



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 07:10 pm BST

PDB ID : 4KCG  
Title : Human dCK C4S-S74E mutant in complex with UDP and the DI-39 inhibitor  
Authors : Nomme, J.; Lavie, A.  
Deposited on : 2013-04-24  
Resolution : 2.09 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.

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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 : 2.11  
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

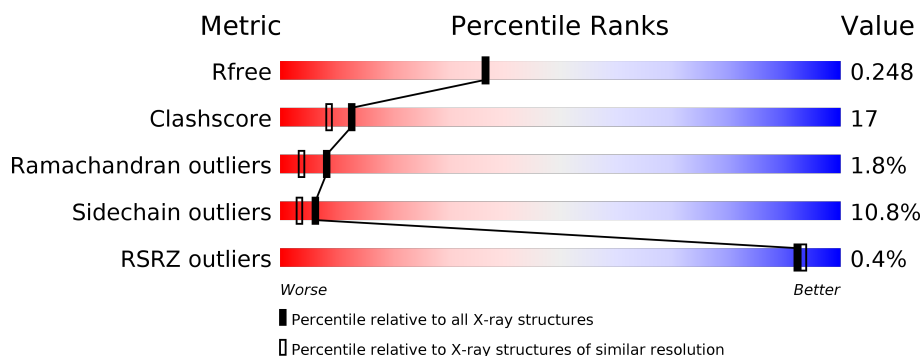
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.09 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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  $\geq 3$ , 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	280	<div> <div style="width: 52%; background-color: green;"></div> <div style="width: 26%; background-color: yellow;"></div> <div style="width: 18%; background-color: grey;"></div> </div>
1	B	280	<div> <div style="width: 48%; background-color: green;"></div> <div style="width: 30%; background-color: yellow;"></div> <div style="width: 18%; background-color: grey;"></div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4027 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 Deoxycytidine kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	230	Total	C	N	O	S	0	3	0
			1910	1225	315	362	8			
1	B	230	Total	C	N	O	S	0	4	0
			1905	1224	315	358	8			

There are 50 discrepancies between the modelled and reference sequences:

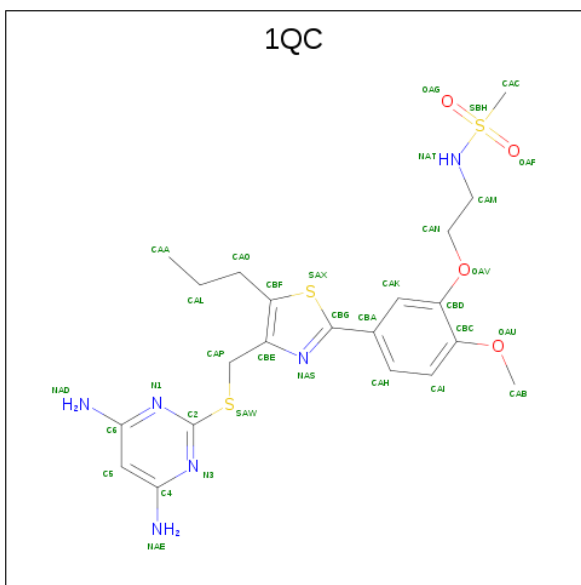
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	INITIATING METHIONINE	UNP P27707
A	-18	GLY	-	EXPRESSION TAG	UNP P27707
A	-17	SER	-	EXPRESSION TAG	UNP P27707
A	-16	SER	-	EXPRESSION TAG	UNP P27707
A	-15	HIS	-	EXPRESSION TAG	UNP P27707
A	-14	HIS	-	EXPRESSION TAG	UNP P27707
A	-13	HIS	-	EXPRESSION TAG	UNP P27707
A	-12	HIS	-	EXPRESSION TAG	UNP P27707
A	-11	HIS	-	EXPRESSION TAG	UNP P27707
A	-10	HIS	-	EXPRESSION TAG	UNP P27707
A	-9	SER	-	EXPRESSION TAG	UNP P27707
A	-8	SER	-	EXPRESSION TAG	UNP P27707
A	-7	GLY	-	EXPRESSION TAG	UNP P27707
A	-6	LEU	-	EXPRESSION TAG	UNP P27707
A	-5	VAL	-	EXPRESSION TAG	UNP P27707
A	-4	PRO	-	EXPRESSION TAG	UNP P27707
A	-3	ARG	-	EXPRESSION TAG	UNP P27707
A	-2	GLY	-	EXPRESSION TAG	UNP P27707
A	-1	SER	-	EXPRESSION TAG	UNP P27707
A	0	HIS	-	EXPRESSION TAG	UNP P27707
A	9	SER	CYS	ENGINEERED MUTATION	UNP P27707
A	45	SER	CYS	ENGINEERED MUTATION	UNP P27707
A	59	SER	CYS	ENGINEERED MUTATION	UNP P27707
A	74	GLU	SER	ENGINEERED MUTATION	UNP P27707
A	146	SER	CYS	ENGINEERED MUTATION	UNP P27707

