



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 07:43 am BST

PDB ID : 4V0R
Title : DENGUE VIRUS FULL LENGTH NS5 COMPLEXED WITH GTP AND SAH
Authors : Zhao, Y.; Soh, S.; Zheng, J.; Phoo, W.W.; Swaminathan, K.; Cornvik, T.C.; Lim, S.P.; Shi, P.-Y.; Lescar, J.; Vasudevan, S.G.; Luo, D.
Deposited on : 2014-09-18
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

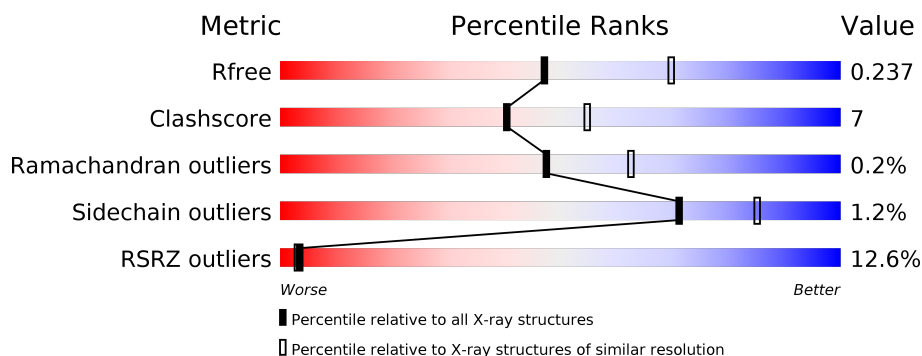
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	892	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 7332 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 NS5 POLYMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	852	Total	C	N	O	S	0	1	0
			6849	4314	1228	1260	47			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	5	MET	GLN	conflict	UNP Q6DLV0
A	72	ILE	VAL	conflict	UNP Q6DLV0
A	374	GLU	GLY	conflict	UNP Q6DLV0
A	418	TYR	TRP	conflict	UNP Q6DLV0

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

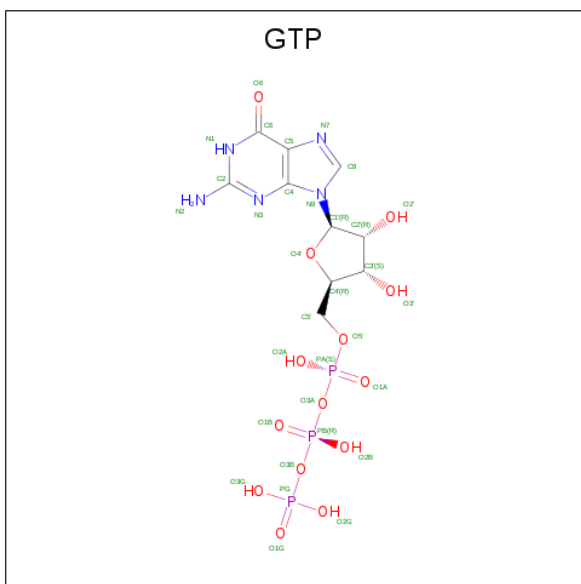
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		

- Molecule 3 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: C₁₄H₂₀N₆O₅S).



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

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{14}\text{P}_3$).

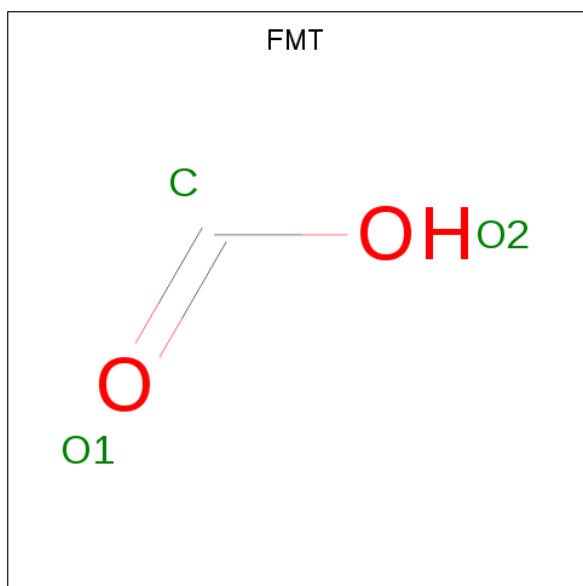


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Mg	0	0
			2	2		

- Molecule 6 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			3	1	2		
6	A	1	Total	C	O	0	0
			3	1	2		
6	A	1	Total	C	O	0	0
			3	1	2		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



