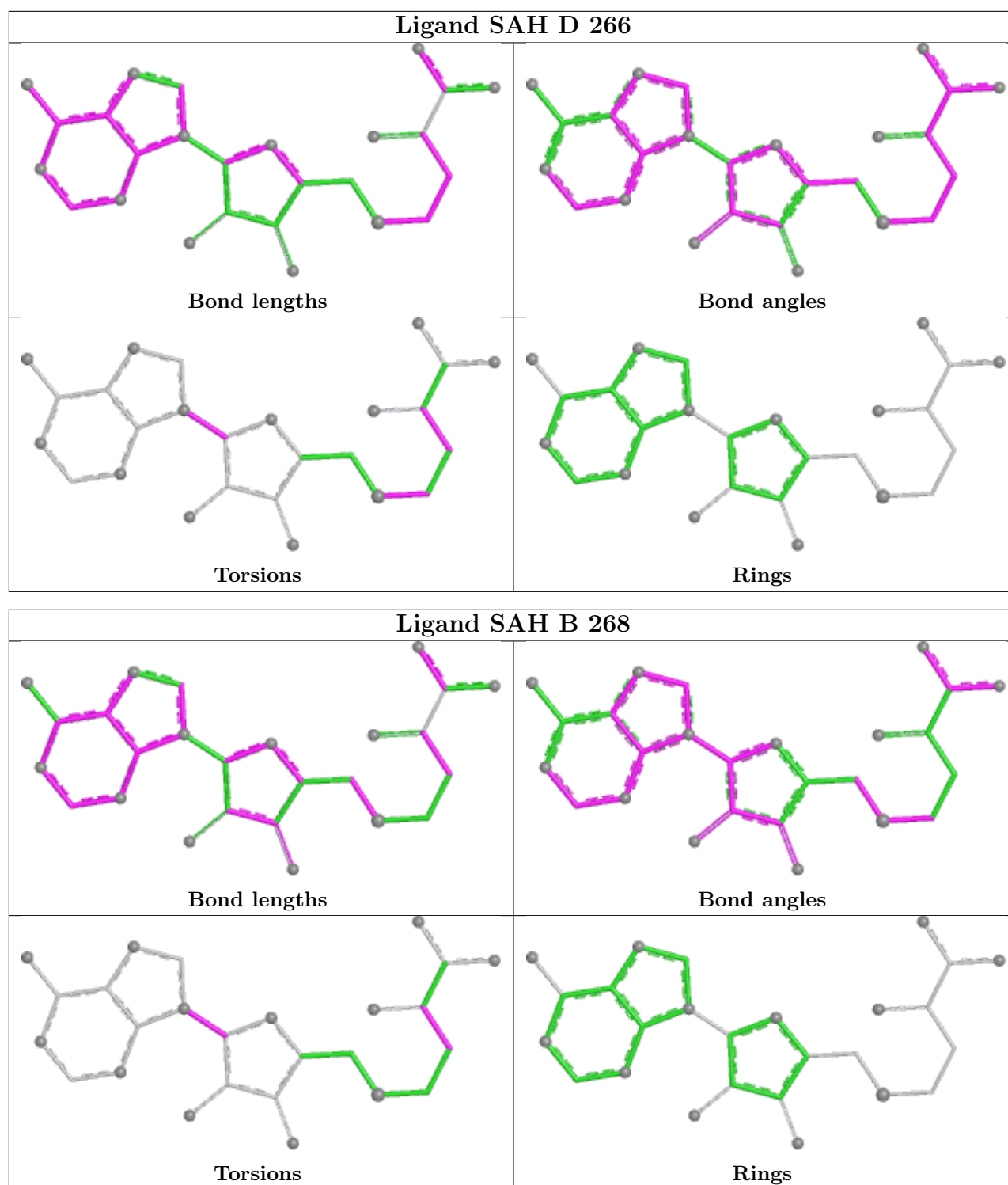
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand SAH C 266



