wwPDB X-ray Structure Validation Summary Report (i)

May 29, 2020 – 10:57 pm BST

PDB ID	:	3SFG
Title	:	crystal structure of murine norovirus RNA dependent RNA polymerase in complex with 2thiouridine(2TU)
Authors	:	Kim, K.H.; Alam, I.
Deposited on	:	2011-06-13
Resolution	:	2.21 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

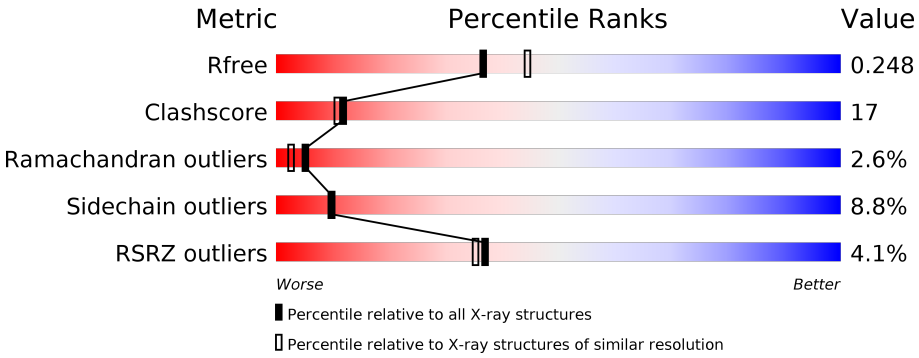
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.21 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 <=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	517	4% 65% 20% 7% • 7%
1	B	517	3% 65% 22% 5% • 8%
1	C	517	4% 67% 23% • • 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	2TU	C	601	-	-	X	-
3	SO4	B	607	-	-	X	-
4	GOL	A	613	-	-	X	-
4	GOL	A	615	-	-	X	-
4	GOL	B	614	-	-	X	-
4	GOL	B	616	-	-	X	-
4	GOL	C	613	-	-	X	-
4	GOL	C	617	-	-	X	-
4	GOL	C	618	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 12359 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 RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	480	Total	C	N	O	S	0	1	0
			3826	2421	674	706	25			
1	B	474	Total	C	N	O	S	0	1	0
			3774	2390	663	696	25			
1	C	488	Total	C	N	O	S	0	0	0
			3872	2448	681	718	25			

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	510	ALA	-	EXPRESSION TAG	UNP Q80J95
A	511	ALA	-	EXPRESSION TAG	UNP Q80J95
A	512	ALA	-	EXPRESSION TAG	UNP Q80J95
A	513	LEU	-	EXPRESSION TAG	UNP Q80J95
A	514	GLU	-	EXPRESSION TAG	UNP Q80J95
A	515	HIS	-	EXPRESSION TAG	UNP Q80J95
A	516	HIS	-	EXPRESSION TAG	UNP Q80J95
A	517	HIS	-	EXPRESSION TAG	UNP Q80J95
A	518	HIS	-	EXPRESSION TAG	UNP Q80J95
A	519	HIS	-	EXPRESSION TAG	UNP Q80J95
A	520	HIS	-	EXPRESSION TAG	UNP Q80J95
B	510	ALA	-	EXPRESSION TAG	UNP Q80J95
B	511	ALA	-	EXPRESSION TAG	UNP Q80J95
B	512	ALA	-	EXPRESSION TAG	UNP Q80J95
B	513	LEU	-	EXPRESSION TAG	UNP Q80J95
B	514	GLU	-	EXPRESSION TAG	UNP Q80J95
B	515	HIS	-	EXPRESSION TAG	UNP Q80J95
B	516	HIS	-	EXPRESSION TAG	UNP Q80J95
B	517	HIS	-	EXPRESSION TAG	UNP Q80J95
B	518	HIS	-	EXPRESSION TAG	UNP Q80J95
B	519	HIS	-	EXPRESSION TAG	UNP Q80J95
B	520	HIS	-	EXPRESSION TAG	UNP Q80J95
C	510	ALA	-	EXPRESSION TAG	UNP Q80J95

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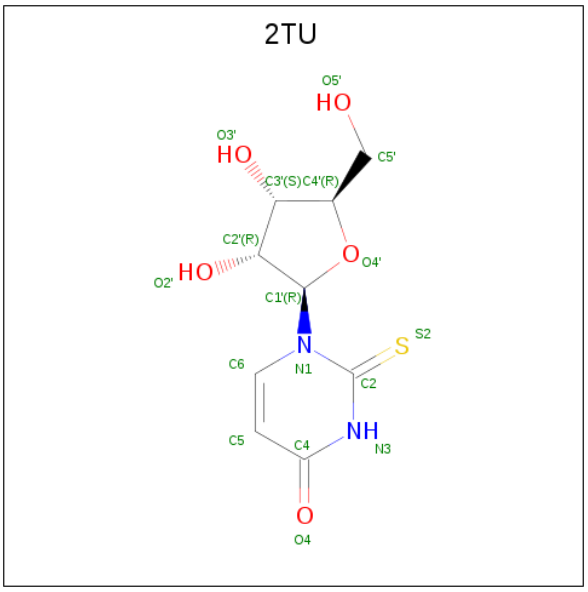
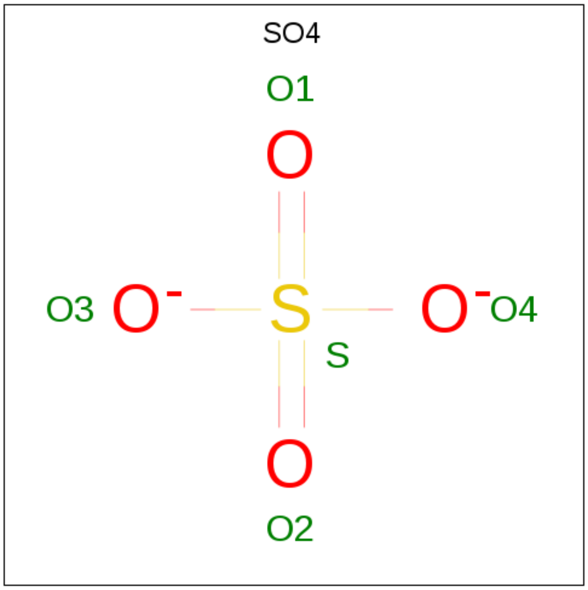
Chain	Residue	Modelled	Actual	Comment	Reference
C	511	ALA	-	EXPRESSION TAG	UNP Q80J95
C	512	ALA	-	EXPRESSION TAG	UNP Q80J95
C	513	LEU	-	EXPRESSION TAG	UNP Q80J95
C	514	GLU	-	EXPRESSION TAG	UNP Q80J95
C	515	HIS	-	EXPRESSION TAG	UNP Q80J95
C	516	HIS	-	EXPRESSION TAG	UNP Q80J95
C	517	HIS	-	EXPRESSION TAG	UNP Q80J95
C	518	HIS	-	EXPRESSION TAG	UNP Q80J95
C	519	HIS	-	EXPRESSION TAG	UNP Q80J95
C	520	HIS	-	EXPRESSION TAG	UNP Q80J95