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

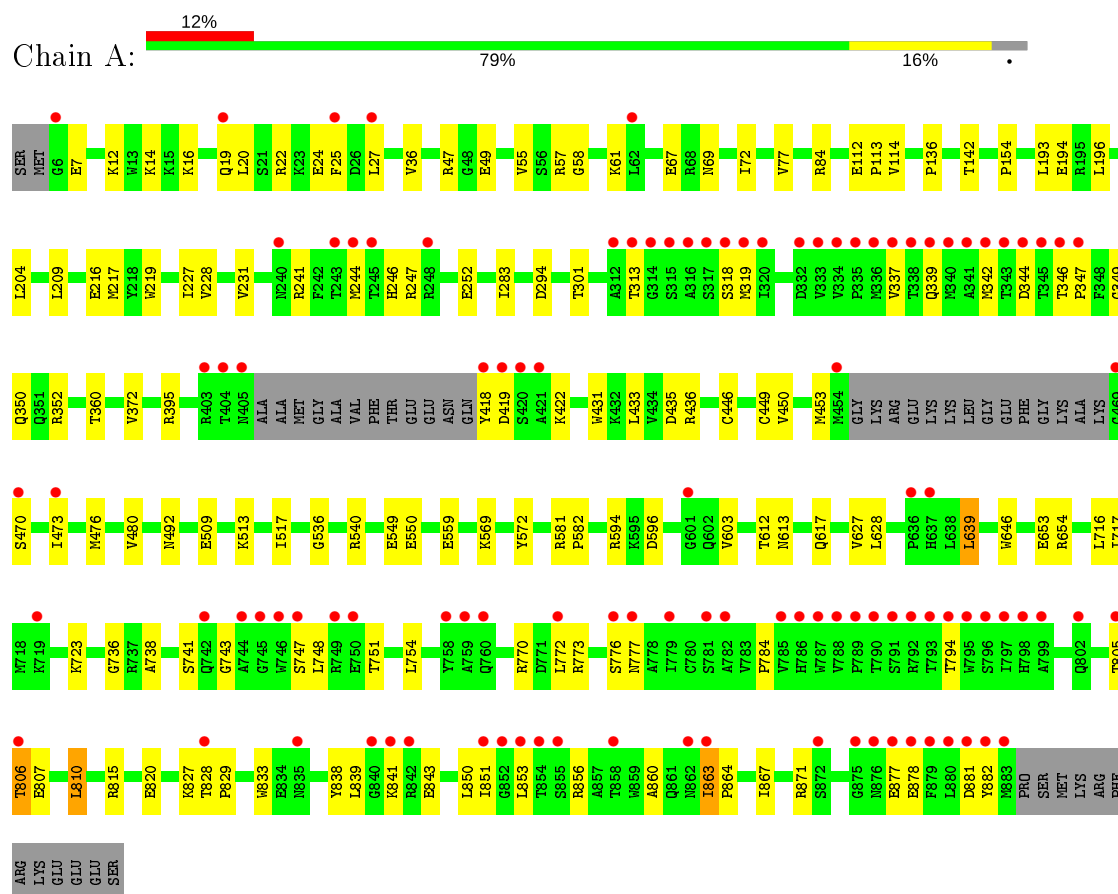
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	406	Total	O	0	0
			406	406		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: NS5 POLYMERASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	94.86 Å 150.97 Å 69.28 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.88 – 2.40 28.77 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.88-2.40) 99.7 (28.77-2.40)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.03 (at 2.39 Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.188 , 0.237 0.189 , 0.237	Depositor DCC
R_{free} test set	1984 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	27.5	Xtriage
Anisotropy	0.813	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 54.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7332	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% 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: GOL, MG, SAH, FMT, ZN, GTP

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	0.24	0/7014	0.45	0/9489

There are no bond length outliers.

