



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 08:48 PM EDT

PDB ID : 3WFR  
Title : tRNA processing enzyme complex 2  
Authors : Yamashita, S.; Takeshita, D.; Tomita, K.  
Deposited on : 2013-07-23  
Resolution : 3.50 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>.

---

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
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)	:	2.36.2

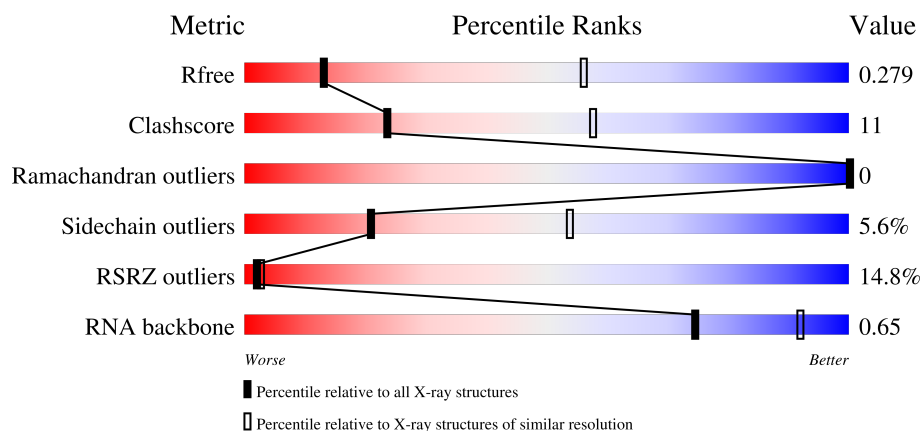
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 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	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)
RNA backbone	3102	1002 (4.00-3.00)

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	74	<div> <div>74%</div> <div> <div></div> <div>76%</div> <div>24%</div> </div> </div>
1	B	74	<div> <div>82%</div> <div> <div></div> <div>61%</div> <div>36%</div> <div>.</div> </div> </div>
2	C	75	<div> <div>81%</div> <div> <div></div> <div>65%</div> <div>31%</div> <div>.</div> </div> </div>
2	D	75	<div> <div>83%</div> <div> <div></div> <div>69%</div> <div>21%</div> <div>9%</div> </div> </div>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	E	512	<div><div><div></div><div></div><div></div><div></div></div><div><div>2%</div><div>63%</div><div>21%</div><div>•</div><div>14%</div></div></div>
3	F	512	<div><div><div></div><div></div><div></div><div></div></div><div><div>2%</div><div>64%</div><div>20%</div><div>•</div><div>14%</div></div></div>
3	G	512	<div><div><div></div><div></div><div></div><div></div></div><div><div>4%</div><div>64%</div><div>23%</div><div>•</div><div>10%</div></div></div>
3	H	512	<div><div><div></div><div></div><div></div><div></div></div><div><div>2%</div><div>63%</div><div>24%</div><div>•</div><div>10%</div></div></div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 20831 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 RNA chain called RNA (74-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	74	Total	C	N	O	P	0	2	0
			1587	706	284	522	75			
1	B	74	Total	C	N	O	P	0	2	0
			1587	706	284	522	75			

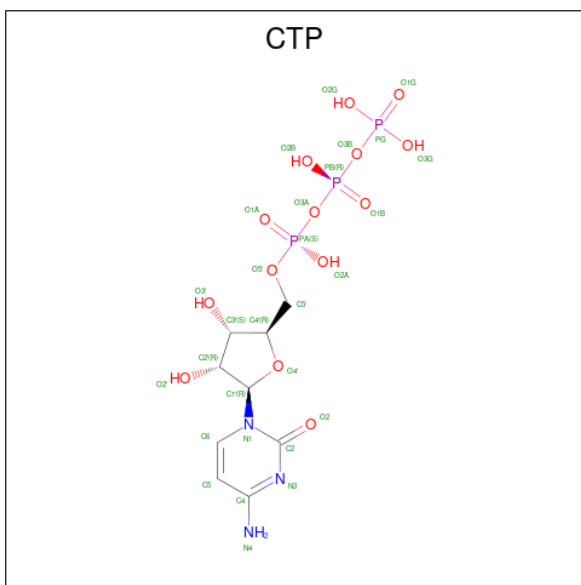
- Molecule 2 is a RNA chain called RNA (75-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	75	Total	C	N	O	P	0	2	0
			1605	714	285	530	76			
2	D	75	Total	C	N	O	P	0	2	0
			1605	714	285	530	76			

- Molecule 3 is a protein called Poly A polymerase.

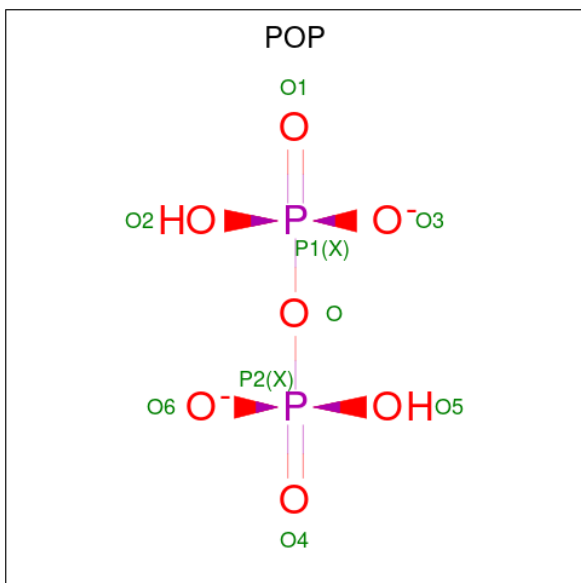
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	439	Total	C	N	O	S	0	0	0
			3491	2249	598	637	7			
3	F	439	Total	C	N	O	S	0	0	0
			3494	2252	598	637	7			
3	G	461	Total	C	N	O	S	0	0	0
			3645	2346	628	664	7			
3	H	463	Total	C	N	O	S	0	0	0
			3661	2356	632	666	7			

- Molecule 4 is CYTIDINE-5'-TRIPHOSPHATE (three-letter code: CTP) (formula:  $\text{C}_9\text{H}_{16}\text{N}_3\text{O}_{14}\text{P}_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	E	1	Total 29	C 9	N 3	O 14	P 3	0	1
4	F	1	Total 29	C 9	N 3	O 14	P 3	0	1
4	G	1	Total 29	C 9	N 3	O 14	P 3	0	1
4	H	1	Total 29	C 9	N 3	O 14	P 3	0	1

- Molecule 5 is PYROPHOSPHATE 2- (three-letter code: POP) (formula:  $\text{H}_2\text{O}_7\text{P}_2$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	1	Total O P 9 7 2	0	1
5	F	1	Total O P 9 7 2	0	1
5	G	1	Total O P 9 7 2	0	1
5	H	1	Total O P 9 7 2	0	1

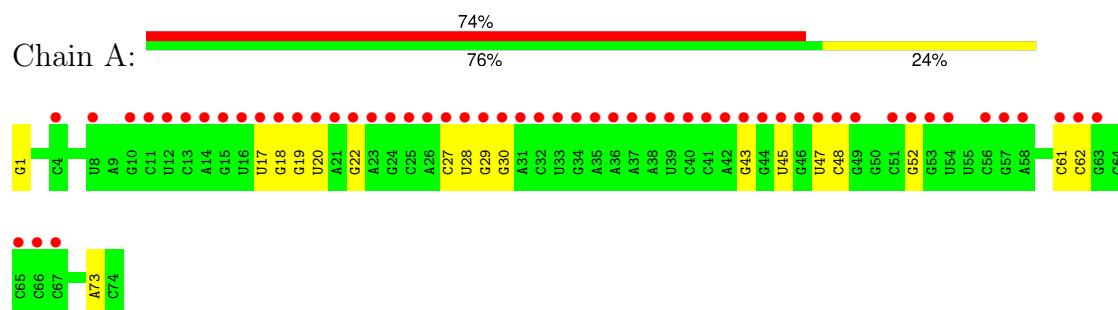
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	E	1	Total Mg 1 1	0	0
6	F	1	Total Mg 1 1	0	0
6	G	1	Total Mg 1 1	0	0
6	H	1	Total Mg 1 1	0	0

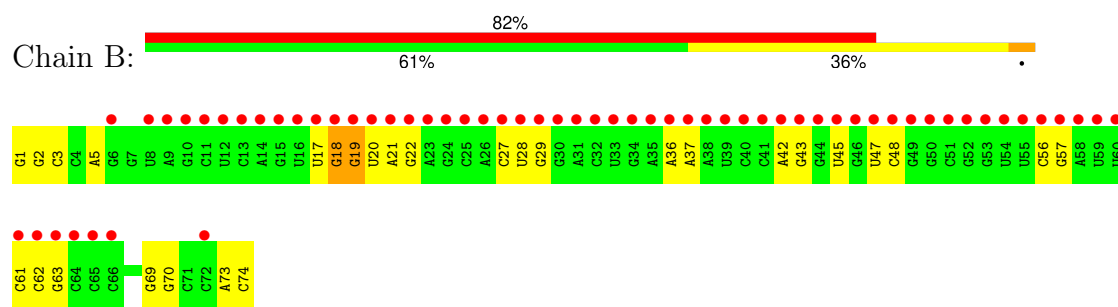
### 3 Residue-property plots [i](#)

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.

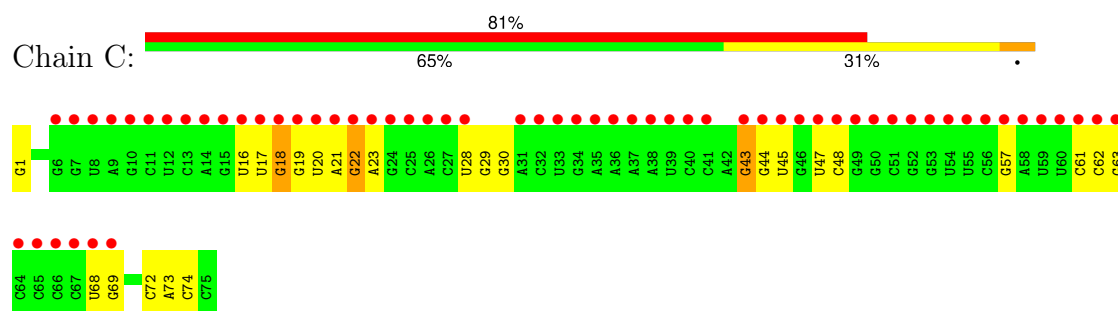
- Molecule 1: RNA (74-MER)



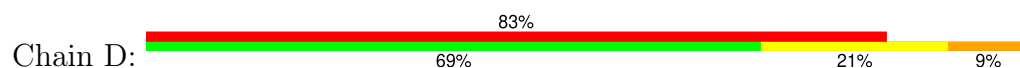
- Molecule 1: RNA (74-MER)

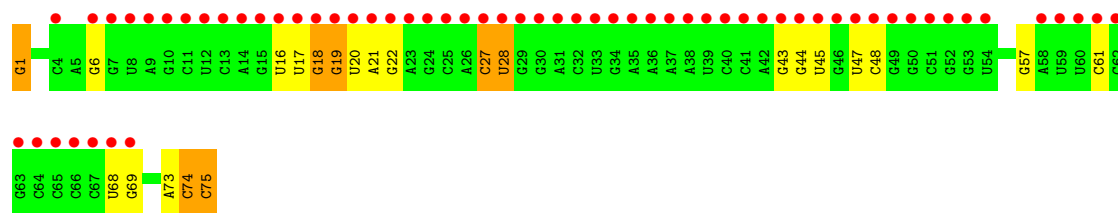


- Molecule 2: RNA (75-MER)