- Molecule 2 is 1-(beta-D-ribofuranosyl)-2-thioxo-2,3-dihydropyrimidin-4(1H)-one (three-letter code: 2TU) (formula: $C_9H_{12}N_2O_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			17	9	2	5	1		
2	B	1	Total	C	N	O	S	0	0
			17	9	2	5	1		
2	C	1	Total	C	N	O	S	0	0
			17	9	2	5	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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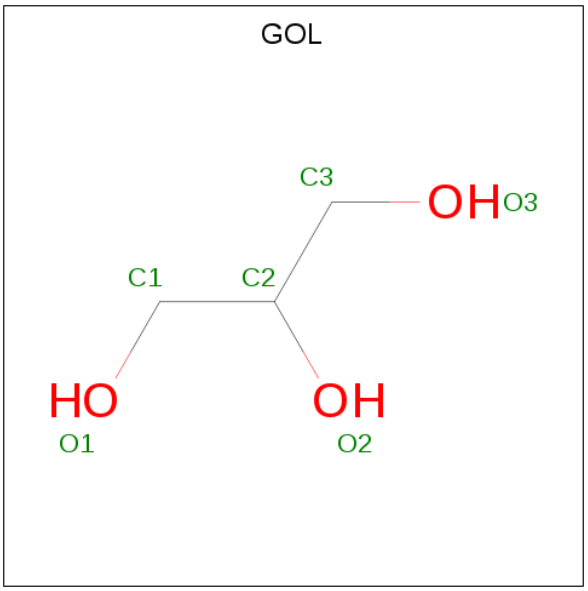
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Mg 1 1	0	0
5	A	1	Total Mg 1 1	0	0
5	C	1	Total Mg 1 1	0	0

- Molecule 6 is water.

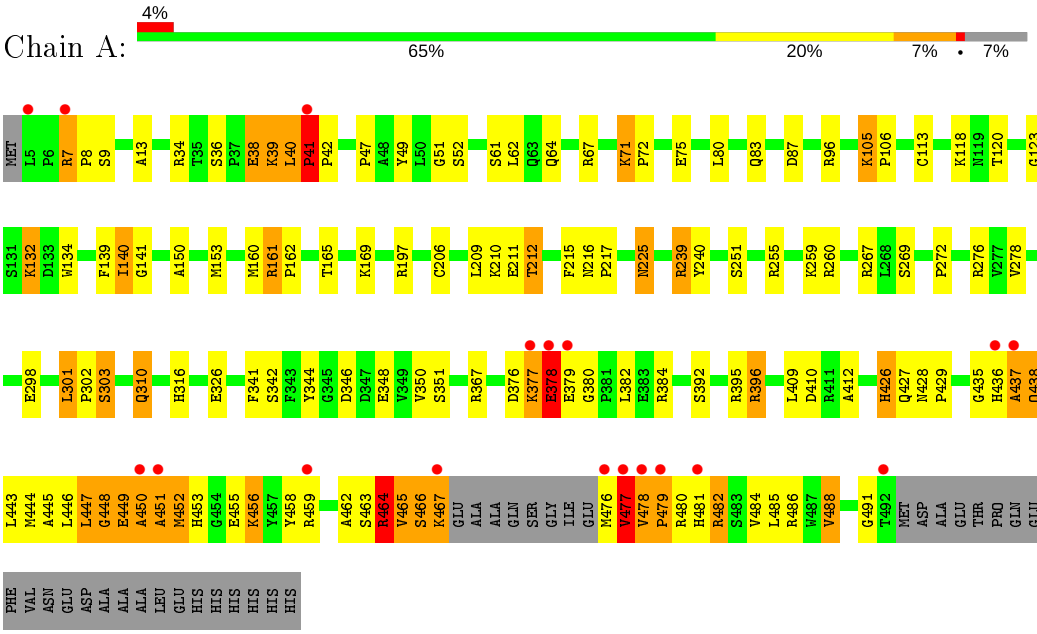
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	212	Total O 212 212	0	0
6	B	168	Total O 168 168	0	0
6	C	163	Total O 163 163	0	0

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.

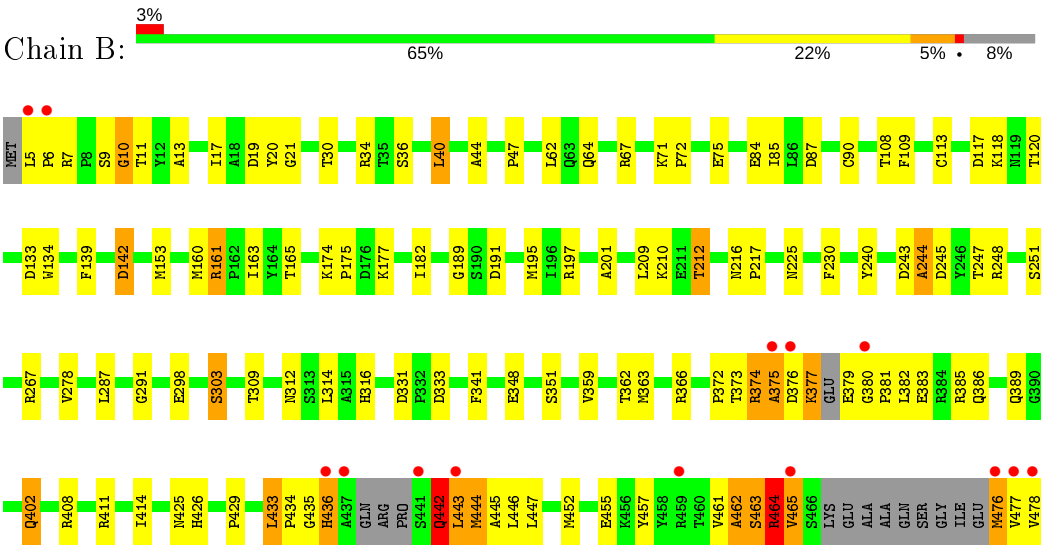
- Molecule 1: RNA polymerase

Chain A:



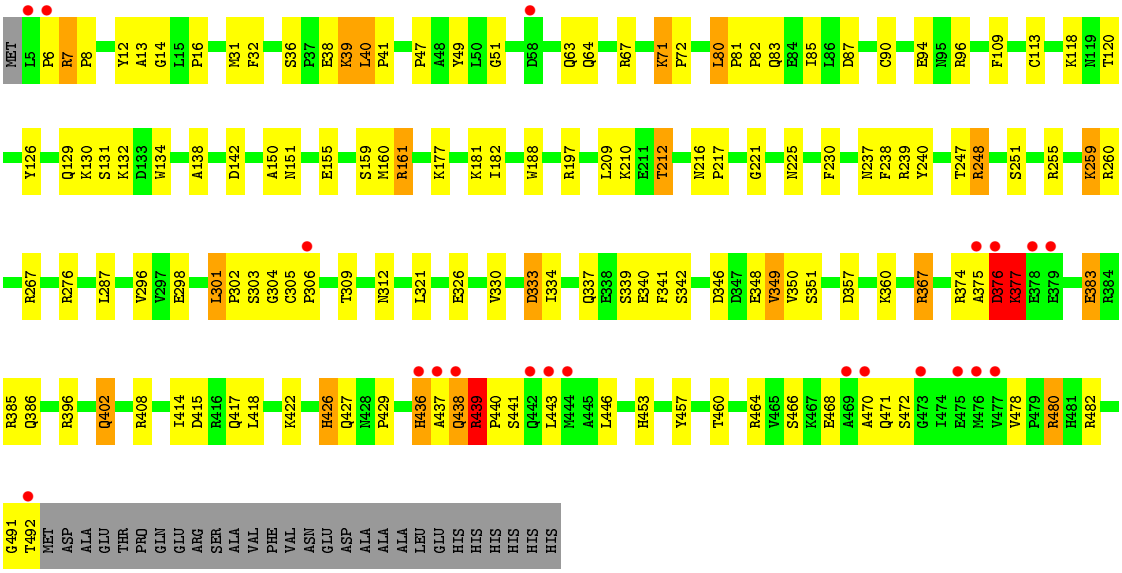
- Molecule 1: RNA polymerase

Chain B:



- Molecule 1: RNA polymerase

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	120.79Å 195.97Å 109.33Å 90.00° 114.86° 90.00°	Depositor
Resolution (Å)	31.62 – 2.21 31.62 – 2.21	Depositor EDS
% Data completeness (in resolution range)	99.0 (31.62-2.21) 98.8 (31.62-2.21)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.46	Depositor
$< I/\sigma(I) >$ [1]	1.17 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.7.1_743	Depositor
R, R_{free}	0.203 , 0.253 0.200 , 0.248	Depositor DCC
R_{free} test set	2000 reflections (1.76%)	wwPDB-VP
Wilson B-factor (Å^2)	26.1	Xtriage
Anisotropy	0.295	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 45.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12359	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 2TU, GOL, MG, SO4

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	0.49	0/3921	0.65	1/5313 (0.0%)
1	B	0.45	0/3866	0.58	0/5236
1	C	0.46	0/3968	0.57	0/5378
All	All	0.47	0/11755	0.60	1/15927 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
1	B	0	1
All	All	0	7

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	447	LEU	CA-CB-CG	6.14	129.42	115.30

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	40	LEU	Peptide
1	A	41	PRO	Peptide
1	A	439	ARG	Peptide
1	A	440	PRO	Peptide

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Mol	Chain	Res	Type	Group
1	A	450	ALA	Peptide

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	3826	0	3786	165	1
1	B	3774	0	3730	132	0
1	C	3872	0	3829	106	0
2	A	17	0	12	1	0
2	B	17	0	12	3	0
2	C	17	0	12	7	0
3	A	45	0	0	4	0
3	B	40	0	0	4	0
3	C	55	0	0	1	0
4	A	72	0	96	19	1
4	B	42	0	56	20	0
4	C	36	0	48	14	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
6	A	212	0	0	15	0
6	B	168	0	0	7	0
6	C	163	0	0	3	0
All	All	12359	0	11581	405	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 17.

The worst 5 of 405 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:440:PRO:CB	1:A:441:SER:HB2	1.76	1.16
1:A:466:SER:CB	1:A:467:LYS:HA	1.80	1.11
1:A:39:LYS:HD3	1:A:40:LEU:H	1.06	1.10
1:A:466:SER:HB2	1:A:467:LYS:CA	1.87	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:SER:HB2	1:A:467:LYS:HA	1.07	1.03

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)
1:A:9:SER:O	4:A:613:GOL:O1[2_655]	2.12	0.08

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	477/517 (92%)	442 (93%)	20 (4%)	15 (3%)	4 2
1	B	467/517 (90%)	434 (93%)	21 (4%)	12 (3%)	5 3
1	C	486/517 (94%)	458 (94%)	18 (4%)	10 (2%)	7 4
All	All	1430/1551 (92%)	1334 (93%)	59 (4%)	37 (3%)	5 3

5 of 37 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	378	GLU
1	A	436	HIS
1	A	440	PRO
1	A	442	GLN
1	A	449	GLU

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	412/440 (94%)	373 (90%)	39 (10%)	8 8
1	B	406/440 (92%)	373 (92%)	33 (8%)	11 12
1	C	416/440 (94%)	378 (91%)	38 (9%)	9 9
All	All	1234/1320 (94%)	1124 (91%)	110 (9%)	10 9

