



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 18, 2024 – 09:22 PM EST

PDB ID : 4HO5  
Title : Crystal structure of glucose 1-phosphate thymidyltransferase from *Aneurini-bacillus thermoaerophilus* complexed with TDP-glucose  
Authors : Chen, T.J.; Chien, W.T.; Lin, C.C.; Wang, W.C.  
Deposited on : 2012-10-22  
Resolution : 1.70 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](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

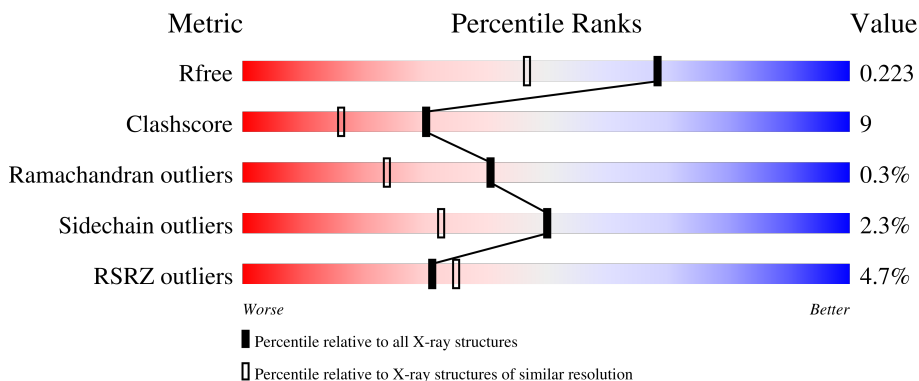
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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  $\geq 3$ , 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	297	
1	B	297	

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 5191 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.

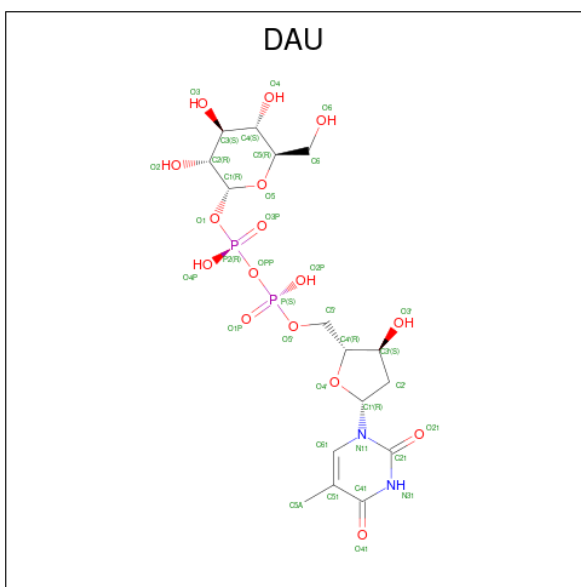
- Molecule 1 is a protein called Glucose-1-phosphate thymidyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	288	Total	C	N	O	S	0	0	0
			2256	1449	370	430	7			
1	B	289	Total	C	N	O	S	0	0	0
			2262	1452	371	432	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	297	GLY	-	expression tag	UNP Q9AGY4
B	297	GLY	-	expression tag	UNP Q9AGY4

- Molecule 2 is 2'DEOXY-THYMIDINE-5'-DIPHOSPHO-ALPHA-D-GLUCOSE (three-letter code: DAU) (formula: C<sub>16</sub>H<sub>26</sub>N<sub>2</sub>O<sub>16</sub>P<sub>2</sub>).



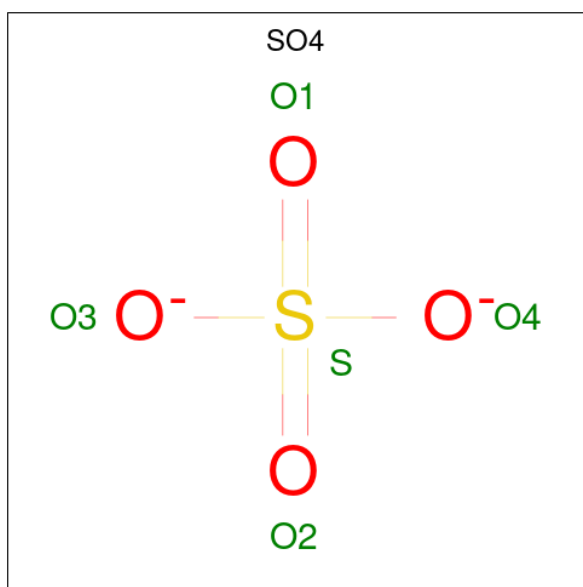
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total	C	N	O	P	0	0
			36	16	2	16	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			P
2	A	1	Total 36	C 16	N 2	O 16	P 2	0	0
2	B	1	Total 36	C 16	N 2	O 16	P 2	0	0
2	B	1	Total 36	C 16	N 2	O 16	P 2	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	258	Total 258	O 258	0	0

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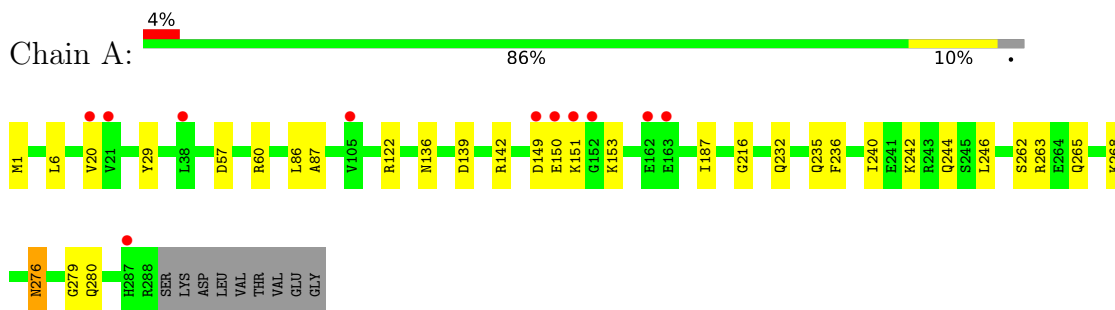
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
4	B	246	Total 246	O 246	0	0