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	6849	0	6754	99	0
2	A	2	0	0	0	0
3	A	26	0	19	1	0
4	A	32	0	12	1	0
5	A	2	0	0	0	0
6	A	9	0	3	0	0
7	A	6	0	8	0	0
8	A	406	0	0	13	1
All	All	7332	0	6796	99	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (99) 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:418:TYR:N	8:A:2257:HOH:O	2.02	0.93
1:A:827:LYS:NZ	8:A:2398:HOH:O	2.06	0.89
1:A:509:GLU:OE1	8:A:2286:HOH:O	2.00	0.79
1:A:244:MET:HE1	1:A:247:ARG:HE	1.49	0.77
1:A:784:PRO:HA	1:A:878:GLU:O	1.87	0.74
1:A:347:PRO:HB2	1:A:582:PRO:HG3	1.70	0.73
1:A:194:GLU:OE2	8:A:2140:HOH:O	2.05	0.72
1:A:777:ASN:HB3	1:A:882:TYR:HB3	1.72	0.71
1:A:241:ARG:HA	1:A:244:MET:HG2	1.73	0.70
1:A:716:LEU:HD21	1:A:839:LEU:HD23	1.73	0.69
1:A:805:THR:HG23	1:A:807:GLU:H	1.56	0.69
1:A:350:GLN:NE2	1:A:453:MET:O	2.26	0.68
1:A:360:THR:O	1:A:594:ARG:NH2	2.27	0.68
1:A:346:THR:HG23	1:A:349:GLY:H	1.59	0.67
1:A:843:GLU:OE1	1:A:843:GLU:N	2.27	0.67
1:A:867:ILE:HG22	1:A:871:ARG:HD3	1.78	0.65
1:A:136:PRO:O	8:A:2103:HOH:O	2.14	0.65
1:A:7:GLU:HB3	1:A:12:LYS:HZ1	1.62	0.65
1:A:738:ALA:O	8:A:2209:HOH:O	2.14	0.65
1:A:435:ASP:OD2	8:A:2266:HOH:O	2.15	0.64
1:A:67:GLU:O	8:A:2038:HOH:O	2.15	0.64
1:A:433:LEU:HD23	1:A:436:ARG:HH21	1.62	0.64
1:A:860:ALA:O	1:A:863:ILE:HG12	1.98	0.64
1:A:748:LEU:HA	1:A:751:THR:HG22	1.80	0.63
1:A:228:VAL:HG23	8:A:2140:HOH:O	1.99	0.63
1:A:863:ILE:HG13	1:A:864:PRO:HD3	1.80	0.63
1:A:476:MET:O	1:A:480:VAL:HG23	1.99	0.62
1:A:653:GLU:OE1	1:A:654:ARG:NH1	2.32	0.61
1:A:572:TYR:OH	1:A:603:VAL:O	2.19	0.61
1:A:55:VAL:HG21	1:A:114:VAL:HB	1.84	0.59
1:A:7:GLU:HB3	1:A:12:LYS:NZ	2.18	0.58
1:A:67:GLU:OE2	1:A:352:ARG:NE	2.29	0.57
1:A:372:VAL:HG11	1:A:628:LEU:HD11	1.87	0.57
1:A:446:CYS:SG	1:A:449:CYS:HB2	2.45	0.56
1:A:14:LYS:HG2	1:A:154:PRO:HG3	1.88	0.55
1:A:217:MET:HE1	1:A:231:VAL:HA	1.88	0.55
1:A:594:ARG:NH1	1:A:596:ASP:OD1	2.39	0.55
1:A:867:ILE:O	1:A:871:ARG:HG3	2.07	0.54
1:A:69:ASN:HA	1:A:72:ILE:HD11	1.90	0.54
1:A:773:ARG:O	1:A:777:ASN:ND2	2.42	0.53
1:A:559:GLU:CD	1:A:559:GLU:H	2.12	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:ARG:NH1	4:A:1884:GTP:O6	2.41	0.52
1:A:339:GLN:HA	1:A:342:MET:HE2	1.92	0.52
1:A:337:VAL:HG13	1:A:736:GLY:HA2	1.91	0.52
1:A:770:ARG:NH2	1:A:841:LYS:HA	2.25	0.52
1:A:877:GLU:OE1	1:A:877:GLU:N	2.43	0.52
1:A:850:LEU:HG	1:A:853:LEU:HD12	1.92	0.51