5 of 110 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	212	THR
1	B	402[B]	GLN
1	C	402	GLN
1	B	260	ARG
1	B	379	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	442	GLN
1	C	426	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 59 ligands modelled in this entry, 3 are monoatomic - leaving 56 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	SO4	A	605	-	4,4,4	0.13	0	6,6,6	0.12	0
4	GOL	A	618	-	5,5,5	0.36	0	5,5,5	0.24	0
3	SO4	C	606	-	4,4,4	0.22	0	6,6,6	0.21	0
4	GOL	C	618	-	5,5,5	0.40	0	5,5,5	0.49	0
4	GOL	C	613	-	5,5,5	0.24	0	5,5,5	0.47	0
3	SO4	C	612	-	4,4,4	0.17	0	6,6,6	0.13	0
3	SO4	C	609	-	4,4,4	0.13	0	6,6,6	0.19	0
4	GOL	A	620	-	5,5,5	0.29	0	5,5,5	0.63	0
3	SO4	A	608	-	4,4,4	0.33	0	6,6,6	0.17	0
4	GOL	A	616	-	5,5,5	0.38	0	5,5,5	0.58	0
3	SO4	A	603	-	4,4,4	0.20	0	6,6,6	0.15	0
3	SO4	C	608	-	4,4,4	0.19	0	6,6,6	0.13	0
3	SO4	A	610	-	4,4,4	0.14	0	6,6,6	0.12	0
3	SO4	C	602	-	4,4,4	0.19	0	6,6,6	0.06	0
3	SO4	C	610	-	4,4,4	0.25	0	6,6,6	0.14	0
3	SO4	C	605	-	4,4,4	0.14	0	6,6,6	0.10	0
4	GOL	A	622	-	5,5,5	0.43	0	5,5,5	0.51	0
3	SO4	B	605	-	4,4,4	0.17	0	6,6,6	0.08	0
4	GOL	A	614	-	5,5,5	0.27	0	5,5,5	0.62	0
4	GOL	A	613	-	5,5,5	0.27	0	5,5,5	0.59	0
4	GOL	C	614	-	5,5,5	0.34	0	5,5,5	0.38	0
2	2TU	A	601	-	14,18,18	1.18	1 (7%)	14,26,26	1.70	1 (7%)
4	GOL	B	612	-	5,5,5	0.46	0	5,5,5	0.46	0
3	SO4	C	607	-	4,4,4	0.19	0	6,6,6	0.09	0
3	SO4	C	603	-	4,4,4	0.26	0	6,6,6	0.17	0
3	SO4	B	604	-	4,4,4	0.21	0	6,6,6	0.19	0
4	GOL	C	616	-	5,5,5	0.38	0	5,5,5	0.65	0
3	SO4	B	607	-	4,4,4	0.22	0	6,6,6	0.41	0
4	GOL	B	610	-	5,5,5	0.46	0	5,5,5	0.41	0
4	GOL	A	621	-	5,5,5	0.42	0	5,5,5	0.24	0
2	2TU	C	601	-	14,18,18	1.19	1 (7%)	14,26,26	1.81	1 (7%)
3	SO4	B	606	-	4,4,4	0.19	0	6,6,6	0.18	0
3	SO4	C	611	-	4,4,4	0.27	0	6,6,6	0.20	0
3	SO4	B	602	-	4,4,4	0.25	0	6,6,6	0.10	0
4	GOL	A	619	-	5,5,5	0.47	0	5,5,5	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	GOL	B	615	-	5,5,5	0.36	0	5,5,5	0.63	0
4	GOL	A	615	-	5,5,5	0.40	0	5,5,5	1.16	1 (20%)
3	SO4	A	604	-	4,4,4	0.22	0	6,6,6	0.06	0
4	GOL	B	611	-	5,5,5	0.47	0	5,5,5	0.73	0
2	2TU	B	601	-	14,18,18	0.86	1 (7%)	14,26,26	1.72	1 (7%)
4	GOL	A	612	-	5,5,5	0.40	0	5,5,5	0.36	0
3	SO4	B	609	-	4,4,4	0.16	0	6,6,6	0.18	0
4	GOL	C	617	-	5,5,5	0.38	0	5,5,5	0.20	0
4	GOL	B	613	-	5,5,5	0.30	0	5,5,5	0.69	0
4	GOL	A	617	-	5,5,5	0.41	0	5,5,5	0.23	0
4	GOL	B	616	-	5,5,5	0.36	0	5,5,5	0.64	0
3	SO4	A	609	-	4,4,4	0.23	0	6,6,6	0.21	0
3	SO4	A	607	-	4,4,4	0.20	0	6,6,6	0.15	0
3	SO4	B	603	-	4,4,4	0.23	0	6,6,6	0.07	0
3	SO4	B	608	-	4,4,4	0.20	0	6,6,6	0.12	0
4	GOL	C	615	-	5,5,5	0.32	0	5,5,5	0.61	0
4	GOL	A	611	-	5,5,5	0.37	0	5,5,5	0.54	0
3	SO4	C	604	-	4,4,4	0.16	0	6,6,6	0.18	0
3	SO4	A	606	-	4,4,4	0.16	0	6,6,6	0.08	0
4	GOL	B	614	-	5,5,5	0.36	0	5,5,5	0.51	0
3	SO4	A	602	-	4,4,4	0.18	0	6,6,6	0.17	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	GOL	A	618	-	-	2/4/4/4	-
4	GOL	C	618	-	-	4/4/4/4	-
4	GOL	C	613	-	-	2/4/4/4	-
4	GOL	A	614	-	-	2/4/4/4	-
4	GOL	A	620	-	-	2/4/4/4	-
4	GOL	C	616	-	-	4/4/4/4	-
4	GOL	A	616	-	-	4/4/4/4	-
4	GOL	A	622	-	-	4/4/4/4	-
4	GOL	A	613	-	-	2/4/4/4	-
4	GOL	C	614	-	-	4/4/4/4	-
2	2TU	A	601	-	-	2/4/22/22	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	B	612	-	-	4/4/4/4	-
4	GOL	B	610	-	-	4/4/4/4	-
4	GOL	A	621	-	-	4/4/4/4	-
2	2TU	C	601	-	-	2/4/22/22	0/2/2/2
4	GOL	A	619	-	-	2/4/4/4	-
4	GOL	B	615	-	-	2/4/4/4	-
4	GOL	A	615	-	-	2/4/4/4	-
4	GOL	B	611	-	-	2/4/4/4	-
2	2TU	B	601	-	-	2/4/22/22	0/2/2/2
4	GOL	A	612	-	-	2/4/4/4	-
4	GOL	C	617	-	-	2/4/4/4	-
4	GOL	B	613	-	-	2/4/4/4	-
4	GOL	A	617	-	-	2/4/4/4	-
4	GOL	B	616	-	-	0/4/4/4	-
4	GOL	C	615	-	-	4/4/4/4	-
4	GOL	A	611	-	-	3/4/4/4	-
4	GOL	B	614	-	-	1/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	2TU	C2-S2	3.53	1.74	1.66
2	A	601	2TU	C2-S2	3.45	1.73	1.66
2	B	601	2TU	C2-S2	2.33	1.71	1.66

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	601	2TU	C2-N3-C4	6.41	120.86	114.74
2	A	601	2TU	C2-N3-C4	5.91	120.38	114.74
2	B	601	2TU	C2-N3-C4	5.86	120.34	114.74
4	A	615	GOL	C3-C2-C1	-2.04	103.78	111.70

There are no chirality outliers.

5 of 72 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	618	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
4	A	620	GOL	O1-C1-C2-C3
4	A	616	GOL	O1-C1-C2-C3
4	A	622	GOL	O1-C1-C2-C3
4	A	613	GOL	O1-C1-C2-C3

There are no ring outliers.