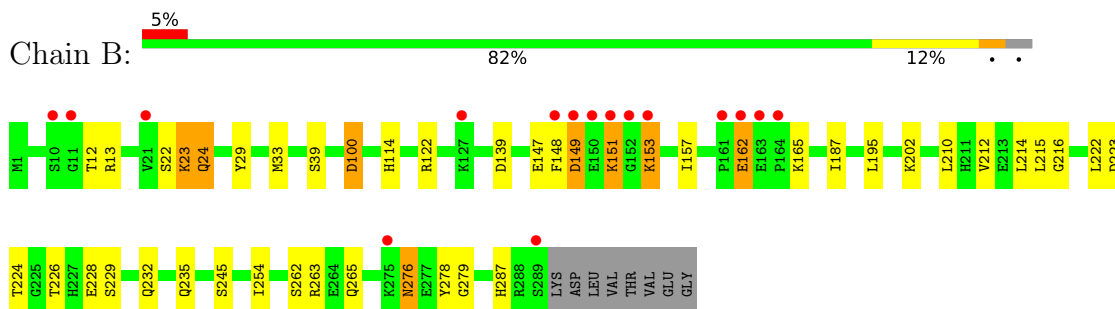
### 3 Residue-property plots [i](#)

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

- Molecule 1: Glucose-1-phosphate thymidyltransferase



- Molecule 1: Glucose-1-phosphate thymidyltransferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	114.30Å 90.56Å 87.52Å 90.00° 124.96° 90.00°	Depositor
Resolution (Å)	30.00 – 1.70 28.44 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.1 (30.00-1.70) 99.1 (28.44-1.70)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.94 (at 1.70Å)	Xtrriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.192 , 0.223 0.191 , 0.223	Depositor DCC
$R_{free}$ test set	3994 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.1	Xtrriage
Anisotropy	0.052	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 44.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5191	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.89% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: DAU, 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	0.92	0/2299	0.66	0/3107
1	B	0.92	1/2305 (0.0%)	0.66	0/3115
All	All	0.92	1/4604 (0.0%)	0.66	0/6222

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	23	LYS	CB-CG	-6.76	1.34	1.52

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	2256	0	2277	34	1
1	B	2262	0	2282	48	1
2	A	72	0	48	3	0
2	B	72	0	48	5	0
3	A	15	0	0	0	0
3	B	10	0	0	0	0
4	A	258	0	0	13	1
4	B	246	0	0	14	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5191	0	4655	87	4

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 (87) 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:B:122:ARG:HD3	4:B:578:HOH:O	1.32	1.26
1:A:242:LYS:HB3	4:A:650:HOH:O	1.09	1.26
1:A:280:GLN:HG2	4:A:582:HOH:O	1.35	1.24
1:A:268:LYS:HG2	4:A:487:HOH:O	1.33	1.23
1:A:242:LYS:HG2	4:A:529:HOH:O	1.37	1.17
1:B:245:SER:HA	4:B:639:HOH:O	1.53	1.07
1:A:216:GLY:N	4:A:590:HOH:O	1.60	1.04
1:A:20:VAL:HB	4:A:484:HOH:O	1.58	1.01
1:A:139:ASP:HB2	1:A:142:ARG:HH11	1.28	0.99
2:B:300:DAU:O6	4:B:547:HOH:O	1.77	0.94
1:A:1:MET:O	4:A:655:HOH:O	1.87	0.93
1:A:262:SER:H	1:A:265:GLN:HE21	1.23	0.85
1:B:100:ASP:OD1	4:B:637:HOH:O	1.97	0.82
1:B:216:GLY:N	4:B:629:HOH:O	2.15	0.79
1:A:150:GLU:H	1:A:150:GLU:CD	1.85	0.78
1:B:224:THR:HG22	1:B:224:THR:O	1.83	0.77
1:B:23:LYS:CE	1:B:224:THR:HG22	2.17	0.74
1:A:139:ASP:HB2	1:A:142:ARG:NH1	2.03	0.73
1:B:33:MET:SD	1:B:224:THR:HG21	2.30	0.71
1:B:33:MET:CE	1:B:224:THR:HG21	2.22	0.69
1:B:245:SER:CB	4:B:639:HOH:O	2.41	0.69
1:B:187:ILE:HD11	1:B:195:LEU:HB3	1.73	0.69
1:B:215:LEU:HA	4:B:629:HOH:O	1.94	0.67
1:B:232:GLN:HA	1:B:235:GLN:HE21	1.59	0.67
1:B:114:HIS:CE1	2:B:301:DAU:HC5	2.30	0.66
1:A:139:ASP:CB	1:A:142:ARG:HD3	2.25	0.65
1:A:232:GLN:HA	1:A:235:GLN:HE21	1.62	0.65
1:A:136:ASN:OD1	1:B:245:SER:OG	2.09	0.65
1:B:23:LYS:HE2	1:B:224:THR:HG22	1.78	0.65
1:B:224:THR:O	1:B:224:THR:CG2	2.43	0.65
1:B:24:GLN:HE21	1:B:24:GLN:H	1.46	0.63
1:A:139:ASP:HB3	1:A:142:ARG:HD3	1.81	0.62
1:B:202:LYS:NZ	4:B:638:HOH:O	2.22	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:LEU:O	4:B:628:HOH:O	2.16	0.61
1:B:215:LEU:CA	4:B:629:HOH:O	2.47	0.60
1:A:242:LYS:HD3	4:A:650:HOH:O	2.01	0.60
2:B:301:DAU:O1P	4:B:468:HOH:O	2.16	0.59
1:A:122:ARG:NH1	4:A:614:HOH:O	2.37	0.58
2:A:301:DAU:O2P	2:A:301:DAU:O3P	2.22	0.57
1:B:24:GLN:H	1:B:24:GLN:NE2	2.03	0.56
1:B:162:GLU:OE2	1:B:162:GLU:HA	2.05	0.56
1:A:20:VAL:CB	4:A:484:HOH:O	2.34	0.56
1:B:263:ARG:NH2	1:B:287:HIS:HD2	2.03	0.56
1:B:262:SER:H	1:B:265:GLN:NE2	2.03	0.55
1:A:149:ASP:HB2	1:A:153:LYS:H	1.72	0.54
1:B:33:MET:CE	1:B:224:THR:CG2	2.85	0.54
1:B:232:GLN:HA	1:B:235:GLN:NE2	2.22	0.54
1:A:139:ASP:HB2	1:A:142:ARG:HD3	1.89	0.54
1:B:148:PHE:CE1	1:B:214:LEU:HD21	2.42	0.54
1:B:226:THR:OG1	1:B:228:GLU:HG2	2.08	0.54
1:B:223:ASP:HB3	1:B:229:SER:HB2	1.90	0.53
1:A:149:ASP:HB3	1:A:151:LYS:H	1.73	0.53
1:A:232:GLN:NE2	4:A:577:HOH:O	2.42	0.53
1:B:148:PHE:CZ	1:B:214:LEU:HD21	2.44	0.52
1:B:149:ASP:HB3	1:B:151:LYS:H	1.76	0.51
1:A:57:ASP:HA	1:A:60:ARG:HD2	1.92	0.50
1:B:276:ASN:C	1:B:276:ASN:HD22	2.15	0.50
1:B:228:GLU:CD	1:B:228:GLU:H	2.14	0.50
1:A:263:ARG:HD2	4:A:579:HOH:O	2.13	0.48
1:B:23:LYS:HE2	1:B:224:THR:CG2	2.42	0.48
1:B:33:MET:HE1	1:B:224:THR:CG2	2.44	0.48
2:B:301:DAU:O1P	2:B:301:DAU:O4P	2.31	0.47
1:B:187:ILE:HD11	1:B:195:LEU:CB	2.40	0.47
1:B:276:ASN:ND2	1:B:279:GLY:H	2.12	0.47
1:A:276:ASN:ND2	1:A:279:GLY:H	2.12	0.47
1:B:139:ASP:N	4:B:545:HOH:O	1.94	0.47
2:B:300:DAU:O2P	2:B:300:DAU:O4P	2.34	0.46
1:B:100:ASP:CG	4:B:637:HOH:O	2.50	0.46
1:B:157:ILE:HD11	1:B:210:LEU:CD2	2.45	0.46
1:A:276:ASN:HD22	1:A:276:ASN:C	2.20	0.45
1:A:262:SER:H	1:A:265:GLN:NE2	2.04	0.45
1:B:148:PHE:CE2	1:B:212:VAL:HG11	2.52	0.44
1:A:242:LYS:CD	4:A:650:HOH:O	2.58	0.44
1:B:263:ARG:NH2	1:B:287:HIS:CD2	2.84	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:LEU:C	4:B:629:HOH:O	2.52	0.43
1:A:232:GLN:HA	1:A:235:GLN:NE2	2.30	0.43
1:B:157:ILE:HD11	1:B:210:LEU:HD21	2.01	0.43
1:A:236:PHE:CE2	1:A:240:ILE:HD11	2.54	0.43
1:A:244:GLN:HE21	1:A:246:LEU:HB2	1.84	0.42
1:B:149:ASP:HB2	1:B:153:LYS:H	1.84	0.42
1:B:276:ASN:HD21	1:B:278:TYR:HB3	1.83	0.42
2:A:301:DAU:HC1	2:A:301:DAU:O6	2.19	0.42
1:A:87:ALA:CB	1:A:187:ILE:HD11	2.49	0.42
1:B:39:SER:HB2	1:B:254:ILE:CD1	2.50	0.42
1:A:6:LEU:HG	2:A:300:DAU:O21	2.21	0.41
1:B:147:GLU:CD	1:B:165:LYS:HD3	2.41	0.41
1:A:6:LEU:HD23	1:A:86:LEU:HD22	2.03	0.41