Ligand SAH A 268





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	261/263 (99%)	-1.75	0 100 100	19, 48, 80, 92	3 (1%)
1	B	258/263 (98%)	-1.73	0 100 100	20, 48, 80, 93	4 (1%)
1	C	259/263 (98%)	-1.73	0 100 100	34, 53, 85, 101	0
1	D	259/263 (98%)	-1.73	0 100 100	34, 54, 86, 102	0
2	E	8/9 (88%)	-1.16	0 100 100	91, 105, 112, 115	0
2	F	8/9 (88%)	-0.99	0 100 100	92, 108, 121, 124	0
All	All	1053/1070 (98%)	-1.73	0 100 100	19, 51, 86, 124	7 (0%)

There are no RSRZ outliers to report.

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, 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
2	G3A	E	0	50/50	0.99	0.04	72,81,99,105	0
2	G3A	F	0	50/50	0.99	0.04	84,95,114,120	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

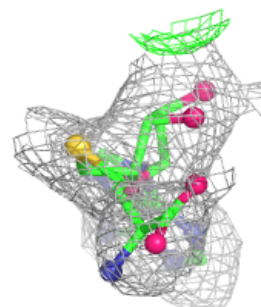
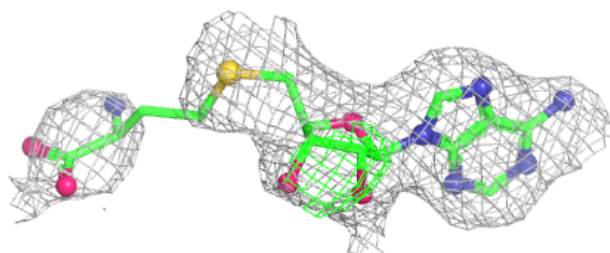
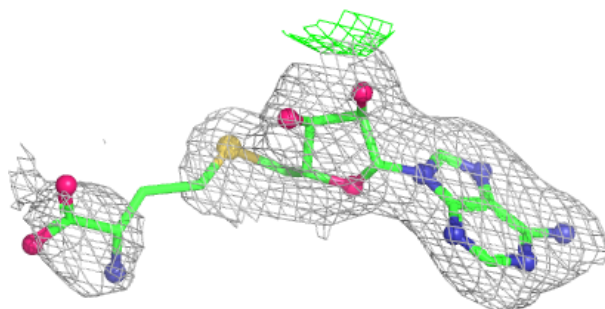
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	A	267	5/5	0.98	0.04	143,143,143,143	0
3	SO4	D	264	5/5	0.98	0.07	126,126,127,127	0
5	GOL	A	269	6/6	0.98	0.15	95,95,95,95	0
3	SO4	B	265	5/5	0.99	0.03	97,98,98,98	0
3	SO4	B	266	5/5	0.99	0.03	104,104,104,104	0
3	SO4	C	264	5/5	0.99	0.05	123,123,123,123	0
3	SO4	C	265	5/5	0.99	0.04	109,110,110,110	0
3	SO4	A	265	5/5	0.99	0.04	98,98,98,98	0
3	SO4	A	264	5/5	0.99	0.03	97,97,97,97	0
5	GOL	B	269	6/6	0.99	0.09	74,74,74,74	0
3	SO4	B	267	5/5	1.00	0.03	61,61,61,62	0
3	SO4	D	265	5/5	1.00	0.04	104,104,104,104	0
4	SAH	A	268	26/26	1.00	0.02	50,58,70,70	0
4	SAH	B	268	26/26	1.00	0.02	48,55,66,67	0
4	SAH	C	266	26/26	1.00	0.03	45,53,65,65	0
4	SAH	D	266	26/26	1.00	0.03	44,53,67,67	0
3	SO4	A	266	5/5	1.00	0.02	54,54,54,54	0
3	SO4	B	264	5/5	1.00	0.04	105,105,105,105	0