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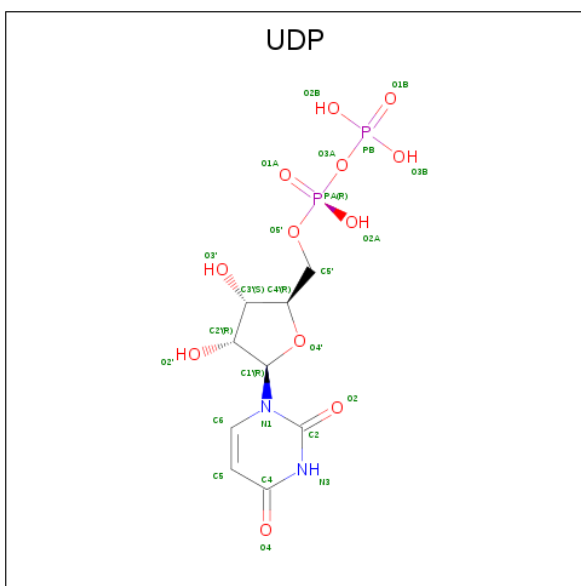
Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	INITIATING METHIONINE	UNP P27707
B	-18	GLY	-	EXPRESSION TAG	UNP P27707
B	-17	SER	-	EXPRESSION TAG	UNP P27707
B	-16	SER	-	EXPRESSION TAG	UNP P27707
B	-15	HIS	-	EXPRESSION TAG	UNP P27707
B	-14	HIS	-	EXPRESSION TAG	UNP P27707
B	-13	HIS	-	EXPRESSION TAG	UNP P27707
B	-12	HIS	-	EXPRESSION TAG	UNP P27707
B	-11	HIS	-	EXPRESSION TAG	UNP P27707
B	-10	HIS	-	EXPRESSION TAG	UNP P27707
B	-9	SER	-	EXPRESSION TAG	UNP P27707
B	-8	SER	-	EXPRESSION TAG	UNP P27707
B	-7	GLY	-	EXPRESSION TAG	UNP P27707
B	-6	LEU	-	EXPRESSION TAG	UNP P27707
B	-5	VAL	-	EXPRESSION TAG	UNP P27707
B	-4	PRO	-	EXPRESSION TAG	UNP P27707
B	-3	ARG	-	EXPRESSION TAG	UNP P27707
B	-2	GLY	-	EXPRESSION TAG	UNP P27707
B	-1	SER	-	EXPRESSION TAG	UNP P27707
B	0	HIS	-	EXPRESSION TAG	UNP P27707
B	9	SER	CYS	ENGINEERED MUTATION	UNP P27707
B	45	SER	CYS	ENGINEERED MUTATION	UNP P27707
B	59	SER	CYS	ENGINEERED MUTATION	UNP P27707
B	74	GLU	SER	ENGINEERED MUTATION	UNP P27707
B	146	SER	CYS	ENGINEERED MUTATION	UNP P27707

- Molecule 2 is N-{2-[5-(4-[(4,6-diaminopyrimidin-2-yl)sulfanyl]methyl)-5-propyl-1,3-thiazol-2-yl)-2-methoxyphenoxy]ethyl}methanesulfonamide (three-letter code: 1QC) (formula: C<sub>21</sub>H<sub>28</sub>N<sub>6</sub>O<sub>4</sub>S<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 34	C 21	N 6	O 4	S 3	0	0
2	B	1	Total 34	C 21	N 6	O 4	S 3	0	0

- Molecule 3 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula:  $\text{C}_9\text{H}_{14}\text{N}_2\text{O}_{12}\text{P}_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 25	C 9	N 2	O 12	P 2	0	0
3	B	1	Total 25	C 9	N 2	O 12	P 2	0	0

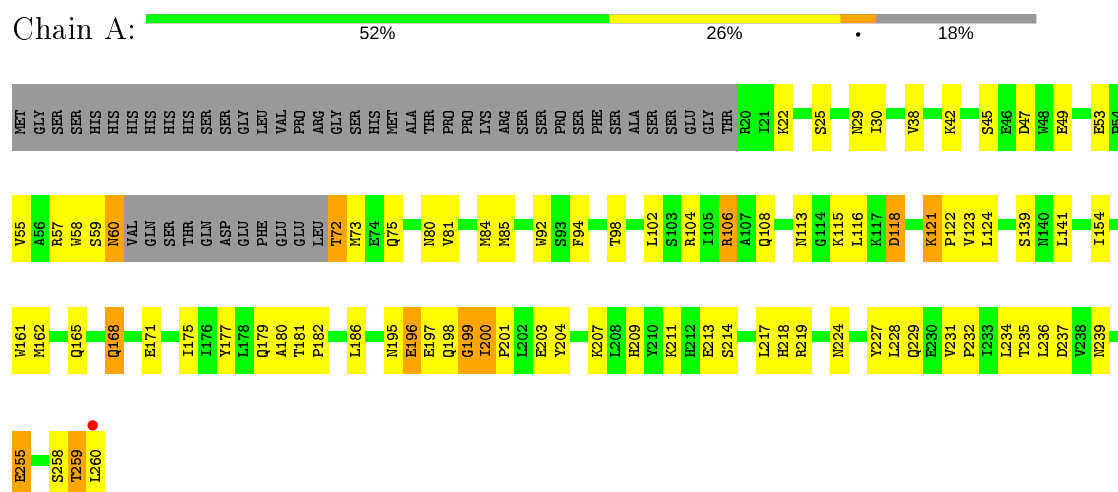
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	40	Total 40	O 40	0	0
4	B	54	Total 54	O 54	0	0

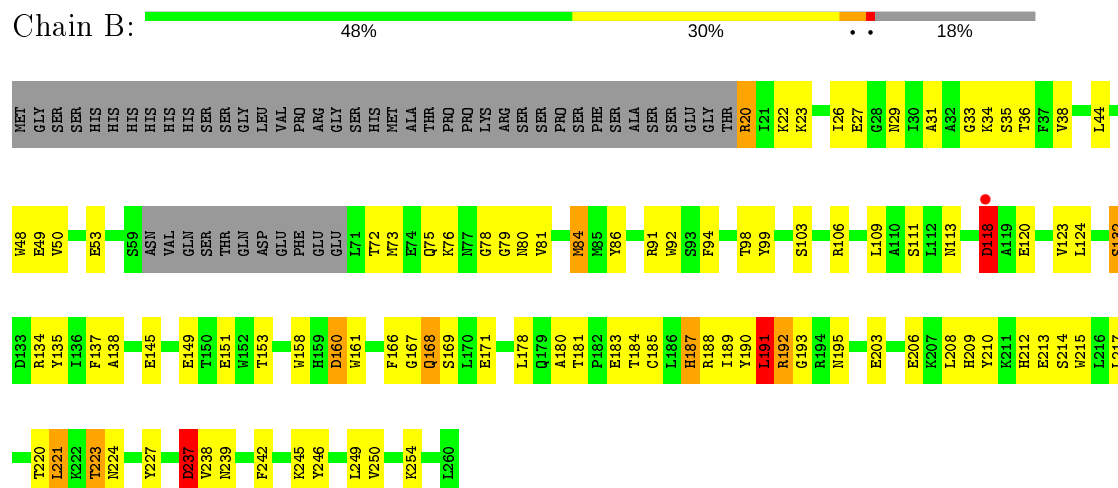
### 3 Residue-property plots

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: Deoxycytidine kinase



#### • Molecule 1: Deoxycytidine kinase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.73 Å 68.73 Å 120.59 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.61 – 2.09 27.61 – 2.09	Depositor EDS
% Data completeness (in resolution range)	96.4 (27.61-2.09) 96.5 (27.61-2.09)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.20 (at 2.10 Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.177 , 0.248 0.178 , 0.248	Depositor DCC
$R_{free}$ test set	1617 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	52.5	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 39.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.478 for h,-k,-l	Xtriage
Reported twinning fraction	0.504 for H, K, L 0.496 for -H, K, -L	Depositor
Outliers	0 of 32256 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	4027	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.09% 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: UDP, 1QC