All (4) 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)
4:A:413:HOH:O	4:A:413:HOH:O[2_656]	1.45	0.75
4:B:432:HOH:O	4:B:432:HOH:O[2_656]	1.65	0.55
1:B:235:GLN:OE1	1:B:235:GLN:OE1[2_656]	1.83	0.37
1:A:235:GLN:OE1	1:A:235:GLN:OE1[2_656]	2.11	0.09

## 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	286/297 (96%)	284 (99%)	1 (0%)	1 (0%)	41	24
1	B	287/297 (97%)	283 (99%)	3 (1%)	1 (0%)	41	24
All	All	573/594 (96%)	567 (99%)	4 (1%)	2 (0%)	41	24

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	TYR
1	B	29	TYR

### 5.3.2 Protein sidechains [i](#)

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	243/251 (97%)	242 (100%)	1 (0%)	91	87
1	B	244/251 (97%)	234 (96%)	10 (4%)	30	12
All	All	487/502 (97%)	476 (98%)	11 (2%)	50	33

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	276	ASN
1	B	12	THR
1	B	13	ARG
1	B	22	SER
1	B	24	GLN
1	B	100	ASP
1	B	149	ASP
1	B	151	LYS
1	B	153	LYS
1	B	162	GLU
1	B	276	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	GLN
1	A	211	HIS
1	A	232	GLN
1	A	235	GLN

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Mol	Chain	Res	Type
1	A	244	GLN
1	A	265	GLN
1	A	276	ASN
1	B	24	GLN
1	B	232	GLN
1	B	235	GLN
1	B	244	GLN
1	B	265	GLN
1	B	276	ASN
1	B	287	HIS

### 5.3.3 RNA [i](#)

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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

9 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	304	-	4,4,4	0.28	0	6,6,6	0.52	0
2	DAU	B	300	-	35,38,38	1.36	5 (14%)	53,58,58	2.18	11 (20%)
2	DAU	B	301	-	35,38,38	1.36	3 (8%)	53,58,58	2.17	17 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SO4	A	302	-	4,4,4	0.30	0	6,6,6	0.36	0
3	SO4	A	303	-	4,4,4	0.15	0	6,6,6	0.29	0
3	SO4	B	302	-	4,4,4	0.22	0	6,6,6	0.31	0
3	SO4	B	303	-	4,4,4	0.16	0	6,6,6	0.23	0
2	DAU	A	301	-	35,38,38	1.39	5 (14%)	53,58,58	1.73	12 (22%)
2	DAU	A	300	-	35,38,38	1.31	5 (14%)	53,58,58	1.76	10 (18%)