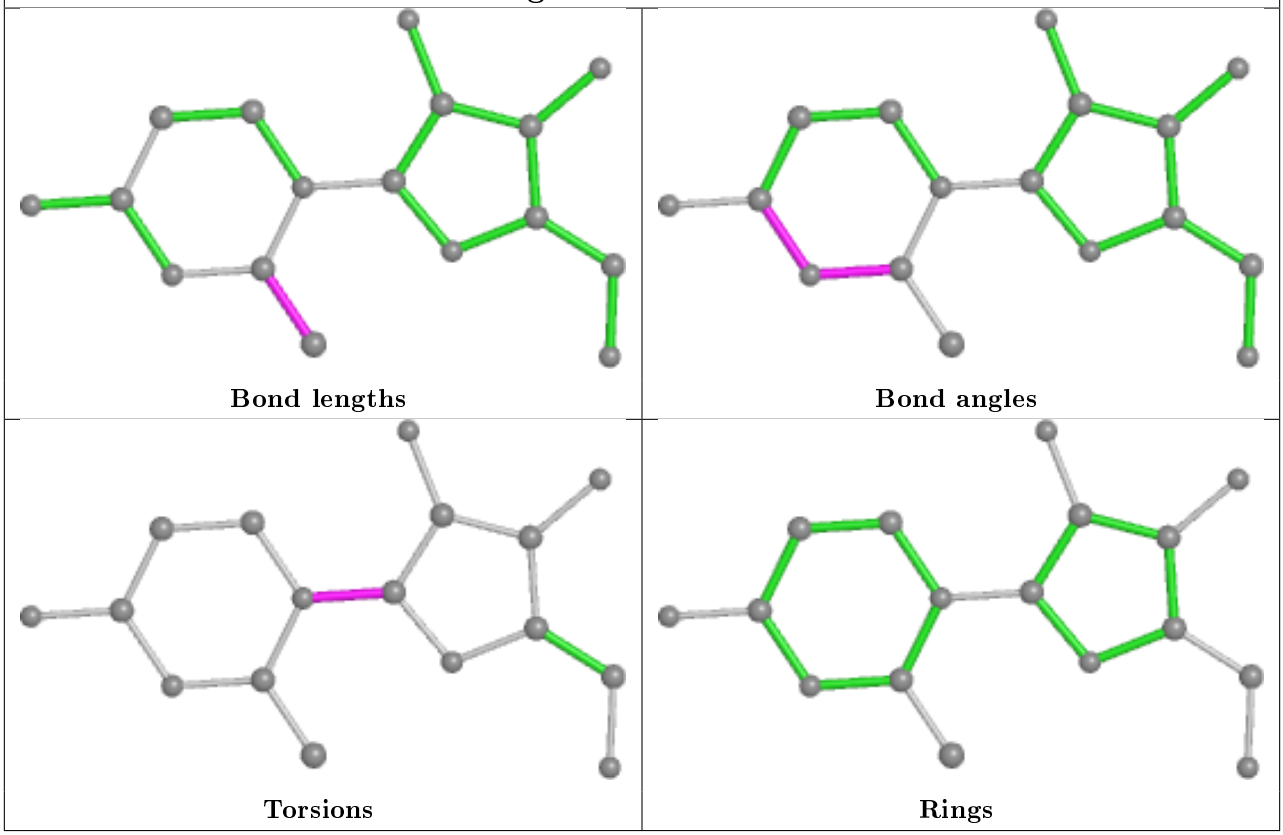
27 monomers are involved in 74 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	618	GOL	4	0
4	C	613	GOL	4	0
4	A	620	GOL	1	0
3	A	608	SO4	1	0
4	A	614	GOL	2	0
4	A	613	GOL	4	1
2	A	601	2TU	1	0
4	C	616	GOL	1	0
3	B	607	SO4	3	0
4	B	610	GOL	2	0
2	C	601	2TU	7	0
4	A	619	GOL	2	0
4	A	615	GOL	5	0
4	B	611	GOL	1	0
2	B	601	2TU	3	0
4	A	612	GOL	2	0
3	B	609	SO4	1	0
4	C	617	GOL	4	0
4	B	613	GOL	2	0
4	A	617	GOL	3	0
4	B	616	GOL	11	0
3	A	609	SO4	1	0
3	A	607	SO4	1	0
4	C	615	GOL	1	0
3	C	604	SO4	1	0
3	A	606	SO4	1	0
4	B	614	GOL	4	0

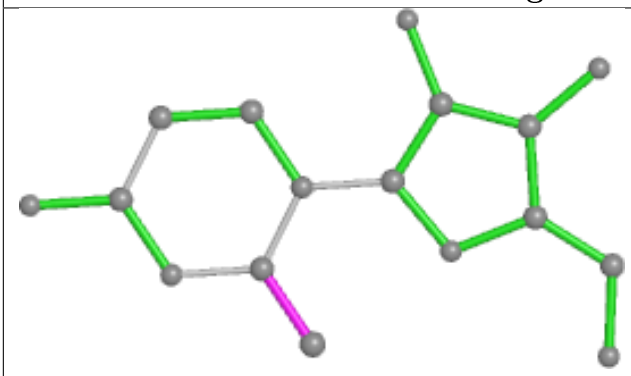
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