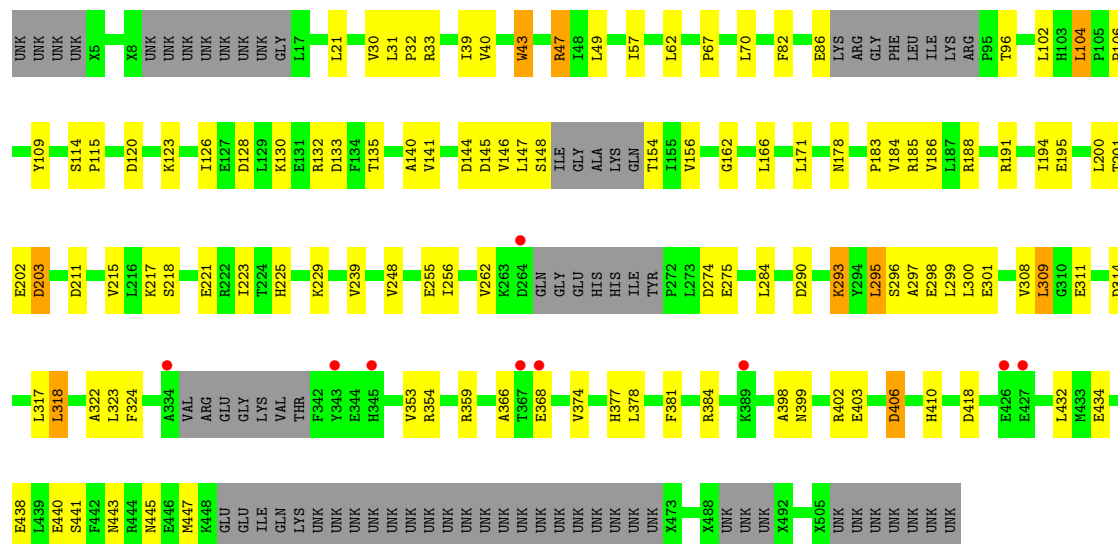


- Molecule 2: RNA (75-MER)

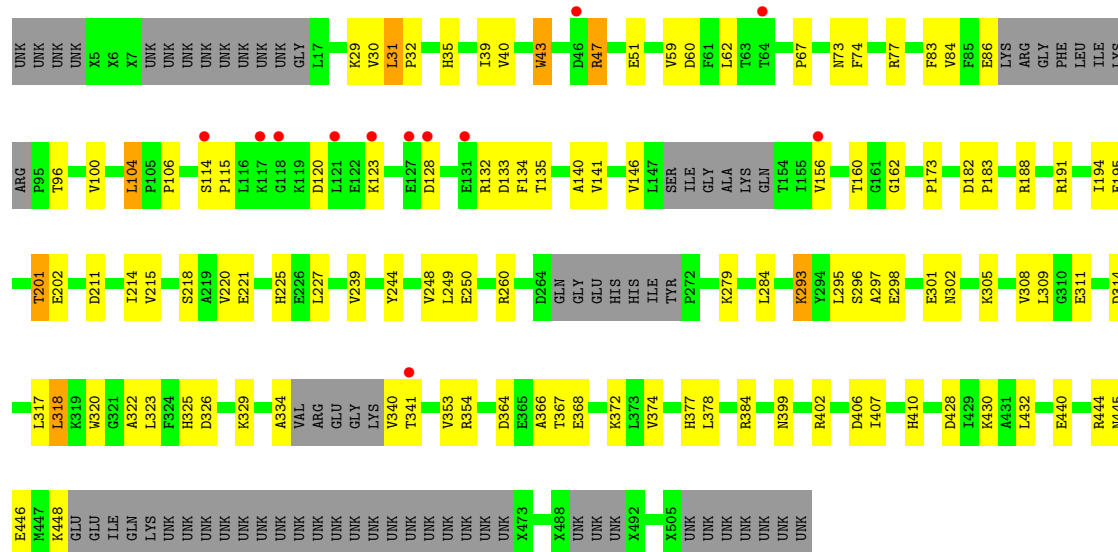




• Molecule 3: Poly A polymerase



• Molecule 3: Poly A polymerase



• Molecule 3: Poly A polymerase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	152.81Å 154.59Å 174.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 3.50 48.90 – 3.50	Depositor EDS
% Data completeness (in resolution range)	70.2 (19.98-3.50) 70.4 (48.90-3.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.76 (at 3.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1389)	Depositor
R, $R_{free}$	0.224 , 0.269 0.236 , 0.279	Depositor DCC
$R_{free}$ test set	1856 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.4	Xtriage
Anisotropy	0.371	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 89.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.026 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	20831	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	128.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 30.25 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3511e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: POP, CTP, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.44	6/1773 (0.3%)	0.76	4/2761 (0.1%)
1	B	0.41	3/1773 (0.2%)	0.78	6/2761 (0.2%)
2	C	0.56	5/1792 (0.3%)	0.73	2/2790 (0.1%)
2	D	1.65	6/1792 (0.3%)	0.82	6/2790 (0.2%)
3	E	0.22	0/3391	0.39	0/4567
3	F	0.23	0/3399	0.40	0/4579
3	G	0.29	1/3497 (0.0%)	0.43	1/4709 (0.0%)
3	H	0.25	1/3508 (0.0%)	0.42	1/4722 (0.0%)
All	All	0.58	22/20925 (0.1%)	0.57	20/29679 (0.1%)

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	74[A]	C	O3'-P	47.79	2.18	1.61
2	D	74[B]	C	O3'-P	47.79	2.18	1.61
2	C	74[A]	C	O3'-P	11.87	1.75	1.61
2	C	74[B]	C	O3'-P	11.87	1.75	1.61
1	A	1	G	OP3-P	-10.57	1.48	1.61
2	C	1	G	OP3-P	-10.55	1.48	1.61
1	B	1	G	OP3-P	-10.54	1.48	1.61
2	D	1	G	OP3-P	-10.51	1.48	1.61
2	C	43	G	C1'-N9	-5.89	1.38	1.46
1	A	43	G	C1'-N9	-5.88	1.38	1.46
2	D	43	G	C1'-N9	-5.88	1.38	1.46
2	C	28	U	C1'-N1	5.68	1.57	1.48
2	D	28	U	C1'-N1	5.67	1.57	1.48
1	A	28	U	C1'-N1	5.64	1.57	1.48
1	B	28	U	C1'-N1	5.63	1.57	1.48
1	A	73[A]	A	O3'-P	5.61	1.67	1.61
1	A	73[B]	A	O3'-P	5.61	1.67	1.61
3	G	95	PRO	N-CD	5.23	1.55	1.47

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	27	C	C1'-N1	5.13	1.56	1.48
2	D	27	C	C1'-N1	5.06	1.56	1.48
1	B	27	C	C1'-N1	5.06	1.56	1.48
3	H	95	PRO	N-CD	5.02	1.54	1.47

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	74[A]	C	P-O3'-C3'	-10.64	106.93	119.70
2	D	74[B]	C	P-O3'-C3'	-10.64	106.93	119.70
2	D	74[A]	C	O3'-P-O5'	9.36	121.78	104.00
2	D	74[B]	C	O3'-P-O5'	9.36	121.78	104.00
1	A	73[A]	A	P-O3'-C3'	-8.88	109.04	119.70
1	A	73[B]	A	P-O3'-C3'	-8.88	109.04	119.70
1	B	73[A]	A	OP2-P-O3'	-8.63	86.21	105.20
1	B	73[B]	A	OP2-P-O3'	-8.63	86.21	105.20
2	C	74[A]	C	P-O3'-C3'	-7.38	110.84	119.70
2	C	74[B]	C	P-O3'-C3'	-7.38	110.84	119.70
1	B	73[A]	A	O3'-P-O5'	6.33	116.02	104.00
1	B	73[B]	A	O3'-P-O5'	6.33	116.02	104.00
2	D	74[A]	C	OP2-P-O3'	-6.21	91.54	105.20
2	D	74[B]	C	OP2-P-O3'	-6.21	91.54	105.20
3	H	94	ARG	C-N-CD	5.90	140.79	128.40
1	B	73[A]	A	OP1-P-O3'	5.87	118.11	105.20
1	B	73[B]	A	OP1-P-O3'	5.87	118.11	105.20
1	A	73[A]	A	O3'-P-O5'	5.81	115.05	104.00
1	A	73[B]	A	O3'-P-O5'	5.81	115.05	104.00
3	G	94	ARG	C-N-CD	5.61	140.17	128.40

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	1587	0	800	2	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1587	0	801	9	0
2	C	1605	0	812	10	0
2	D	1605	0	813	21	0
3	E	3491	0	3375	77	0
3	F	3494	0	3382	85	0
3	G	3645	0	3501	122	0
3	H	3661	0	3517	145	0
4	E	29	0	8	1	0
4	F	29	0	8	0	0
4	G	29	0	3	0	0
4	H	29	0	7	0	0
5	E	9	0	0	0	0
5	F	9	0	0	0	0
5	G	9	0	0	2	0
5	H	9	0	0	1	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
6	G	1	0	0	0	0
6	H	1	0	0	0	0
All	All	20831	0	17027	423	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 11.

All (423) 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)
3:F:31:LEU:HD12	3:F:32:PRO:N	1.59	1.17
3:G:149:ILE:HG13	3:H:433:MET:CE	1.75	1.15
3:H:86:GLU:OE1	3:H:96:THR:HB	1.45	1.14
3:H:93:LYS:HD2	3:H:131:GLU:HB3	1.28	1.14
3:G:93:LYS:NZ	3:G:131:GLU:HG3	1.67	1.09
3:H:93:LYS:CD	3:H:131:GLU:HB3	1.83	1.09
3:G:149:ILE:HG13	3:H:433:MET:HE1	1.10	1.08
3:F:334:ALA:HB3	3:F:341:THR:OG1	1.55	1.07
3:G:17:LEU:HD13	3:G:149:ILE:CG2	1.83	1.07
3:G:93:LYS:HZ3	3:G:131:GLU:CG	1.70	1.03
3:G:17:LEU:CD1	3:G:149:ILE:HG23	1.90	1.02
3:H:93:LYS:HD2	3:H:131:GLU:CB	1.89	1.01
3:E:33:ARG:HE	3:H:31:LEU:HD23	1.20	1.00
3:E:33:ARG:NE	3:H:31:LEU:HD23	1.75	1.00