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	0.58	0/1965	0.76	0/2661
1	B	0.59	0/1962	0.78	1/2654 (0.0%)
All	All	0.59	0/3927	0.77	1/5315 (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	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	191	LEU	CA-CB-CG	5.38	127.67	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	118	ASP	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	1910	0	1837	55	0
1	B	1905	0	1847	76	0
2	A	34	0	28	1	0
2	B	34	0	28	3	0
3	A	25	0	11	0	0
3	B	25	0	11	2	0
4	A	40	0	0	5	0
4	B	54	0	0	6	0
All	All	4027	0	3762	128	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 17.

All (128) 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:237:ASP:OD2	1:B:239:ASN:HB2	1.46	1.13
1:B:75:GLN:HG3	4:B:443:HOH:O	1.68	0.91
1:A:94:PHE:O	1:A:98:THR:HG23	1.73	0.87
1:A:45:SER:O	4:A:407:HOH:O	1.96	0.84
1:B:78:GLY:HA2	1:B:81:VAL:HG12	1.59	0.82
1:B:215:TRP:HB2	1:B:221:LEU:HD22	1.61	0.80
1:B:48:TRP:O	4:B:453:HOH:O	1.99	0.79
1:A:237:ASP:OD2	1:A:239:ASN:ND2	2.17	0.77
1:B:75:GLN:O	1:B:79:GLY:N	2.16	0.74
1:B:181:THR:OG1	1:B:184:THR:N	2.15	0.74
1:B:26:ILE:HD12	1:B:38:VAL:HG12	1.70	0.73
1:A:42:LYS:O	4:A:407:HOH:O	2.08	0.70
1:B:120:GLU:N	1:B:120:GLU:OE1	2.23	0.69
1:B:166:PHE:HB3	1:B:169:SER:OG	1.93	0.68
1:A:49:GLU:HB3	1:A:124:LEU:HD12	1.76	0.68
1:B:167:GLY:O	1:B:168:GLN:HB2	1.93	0.67
2:B:301:1QC:OAU	2:B:301:1QC:H7	1.93	0.67
1:A:180:ALA:O	1:A:181:THR:HG23	1.95	0.66
1:A:228:LEU:HA	1:A:231:VAL:HB	1.77	0.66
1:B:242:PHE:HB2	1:B:249:LEU:HD11	1.76	0.66
1:B:94:PHE:O	1:B:98:THR:HG23	1.97	0.64
1:A:113:ASN:HB2	4:A:428:HOH:O	1.98	0.64
1:B:31:ALA:HB3	1:B:189:ILE:HG13	1.82	0.62
1:A:25:SER:HB3	1:A:175:ILE:HG12	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:ARG:HB2	3:B:302:UDP:H4'	1.83	0.60
1:B:242:PHE:CB	1:B:249:LEU:HD11	2.32	0.59
1:B:238:VAL:HB	1:B:242:PHE:CE2	2.38	0.58
1:B:27:GLU:OE2	4:B:402:HOH:O	2.17	0.58
1:A:199:GLY:O	1:A:200:ILE:O	2.21	0.58
1:B:238:VAL:HB	1:B:242:PHE:HE2	1.69	0.58
1:A:219:ARG:NH2	1:A:229:GLN:O	2.36	0.58
1:A:102:LEU:HD12	1:B:158:TRP:HD1	1.69	0.57
1:A:168:GLN:HE21	1:A:168:GLN:HA	1.70	0.57
1:B:188:ARG:HA	1:B:191:LEU:HB3	1.87	0.57
1:A:201:PRO:HG2	1:A:204:TYR:HB2	1.85	0.56
1:B:220:THR:OG1	1:B:221:LEU:N	2.36	0.56
1:B:23:LYS:NZ	1:B:23:LYS:HB2	2.20	0.56
1:B:134:ARG:HA	1:B:138:ALA:HB3	1.88	0.56
1:A:116:LEU:HB3	1:A:122:PRO:HB3	1.87	0.56
1:B:188:ARG:HA	1:B:191:LEU:CB	2.37	0.55
1:B:26:ILE:HD12	1:B:38:VAL:CG1	2.36	0.55
1:A:102:LEU:CD1	1:B:158:TRP:HD1	2.19	0.55
1:B:210:TYR:O	1:B:214[A]:SER:HB3	2.07	0.55
1:B:180:ALA:HB1	1:B:184:THR:HB	1.89	0.54
1:A:177:TYR:CD2	1:A:235:THR:HG23	2.43	0.54
1:B:35:SER:HA	1:B:38:VAL:HG22	1.89	0.54
1:A:47:ASP:HB3	1:A:121:LYS:O	2.08	0.53
1:A:106:ARG:HH21	1:B:161:TRP:HB2	1.74	0.53
1:B:132:SER:O	1:B:137:PHE:HD1	1.91	0.53
1:B:190:TYR:C	1:B:192:ARG:H	2.12	0.52
1:B:242:PHE:O	1:B:246:TYR:HB3	2.09	0.52
1:A:22:LYS:HB2	1:A:123:VAL:HG22	1.91	0.52
1:B:242:PHE:HB2	1:B:249:LEU:CD1	2.38	0.52
1:A:104:ARG:O	1:A:108:GLN:HG3	2.10	0.52
1:A:217:LEU:HD23	1:A:218:HIS:CE1	2.45	0.52
1:A:161:TRP:HZ2	1:B:109:LEU:HD12	1.74	0.52