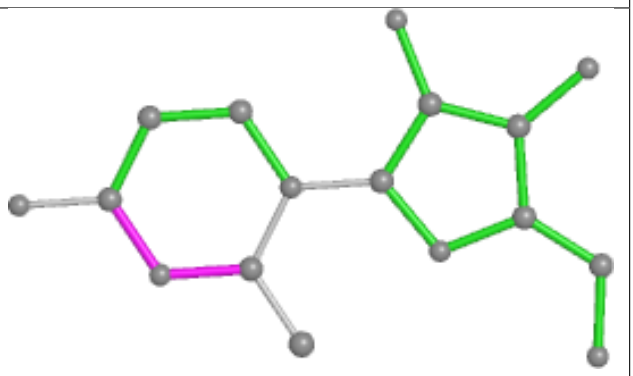
Ligand 2TU A 601



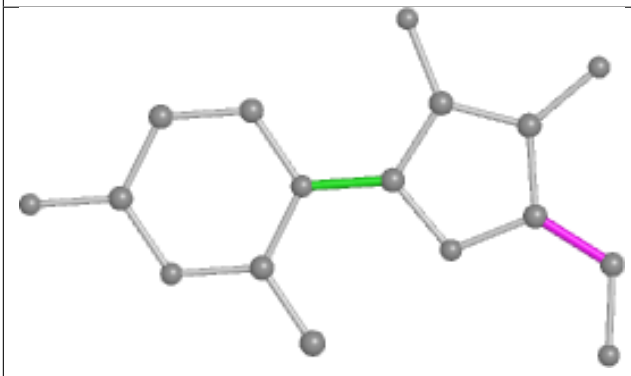
Ligand 2TU C 601



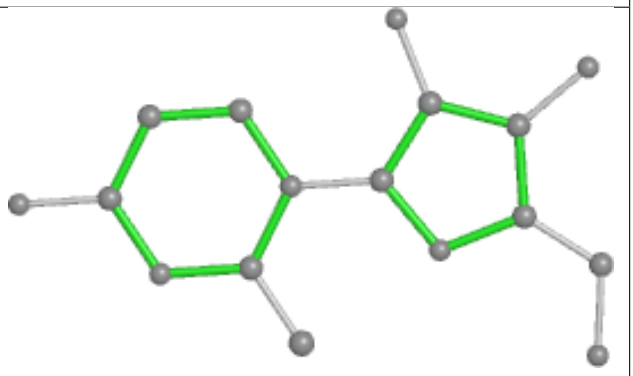
Bond lengths



Bond angles

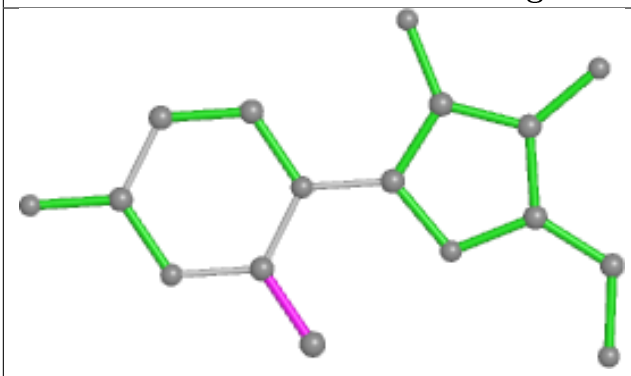


Torsions

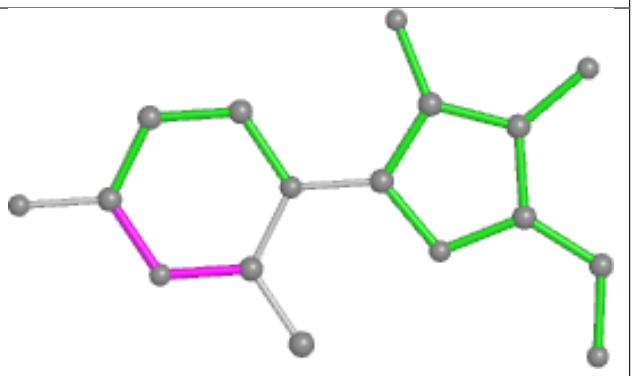


Rings

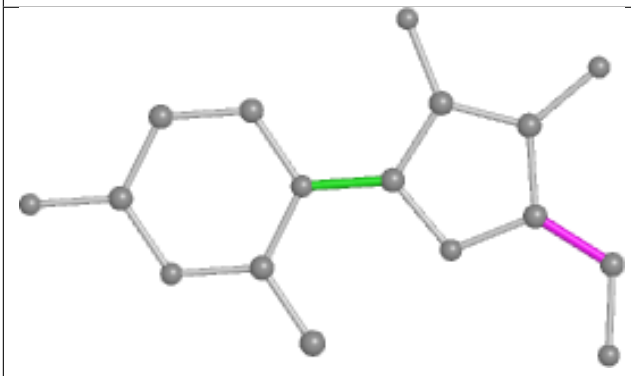
Ligand 2TU B 601



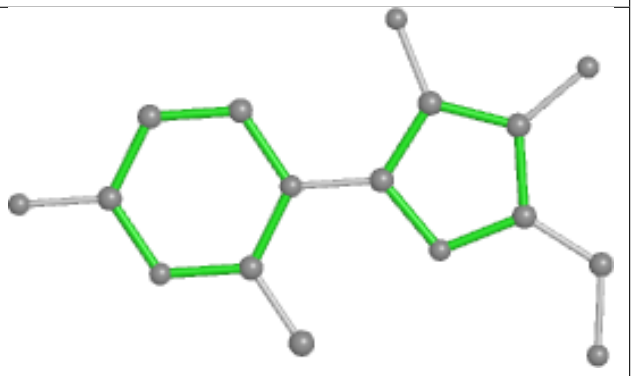
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	480/517 (92%)	-0.31	21 (4%)	34	32	15, 27, 66, 107	0
1	B	474/517 (91%)	-0.20	17 (3%)	42	41	19, 32, 66, 112	0
1	C	488/517 (94%)	-0.28	21 (4%)	35	33	18, 32, 66, 105	0
All	All	1442/1551 (92%)	-0.26	59 (4%)	37	35	15, 31, 66, 112	0

The worst 5 of 59 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	5	LEU	8.0
1	B	476	MET	7.7
1	C	437	ALA	7.2
1	A	441	SER	7.0
1	B	479	PRO	6.9