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:17:LEU:HD13	3:G:149:ILE:HG23	1.41	1.00
3:E:399:ASN:O	3:E:403:GLU:HG2	1.65	0.97
2:D:1:G:C4	3:H:83:PHE:CE1	2.54	0.95
3:H:90:PHE:HB2	3:H:91:LEU:CD1	1.97	0.95
3:G:93:LYS:NZ	3:G:131:GLU:CG	2.28	0.94
3:G:93:LYS:HZ3	3:G:131:GLU:CD	1.72	0.92
3:F:31:LEU:HD12	3:F:32:PRO:CD	1.99	0.92
3:G:93:LYS:HZ1	3:G:131:GLU:HG3	1.34	0.91
3:G:344:GLU:HG2	3:G:347:LYS:HD2	1.52	0.91
3:F:340:VAL:HG12	3:F:341:THR:HG23	1.53	0.90
3:G:20:TYR:CD1	3:G:149:ILE:HD11	2.07	0.88
3:H:86:GLU:OE1	3:H:96:THR:CB	2.23	0.86
3:G:93:LYS:NZ	3:G:131:GLU:CD	2.30	0.83
3:F:308:VAL:HG12	3:F:309:LEU:HD13	1.60	0.83
3:F:445:ASN:OD1	3:F:446:GLU:N	2.12	0.82
3:G:206:GLU:HA	3:G:209:LYS:HG3	1.61	0.82
2:D:1:G:C4	3:H:83:PHE:HE1	1.94	0.81
3:G:445:ASN:OD1	3:G:446:GLU:N	2.14	0.80
3:H:93:LYS:HD2	3:H:131:GLU:CG	2.11	0.79
3:G:17:LEU:HD13	3:G:149:ILE:HG22	1.60	0.79
3:G:205:TYR:O	3:G:209:LYS:HG2	1.84	0.78
3:F:31:LEU:CD1	3:F:32:PRO:HD2	2.13	0.78
3:G:206:GLU:HA	3:G:209:LYS:CG	2.14	0.78
3:G:308:VAL:CG1	3:G:309:LEU:HD13	2.14	0.78
2:D:74[B]:C:H1'	3:H:97:ILE:CD1	2.14	0.77
3:G:308:VAL:HG12	3:G:309:LEU:HD13	1.65	0.77
3:G:86:GLU:HB3	3:G:96:THR:HA	1.66	0.76
3:G:20:TYR:CG	3:G:149:ILE:HD11	2.19	0.76
3:G:106:PRO:HG3	3:H:301:GLU:HA	1.68	0.76
2:D:74[B]:C:H1'	3:H:97:ILE:HD12	1.66	0.76
3:H:93:LYS:CE	3:H:131:GLU:HB3	2.16	0.76
3:G:206:GLU:O	3:G:209:LYS:HG3	1.87	0.75
3:H:90:PHE:HB2	3:H:91:LEU:HD12	1.67	0.74
3:H:89:GLY:O	3:H:92:ILE:HD12	1.87	0.73
3:G:30:VAL:CG1	3:G:73:ASN:HB2	2.17	0.73
3:G:17:LEU:HD12	3:G:149:ILE:HG23	1.70	0.73
3:H:93:LYS:HD2	3:H:131:GLU:CD	2.08	0.73
3:E:106:PRO:HG3	3:F:301:GLU:HA	1.71	0.71
3:G:133:ASP:OD2	3:G:188:ARG:NH1	2.23	0.71
3:F:308:VAL:HG11	3:F:366:ALA:HB2	1.73	0.71
3:H:90:PHE:HB2	3:H:91:LEU:HD13	1.72	0.71

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:340:VAL:HG12	3:F:341:THR:N	2.04	0.70
3:H:93:LYS:HD2	3:H:131:GLU:OE2	1.92	0.70
3:H:93:LYS:HZ1	3:H:181:ARG:HD2	1.58	0.69
3:E:438:GLU:OE2	3:F:29:LYS:NZ	2.26	0.69
3:H:194:ILE:HG13	3:H:239:VAL:HG22	1.75	0.69
3:G:17:LEU:CD1	3:G:149:ILE:CG2	2.59	0.69
3:G:301:GLU:HA	3:H:106:PRO:HG3	1.75	0.69
3:H:177:GLU:O	3:H:181:ARG:HG3	1.93	0.69
3:F:31:LEU:HD11	3:F:35:HIS:HB2	1.76	0.68
3:H:188:ARG:NH2	5:H:602[B]:POP:O2	2.27	0.68
3:F:31:LEU:HD12	3:F:31:LEU:C	2.15	0.67
3:F:31:LEU:CD1	3:F:32:PRO:CD	2.70	0.66
2:D:18:G:O2'	2:D:57:G:N2	2.28	0.66
3:G:206:GLU:CA	3:G:209:LYS:HG3	2.24	0.66
3:E:144:ASP:OD1	3:H:33:ARG:NH1	2.29	0.66
3:E:406:ASP:OD1	3:E:406:ASP:N	2.25	0.66
3:F:194:ILE:HG13	3:F:239:VAL:HG22	1.78	0.66
3:E:398:ALA:O	3:E:402:ARG:HG3	1.96	0.66
3:G:149:ILE:CG1	3:H:433:MET:HE1	2.05	0.65
3:G:194:ILE:HG13	3:G:239:VAL:HG22	1.78	0.65
3:H:29:LYS:HE2	3:H:77:ARG:CZ	2.25	0.65
2:D:1:G:N3	3:H:83:PHE:CE1	2.63	0.65
3:G:250:GLU:OE2	3:G:260:ARG:NH2	2.30	0.65
3:G:149:ILE:HG13	3:H:433:MET:HE3	1.78	0.65
3:F:86:GLU:HG3	3:F:96:THR:HG22	1.79	0.65
3:H:482:UNK:O	3:H:486:UNK:N	2.30	0.64
3:E:148:SER:H	3:F:430:LYS:HE2	1.61	0.64
3:G:30:VAL:HG11	3:G:73:ASN:HB2	1.79	0.64
2:C:73:A:C2	3:G:92:ILE:CG2	2.81	0.64
3:G:93:LYS:NZ	3:G:131:GLU:OE1	2.29	0.64
3:H:250:GLU:OE2	3:H:260:ARG:NH2	2.31	0.64
2:D:1:G:C5	3:H:83:PHE:HE1	2.16	0.64
3:G:497:UNK:O	3:G:501:UNK:N	2.31	0.64
3:E:225:HIS:NE2	3:E:311:GLU:OE2	2.31	0.64
3:F:284:LEU:HD22	3:F:322:ALA:HB2	1.80	0.63
3:F:308:VAL:HG21	3:F:317:LEU:HD11	1.79	0.63
3:E:133:ASP:OD2	3:E:188:ARG:NH1	2.32	0.63
3:H:133:ASP:OD2	3:H:188:ARG:NH1	2.32	0.62
3:G:344:GLU:HG2	3:G:347:LYS:CD	2.28	0.62
3:E:308:VAL:O	3:E:309:LEU:HB2	1.99	0.62
2:D:1:G:C2	3:H:83:PHE:HE1	2.17	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:33:ARG:NH1	3:H:144:ASP:OD1	2.33	0.62
3:G:206:GLU:HA	3:G:209:LYS:CD	2.29	0.62
3:H:94:ARG:NE	3:H:128:ASP:OD2	2.30	0.62
3:E:308:VAL:HG21	3:E:317:LEU:HD11	1.81	0.62
3:F:31:LEU:HD13	3:F:32:PRO:HD2	1.82	0.61
3:F:354:ARG:NH1	3:F:368:GLU:OE1	2.33	0.61
3:G:188:ARG:NH2	5:G:602[B]:POP:O5	2.33	0.61
3:H:91:LEU:HD12	3:H:91:LEU:N	2.15	0.61
3:H:94:ARG:HH21	3:H:128:ASP:HB2	1.64	0.61
3:H:308:VAL:O	3:H:309:LEU:HB2	2.01	0.61
3:E:441:SER:O	3:E:445:ASN:ND2	2.33	0.61
3:H:133:ASP:HB3	3:H:185:ARG:HD3	1.83	0.61
3:E:298:GLU:HG2	3:E:299:LEU:HD12	1.84	0.60
3:F:340:VAL:CG1	3:F:341:THR:N	2.64	0.60
3:E:191:ARG:NH1	3:E:195:GLU:OE1	2.33	0.60
3:G:149:ILE:CG1	3:H:433:MET:CE	2.67	0.60
1:B:29:G:C2	1:B:42:A:C2	2.89	0.60
3:H:353:VAL:HG21	3:H:374:VAL:HG21	1.83	0.60
3:G:30:VAL:HG12	3:G:30:VAL:O	2.01	0.60
3:G:297:ALA:HB1	3:H:104:LEU:HD11	1.83	0.60
3:E:183:PRO:HG2	3:E:218:SER:HB3	1.83	0.60
3:G:307:ARG:NH2	3:G:310:GLY:O	2.34	0.59
3:H:84:VAL:HG13	3:H:84:VAL:O	2.01	0.59
3:H:39:ILE:HD12	3:H:146:VAL:HG21	1.83	0.59
3:E:141:VAL:HG12	3:E:156:VAL:HG12	1.85	0.59
3:E:297:ALA:HB1	3:F:104:LEU:HD11	1.83	0.59
2:D:1:G:C5	3:H:83:PHE:CE1	2.89	0.59
3:G:183:PRO:HG2	3:G:218:SER:HB3	1.85	0.59
3:G:498:UNK:O	3:G:502:UNK:N	2.35	0.59
3:H:308:VAL:HG21	3:H:317:LEU:HD11	1.83	0.59
3:E:438:GLU:CD	3:F:29:LYS:NZ	2.57	0.59
3:H:284:LEU:HD22	3:H:322:ALA:HB2	1.85	0.58
3:E:438:GLU:OE1	3:F:29:LYS:NZ	2.34	0.58
3:G:30:VAL:CG2	3:G:77:ARG:HD3	2.34	0.58
3:F:250:GLU:OE2	3:F:260:ARG:NH2	2.33	0.58
3:E:40:VAL:HG13	3:E:140:ALA:HB2	1.85	0.58
3:H:295:LEU:HD21	3:H:409:PRO:HB3	1.86	0.58
1:B:19:G:O6	1:B:56:C:N4	2.34	0.58
3:E:39:ILE:HD12	3:E:146:VAL:HG21	1.86	0.58
3:H:97:ILE:HD11	3:H:112:ASP:HB3	1.84	0.58
3:H:376:HIS:HD1	3:H:404:CYS:HG	1.50	0.58