1:A:283:ILE:HD11	1:A:450:VAL:HG21	1.92	0.50
1:A:209:LEU:HD23	8:A:2029:HOH:O	2.10	0.50
1:A:20:LEU:HG	1:A:24:GLU:HG2	1.93	0.50
1:A:810:LEU:HG	1:A:833:TRP:NE1	2.27	0.50
1:A:36:VAL:O	1:A:57:ARG:NH2	2.46	0.49
1:A:16:LYS:O	1:A:19:GLN:HG2	2.13	0.49
1:A:627:VAL:HG21	1:A:646:TRP:CD1	2.47	0.49
1:A:193:LEU:HD13	1:A:204:LEU:HD11	1.95	0.49
1:A:112:GLU:HG3	1:A:113:PRO:HD2	1.96	0.48
1:A:492:ASN:ND2	8:A:2281:HOH:O	2.29	0.47
1:A:549:GLU:OE2	1:A:612:THR:OG1	2.30	0.47
1:A:810:LEU:HG	1:A:833:TRP:CE2	2.49	0.47
1:A:449:CYS:HA	1:A:480:VAL:CG2	2.45	0.47
1:A:61:LYS:NZ	1:A:216:GLU:OE2	2.38	0.47
1:A:20:LEU:HD23	1:A:25:PHE:HA	1.97	0.46
1:A:204:LEU:HD12	1:A:227:ILE:HG23	1.96	0.46
1:A:772:LEU:O	1:A:776:SER:N	2.48	0.46
1:A:509:GLU:HG3	1:A:513:LYS:HB2	1.96	0.46
1:A:252:GLU:CD	1:A:352:ARG:HH12	2.17	0.46
1:A:67:GLU:HG2	8:A:2040:HOH:O	2.15	0.46
1:A:550:GLU:OE2	1:A:569:LYS:NZ	2.38	0.46
1:A:851:ILE:HA	1:A:856:ARG:HD2	1.98	0.45
1:A:806:THR:HG22	1:A:807:GLU:HG3	1.99	0.45
1:A:777:ASN:CB	1:A:882:TYR:HB3	2.44	0.45
1:A:815:ARG:O	1:A:820:GLU:HG3	2.16	0.45
1:A:863:ILE:O	1:A:867:ILE:HG12	2.17	0.44
1:A:395:ARG:HG3	1:A:431:TRP:CZ2	2.53	0.43
1:A:509:GLU:HG2	1:A:517:ILE:HD11	2.01	0.43
1:A:536:GLY:O	1:A:540:ARG:HG2	2.19	0.43
1:A:196:LEU:HB3	1:A:219:TRP:CH2	2.53	0.43
1:A:470:SER:O	1:A:473:ILE:HG22	2.18	0.43
1:A:717:ILE:HG12	1:A:723:LYS:HG2	2.01	0.43
1:A:294:ASP:OD2	1:A:581:ARG:NH2	2.44	0.42
1:A:58:GLY:HA3	3:A:1051:SAH:OXT	2.19	0.42
1:A:613:ASN:O	1:A:617:GLN:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:THR:HG23	1:A:349:GLY:N	2.32	0.42
1:A:449:CYS:HA	1:A:480:VAL:HG22	2.00	0.42
1:A:639:LEU:H	1:A:639:LEU:HD22	1.84	0.42
1:A:217:MET:CE	1:A:231:VAL:HA	2.49	0.42
1:A:342:MET:HG3	1:A:342:MET:O	2.19	0.42
1:A:770:ARG:NH2	1:A:839:LEU:O	2.52	0.42
1:A:47:ARG:NH2	1:A:49:GLU:OE2	2.52	0.42
1:A:344:ASP:O	1:A:344:ASP:OD1	2.38	0.42
1:A:770:ARG:HG3	1:A:838:TYR:CD1	2.55	0.42
1:A:77:VAL:HG22	1:A:142:THR:HB	2.02	0.41
1:A:741:SER:HA	1:A:754:LEU:HD23	2.02	0.41
1:A:27:LEU:HG	1:A:246:HIS:CD2	2.56	0.41
1:A:419:ASP:OD1	1:A:422:LYS:N	2.51	0.41
1:A:646:TRP:CZ2	1:A:654:ARG:HG3	2.56	0.41
1:A:828:THR:HA	1:A:829:PRO:HD3	1.73	0.41
1:A:881:ASP:OD1	1:A:882:TYR:N	2.53	0.41
1:A:84:ARG:HG3	8:A:2052:HOH:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:2101:HOH:O	8:A:2246:HOH:O[3_445]	2.00	0.20