1:B:151:GLU:OE2	4:B:407:HOH:O	2.19	0.52
1:B:76:LYS:O	1:B:80:ASN:N	2.43	0.51
1:A:171:GLU:HG3	1:A:227:TYR:CZ	2.45	0.51
1:A:181:THR:HB	1:A:182:PRO:HD2	1.93	0.51
1:B:103:SER:HA	1:B:106:ARG:HG2	1.93	0.51
1:B:134:ARG:NH2	1:B:160:ASP:OD2	2.41	0.51
1:A:118:ASP:O	1:A:118:ASP:OD2	2.30	0.50
1:B:84[A]:MET:HG2	1:B:92:TRP:CD1	2.45	0.50
1:A:201:PRO:O	1:A:204:TYR:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:GLU:HA	1:B:206:GLU:OE2	2.11	0.50
1:A:255:GLU:O	1:A:259:THR:HG23	2.12	0.50
1:B:167:GLY:O	1:B:168:GLN:CB	2.60	0.49
1:A:102:LEU:HD12	1:A:162:MET:CE	2.42	0.49
1:A:55:VAL:HG11	2:A:301:1QC:NAD	2.27	0.49
1:B:34:LYS:HA	1:B:178:LEU:HD12	1.95	0.49
1:B:29:ASN:HB3	1:B:185:CYS:SG	2.53	0.49
1:B:84[A]:MET:HG2	1:B:92:TRP:NE1	2.28	0.49
1:B:145:GLU:HA	4:B:435:HOH:O	2.12	0.48
1:B:187:HIS:O	1:B:191:LEU:HB2	2.12	0.48
1:B:190:TYR:O	1:B:192:ARG:N	2.46	0.48
1:A:49:GLU:HB3	1:A:124:LEU:CD1	2.42	0.48
1:B:192:ARG:HG2	1:B:193:GLY:N	2.29	0.48
1:B:86:TYR:CD2	2:B:301:1QC:H14	2.49	0.48
1:A:204:TYR:OH	4:A:410:HOH:O	2.19	0.47
1:B:166:PHE:HB3	1:B:169:SER:HG	1.80	0.47
1:B:33:GLY:O	1:B:36:THR:HB	2.15	0.46
1:A:171:GLU:HB3	4:A:421:HOH:O	2.15	0.46
1:A:59:SER:C	1:A:60:ASN:HD22	2.19	0.46
1:A:80:ASN:O	1:A:84[A]:MET:HG3	2.15	0.46
1:B:190:TYR:C	1:B:192:ARG:N	2.68	0.46
1:B:135:TYR:CZ	1:B:223:THR:HB	2.51	0.46
1:A:81:VAL:HA	1:A:84[A]:MET:SD	2.56	0.45
1:B:134:ARG:HH12	1:B:160:ASP:CG	2.19	0.45
1:B:134:ARG:NH1	1:B:160:ASP:OD2	2.46	0.45
1:A:141:LEU:HA	1:A:141:LEU:HD23	1.78	0.45
1:A:84[A]:MET:HE2	1:A:92:TRP:CZ2	2.52	0.44
1:A:154:ILE:HG23	1:B:99:TYR:CD1	2.52	0.44
1:A:53:GLU:O	1:A:57:ARG:HG3	2.17	0.44
1:A:161:TRP:CE2	1:A:165:GLN:HG3	2.53	0.44
1:A:196:GLU:H	1:A:196:GLU:HG3	1.70	0.44
1:B:180:ALA:HB3	1:B:185:CYS:SG	2.57	0.44
1:A:234:LEU:HD21	1:A:236:LEU:HD21	1.99	0.44
1:B:181:THR:C	1:B:183:GLU:N	2.69	0.44
1:B:168:GLN:CG	1:B:171:GLU:OE1	2.65	0.44
1:B:91:ARG:HG3	1:B:92:TRP:CE2	2.53	0.44
1:B:168:GLN:HG3	1:B:171:GLU:OE1	2.18	0.43
1:A:29:ASN:OD1	1:A:30:ILE:N	2.50	0.43
1:A:49:GLU:HG2	1:A:115:LYS:HD3	2.00	0.43
1:A:213:GLU:O	1:A:217:LEU:N	2.52	0.42
1:B:208:LEU:O	1:B:212:HIS:N	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:TRP:HD1	1:A:75:GLN:NE2	2.17	0.42
1:A:72:THR:OG1	1:A:75:GLN:HB2	2.19	0.42
1:B:149:GLU:O	1:B:153:THR:OG1	2.28	0.42
1:B:168:GLN:HA	1:B:171:GLU:CG	2.50	0.42
1:B:26:ILE:CD1	1:B:38:VAL:HG12	2.42	0.42
1:A:197:GLU:O	1:A:199:GLY:N	2.53	0.42
1:B:209:HIS:NE2	1:B:213:GLU:HG3	2.35	0.41
1:B:48:TRP:CD1	1:B:123:VAL:HB	2.55	0.41
1:B:72:THR:HG23	4:B:443:HOH:O	2.19	0.41
1:A:29:ASN:ND2	1:A:209:HIS:HB2	2.36	0.41
1:B:31:ALA:HB2	1:B:192:ARG:NH1	2.35	0.41
1:A:231:VAL:HA	1:A:232:PRO:HD3	1.78	0.41
2:B:301:1QC:OAU	2:B:301:1QC:CAN	2.66	0.41
1:A:102:LEU:HD12	1:A:162:MET:HE2	2.03	0.41
1:B:44:LEU:HD13	1:B:250:VAL:HG11	2.02	0.41
1:B:38:VAL:O	1:B:50:VAL:HG21	2.21	0.40
1:A:84[B]:MET:SD	1:A:92:TRP:CZ2	3.14	0.40
1:B:20:ARG:HH12	1:B:118:ASP:HA	1.87	0.40
1:A:201:PRO:C	1:A:203:GLU:N	2.71	0.40
1:A:217:LEU:HD23	1:A:218:HIS:ND1	2.36	0.40
1:B:23:LYS:HZ2	1:B:23:LYS:HB2	1.86	0.40
1:B:33:GLY:H	3:B:302:UDP:PB	2.44	0.40

There are no symmetry-related clashes.