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:183:PRO:HG3	3:E:217:LYS:HB3	1.84	0.58
3:F:183:PRO:HG2	3:F:218:SER:HB3	1.86	0.58
3:H:128:ASP:OD1	3:H:132:ARG:NH1	2.37	0.58
3:G:148:SER:HA	3:H:430:LYS:HD2	1.86	0.58
3:G:350:ALA:HB2	3:G:375:ARG:HB2	1.85	0.57
3:H:62:LEU:HD11	3:H:132:ARG:HH12	1.68	0.57
3:G:201:THR:OG1	3:G:202:GLU:N	2.37	0.57
3:G:206:GLU:C	3:G:209:LYS:HG3	2.25	0.57
3:E:290:ASP:HB3	3:E:293:LYS:HE3	1.86	0.57
3:F:40:VAL:HG13	3:F:140:ALA:HB2	1.87	0.57
3:E:104:LEU:HD11	3:F:297:ALA:HB1	1.85	0.56
2:D:1:G:C2	3:H:83:PHE:CE1	2.93	0.56
3:E:135:THR:HB	3:E:162:GLY:HA2	1.87	0.56
3:F:191:ARG:NH1	3:F:195:GLU:OE1	2.38	0.56
3:G:93:LYS:HB3	3:G:94:ARG:HD2	1.86	0.56
3:G:290:ASP:O	3:G:293:LYS:HG2	2.05	0.56
3:G:94:ARG:HD2	3:G:94:ARG:N	2.19	0.56
3:E:188:ARG:NH2	4:E:601[A]:CTP:O2A	2.39	0.56
3:G:342:PHE:N	3:G:342:PHE:CD1	2.73	0.56
3:E:186:VAL:HG11	3:E:215:VAL:HG22	1.87	0.56
3:H:93:LYS:NZ	3:H:181:ARG:HH11	2.03	0.56
3:H:331:GLN:HG3	3:H:352:ILE:HD11	1.86	0.56
3:E:128:ASP:OD1	3:E:132:ARG:NH1	2.38	0.56
3:E:255:GLU:OE1	3:E:359:ARG:NH2	2.38	0.56
3:G:120:ASP:HB3	3:G:123:LYS:HE3	1.87	0.56
3:F:74:PHE:HD2	3:F:100:VAL:HG21	1.70	0.56
3:F:318:LEU:HG	3:F:410:HIS:HB3	1.88	0.56
3:G:183:PRO:HG3	3:G:217:LYS:HB3	1.88	0.55
1:B:18:G:O2'	1:B:57:G:N2	2.31	0.55
3:E:194:ILE:HG13	3:E:239:VAL:HG22	1.89	0.55
3:F:201:THR:OG1	3:F:202:GLU:N	2.38	0.55
2:D:74[A]:C:O4'	3:H:97:ILE:HD13	2.06	0.55
3:G:39:ILE:HD12	3:G:146:VAL:HG21	1.87	0.55
3:E:399:ASN:O	3:E:403:GLU:CG	2.50	0.55
3:F:31:LEU:HD12	3:F:32:PRO:HD2	1.72	0.55
3:F:302:ASN:HA	3:F:305:LYS:HD2	1.89	0.55
2:D:75[B]:C:O2'	3:H:133:ASP:OD1	2.24	0.55
3:E:33:ARG:NE	3:H:31:LEU:CD2	2.61	0.55
3:E:353:VAL:HG21	3:E:374:VAL:HG21	1.87	0.55
3:E:301:GLU:HA	3:F:106:PRO:HG3	1.87	0.55
3:G:284:LEU:HD22	3:G:322:ALA:HB2	1.89	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:94:ARG:NH2	3:G:132:ARG:HG2	2.22	0.55
3:F:67:PRO:HG2	3:F:115:PRO:HG3	1.89	0.54
3:E:49:LEU:HD21	3:E:166:LEU:HD22	1.90	0.54
3:F:31:LEU:CD1	3:F:35:HIS:HB2	2.37	0.54
3:F:183:PRO:HB3	3:F:214:ILE:HG13	1.89	0.54
3:G:398:ALA:O	3:G:402:ARG:HB2	2.08	0.54
3:H:183:PRO:HG2	3:H:218:SER:HB3	1.89	0.54
3:E:314:ASP:OD2	3:E:410:HIS:NE2	2.34	0.54
3:H:295:LEU:CD2	3:H:409:PRO:HB3	2.38	0.54
2:D:1:G:N3	3:H:83:PHE:CZ	2.76	0.53
3:H:67:PRO:HG2	3:H:115:PRO:HG3	1.90	0.53
3:H:93:LYS:HZ2	3:H:181:ARG:HH11	1.56	0.53
3:E:284:LEU:HD22	3:E:322:ALA:HB2	1.90	0.53
3:F:47:ARG:NH1	3:F:51:GLU:O	2.42	0.53
2:D:1:G:N3	3:H:83:PHE:HE1	2.06	0.53
3:F:39:ILE:HD12	3:F:146:VAL:HG21	1.90	0.53
3:F:326:ASP:HB3	3:F:329:LYS:HG3	1.90	0.53
3:H:203:ASP:OD1	3:H:203:ASP:N	2.40	0.53
3:H:285:GLU:HG2	3:H:319:LYS:HE2	1.90	0.53
2:C:72:C:H4'	3:G:221:GLU:HG3	1.91	0.53
3:E:256:ILE:HD11	3:E:324:PHE:HE1	1.74	0.53
3:E:354:ARG:NH1	3:E:368:GLU:OE2	2.42	0.53
3:F:308:VAL:O	3:F:309:LEU:HB2	2.08	0.52
3:H:30:VAL:HG11	3:H:73:ASN:HB2	1.91	0.52
3:H:481:UNK:O	3:H:485:UNK:N	2.41	0.52
3:G:442:PHE:HA	3:G:446:GLU:HB2	1.91	0.52
3:F:128:ASP:OD2	3:F:132:ARG:NH1	2.43	0.52
3:E:215:VAL:HG21	3:E:248:VAL:HG13	1.92	0.52
3:F:340:VAL:HG12	3:F:341:THR:CG2	2.35	0.52
3:G:329:LYS:HG2	3:G:345:HIS:HD2	1.74	0.52
3:H:321:GLY:HA3	3:H:373:LEU:HD23	1.91	0.52
3:H:404:CYS:HB2	3:H:407:ILE:HG12	1.90	0.52
3:G:94:ARG:N	3:G:94:ARG:CD	2.73	0.52
3:H:90:PHE:CB	3:H:91:LEU:HD13	2.39	0.52
3:G:308:VAL:HG13	3:G:309:LEU:HD13	1.91	0.51
3:H:49:LEU:HD21	3:H:166:LEU:HD22	1.92	0.51
3:H:91:LEU:CD1	3:H:91:LEU:N	2.73	0.51
3:H:302:ASN:HA	3:H:305:LYS:HD2	1.91	0.51
3:G:101:VAL:HG22	3:G:110:ARG:HG3	1.92	0.51
2:D:19:G:C6	3:H:474:UNK:HA	2.45	0.51
3:F:227:LEU:HB3	3:F:320:TRP:HZ2	1.75	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:406:ASP:OD1	3:F:406:ASP:N	2.34	0.51
3:G:346:ASP:OD2	3:G:378:LEU:HD21	2.10	0.51
3:F:30:VAL:HG11	3:F:73:ASN:HB2	1.93	0.51
3:G:215:VAL:HG21	3:G:248:VAL:HG13	1.93	0.51
3:H:215:VAL:HG21	3:H:248:VAL:HG13	1.92	0.51
3:H:326:ASP:HB3	3:H:329:LYS:HG3	1.93	0.51
3:F:135:THR:HB	3:F:162:GLY:HA2	1.93	0.51
3:G:346:ASP:OD1	3:G:347:LYS:N	2.43	0.51
3:F:133:ASP:OD2	3:F:188:ARG:NH1	2.44	0.50
3:H:57:ILE:HD12	3:H:109:TYR:HE1	1.75	0.50
3:E:384:ARG:HD3	3:E:432:LEU:HB2	1.92	0.50
1:B:29:G:C6	1:B:42:A:N1	2.80	0.50
3:F:334:ALA:CB	3:F:341:THR:OG1	2.43	0.50
3:G:346:ASP:OD1	3:G:347:LYS:HG3	2.11	0.50
2:C:68:U:H2'	2:C:69:G:H8	1.77	0.50
3:G:353:VAL:HG21	3:G:374:VAL:HG21	1.93	0.50
3:E:120:ASP:HB3	3:E:123:LYS:HB3	1.94	0.50
3:F:120:ASP:HB3	3:F:123:LYS:HB3	1.94	0.50
3:E:443:ASN:ND2	3:E:447:MET:SD	2.84	0.49
3:F:225:HIS:NE2	3:F:311:GLU:OE2	2.44	0.49
3:H:62:LEU:HD23	3:H:114:SER:HB2	1.94	0.49
3:H:379:ARG:NH1	3:H:403:GLU:OE1	2.41	0.49
1:B:62:C:H2'	1:B:63:G:H8	1.78	0.49
3:G:308:VAL:HG21	3:G:317:LEU:HD11	1.94	0.49
3:G:326:ASP:HB3	3:G:329:LYS:HG3	1.94	0.49
3:G:345:HIS:ND1	3:G:346:ASP:N	2.60	0.49
3:G:45:ARG:HG3	3:G:136:ALA:HB1	1.94	0.49
3:H:201:THR:OG1	3:H:202:GLU:N	2.45	0.49
3:G:224:THR:OG1	3:G:360:LEU:O	2.25	0.49
3:H:95:PRO:HG2	3:H:96:THR:N	2.28	0.49
3:F:298:GLU:OE2	3:F:444:ARG:HD3	2.13	0.49
3:F:340:VAL:CG1	3:F:341:THR:H	2.26	0.49
2:D:74[A]:C:H1'	3:H:97:ILE:CD1	2.42	0.49
3:H:132:ARG:HD3	3:H:138:ALA:HA	1.94	0.49
3:F:445:ASN:O	3:F:448:LYS:HE2	2.14	0.48
3:G:259:LEU:HD21	3:G:327:ILE:HD12	1.94	0.48
3:F:314:ASP:OD2	3:F:410:HIS:NE2	2.43	0.48
3:H:274:ASP:OD1	3:H:275:GLU:N	2.44	0.48
3:E:318:LEU:HG	3:E:410:HIS:HB3	1.95	0.48
3:H:130:LYS:HD3	3:H:159:PRO:HB2	1.94	0.48
2:D:73:A:H5'	3:H:87:LYS:HE3	1.96	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:438:GLU:OE2	3:F:29:LYS:CE	2.62	0.48
3:E:438:GLU:CD	3:F:29:LYS:HZ1	2.16	0.48
3:F:211:ASP:N	3:F:211:ASP:OD1	2.47	0.48
3:H:211:ASP:N	3:H:211:ASP:OD1	2.45	0.48
2:C:18:G:O2'	2:C:57:G:N2	2.39	0.47
2:C:73:A:N1	3:G:92:ILE:HG23	2.29	0.47
3:F:62:LEU:HD23	3:F:114:SER:HB2	1.95	0.47
3:G:86:GLU:O	3:G:87:LYS:HE2	2.14	0.47
3:G:104:LEU:HD11	3:H:297:ALA:HB1	1.96	0.47
3:H:135:THR:HG22	3:H:160:THR:HB	1.96	0.47
3:H:384:ARG:HD3	3:H:432:LEU:HB2	1.95	0.47
3:E:171:LEU:HB3	3:E:200:LEU:HD23	1.95	0.47
3:H:43:TRP:CD1	3:H:59:VAL:HG22	2.49	0.47
3:E:211:ASP:OD1	3:E:211:ASP:N	2.48	0.47
3:E:225:HIS:CE1	3:E:229:LYS:HD2	2.49	0.47
3:E:381:PHE:HZ	3:E:418:ASP:HB3	1.79	0.47
3:F:372:LYS:HG2	3:F:407:ILE:HD13	1.96	0.47
3:H:29:LYS:HE2	3:H:77:ARG:NH2	2.28	0.47
3:G:221:GLU:H	3:G:221:GLU:HG2	1.34	0.47
2:D:74[A]:C:H1'	3:H:97:ILE:HD12	1.96	0.47
3:E:201:THR:OG1	3:E:202:GLU:N	2.48	0.47
3:H:93:LYS:NZ	3:H:181:ARG:CD	2.78	0.47
3:H:184:VAL:HG23	3:H:223:ILE:HD13	1.96	0.47
3:G:45:ARG:NH2	5:G:602[B]:POP:O4	2.48	0.46
3:G:94:ARG:HH22	3:G:132:ARG:HG2	1.80	0.46