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	847/892 (95%)	812 (96%)	33 (4%)	2 (0%)	47 62

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	747	SER
1	A	743	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	742/781 (95%)	733 (99%)	9 (1%)	71 85

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	301	THR
1	A	313	THR
1	A	318	SER
1	A	319	MET
1	A	639	LEU
1	A	794	THR
1	A	806	THR
1	A	810	LEU
1	A	863	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	321	ASN
1	A	350	GLN
1	A	777	ASN
1	A	786	HIS
1	A	876	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	SAH	A	1051	-	21,28,28	1.19	2 (9%)	20,40,40	1.70	2 (10%)
6	FMT	A	1889	-	0,2,2	0.00	-	0,1,1	0.00	-
6	FMT	A	1888	-	0,2,2	0.00	-	0,1,1	0.00	-
7	GOL	A	1890	-	5,5,5	0.37	0	5,5,5	0.19	0
6	FMT	A	1887	-	0,2,2	0.00	-	0,1,1	0.00	-
4	GTP	A	1884	5	26,34,34	0.97	1 (3%)	33,54,54	1.77	7 (21%)

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
7	GOL	A	1890	-	-	4/4/4/4	-
3	SAH	A	1051	-	-	0/7/31/31	0/3/3/3
4	GTP	A	1884	5	-	7/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1051	SAH	C2-N3	3.93	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1884	GTP	C6-N1	3.06	1.38	1.33
3	A	1051	SAH	C2-N1	2.50	1.38	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1051	SAH	N3-C2-N1	-5.39	120.25	128.68
4	A	1884	GTP	N3-C2-N1	-5.29	120.17	127.22
4	A	1884	GTP	C2-N3-C4	4.35	120.32	115.36
3	A	1051	SAH	C5'-SD-CG	-4.09	90.01	102.27
4	A	1884	GTP	PB-O3B-PG	-3.67	120.22	132.83
4	A	1884	GTP	PA-O3A-PB	-2.92	122.80	132.83
4	A	1884	GTP	C5-C6-N1	-2.77	119.65	123.43
4	A	1884	GTP	C3'-C2'-C1'	2.65	104.96	100.98
4	A	1884	GTP	C6-N1-C2	2.47	119.85	115.93

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1890	GOL	O1-C1-C2-C3
7	A	1890	GOL	C1-C2-C3-O3
7	A	1890	GOL	O2-C2-C3-O3
4	A	1884	GTP	C5'-O5'-PA-O1A
4	A	1884	GTP	C5'-O5'-PA-O2A
7	A	1890	GOL	O1-C1-C2-O2
4	A	1884	GTP	O4'-C4'-C5'-O5'
4	A	1884	GTP	C3'-C4'-C5'-O5'
4	A	1884	GTP	PA-O3A-PB-O2B
4	A	1884	GTP	C5'-O5'-PA-O3A
4	A	1884	GTP	PA-O3A-PB-O1B

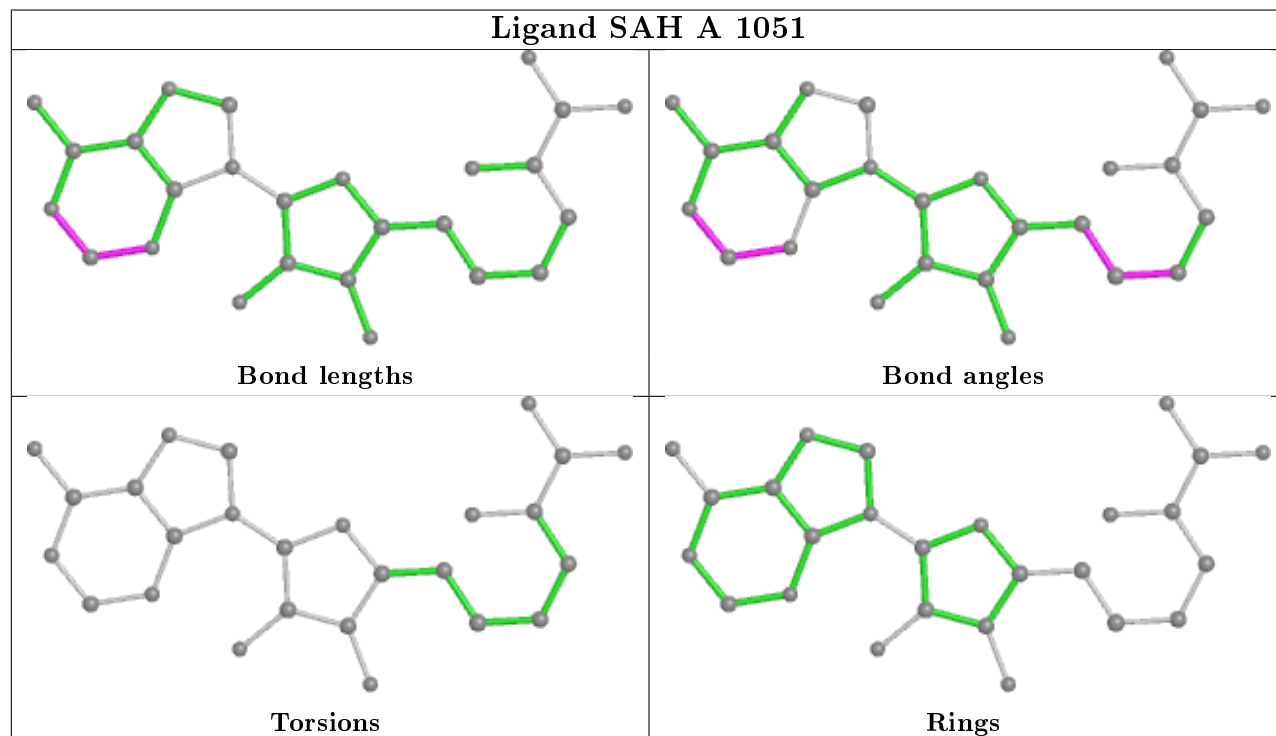
There are no ring outliers.