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	DAU	B	301	-	-	11/23/55/55	0/3/3/3
2	DAU	A	301	-	-	1/23/55/55	0/3/3/3
2	DAU	A	300	-	-	2/23/55/55	0/3/3/3
2	DAU	B	300	-	-	4/23/55/55	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	DAU	C41-C51	-4.29	1.37	1.44
2	B	301	DAU	C41-C51	-4.10	1.38	1.44
2	B	300	DAU	C61-C51	3.47	1.40	1.34
2	B	300	DAU	C41-C51	-3.40	1.39	1.44
2	B	300	DAU	C21-N11	-3.35	1.33	1.38
2	A	300	DAU	C41-N31	-3.33	1.32	1.38
2	A	301	DAU	C61-C51	3.25	1.39	1.34
2	B	300	DAU	C61-N11	-3.18	1.32	1.38
2	B	301	DAU	C61-C51	3.15	1.39	1.34
2	A	300	DAU	C21-N11	-3.04	1.33	1.38
2	B	300	DAU	C41-N31	-3.01	1.33	1.38
2	A	301	DAU	C41-N31	-2.90	1.33	1.38
2	B	301	DAU	O21-C21	2.61	1.27	1.23
2	A	301	DAU	C21-N11	-2.54	1.34	1.38
2	A	300	DAU	C61-N11	-2.49	1.33	1.38
2	A	300	DAU	O2-C2	2.15	1.48	1.43
2	A	301	DAU	O41-C41	2.11	1.27	1.23
2	A	300	DAU	C61-C51	2.00	1.37	1.34

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	300	DAU	C41-N31-C21	-6.60	118.80	127.35
2	B	300	DAU	C51-C41-N31	5.96	120.40	115.31
2	B	301	DAU	C41-N31-C21	-5.51	120.22	127.35
2	B	301	DAU	P-OPP-P2	-5.40	114.29	132.83
2	B	300	DAU	P-OPP-P2	-5.31	114.61	132.83
2	A	300	DAU	C41-N31-C21	-5.15	120.68	127.35
2	A	300	DAU	C51-C41-N31	5.13	119.69	115.31
2	B	300	DAU	C51-C61-N11	-4.77	118.43	123.34
2	B	301	DAU	N31-C21-N11	4.69	121.11	114.89
2	B	301	DAU	C51-C41-N31	4.64	119.27	115.31
2	B	301	DAU	C51-C61-N11	-4.62	118.58	123.34
2	A	301	DAU	P-OPP-P2	-4.57	117.14	132.83
2	B	300	DAU	N31-C21-N11	4.55	120.93	114.89
2	A	301	DAU	C51-C41-N31	4.30	118.98	115.31
2	A	300	DAU	N31-C21-N11	4.09	120.32	114.89
2	A	300	DAU	C5A-C51-C41	3.88	123.04	118.77
2	A	301	DAU	C41-N31-C21	-3.88	122.33	127.35
2	A	300	DAU	C51-C61-N11	-3.71	119.52	123.34
2	A	301	DAU	N31-C21-N11	3.61	119.68	114.89
2	B	301	DAU	C5A-C51-C61	-3.56	118.09	122.85
2	B	300	DAU	O41-C41-C51	-3.46	120.89	124.90
2	A	301	DAU	O41-C41-C51	-3.42	120.94	124.90
2	B	300	DAU	C5A-C51-C41	3.41	122.52	118.77
2	A	301	DAU	C51-C61-N11	-3.22	120.02	123.34
2	A	301	DAU	O5-C1-O1	3.08	115.40	111.36
2	B	300	DAU	C5A-C51-C61	-3.08	118.73	122.85
2	B	301	DAU	C3-C4-C5	3.04	115.66	110.24
2	A	300	DAU	C5A-C51-C61	-3.01	118.83	122.85
2	B	301	DAU	O21-C21-N31	-2.90	116.09	121.50
2	B	301	DAU	C61-C51-C41	2.85	120.42	118.03
2	B	301	DAU	C2-C3-C4	2.82	115.75	110.82
2	A	301	DAU	O1-C1-C2	2.81	113.53	108.38
2	B	301	DAU	O5'-P-O1P	-2.77	98.23	109.07
2	B	301	DAU	O5-C5-C6	2.67	113.06	106.44
2	A	300	DAU	O41-C41-C51	-2.57	121.92	124.90
2	A	301	DAU	C5A-C51-C41	2.56	121.59	118.77
2	B	301	DAU	O5-C1-C2	-2.51	105.04	110.35
2	B	301	DAU	C5A-C51-C41	2.47	121.49	118.77
2	B	300	DAU	O21-C21-N11	-2.42	119.56	122.79
2	A	301	DAU	C5A-C51-C61	-2.39	119.66	122.85
2	A	300	DAU	O21-C21-N11	-2.38	119.62	122.79
2	A	300	DAU	C6-C5-C4	-2.37	107.46	113.00
2	B	300	DAU	O2P-P-O1P	2.33	123.74	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	DAU	OPP-P2-O1	-2.30	97.85	102.48
2	A	301	DAU	P2-O1-C1	2.27	128.53	119.74
2	B	301	DAU	O5-C5-C4	2.27	113.82	109.69
2	A	300	DAU	O4'-C1'-N11	-2.16	104.00	107.86
2	A	301	DAU	O21-C21-N11	-2.11	119.98	122.79
2	B	300	DAU	O4P-P2-O3P	2.10	122.64	112.24
2	B	301	DAU	O4P-P2-O3P	2.00	122.15	112.24

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	300	DAU	C1-O1-P2-OPP
2	A	301	DAU	O5-C1-O1-P2
2	B	300	DAU	C1-O1-P2-OPP
2	B	301	DAU	O5-C1-O1-P2
2	B	301	DAU	C5'-O5'-P-OPP
2	B	301	DAU	C5'-O5'-P-O1P
2	B	301	DAU	C5'-O5'-P-O2P
2	B	301	DAU	C4-C5-C6-O6
2	B	301	DAU	O5-C5-C6-O6
2	B	301	DAU	C1-O1-P2-OPP
2	B	300	DAU	C2-C1-O1-P2
2	B	301	DAU	C1-O1-P2-O3P
2	B	301	DAU	P-OPP-P2-O4P
2	B	300	DAU	O5-C5-C6-O6
2	B	301	DAU	P-OPP-P2-O3P
2	A	300	DAU	C1-O1-P2-O4P
2	B	300	DAU	C3'-C4'-C5'-O5'
2	B	301	DAU	C1-O1-P2-O4P

There are no ring outliers.