3:E:31:LEU:HD12	3:E:32:PRO:HD2	1.96	0.46
3:H:186:VAL:HG11	3:H:215:VAL:HG22	1.97	0.46
3:H:375:ARG:HG3	3:H:376:HIS:HD2	1.81	0.46
3:E:86:GLU:HG3	3:E:96:THR:HG22	1.98	0.46
3:G:321:GLY:HA3	3:G:373:LEU:HD23	1.97	0.46
3:E:203:ASP:OD1	3:E:203:ASP:N	2.35	0.46
3:G:43:TRP:CD1	3:G:59:VAL:HG22	2.50	0.46
3:G:96:THR:HG22	3:G:115:PRO:HG2	1.98	0.46
3:G:318:LEU:HG	3:G:410:HIS:HB3	1.98	0.46
3:H:277:THR:HG22	3:H:325:HIS:CE1	2.51	0.46
3:H:93:LYS:NZ	3:H:181:ARG:HD2	2.29	0.46
3:H:443:ASN:HA	3:H:447:MET:HB2	1.97	0.46
3:G:327:ILE:HG22	3:G:349:GLY:HA2	1.97	0.46
3:F:30:VAL:CG1	3:F:73:ASN:HB2	2.46	0.46
3:F:353:VAL:HG21	3:F:374:VAL:HG21	1.97	0.46
3:G:135:THR:HB	3:G:162:GLY:HA2	1.98	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:93:LYS:HZ1	3:H:181:ARG:CD	2.28	0.46
3:G:258:ARG:O	3:G:261:GLU:HG2	2.16	0.45
3:H:295:LEU:HD21	3:H:409:PRO:CB	2.46	0.45
3:E:308:VAL:CG1	3:E:366:ALA:HB2	2.45	0.45
3:F:30:VAL:CG2	3:F:77:ARG:HD3	2.47	0.45
3:G:20:TYR:HB2	3:G:149:ILE:CD1	2.47	0.45
3:G:85:PHE:O	3:G:97:ILE:O	2.33	0.45
3:G:384:ARG:HD3	3:G:432:LEU:HD13	1.98	0.45
3:H:35:HIS:CG	3:H:65:ALA:HB2	2.52	0.45
1:B:5:A:OP1	3:F:364:ASP:HB2	2.16	0.45
3:F:399:ASN:OD1	3:F:402:ARG:NH2	2.34	0.45
3:G:67:PRO:HG2	3:G:115:PRO:HG3	1.97	0.45
2:C:68:U:H2'	2:C:69:G:C8	2.52	0.45
3:E:67:PRO:HG2	3:E:115:PRO:HG3	1.99	0.45
3:H:30:VAL:CG1	3:H:73:ASN:HB2	2.47	0.45
3:H:86:GLU:HB2	3:H:96:THR:HA	1.97	0.45
3:E:145:ASP:HB3	3:E:154:THR:HA	1.99	0.45
3:G:255:GLU:HG2	3:G:352:ILE:HG23	1.99	0.45
3:H:96:THR:O	3:H:115:PRO:HD3	2.17	0.45
2:D:68:U:H2'	2:D:69:G:C8	2.52	0.44
3:E:296:SER:OG	3:E:440:GLU:OE1	2.31	0.44
3:F:284:LEU:HD21	3:F:318:LEU:HD22	1.99	0.44
3:H:126:ILE:HD12	3:H:159:PRO:HB3	1.99	0.44
3:H:183:PRO:HG3	3:H:217:LYS:HB3	1.99	0.44
3:H:441:SER:O	3:H:445:ASN:ND2	2.50	0.44
3:E:184:VAL:HG23	3:E:223:ILE:HD13	2.00	0.44
3:H:87:LYS:HD3	3:H:87:LYS:HA	1.58	0.44
3:E:30:VAL:HG12	3:E:70:LEU:HD12	1.99	0.44
3:E:295:LEU:HB3	3:E:300:LEU:HG	1.99	0.44
3:G:89:GLY:O	3:G:92:ILE:HG13	2.17	0.44
3:H:350:ALA:HB2	3:H:375:ARG:HB2	1.99	0.44
3:G:94:ARG:HH21	3:G:132:ARG:NH1	2.16	0.44
3:G:193:ALA:HA	3:G:198:LEU:HB2	1.99	0.44
2:C:62:C:H2'	2:C:63:G:H8	1.82	0.44
1:B:69:G:H2'	1:B:70:G:H8	1.83	0.44
3:H:93:LYS:HE2	3:H:131:GLU:HB3	1.98	0.44
3:G:256:ILE:HD11	3:G:324:PHE:HE1	1.83	0.44
3:G:387:PHE:CE1	3:G:438:GLU:HG3	2.52	0.44
3:E:40:VAL:HG21	3:E:62:LEU:HD12	2.00	0.43
3:E:43:TRP:HE1	3:E:57:ILE:HG23	1.83	0.43
3:E:274:ASP:OD1	3:E:275:GLU:N	2.50	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:384:ARG:HD3	3:F:432:LEU:HB2	2.00	0.43
3:G:96:THR:O	3:G:115:PRO:HD3	2.18	0.43
3:F:40:VAL:O	3:F:60:ASP:HB2	2.19	0.43
3:G:344:GLU:CG	3:G:347:LYS:HD2	2.35	0.43
1:B:36:A:H2'	1:B:37:A:C8	2.53	0.43
3:F:31:LEU:CD1	3:F:32:PRO:O	2.67	0.43
3:G:102:LEU:HB3	3:G:109:TYR:HB2	2.00	0.43
3:F:135:THR:HG22	3:F:160:THR:HB	2.00	0.43
2:C:22:G:H2'	2:C:23:A:C8	2.54	0.43
3:G:206:GLU:HA	3:G:209:LYS:HD2	1.99	0.43
3:H:126:ILE:O	3:H:130:LYS:HG2	2.18	0.43
3:H:165:ASP:OD1	3:H:172:ARG:NH2	2.49	0.43
2:D:27:C:H2'	2:D:28:U:C6	2.54	0.43
3:F:43:TRP:CD1	3:F:59:VAL:HG22	2.53	0.43
3:H:88:ARG:HE	3:H:88:ARG:HA	1.83	0.43
3:H:82:PHE:CZ	3:H:84:VAL:HB	2.54	0.43
3:F:279:LYS:HD3	3:F:279:LYS:HA	1.90	0.42
3:G:46:ASP:O	3:G:50:GLY:N	2.52	0.42
3:F:120:ASP:HB3	3:F:123:LYS:HE3	2.01	0.42
3:F:296:SER:OG	3:F:440:GLU:OE1	2.33	0.42
3:H:57:ILE:HD12	3:H:109:TYR:CE1	2.54	0.42
3:E:126:ILE:O	3:E:130:LYS:HG2	2.18	0.42
3:G:284:LEU:HD21	3:G:318:LEU:HD22	2.01	0.42
3:H:90:PHE:CD1	3:H:91:LEU:HD13	2.55	0.42
3:E:102:LEU:HB3	3:E:109:TYR:HB2	2.01	0.42
3:F:244:TYR:HB2	3:F:249:LEU:HD23	2.01	0.42
3:G:19:PHE:CE2	3:G:141:VAL:HG11	2.55	0.42
3:G:309:LEU:CD1	3:G:309:LEU:N	2.82	0.42
1:A:52:G:H1	1:A:62:C:H42	1.67	0.42
3:F:364:ASP:HA	3:F:367:THR:HG22	2.00	0.42
3:E:21:LEU:HD12	3:F:293:LYS:HA	2.01	0.42
3:H:252:ILE:O	3:H:359:ARG:NH1	2.52	0.42
1:A:29:G:H2'	1:A:30:G:H8	1.83	0.42
3:G:296:SER:OG	3:G:440:GLU:OE1	2.31	0.42
3:E:47:ARG:HD3	3:E:47:ARG:HA	1.89	0.42
3:G:496:UNK:O	3:G:500:UNK:N	2.52	0.42
3:E:295:LEU:HD12	3:E:295:LEU:HA	1.86	0.42
2:C:29:G:H2'	2:C:30:G:C8	2.55	0.41
3:F:141:VAL:HG12	3:F:156:VAL:HG12	2.00	0.41
3:F:31:LEU:CD1	3:F:32:PRO:N	2.53	0.41
3:F:182:ASP:HA	3:F:183:PRO:HD2	1.91	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:176:ILE:HD11	3:G:203:ASP:HB2	2.02	0.41
3:E:434:GLU:O	3:E:438:GLU:HG2	2.20	0.41
3:H:95:PRO:HG2	3:H:96:THR:H	1.84	0.41
3:H:172:ARG:HA	3:H:173:PRO:HD2	1.95	0.41
3:H:376:HIS:ND1	3:H:404:CYS:SG	2.82	0.41
3:F:134:PHE:HA	3:F:173:PRO:HA	2.02	0.41
3:G:30:VAL:HG13	3:G:73:ASN:CB	2.50	0.41
3:H:92:ILE:HG21	3:H:95:PRO:HA	2.02	0.41
3:G:30:VAL:HG13	3:G:73:ASN:HB2	1.99	0.41
3:H:314:ASP:OD1	3:H:314:ASP:N	2.37	0.41
3:E:308:VAL:HG11	3:E:366:ALA:HB2	2.03	0.41
3:G:30:VAL:HG23	3:G:77:ARG:HD3	2.01	0.41
3:G:329:LYS:HG2	3:G:345:HIS:CD2	2.56	0.41
3:H:84:VAL:O	3:H:84:VAL:HG22	2.21	0.41
1:B:2:G:C6	1:B:3:C:C4	3.09	0.41
3:G:314:ASP:OD1	3:G:314:ASP:N	2.41	0.41
2:D:74[B]:C:C1'	3:H:97:ILE:CD1	2.94	0.41
3:G:205:TYR:O	3:G:209:LYS:CG	2.61	0.41
3:H:73:ASN:O	3:H:76:LYS:HB3	2.21	0.41
3:H:227:LEU:HB3	3:H:320:TRP:HZ2	1.86	0.41
3:H:445:ASN:OD1	3:H:446:GLU:HG3	2.21	0.41
3:F:114:SER:HA	3:F:115:PRO:HD3	1.90	0.41
3:G:184:VAL:HG23	3:G:223:ILE:HD13	2.02	0.41
3:G:186:VAL:HG11	3:G:215:VAL:HG22	2.03	0.41
3:H:364:ASP:O	3:H:368:GLU:HB2	2.21	0.41
3:H:480:UNK:O	3:H:484:UNK:N	2.54	0.41
3:G:182:ASP:HA	3:G:183:PRO:HD2	1.89	0.41
3:H:29:LYS:CE	3:H:77:ARG:NH2	2.84	0.40
3:H:47:ARG:HD3	3:H:47:ARG:HA	1.98	0.40
3:H:295:LEU:HD21	3:H:409:PRO:CA	2.51	0.40
3:H:327:ILE:HD12	3:H:327:ILE:HA	1.96	0.40
2:C:29:G:H2'	2:C:30:G:H8	1.85	0.40
3:E:178:ASN:O	3:E:185:ARG:NH1	2.53	0.40
3:F:215:VAL:HG21	3:F:248:VAL:HG13	2.04	0.40
3:H:93:LYS:CE	3:H:131:GLU:CB	2.92	0.40
3:H:347:LYS:HG2	3:H:375:ARG:NE	2.36	0.40
3:E:114:SER:HA	3:E:115:PRO:HD3	1.86	0.40
3:E:290:ASP:O	3:E:293:LYS:HG3	2.21	0.40
3:H:86:GLU:CB	3:H:96:THR:HA	2.51	0.40
3:H:135:THR:HB	3:H:162:GLY:HA2	2.03	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	E	395/512 (77%)	390 (99%)	5 (1%)	0	100	100
3	F	396/512 (77%)	392 (99%)	4 (1%)	0	100	100
3	G	409/512 (80%)	406 (99%)	3 (1%)	0	100	100
3	H	410/512 (80%)	402 (98%)	8 (2%)	0	100	100
All	All	1610/2048 (79%)	1590 (99%)	20 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	
3	E	353/380 (93%)	337 (96%)	16 (4%)	27	61
3	F	354/380 (93%)	337 (95%)	17 (5%)	25	60
3	G	364/380 (96%)	341 (94%)	23 (6%)	18	51
3	H	365/380 (96%)	340 (93%)	25 (7%)	16	48
All	All	1436/1520 (94%)	1355 (94%)	81 (6%)	21	54