## 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	229/280 (82%)	208 (91%)	18 (8%)	3 (1%)	12	7
1	B	230/280 (82%)	206 (90%)	19 (8%)	5 (2%)	6	2
All	All	459/560 (82%)	414 (90%)	37 (8%)	8 (2%)	8	4

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	200	ILE
1	B	168	GLN
1	A	198	GLN
1	B	191	LEU
1	B	118	ASP
1	B	195	ASN
1	B	237	ASP
1	A	199	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	208/256 (81%)	187 (90%)	21 (10%)	7	4
1	B	207/256 (81%)	183 (88%)	24 (12%)	5	3
All	All	415/512 (81%)	370 (89%)	45 (11%)	6	3

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	VAL
1	A	60	ASN
1	A	72	THR
1	A	73	MET
1	A	85	MET
1	A	106	ARG
1	A	121	LYS
1	A	139	SER
1	A	168	GLN
1	A	179	GLN
1	A	186	LEU
1	A	195	ASN
1	A	196	GLU
1	A	207	LYS
1	A	211	LYS

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Mol	Chain	Res	Type
1	A	214	SER
1	A	224	ASN
1	A	255	GLU
1	A	258	SER
1	A	259	THR
1	A	260	LEU
1	B	20	ARG
1	B	22	LYS
1	B	49	GLU
1	B	53	GLU
1	B	73	MET
1	B	84[A]	MET
1	B	84[B]	MET
1	B	111	SER
1	B	113	ASN
1	B	118	ASP
1	B	124	LEU
1	B	132	SER
1	B	160	ASP
1	B	187	HIS
1	B	191	LEU
1	B	192	ARG
1	B	217	LEU
1	B	221	LEU
1	B	223	THR
1	B	224	ASN
1	B	227	TYR
1	B	237	ASP
1	B	245	LYS
1	B	254	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	75	GLN
1	A	77	ASN
1	A	113	ASN
1	A	168	GLN
1	B	163	ASN

### 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 ⓘ

4 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	UDP	B	302	-	20,26,26	0.83	0	25,40,40	0.89	1 (4%)
3	UDP	A	302	-	20,26,26	0.82	0	25,40,40	0.99	1 (4%)
2	1QC	A	301	-	34,36,36	3.58	9 (26%)	37,50,50	2.54	9 (24%)
2	1QC	B	301	-	34,36,36	3.83	8 (23%)	37,50,50	2.64	11 (29%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	UDP	B	302	-	-	0/14/32/32	0/2/2/2
3	UDP	A	302	-	-	5/14/32/32	0/2/2/2
2	1QC	A	301	-	-	4/19/22/22	0/3/3/3
2	1QC	B	301	-	-	9/19/22/22	0/3/3/3



All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	1QC	SBH-NAT	13.26	1.87	1.60
2	A	301	1QC	CAO-CBF	12.87	1.56	1.50
2	B	301	1QC	CAO-CBF	11.61	1.56	1.50
2	A	301	1QC	CBG-SAX	-8.08	1.62	1.73
2	B	301	1QC	CBF-SAX	-7.56	1.60	1.74
2	B	301	1QC	OAG-SBH	6.80	1.55	1.43
2	A	301	1QC	OAG-SBH	6.45	1.54	1.43
2	A	301	1QC	OAF-SBH	6.00	1.54	1.43
2	A	301	1QC	SBH-NAT	5.88	1.72	1.60
2	A	301	1QC	CBF-SAX	-5.80	1.63	1.74
2	B	301	1QC	OAF-SBH	5.78	1.53	1.43
2	B	301	1QC	CBF-CBE	-4.42	1.33	1.42
2	A	301	1QC	CAP-CBE	4.36	1.55	1.50
2	A	301	1QC	CBF-CBE	-3.86	1.35	1.42
2	B	301	1QC	CAP-CBE	3.20	1.53	1.50
2	B	301	1QC	CBG-SAX	-2.85	1.69	1.73
2	A	301	1QC	C2-SAW	2.26	1.79	1.75

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	1QC	CAC-SBH-NAT	8.52	112.98	107.76
2	B	301	1QC	OAG-SBH-OAF	-8.02	107.32	118.85
2	B	301	1QC	C2-N3-C4	6.17	122.38	115.51
2	B	301	1QC	CAP-SAW-C2	6.07	109.10	102.42
2	A	301	1QC	C2-N3-C4	6.00	122.19	115.51
2	A	301	1QC	C2-N1-C6	5.67	121.82	115.51
2	A	301	1QC	OAG-SBH-OAF	-5.32	111.21	118.85
2	B	301	1QC	C2-N1-C6	4.84	120.90	115.51
2	A	301	1QC	N1-C2-N3	-4.35	118.97	126.95
2	B	301	1QC	N1-C2-N3	-3.88	119.85	126.95
2	B	301	1QC	OAV-CBD-CBC	3.65	123.28	115.73
2	A	301	1QC	CAP-SAW-C2	3.11	105.84	102.42
2	B	301	1QC	CAC-SBH-NAT	3.03	109.61	107.76
2	B	301	1QC	OAV-CBD-CAK	-2.72	117.31	123.58
2	B	301	1QC	CAN-OAV-CBD	2.66	124.19	117.69
2	B	301	1QC	CAO-CBF-CBE	-2.53	125.41	127.47
2	A	301	1QC	C4-C5-C6	-2.41	115.73	117.72
3	B	302	UDP	O3B-PB-O1B	2.30	119.67	110.68
2	B	301	1QC	OAU-CBC-CBD	2.25	118.54	115.41
3	A	302	UDP	O3B-PB-O1B	2.23	119.41	110.68
2	A	301	1QC	CBE-CAP-SAW	2.22	114.90	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	A	301	1QC	NAE-C4-N3	2.13	119.85	116.49

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	302	UDP	C2'-C1'-N1-C6
3	A	302	UDP	O4'-C1'-N1-C6
2	A	301	1QC	CAM-NAT-SBH-CAC
2	A	301	1QC	CAM-NAT-SBH-OAF
2	A	301	1QC	CBE-CAP-SAW-C2
2	B	301	1QC	CAM-NAT-SBH-CAC
2	B	301	1QC	CAM-NAT-SBH-OAG
2	B	301	1QC	CBC-CBD-OAV-CAN
2	B	301	1QC	CAK-CBD-OAV-CAN
2	B	301	1QC	NAT-CAM-CAN-OAV
2	B	301	1QC	CAM-CAN-OAV-CBD
2	A	301	1QC	NAT-CAM-CAN-OAV
3	A	302	UDP	PA-O3A-PB-O1B
2	B	301	1QC	CBE-CAP-SAW-C2
2	B	301	1QC	CAA-CAL-CAO-CBF
2	B	301	1QC	CAM-NAT-SBH-OAF
3	A	302	UDP	PA-O3A-PB-O2B
3	A	302	UDP	PA-O3A-PB-O3B