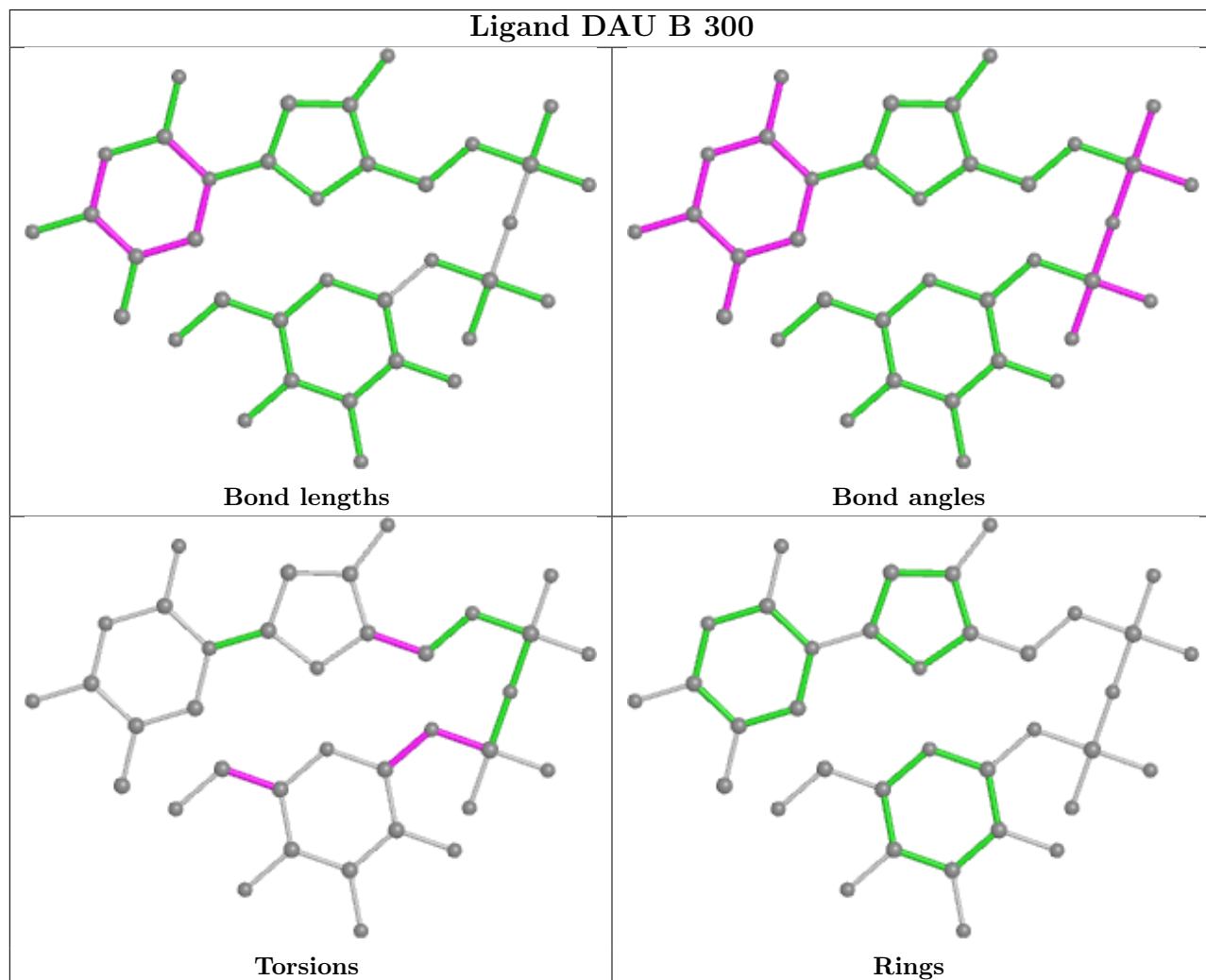
4 monomers are involved in 8 short contacts:

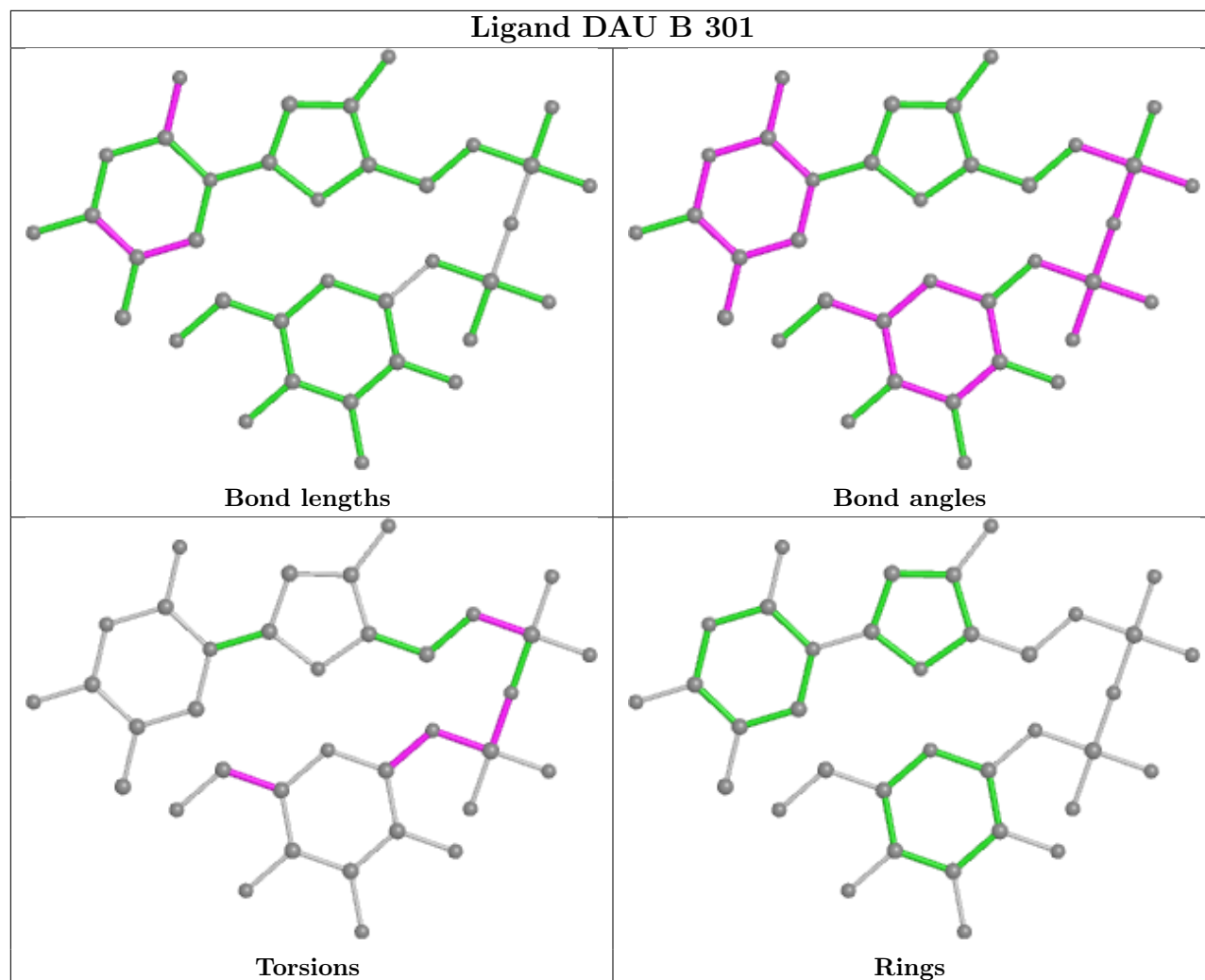
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	300	DAU	2	0
2	B	301	DAU	3	0
2	A	301	DAU	2	0
2	A	300	DAU	1	0