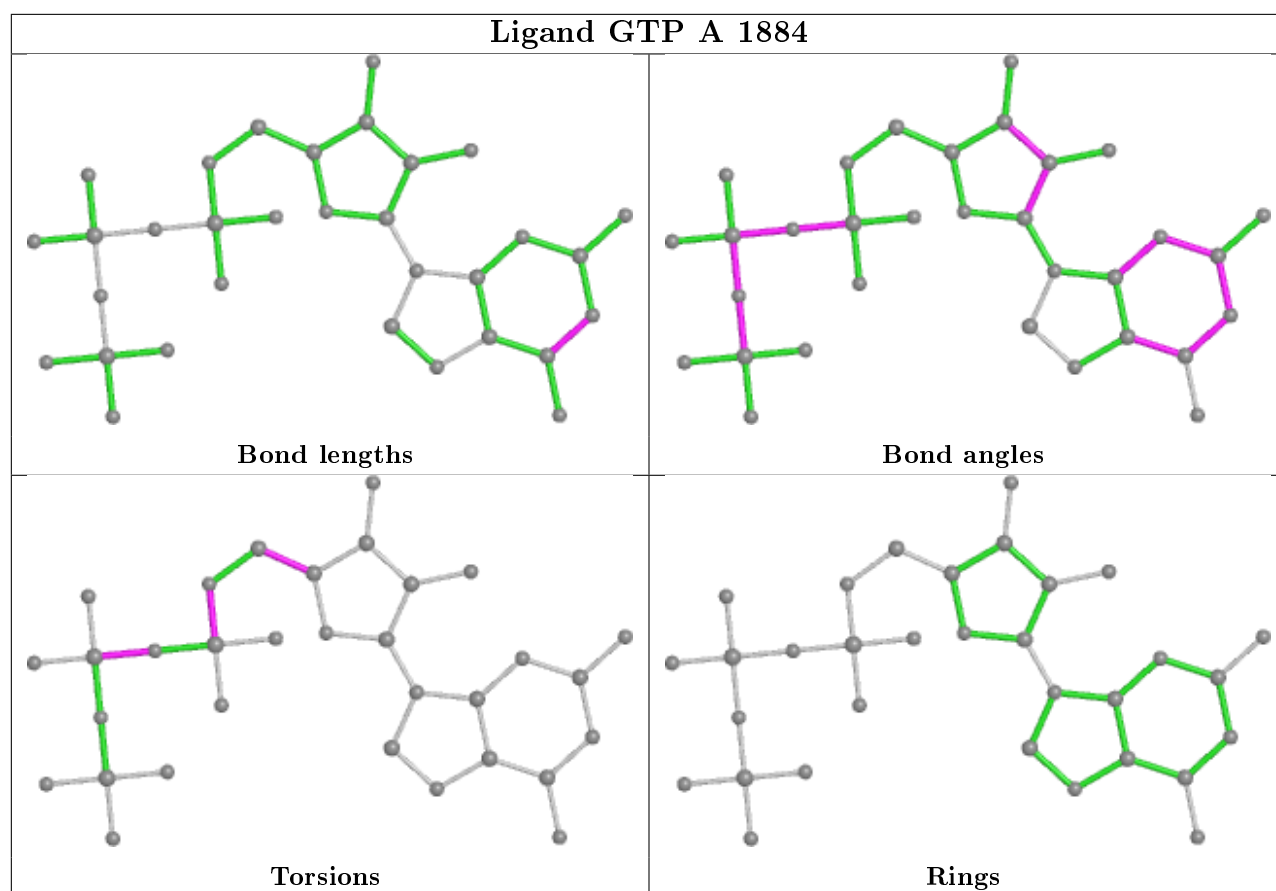
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1051	SAH	1	0
4	A	1884	GTP	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.