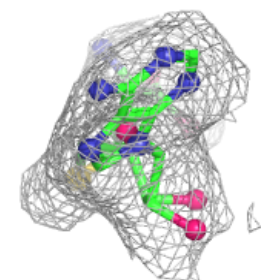
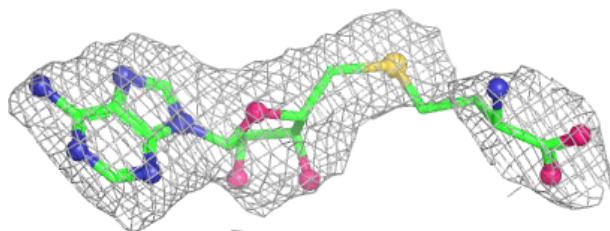
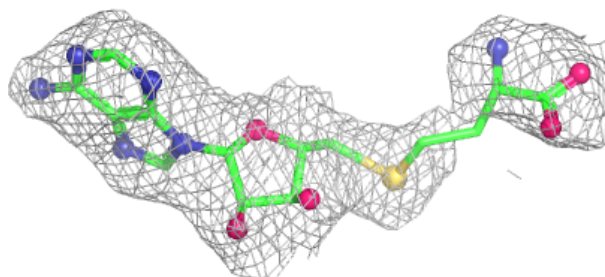
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SAH A 268:

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

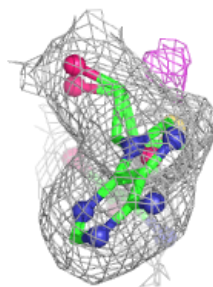
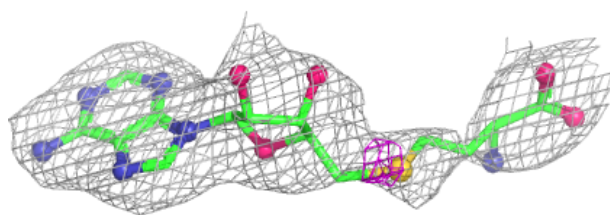
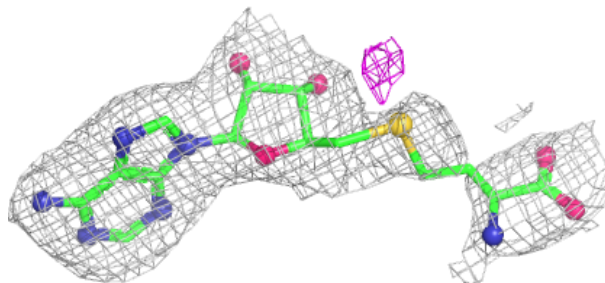
**Electron density around SAH B 268:**

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

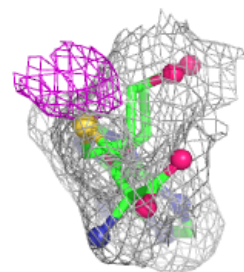
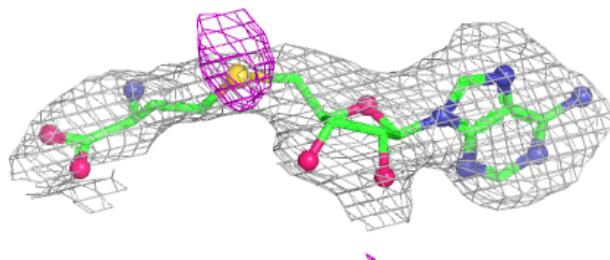
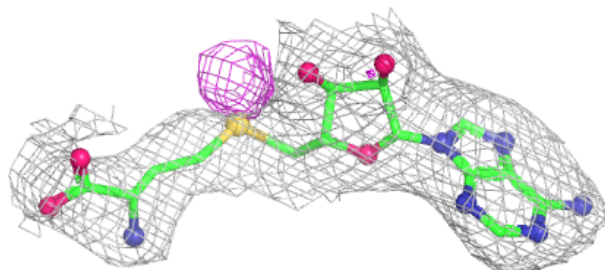


Electron density around SAH C 266:

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

**Electron density around SAH D 266:**

$2mF_o-DF_c$ (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.