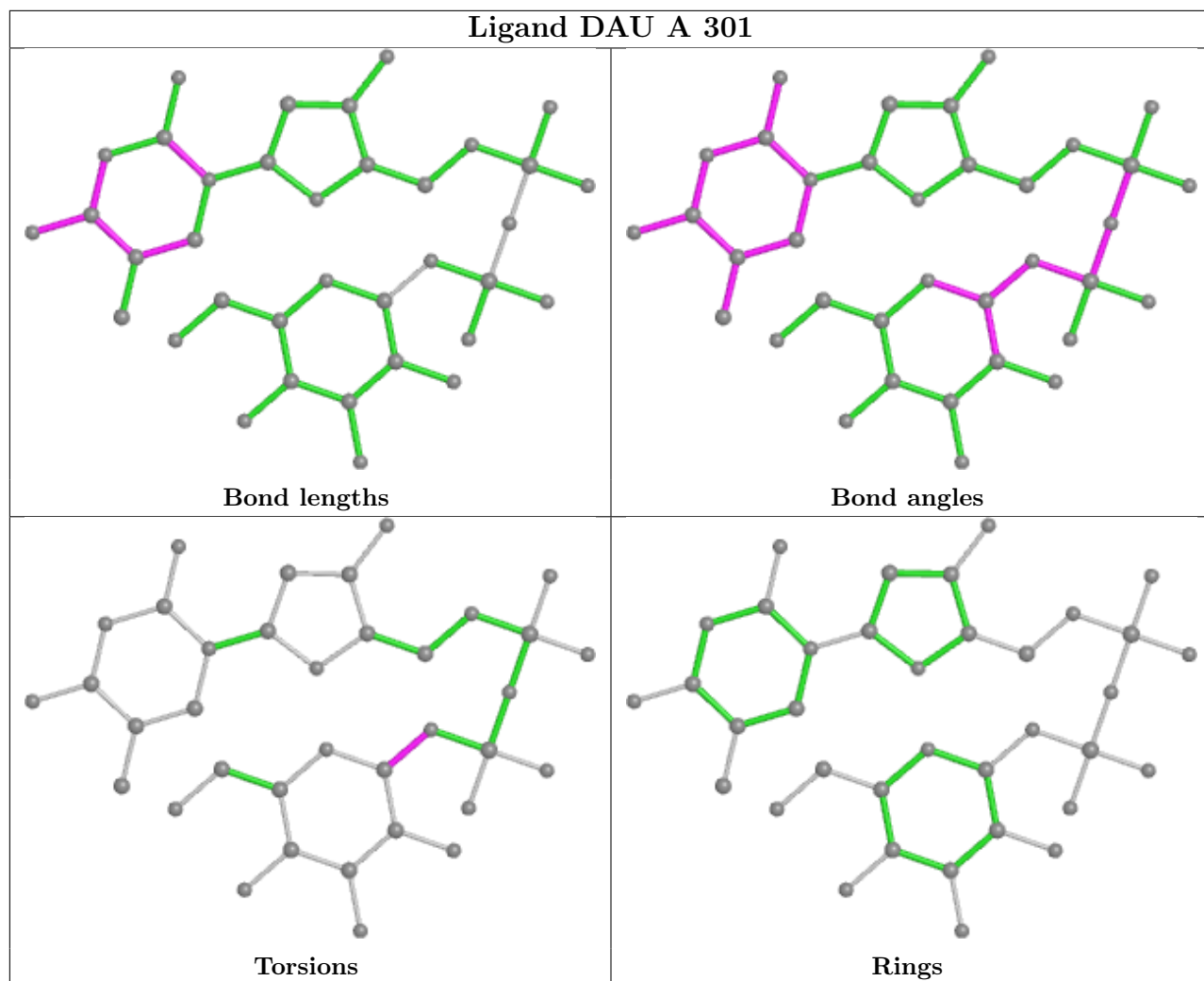
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