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	E	43	TRP
3	E	47	ARG

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
3	E	82	PHE
3	E	104	LEU
3	E	147	LEU
3	E	203	ASP
3	E	221	GLU
3	E	262	VAL
3	E	293	LYS
3	E	295	LEU
3	E	309	LEU
3	E	318	LEU
3	E	323	LEU
3	E	377	HIS
3	E	378	LEU
3	E	406	ASP
3	F	31	LEU
3	F	43	TRP
3	F	47	ARG
3	F	83	PHE
3	F	84	VAL
3	F	104	LEU
3	F	201	THR
3	F	220	VAL
3	F	221	GLU
3	F	293	LYS
3	F	295	LEU
3	F	318	LEU
3	F	323	LEU
3	F	325	HIS
3	F	377	HIS
3	F	378	LEU
3	F	428	ASP
3	G	31	LEU
3	G	43	TRP
3	G	47	ARG
3	G	85	PHE
3	G	86	GLU
3	G	88	ARG
3	G	90	PHE
3	G	93	LYS
3	G	99	SER
3	G	104	LEU
3	G	201	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	G	209	LYS
3	G	210	GLU
3	G	221	GLU
3	G	227	LEU
3	G	293	LYS
3	G	298	GLU
3	G	318	LEU
3	G	325	HIS
3	G	342	PHE
3	G	345	HIS
3	G	361	ARG
3	G	378	LEU
3	H	25	ASP
3	H	31	LEU
3	H	43	TRP
3	H	47	ARG
3	H	59	VAL
3	H	83	PHE
3	H	88	ARG
3	H	90	PHE
3	H	91	LEU
3	H	96	THR
3	H	104	LEU
3	H	203	ASP
3	H	217	LYS
3	H	220	VAL
3	H	221	GLU
3	H	239	VAL
3	H	293	LYS
3	H	295	LEU
3	H	318	LEU
3	H	342	PHE
3	H	377	HIS
3	H	378	LEU
3	H	433	MET
3	H	448	LYS
3	H	451	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	G	376	HIS

## 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	72/74 (97%)	9 (12%)	1 (1%)
1	B	72/74 (97%)	12 (16%)	1 (1%)
2	C	73/75 (97%)	13 (17%)	1 (1%)
2	D	73/75 (97%)	14 (19%)	1 (1%)
All	All	290/298 (97%)	48 (16%)	4 (1%)

All (48) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	17	U
1	A	18	G
1	A	19	G
1	A	20	U
1	A	22	G
1	A	45	U
1	A	47	U
1	A	48	C
1	A	61	C
1	B	17	U
1	B	18	G
1	B	19	G
1	B	20	U
1	B	21	A
1	B	22	G
1	B	43	G
1	B	45	U
1	B	47	U
1	B	48	C
1	B	61	C
1	B	74[B]	C
2	C	16	U
2	C	17	U
2	C	18	G
2	C	19	G
2	C	20	U
2	C	21	A
2	C	22	G
2	C	43	G
2	C	44	G
2	C	45	U
2	C	47	U

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	C	48	C
2	C	61	C
2	D	6	G
2	D	16	U
2	D	17	U
2	D	18	G
2	D	19	G
2	D	20	U
2	D	21	A
2	D	22	G
2	D	44	G
2	D	45	U
2	D	47	U
2	D	48	C
2	D	61	C
2	D	75[B]	C

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	19	G
1	B	19	G
2	C	19	G
2	D	19	G

## 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](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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
4	CTP	F	601[A]	6	29,30,30	1.01	0	43,47,47	0.87	0
5	POP	F	602[B]	6	6,8,8	0.76	0	12,13,13	0.90	0
5	POP	H	602[B]	6	6,8,8	0.75	0	12,13,13	0.92	0
5	POP	E	602[B]	6	6,8,8	0.76	0	12,13,13	0.90	0
5	POP	G	602[B]	6	6,8,8	0.76	0	12,13,13	0.90	0
4	CTP	H	601[A]	6	29,30,30	0.97	0	43,47,47	0.89	1 (2%)
4	CTP	G	601[A]	6	29,30,30	0.99	0	43,47,47	0.88	0
4	CTP	E	601[A]	6	29,30,30	1.01	0	43,47,47	0.88	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	CTP	F	601[A]	6	-	5/22/38/38	0/2/2/2
5	POP	F	602[B]	6	-	0/6/6/6	-
5	POP	H	602[B]	6	-	0/6/6/6	-
5	POP	E	602[B]	6	-	0/6/6/6	-
5	POP	G	602[B]	6	-	0/6/6/6	-
4	CTP	H	601[A]	6	-	7/22/38/38	0/2/2/2
4	CTP	G	601[A]	6	-	5/22/38/38	0/2/2/2
4	CTP	E	601[A]	6	-	6/22/38/38	0/2/2/2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	601[A]	CTP	C3'-C2'-C1'	2.07	105.38	101.46

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	601[A]	CTP	O4'-C4'-C5'-O5'
4	E	601[A]	CTP	C5'-O5'-PA-O1A

*Continued on next page...*

*Continued from previous page...*

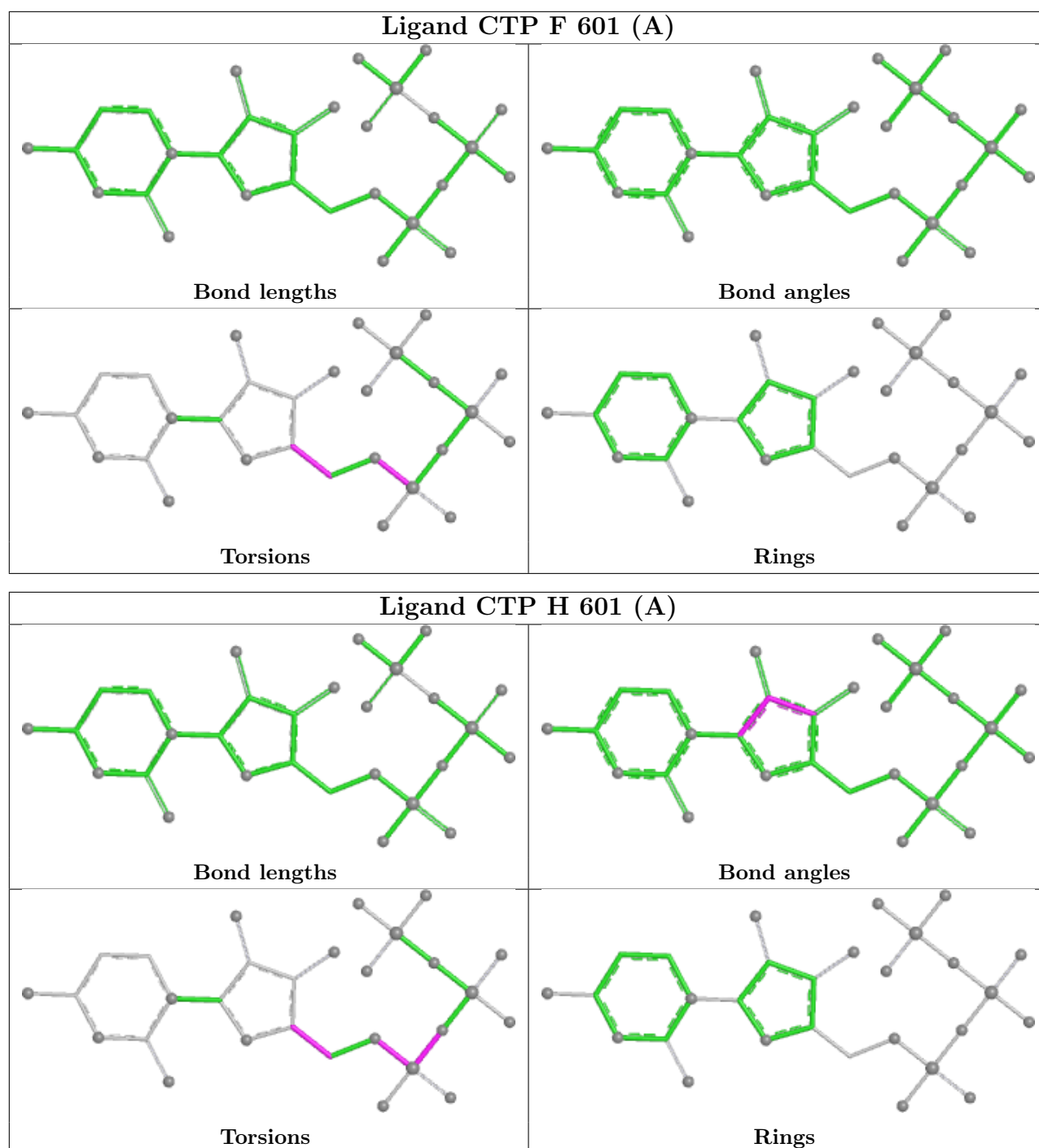
Mol	Chain	Res	Type	Atoms
4	E	601[A]	CTP	C5'-O5'-PA-O2A
4	E	601[A]	CTP	C5'-O5'-PA-O3A
4	F	601[A]	CTP	O4'-C4'-C5'-O5'
4	F	601[A]	CTP	C5'-O5'-PA-O3A
4	G	601[A]	CTP	O4'-C4'-C5'-O5'
4	H	601[A]	CTP	O4'-C4'-C5'-O5'
4	E	601[A]	CTP	C3'-C4'-C5'-O5'
4	G	601[A]	CTP	C3'-C4'-C5'-O5'
4	H	601[A]	CTP	C3'-C4'-C5'-O5'
4	F	601[A]	CTP	C3'-C4'-C5'-O5'
4	H	601[A]	CTP	PB-O3A-PA-O1A
4	F	601[A]	CTP	C5'-O5'-PA-O1A
4	F	601[A]	CTP	C5'-O5'-PA-O2A
4	G	601[A]	CTP	C5'-O5'-PA-O1A
4	G	601[A]	CTP	C5'-O5'-PA-O2A
4	G	601[A]	CTP	C5'-O5'-PA-O3A
4	H	601[A]	CTP	C5'-O5'-PA-O1A
4	H	601[A]	CTP	C5'-O5'-PA-O2A
4	H	601[A]	CTP	C5'-O5'-PA-O3A
4	E	601[A]	CTP	PA-O3A-PB-O1B
4	H	601[A]	CTP	PB-O3A-PA-O2A