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	852/892 (95%)	0.56	107 (12%) 3 3	12, 34, 93, 118	4 (0%)

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	795	TRP	9.9
1	A	878	GLU	8.4
1	A	344	ASP	7.9
1	A	882	TYR	7.9
1	A	469	GLY	7.7
1	A	786	HIS	7.5
1	A	342	MET	7.3
1	A	340	MET	7.3
1	A	314	GLY	6.9
1	A	745	GLY	6.6
1	A	746	TRP	6.5
1	A	418	TYR	6.5
1	A	343	THR	6.5
1	A	636	PRO	6.5
1	A	744	ALA	6.3
1	A	794	THR	6.2
1	A	317	SER	6.2
1	A	316	ALA	6.2
1	A	883	MET	6.0
1	A	337	VAL	5.6
1	A	790	THR	5.6
1	A	315	SER	5.6
1	A	788	VAL	5.5
1	A	454	MET	5.5
1	A	806	THR	5.4
1	A	863	ILE	5.3
1	A	853	LEU	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	345	THR	5.2
1	A	318	SER	5.1
1	A	313	THR	5.1
1	A	796	SER	5.1
1	A	791	SER	5.0
1	A	333	VAL	4.9
1	A	880	LEU	4.9
1	A	245	THR	4.9
1	A	879	PHE	4.8
1	A	637	HIS	4.7
1	A	339	GLN	4.6
1	A	419	ASP	4.5
1	A	792	ARG	4.4
1	A	797	ILE	4.4
1	A	787	TRP	4.3
1	A	312	ALA	4.3
1	A	759	ALA	4.2
1	A	405	ASN	4.2
1	A	6	GLY	4.1
1	A	404	THR	4.1
1	A	336	MET	4.0
1	A	793	THR	3.9
1	A	747	SER	3.9
1	A	852	GLY	3.8
1	A	881	ASP	3.7
1	A	858	THR	3.6
1	A	341	ALA	3.6
1	A	332	ASP	3.5
1	A	346	THR	3.4
1	A	470	SER	3.4
1	A	840	GLY	3.4
1	A	798	HIS	3.4
1	A	335	PRO	3.3
1	A	319	MET	3.2
1	A	855	SER	3.2
1	A	244	MET	3.2
1	A	854	THR	3.1
1	A	789	PRO	3.1
1	A	750	GLU	3.0
1	A	877	GLU	3.0
1	A	805	THR	3.0
1	A	772	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	851	ILE	2.9
1	A	785	VAL	2.9
1	A	719	LYS	2.8
1	A	872	SER	2.7
1	A	19	GLN	2.7
1	A	420	SER	2.7
1	A	749	ARG	2.6
1	A	334	VAL	2.6
1	A	421	ALA	2.6
1	A	742	GLN	2.6
1	A	842	ARG	2.6
1	A	862	ASN	2.5
1	A	243	THR	2.5
1	A	601	GLY	2.5
1	A	347	PRO	2.5
1	A	473	ILE	2.5
1	A	27	LEU	2.4
1	A	835	ASN	2.4
1	A	320	ILE	2.4
1	A	841	LYS	2.4
1	A	779	ILE	2.4
1	A	758	TYR	2.3
1	A	777	ASN	2.3
1	A	828	THR	2.3
1	A	875	GLY	2.3
1	A	802	GLN	2.3
1	A	776	SER	2.3
1	A	760	GLN	2.3
1	A	338	THR	2.3
1	A	782	ALA	2.2
1	A	240	ASN	2.2
1	A	876	ASN	2.2
1	A	799	ALA	2.1
1	A	781	SER	2.1
1	A	403	ARG	2.1
1	A	25	PHE	2.0
1	A	248	ARG	2.0
1	A	62	LEU	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