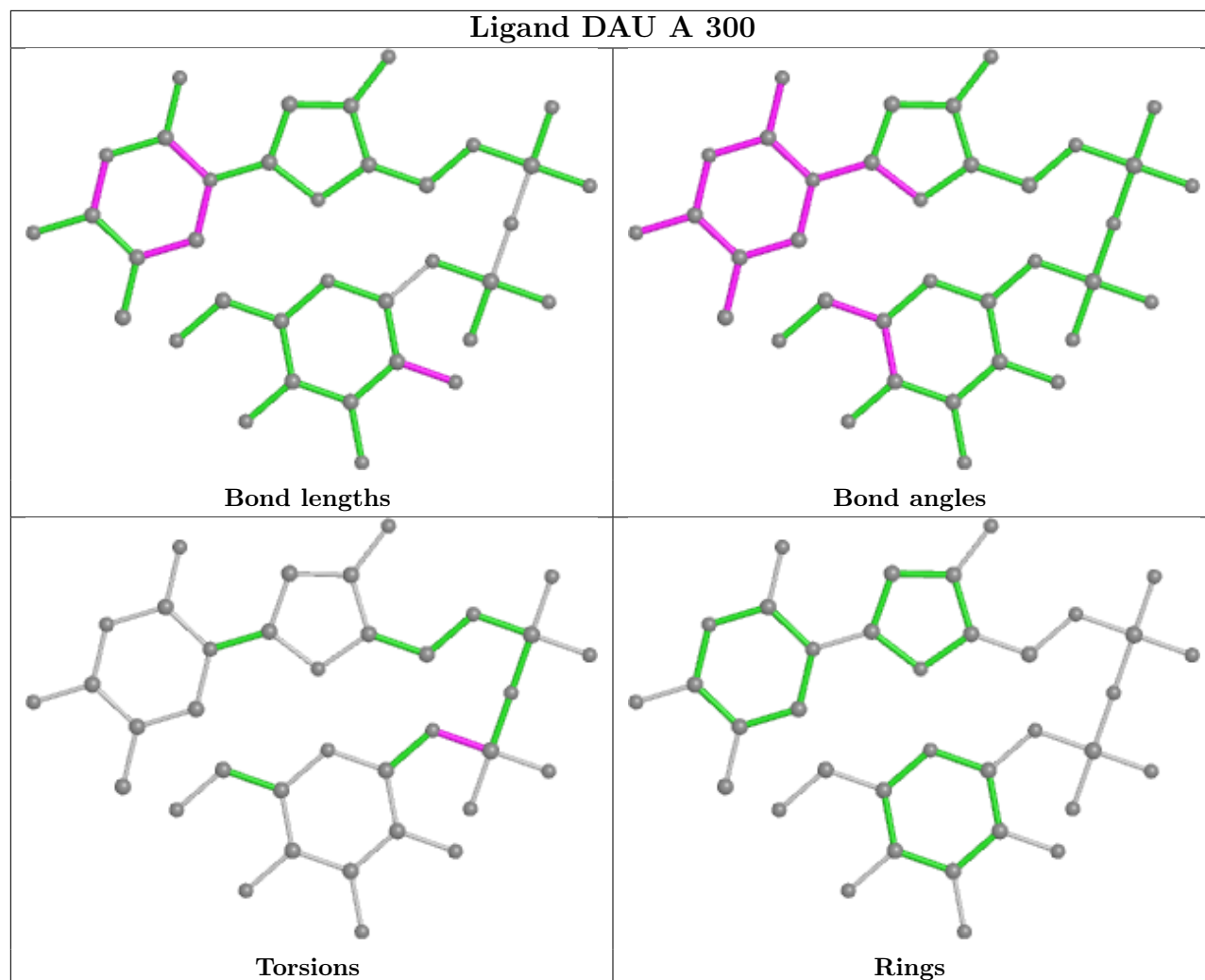


bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	288/297 (96%)	-0.03	11 (3%) 40 45	16, 24, 38, 55	0
1	B	289/297 (97%)	0.21	16 (5%) 25 27	16, 26, 45, 75	0
All	All	577/594 (97%)	0.09	27 (4%) 31 35	16, 26, 43, 75	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	151	LYS	5.9
1	B	149	ASP	5.1
1	B	152	GLY	4.8
1	A	151	LYS	4.3
1	B	150	GLU	4.2
1	B	163	GLU	3.8
1	B	289	SER	3.4
1	B	162	GLU	3.4
1	B	161	PRO	3.2
1	A	150	GLU	3.1
1	B	148	PHE	3.0
1	B	10	SER	2.8
1	B	11	GLY	2.8
1	A	38	LEU	2.7
1	A	20	VAL	2.6
1	A	105	VAL	2.5
1	A	149	ASP	2.4
1	A	152	GLY	2.4
1	B	153	LYS	2.3
1	B	275	LYS	2.3
1	B	164	PRO	2.2
1	A	162	GLU	2.1
1	A	287	HIS	2.1
1	B	21	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	127	LYS	2.1
1	A	163	GLU	2.1
1	A	21	VAL	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

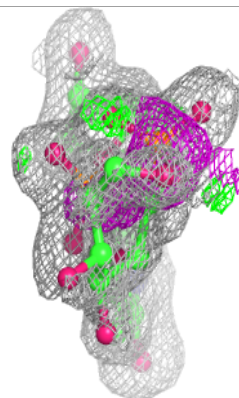
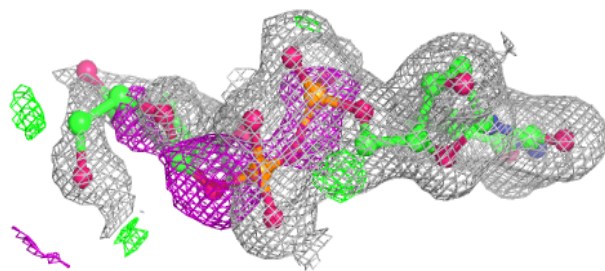
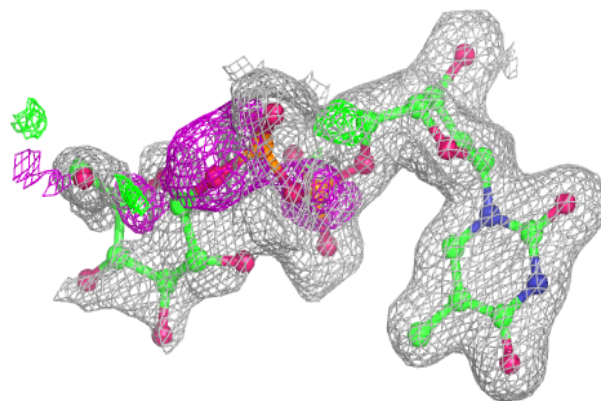
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	DAU	A	301	36/36	0.84	0.16	16,32,72,73	0
3	SO4	A	303	5/5	0.85	0.13	61,63,65,68	0
2	DAU	B	301	36/36	0.90	0.16	16,31,73,74	0
3	SO4	B	303	5/5	0.90	0.21	66,66,68,71	0
3	SO4	A	304	5/5	0.91	0.16	37,38,49,51	0
2	DAU	B	300	36/36	0.93	0.09	23,29,48,53	0
3	SO4	B	302	5/5	0.97	0.18	43,47,47,48	0
2	DAU	A	300	36/36	0.98	0.07	16,23,30,35	0
3	SO4	A	302	5/5	0.99	0.09	31,32,34,41	0