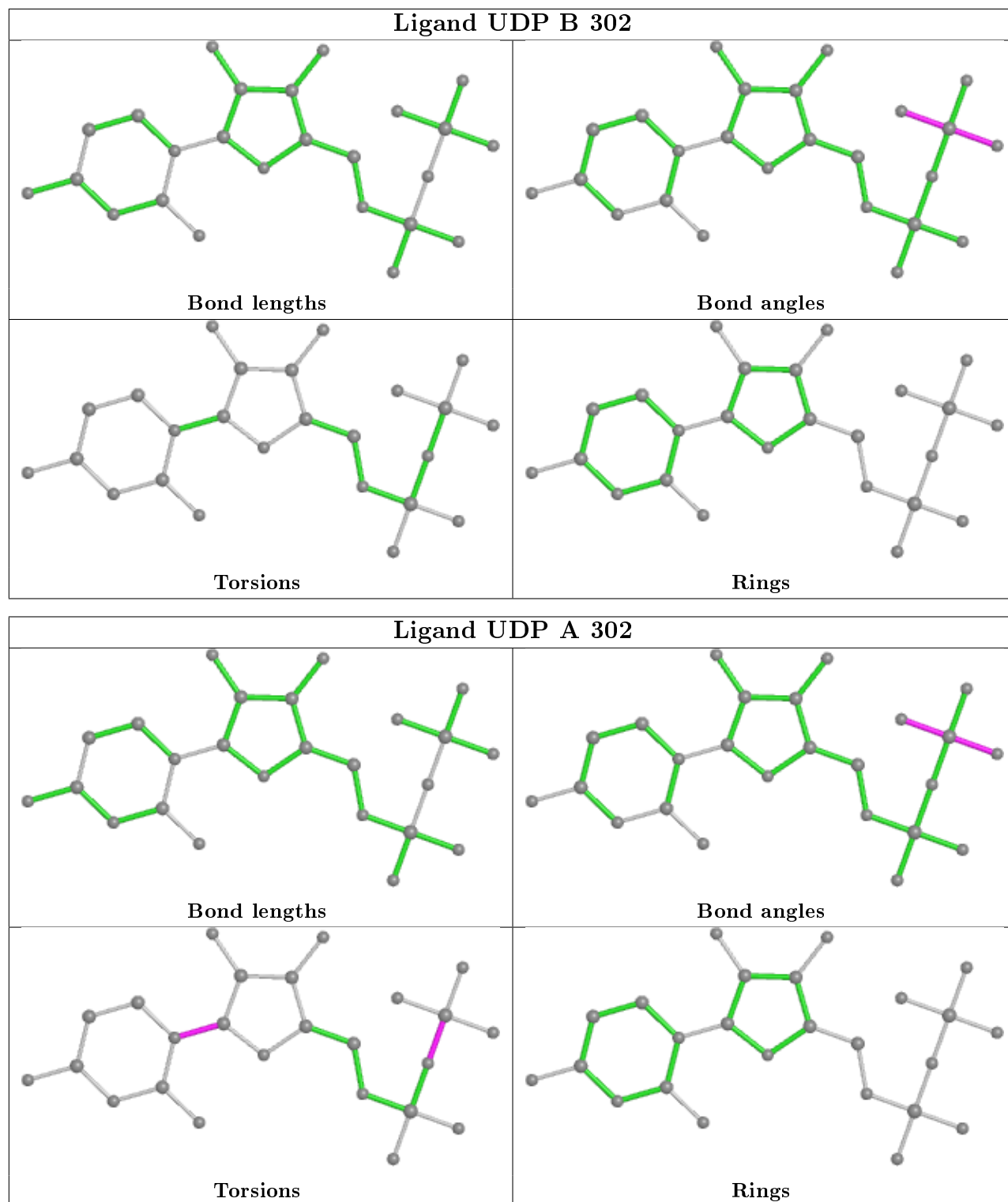
There are no ring outliers.