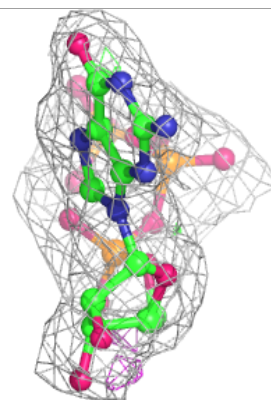
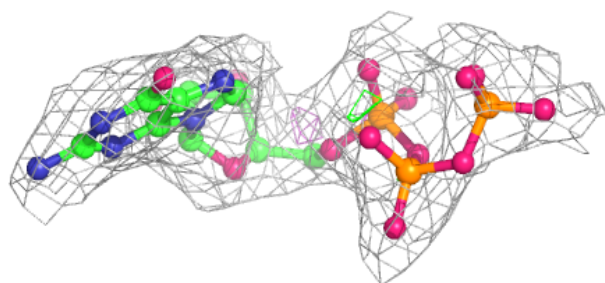
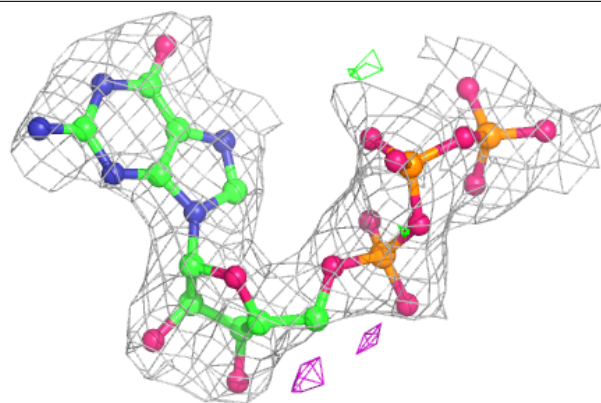
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	MG	A	1885	1/1	0.71	0.17	37,37,37,37	0
5	MG	A	1886	1/1	0.77	0.14	76,76,76,76	0
6	FMT	A	1888	3/3	0.79	0.17	48,48,49,50	0
7	GOL	A	1890	6/6	0.81	0.21	32,40,42,45	0
4	GTP	A	1884	32/32	0.87	0.16	49,56,94,162	0
3	SAH	A	1051	26/26	0.90	0.17	22,30,38,61	0
6	FMT	A	1889	3/3	0.90	0.17	41,41,44,44	0
6	FMT	A	1887	3/3	0.92	0.13	54,54,56,59	0
2	ZN	A	1002	1/1	0.98	0.05	57,57,57,57	0
2	ZN	A	1001	1/1	0.99	0.10	26,26,26,26	0

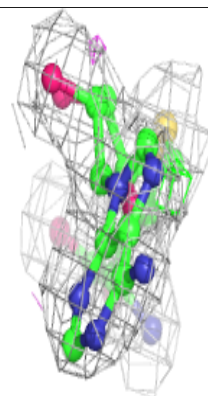
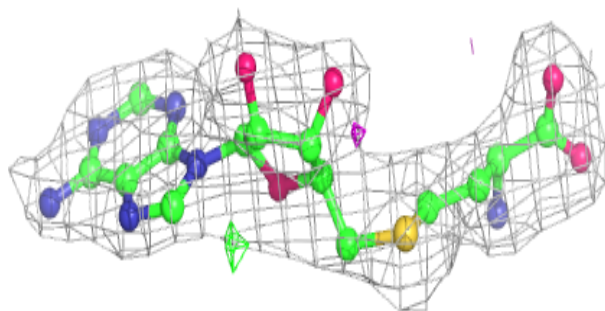
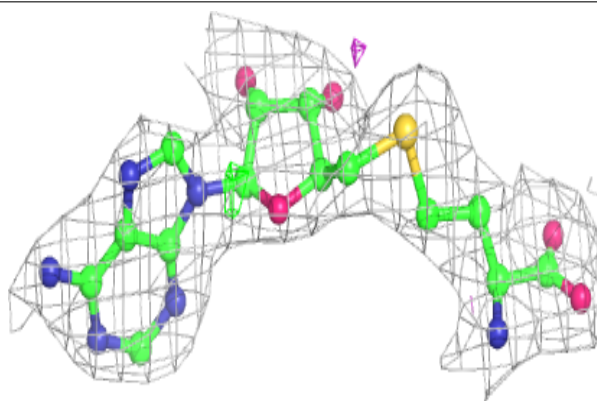
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GTP A 1884:

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

**Electron density around SAH A 1051:**

$2mF_o-DF_c$ (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.