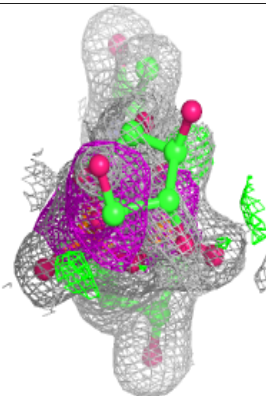
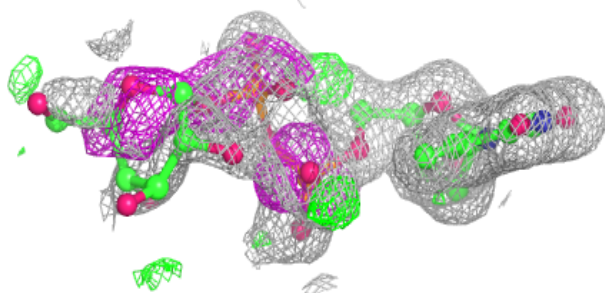
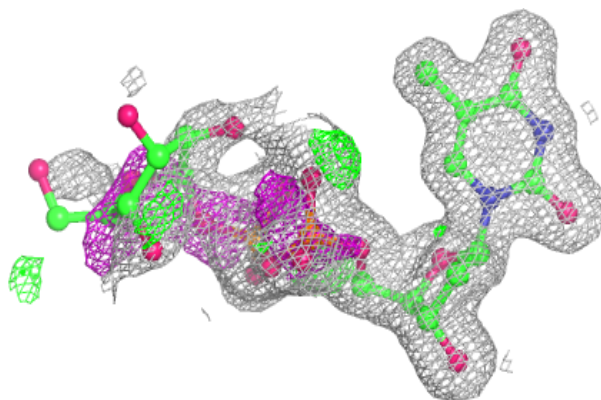
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around DAU A 301:**

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

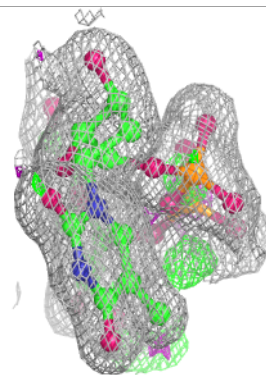
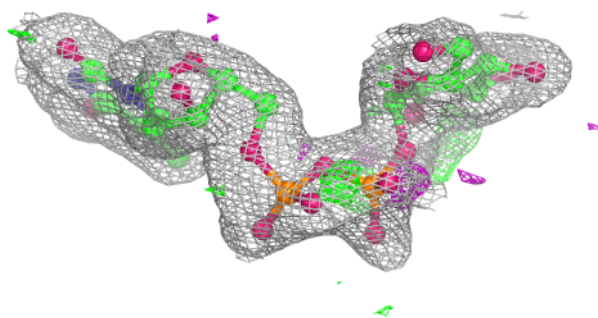
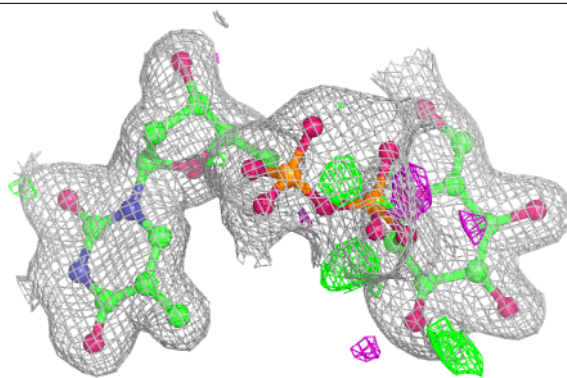
**Electron density around DAU B 301:**

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

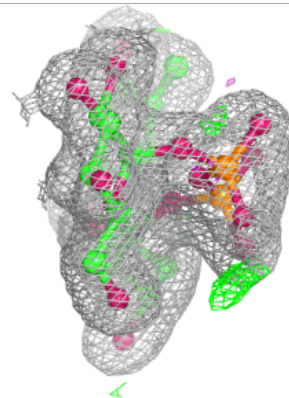
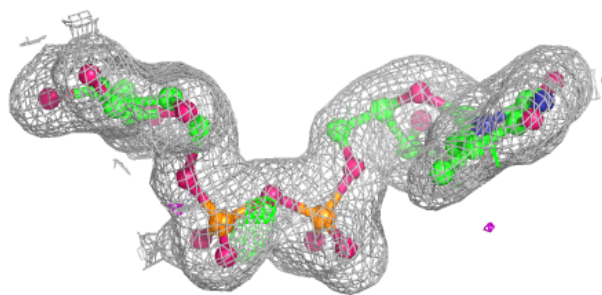
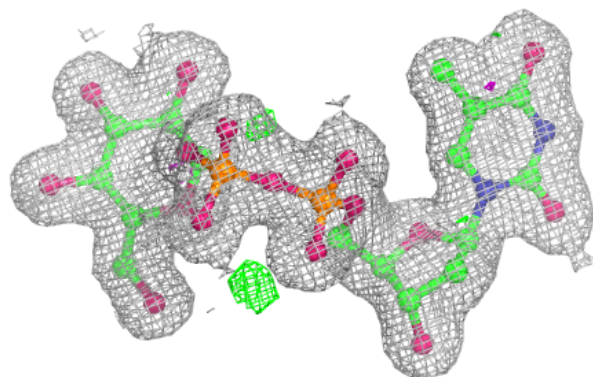


**Electron density around DAU B 300:**

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

**Electron density around DAU A 300:**

$2mF_o-DF_c$  (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.