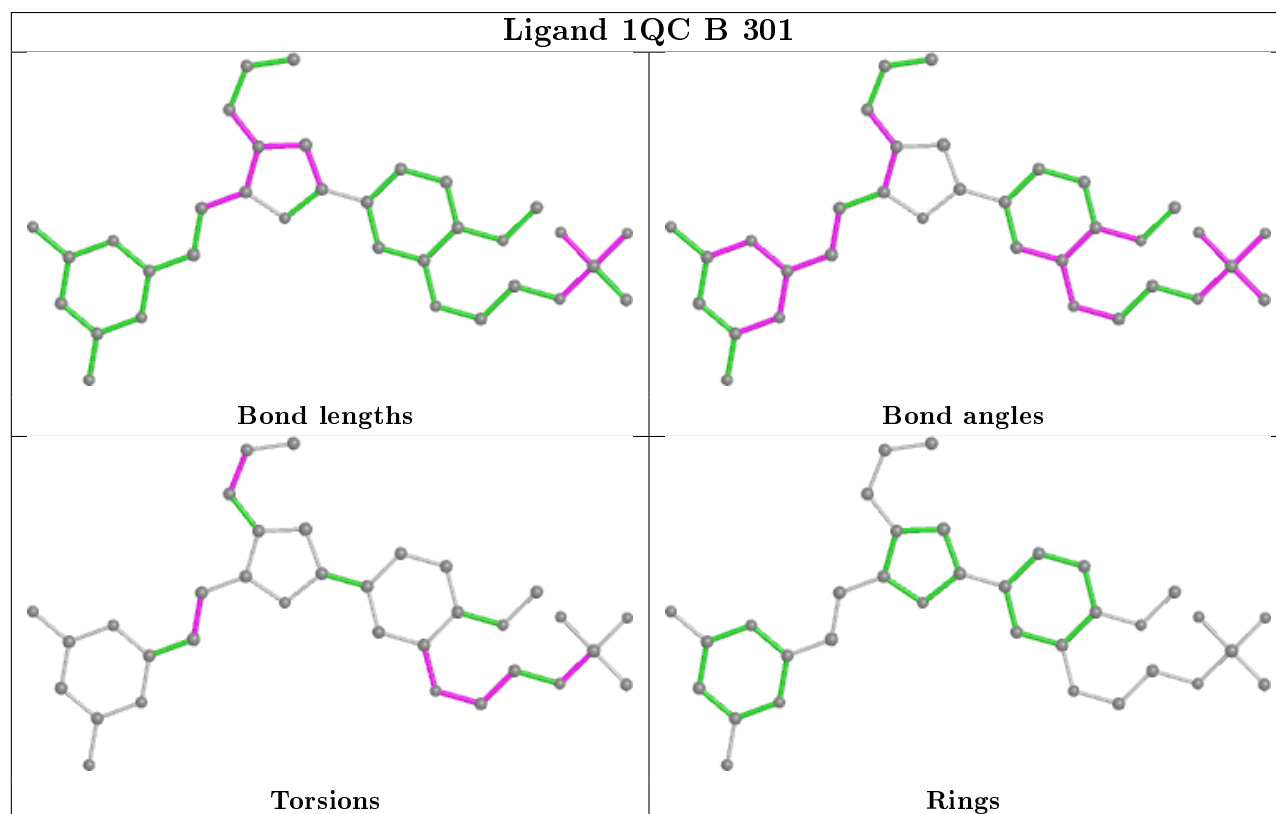
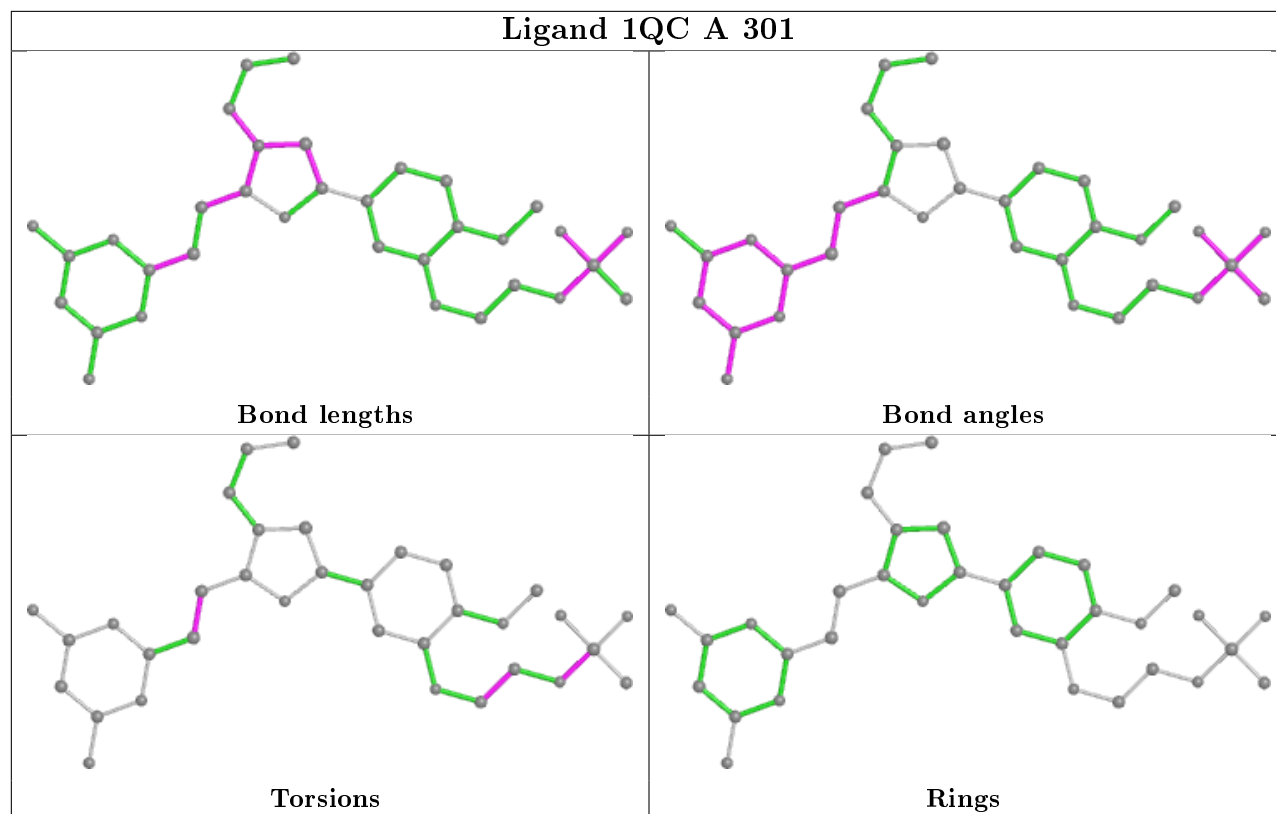
3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	302	UDP	2	0
2	A	301	1QC	1	0
2	B	301	1QC	3	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

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, 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	230/280 (82%)	0.01	1 (0%) 92 93	42, 53, 66, 79	0
1	B	230/280 (82%)	0.02	1 (0%) 92 93	41, 54, 66, 76	0
All	All	460/560 (82%)	0.01	2 (0%) 92 93	41, 54, 66, 79	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	260	LEU	2.7
1	B	118	ASP	2.4

### 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 carbohydrates 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	1QC	B	301	34/34	0.96	0.14	40,51,80,85	0
2	1QC	A	301	34/34	0.97	0.12	40,55,67,74	0
3	UDP	B	302	25/25	0.98	0.09	46,62,66,68	0

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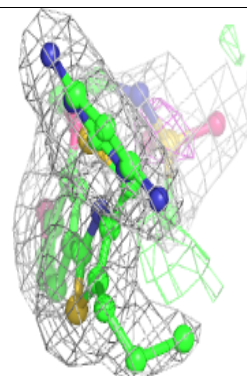
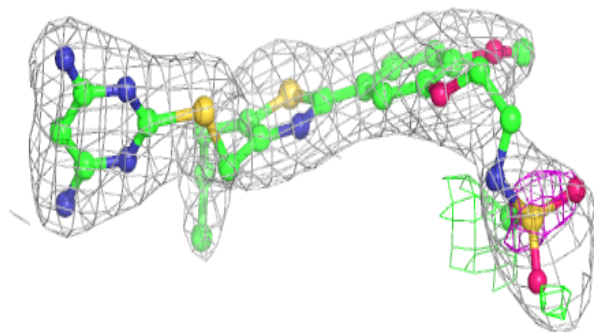
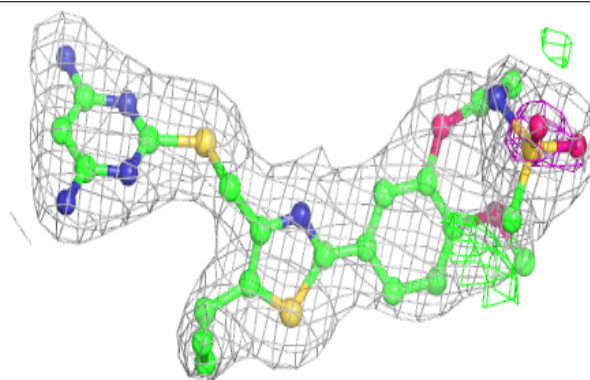
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	UDP	A	302	25/25	0.98	0.10	44,53,61,62	0

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.