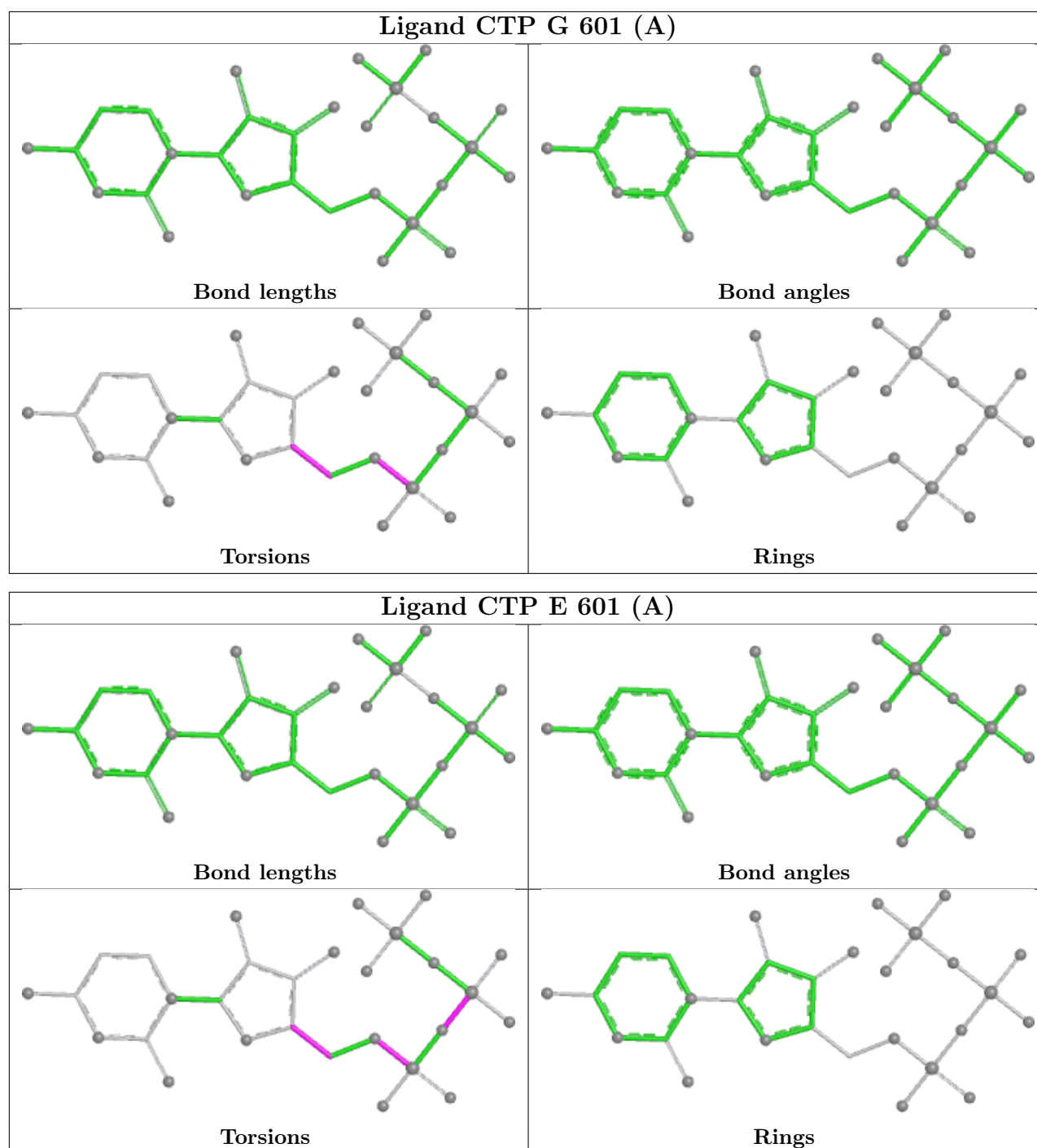
There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	602[B]	POP	1	0
5	G	602[B]	POP	2	0
4	E	601[A]	CTP	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	74/74 (100%)	4.30	55 (74%) 0 0	68, 200, 272, 290	1 (1%)
1	B	74/74 (100%)	4.16	61 (82%) 0 0	99, 203, 276, 312	1 (1%)
2	C	75/75 (100%)	4.04	61 (81%) 0 0	70, 206, 259, 289	1 (1%)
2	D	75/75 (100%)	4.71	62 (82%) 0 0	80, 236, 385, 428	1 (1%)
3	E	405/512 (79%)	0.09	9 (2%) 62 56	40, 79, 143, 171	0
3	F	406/512 (79%)	0.28	12 (2%) 50 44	43, 91, 139, 168	0
3	G	417/512 (81%)	0.30	19 (4%) 32 28	46, 91, 145, 171	0
3	H	418/512 (81%)	0.12	8 (1%) 66 61	42, 79, 138, 164	0
All	All	1944/2346 (82%)	0.83	287 (14%) 2 3	40, 92, 242, 428	4 (0%)

All (287) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	21	A	13.2
1	A	45	U	10.8
2	C	19	G	10.4
2	D	41	C	10.4
2	D	21	A	10.3
1	A	22	G	9.9
2	D	47	U	9.8
1	B	45	U	9.7
2	D	24	G	9.3
1	B	44	G	9.0
2	D	35	A	8.7
2	D	16	U	8.6
1	B	21	A	8.4
2	D	10	G	8.4
2	D	31	A	8.3
2	C	21	A	8.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	57	G	8.2
2	D	22	G	8.2
1	B	19	G	8.1
2	C	36	A	7.9
2	D	26	A	7.8
2	D	42	A	7.7
2	C	46	G	7.6
1	B	20	U	7.6
2	D	34	G	7.6
1	B	47	U	7.6
2	D	43	G	7.6
1	B	18	G	7.5
1	A	37	A	7.4
1	A	27	C	7.4
1	B	53	G	7.3
1	A	35	A	7.2
1	A	15	G	7.1
1	A	36	A	7.0
2	C	22	G	7.0
2	C	53	G	7.0
2	D	36	A	7.0
1	B	54	U	7.0
2	D	51	C	7.0
1	A	20	U	6.9
1	B	40	C	6.9
2	C	54	U	6.9
2	C	18	G	6.9
1	B	56	C	6.9
2	C	35	A	6.9
1	A	47	U	6.8
1	B	52	G	6.7
1	A	32	C	6.7
1	B	32	C	6.7
1	A	53	G	6.7
2	D	45	U	6.6
2	D	15	G	6.6
1	A	16	U	6.6
1	B	46	G	6.6
2	C	45	U	6.5
1	B	58	A	6.5
2	D	12	U	6.4
2	C	39	U	6.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	C	7	G	6.3
2	C	61	C	6.3
2	D	13	C	6.3
2	D	23	A	6.3
1	A	57	G	6.3
1	A	42	A	6.2
1	B	10	G	6.2
1	A	52	G	6.2
1	A	38	A	6.2
1	A	46	G	6.1
2	C	20	U	6.1
2	D	7	G	6.1
1	A	19	G	6.1
2	D	39	U	6.1
2	C	24	G	6.0
1	B	42	A	6.0
1	B	22	G	5.9
3	E	334	ALA	5.9
1	A	26	A	5.9
1	A	10	G	5.9
2	D	46	G	5.9
2	C	27	C	5.9
2	D	32	C	5.9
1	A	18	G	5.9
1	B	29	G	5.8
2	C	37	A	5.8
2	C	52	G	5.7
2	D	17	U	5.7
1	A	30	G	5.6
1	A	39	U	5.5
2	C	34	G	5.5
2	C	47	U	5.5
2	D	63	G	5.5
1	A	31	A	5.4
1	A	29	G	5.4
2	C	59	U	5.4
2	C	60	U	5.4
2	D	25	C	5.4
3	F	118	GLY	5.4
2	D	65	C	5.3
1	B	17	U	5.3
1	A	34	G	5.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	43	G	5.3
2	C	23	A	5.3
1	B	41	C	5.3
1	A	43	G	5.3
2	C	40	C	5.2
1	B	38	A	5.2
2	D	9	A	5.2
2	C	44	G	5.2
2	D	8	U	5.2
2	D	14	A	5.1
2	D	33	U	5.1
1	A	41	C	5.1
1	A	40	C	5.0
2	C	56	C	5.0
2	D	27	C	5.0
1	A	17	U	5.0
1	B	16	U	5.0
2	C	15	G	5.0
3	G	118	GLY	5.0
1	B	15	G	5.0
2	C	57	G	4.9
1	A	14	A	4.9
1	B	39	U	4.8
2	C	58	A	4.8
2	C	38	A	4.8
2	D	61	C	4.8
1	B	37	A	4.7
2	D	20	U	4.7
2	D	50	G	4.7
2	C	16	U	4.7
1	B	34	G	4.6
1	B	61	C	4.6
2	D	58	A	4.6
2	D	6	G	4.6
2	D	18	G	4.6
2	D	40	C	4.6
3	G	334	ALA	4.5
1	B	23	A	4.5
1	A	51	C	4.5
2	C	51	C	4.5
2	C	43	G	4.5
1	B	14	A	4.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	44	G	4.4
1	A	56	C	4.4
2	D	48	C	4.4
1	A	54	U	4.3
1	A	24	G	4.3
1	A	13	C	4.3
2	C	48	C	4.3
2	D	66	C	4.3
2	D	67	C	4.2
1	A	33	U	4.2
1	A	58	A	4.2
1	B	13	C	4.2
2	D	37	A	4.2
2	C	32	C	4.2
1	A	25	C	4.1
1	A	61	C	4.0
2	D	30	G	4.0
2	C	50	G	3.9
3	F	117	LYS	3.9
1	B	26	A	3.9
2	D	38	A	3.8
2	D	52	G	3.8
1	B	24	G	3.8
1	A	63	G	3.8
2	C	64	C	3.8
2	C	26	A	3.8
1	B	31	A	3.7
1	B	49	G	3.7
1	A	11	C	3.7
2	C	65	C	3.7
1	B	55	U	3.7
1	B	33	U	3.7
1	B	30	G	3.6
2	C	62	C	3.6
2	D	49	G	3.6
2	D	11	C	3.5
1	A	28	U	3.5
1	B	63	G	3.5
3	H	93	LYS	3.5
2	C	10	G	3.4
2	C	14	A	3.4
1	A	48	C	3.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
3	F	341	THR	3.4
2	C	17	U	3.4
2	D	44	G	3.4
2	D	68	U	3.4
2	D	19	G	3.4
1	A	12	U	3.3
2	D	53	G	3.3
1	B	36	A	3.3
1	B	35	A	3.3
1	A	66	C	3.3
1	B	65	C	3.3
2	C	66	C	3.3
2	C	6	G	3.2
2	C	67	C	3.2
3	G	159	PRO	3.2
2	D	29	G	3.2
3	G	154	THR	3.2
1	B	51	C	3.1
2	C	9	A	3.1
1	B	48	C	3.1
2	D	28	U	3.1
2	D	64	C	3.1
1	A	23	A	3.1
2	C	8	U	3.1
2	C	25	C	3.1
2	D	59	U	3.0
2	D	60	U	3.0
1	B	60	U	2.9
2	C	41	C	2.9
3	F	156	VAL	2.9
3	H	263	LYS	2.9
2	C	13	C	2.9
3	G	449	GLU	2.9
2	C	68	U	2.9
1	B	50	G	2.9
2	C	33	U	2.9
3	E	426	GLU	2.8
1	B	9	A	2.8
3	F	123	LYS	2.8
1	B	8	U	2.8
1	B	59	U	2.8
2	C	12	U	2.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	C	28	U	2.8
1	B	12	U	2.8
3	G	95	PRO	2.7
1	B	11	C	2.7
1	B	62	C	2.7
2	C	11	C	2.7
2	C	49	G	2.7
1	A	4	C	2.7
1	A	49	G	2.7
3	G	450	GLU	2.7
3	E	368	GLU	2.7
3	G	333	PHE	2.7
3	E	343	TYR	2.6
1	B	64	C	2.5
3	F	46	ASP	2.5
3	H	94	ARG	2.5
3	F	128	ASP	2.5
3	G	69	GLU	2.5
1	A	67	C	2.4
1	A	8	U	2.4
2	D	54	U	2.4
3	G	397	MET	2.4
3	E	345	HIS	2.4
1	B	25	C	2.4
2	C	31	A	2.4
3	H	154	THR	2.4
3	H	326	ASP	2.4
2	D	4	C	2.4
2	C	69	G	2.4
1	A	62	C	2.4
3	G	84	VAL	2.3
1	B	72	C	2.3
1	B	28	U	2.3
3	G	115	PRO	2.3
2	D	69	G	2.3
3	E	264	ASP	2.3
1	B	27	C	2.2
2	D	62	C	2.2
3	H	274	ASP	2.2
3	G	64	THR	2.2
3	H	426	GLU	2.2
3	G	35	HIS	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
3	G	34	GLU	2.1
1	B	6	G	2.1
3	F	64	THR	2.1
3	G	17	LEU	2.1
3	E	367	THR	2.1
3	F	114	SER	2.1
3	E	427	GLU	2.1
3	F	121	LEU	2.1
1	B	66	C	2.1
3	E	389	LYS	2.1
3	G	36	TYR	2.1
3	G	399	ASN	2.1
3	G	117	LYS	2.0
1	A	65	C	2.0
2	C	55	U	2.0
3	F	131	GLU	2.0
3	F	127	GLU	2.0
2	C	63	G	2.0
3	H	393	LYS	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( $\text{\AA}^2$ )	Q<0.9
6	MG	H	603	1/1	0.78	0.23	55,55,55,55	0
6	MG	F	603	1/1	0.80	0.19	81,81,81,81	0
6	MG	G	603	1/1	0.84	0.15	76,76,76,76	0
5	POP	G	602[B]	9/9	0.88	0.26	74,83,97,99	9