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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	2TU	B	601	17/17	0.75	0.30	33,42,47,47	17
2	2TU	A	601	17/17	0.77	0.24	27,38,42,43	17
4	GOL	B	610	6/6	0.79	0.23	44,48,51,53	0
2	2TU	C	601	17/17	0.80	0.28	28,34,41,46	17
4	GOL	A	622	6/6	0.83	0.17	48,51,56,57	0
4	GOL	A	620	6/6	0.84	0.22	38,42,54,60	0
4	GOL	C	617	6/6	0.84	0.14	38,47,53,56	0
3	SO4	B	607	5/5	0.85	0.20	43,43,56,71	0
4	GOL	C	616	6/6	0.86	0.26	49,57,59,67	0
4	GOL	B	613	6/6	0.86	0.16	37,39,40,42	1
3	SO4	A	608	5/5	0.87	0.30	46,52,59,76	0
4	GOL	A	616	6/6	0.87	0.22	36,47,56,58	0
3	SO4	C	611	5/5	0.87	0.24	43,51,62,80	0
4	GOL	B	616	6/6	0.87	0.28	33,37,40,48	0
3	SO4	B	604	5/5	0.88	0.36	48,59,82,90	0
4	GOL	C	614	6/6	0.89	0.16	42,46,47,53	0
4	GOL	A	613	6/6	0.89	0.20	41,46,51,53	0
3	SO4	C	607	5/5	0.89	0.22	73,74,80,97	0
4	GOL	B	615	6/6	0.89	0.14	39,41,45,46	0
3	SO4	A	607	5/5	0.89	0.28	55,59,72,74	0
4	GOL	C	615	6/6	0.89	0.16	36,40,49,51	0
3	SO4	A	606	5/5	0.89	0.22	76,85,95,100	0
4	GOL	B	614	6/6	0.89	0.33	28,35,42,43	0
3	SO4	B	606	5/5	0.90	0.27	61,63,71,81	0
4	GOL	B	612	6/6	0.90	0.17	36,47,51,54	0
4	GOL	A	619	6/6	0.90	0.26	29,35,45,50	0
4	GOL	C	618	6/6	0.91	0.19	42,48,53,54	0
3	SO4	C	608	5/5	0.91	0.35	61,76,86,89	0
3	SO4	B	603	5/5	0.91	0.30	55,65,82,87	0
3	SO4	C	610	5/5	0.92	0.28	37,52,74,77	0
4	GOL	A	612	6/6	0.92	0.22	29,35,40,42	0
3	SO4	A	609	5/5	0.92	0.26	34,50,66,70	0
4	GOL	A	615	6/6	0.92	0.28	23,38,47,50	0
3	SO4	A	602	5/5	0.92	0.12	45,53,61,74	0
4	GOL	A	621	6/6	0.93	0.10	40,43,48,50	0
4	GOL	A	611	6/6	0.93	0.16	34,37,45,47	0
3	SO4	B	609	5/5	0.93	0.32	61,67,86,87	0
4	GOL	B	611	6/6	0.93	0.17	25,42,43,51	0
3	SO4	C	605	5/5	0.93	0.26	74,74,92,93	0
4	GOL	A	618	6/6	0.94	0.12	28,32,33,33	1
4	GOL	A	614	6/6	0.94	0.15	40,44,47,55	0
4	GOL	C	613	6/6	0.94	0.15	34,39,45,47	0
3	SO4	C	602	5/5	0.95	0.15	47,52,67,78	0

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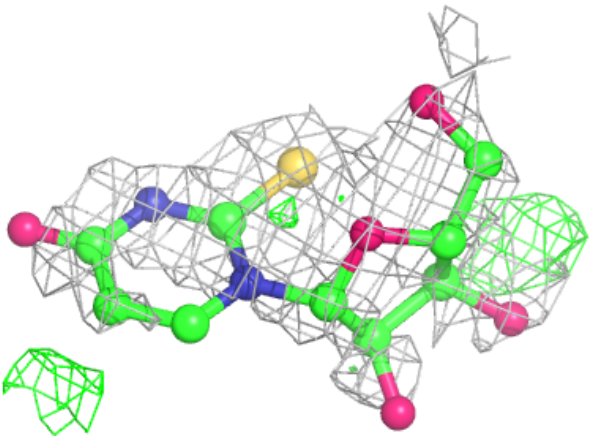
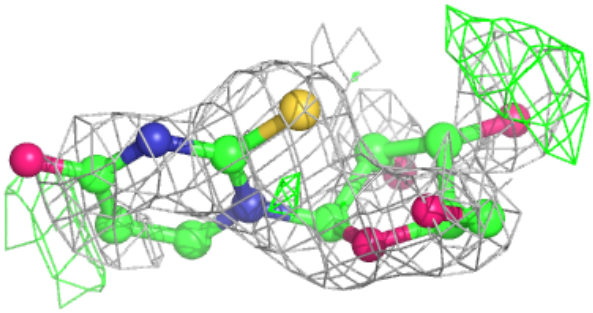
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	A	610	5/5	0.95	0.23	57,61,72,73	0
3	SO4	B	602	5/5	0.95	0.17	42,47,60,66	0
4	GOL	A	617	6/6	0.95	0.13	34,39,40,47	0
3	SO4	B	608	5/5	0.95	0.24	55,56,76,78	0
3	SO4	C	603	5/5	0.96	0.15	37,38,56,63	0
3	SO4	C	606	5/5	0.96	0.13	52,59,69,71	0
3	SO4	B	605	5/5	0.96	0.20	56,57,71,72	0
3	SO4	C	604	5/5	0.97	0.20	55,56,61,68	0
3	SO4	C	612	5/5	0.97	0.26	56,59,72,74	0
3	SO4	A	605	5/5	0.97	0.21	61,61,71,73	0
5	MG	B	617	1/1	0.97	0.34	49,49,49,49	0
3	SO4	A	604	5/5	0.98	0.17	46,46,62,62	0
5	MG	C	619	1/1	0.98	0.06	32,32,32,32	0
5	MG	A	623	1/1	0.98	0.06	29,29,29,29	0
3	SO4	C	609	5/5	0.98	0.21	39,47,54,62	0
3	SO4	A	603	5/5	0.98	0.13	43,44,57,59	0

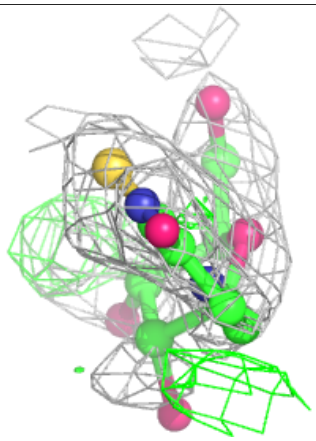
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 2TU B 601:

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

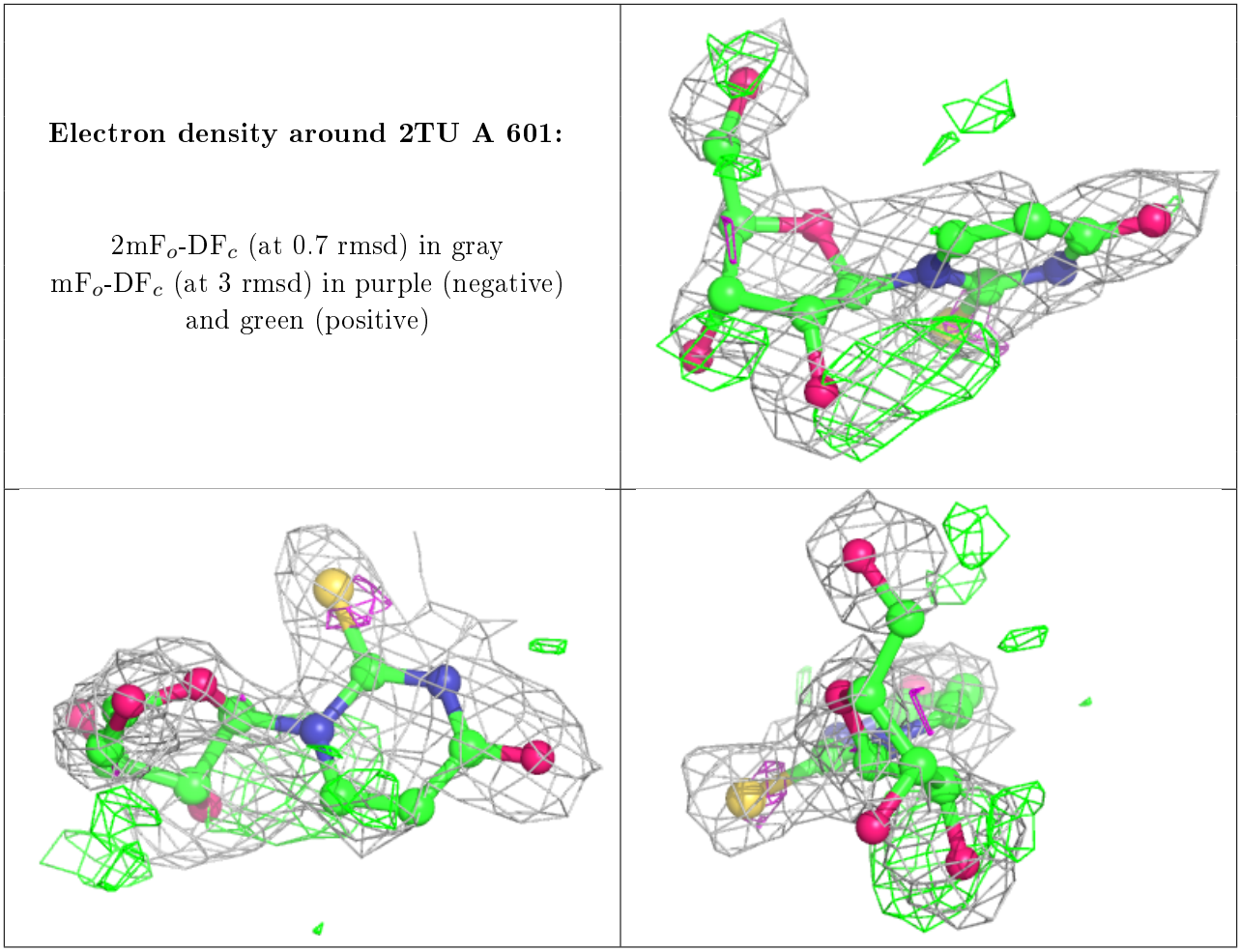






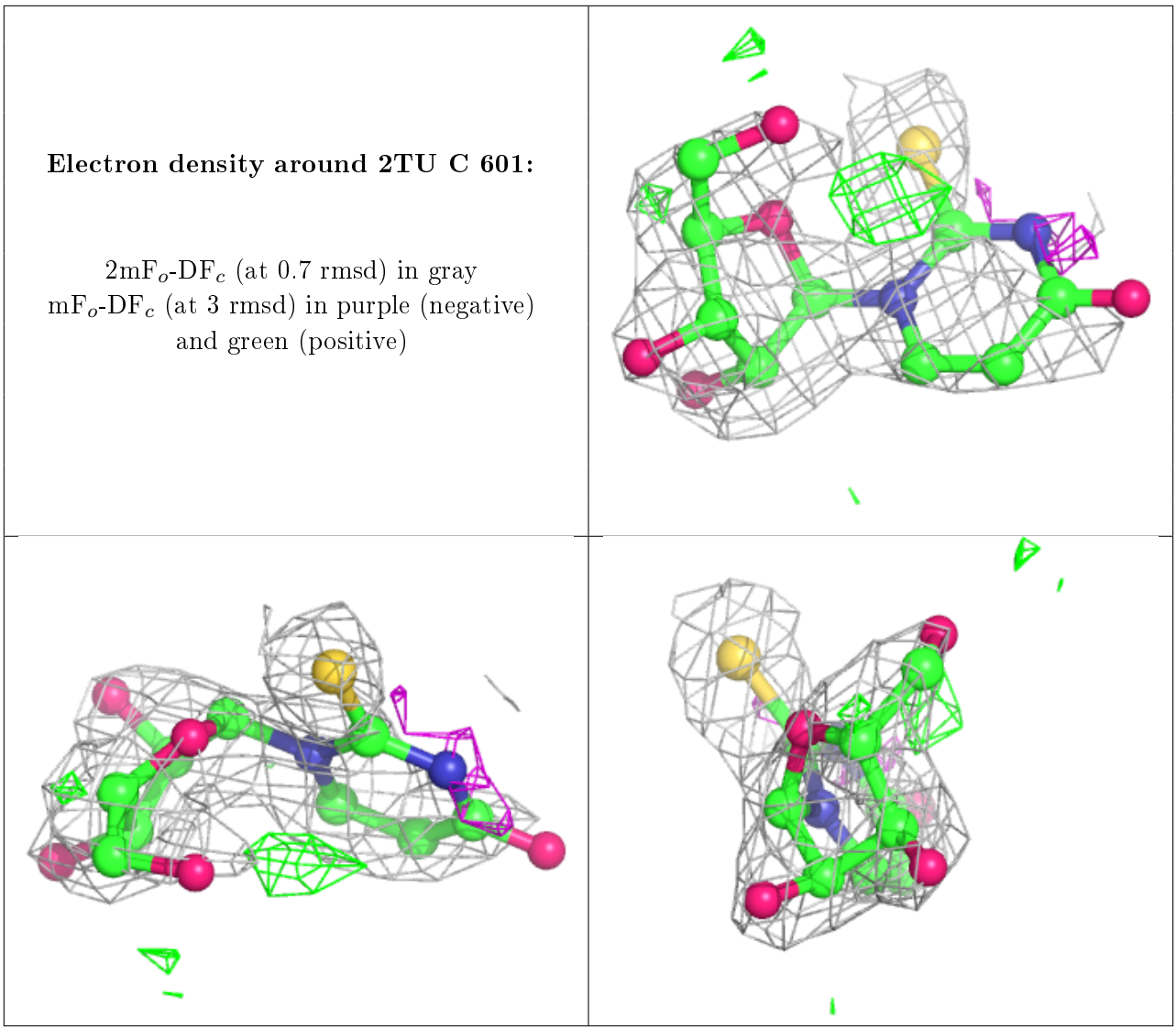
Electron density around 2TU A 601:

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



Electron density around 2TU C 601:

$2mF_o$-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.