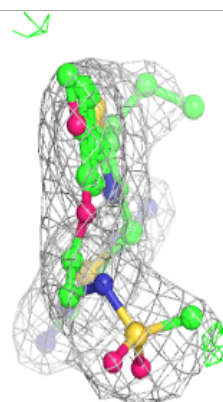
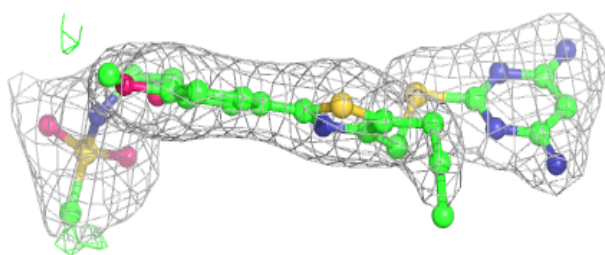
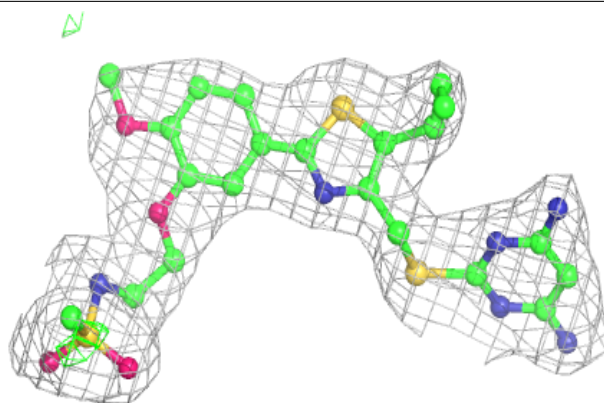
**Electron density around 1QC B 301:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

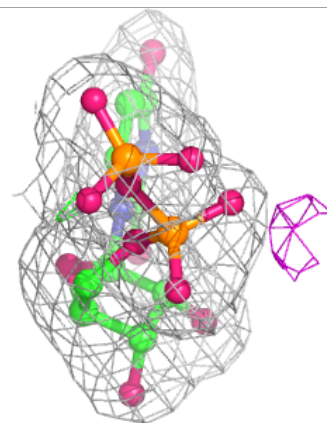
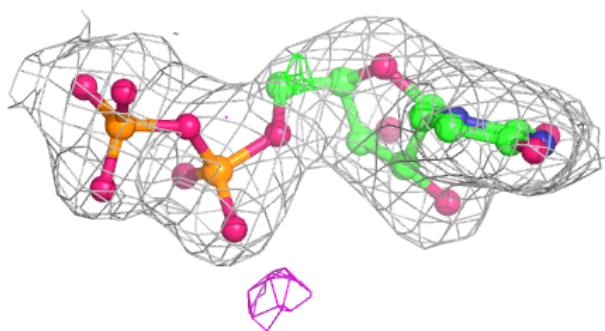
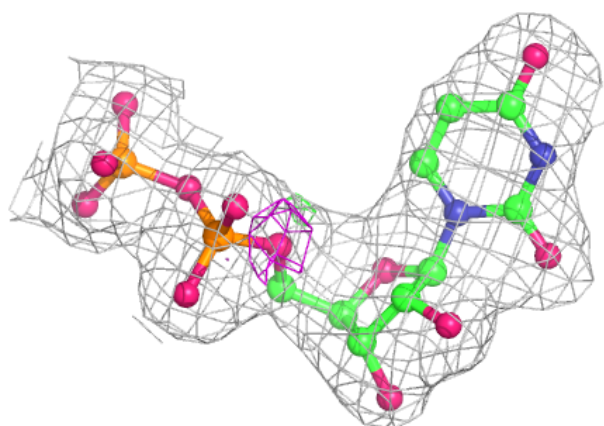


**Electron density around 1QC A 301:**

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

**Electron density around UDP B 302:**

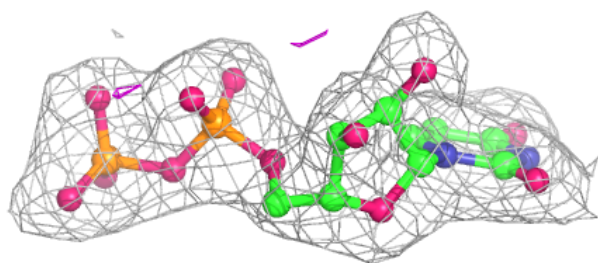
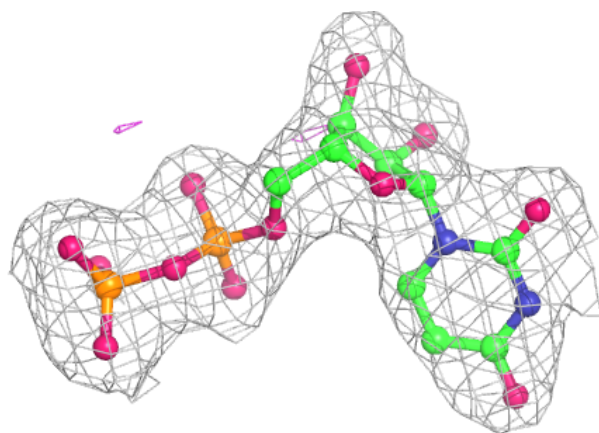
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around UDP A 302:**

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



## 6.5 Other polymers ⓘ

There are no such residues in this entry.