*Continued on next page...*



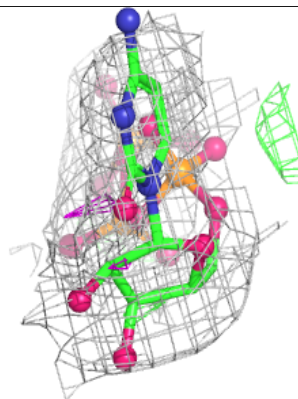
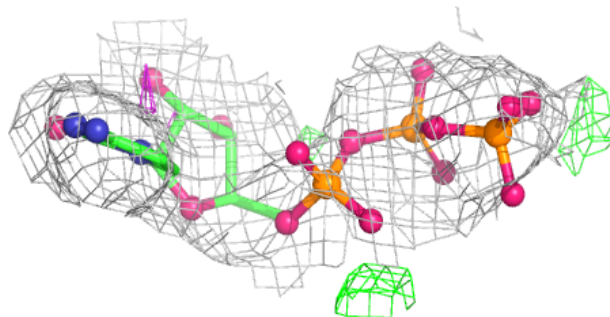
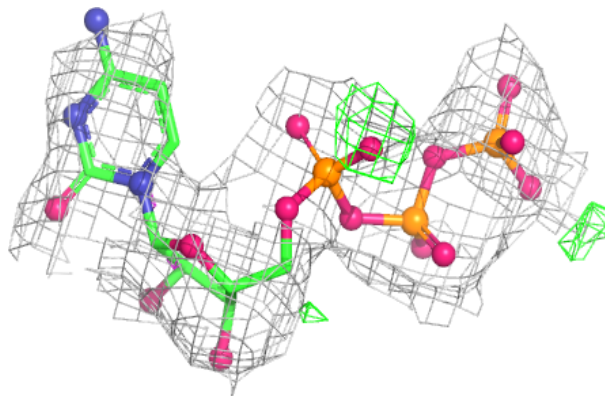
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	CTP	F	601[A]	29/29	0.88	0.27	67,94,121,127	29
5	POP	H	602[B]	9/9	0.90	0.25	37,82,107,108	9
5	POP	F	602[B]	9/9	0.90	0.27	117,118,123,124	9
6	MG	E	603	1/1	0.91	0.23	45,45,45,45	0
4	CTP	H	601[A]	29/29	0.92	0.24	36,57,108,110	29
5	POP	E	602[B]	9/9	0.92	0.25	72,77,119,120	9
4	CTP	G	601[A]	29/29	0.92	0.24	49,72,97,98	29
4	CTP	E	601[A]	29/29	0.93	0.26	40,50,118,120	29

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.

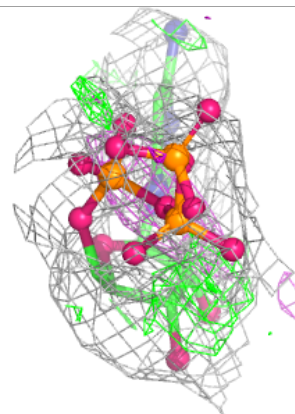
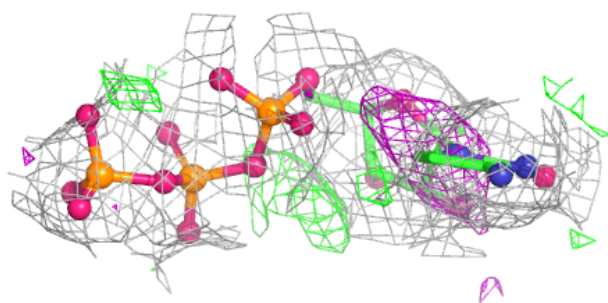
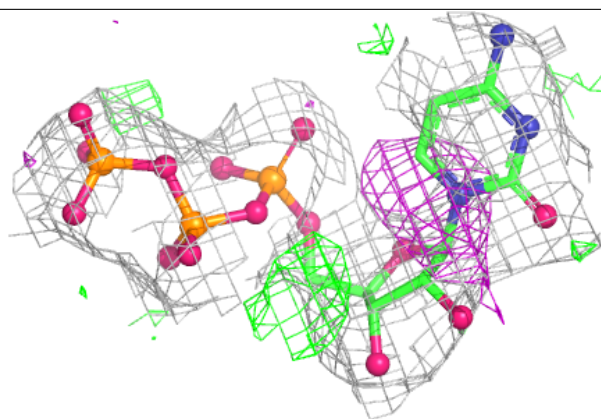
**Electron density around CTP F 601 (A):**

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)



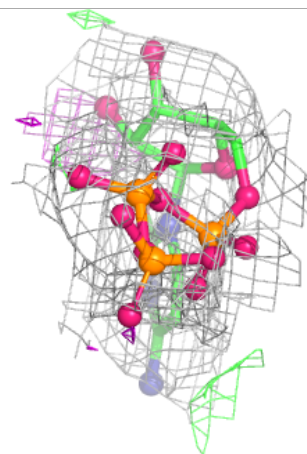
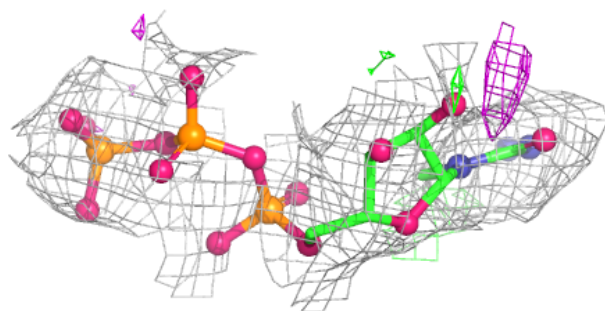
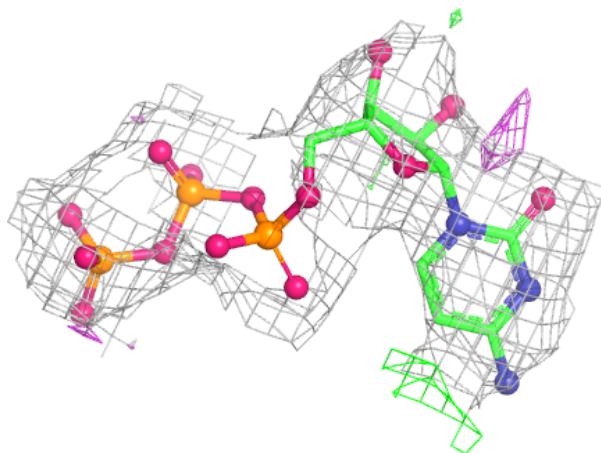
**Electron density around CTP H 601 (A):**

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



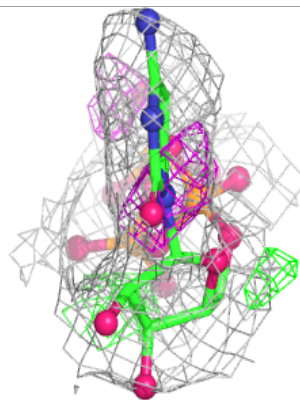
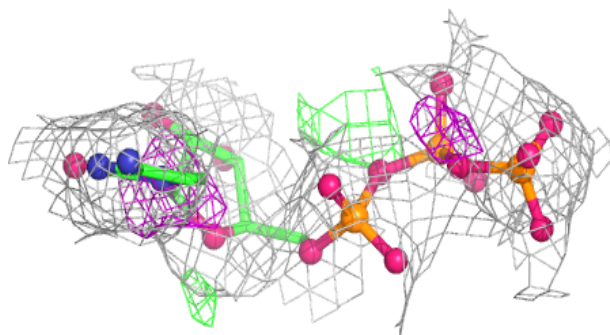
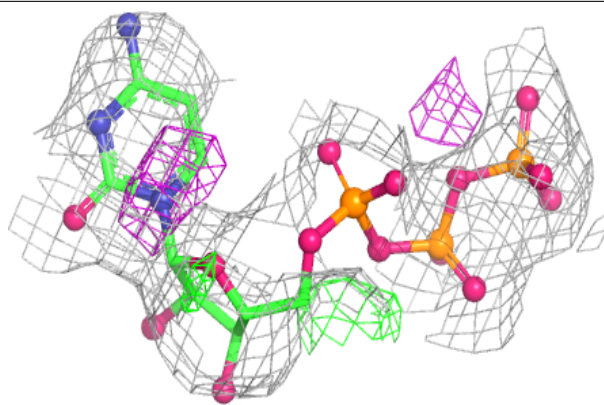
**Electron density around CTP G 601 (A):**

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



**Electron density around CTP E 601 (A):**

$2mF_o-DF_c$  (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.