



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 07:16 am BST

PDB ID : 2CVY  
Title : Structures of Yeast Ribonucleotide Reductase I  
Authors : Xu, H.; Faber, C.; Uchiki, T.; Fairman, J.W.; Racca, J.; Dealwis, C.  
Deposited on : 2005-06-14  
Resolution : 2.40 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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

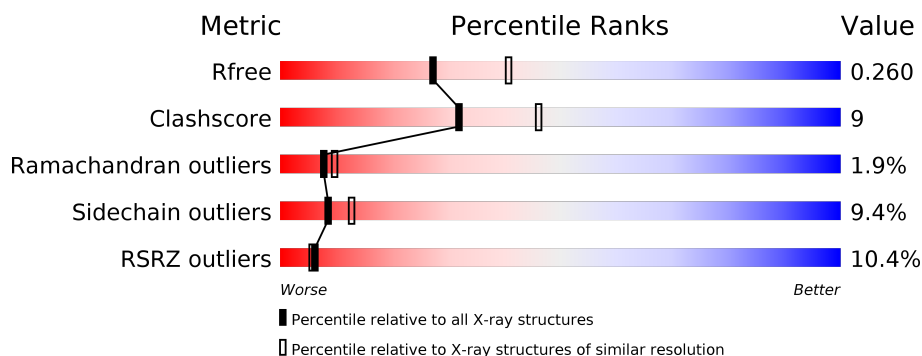
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	888	
2	B	9	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5298 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 Ribonucleoside-diphosphate reductase large chain 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	640	Total	C	N	O	S	0	0	0
			5128	3272	865	960	31			

- Molecule 2 is a protein called 9-per peptide from Ribonucleoside-diphosphate reductase small chain 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	7	Total	C	N	O	0	0	0
			66	44	8	14			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is THYMIDINE-5'-TRIPHOSPHATE (three-letter code: TTP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>2</sub>O<sub>14</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			29	10	2	14	3		

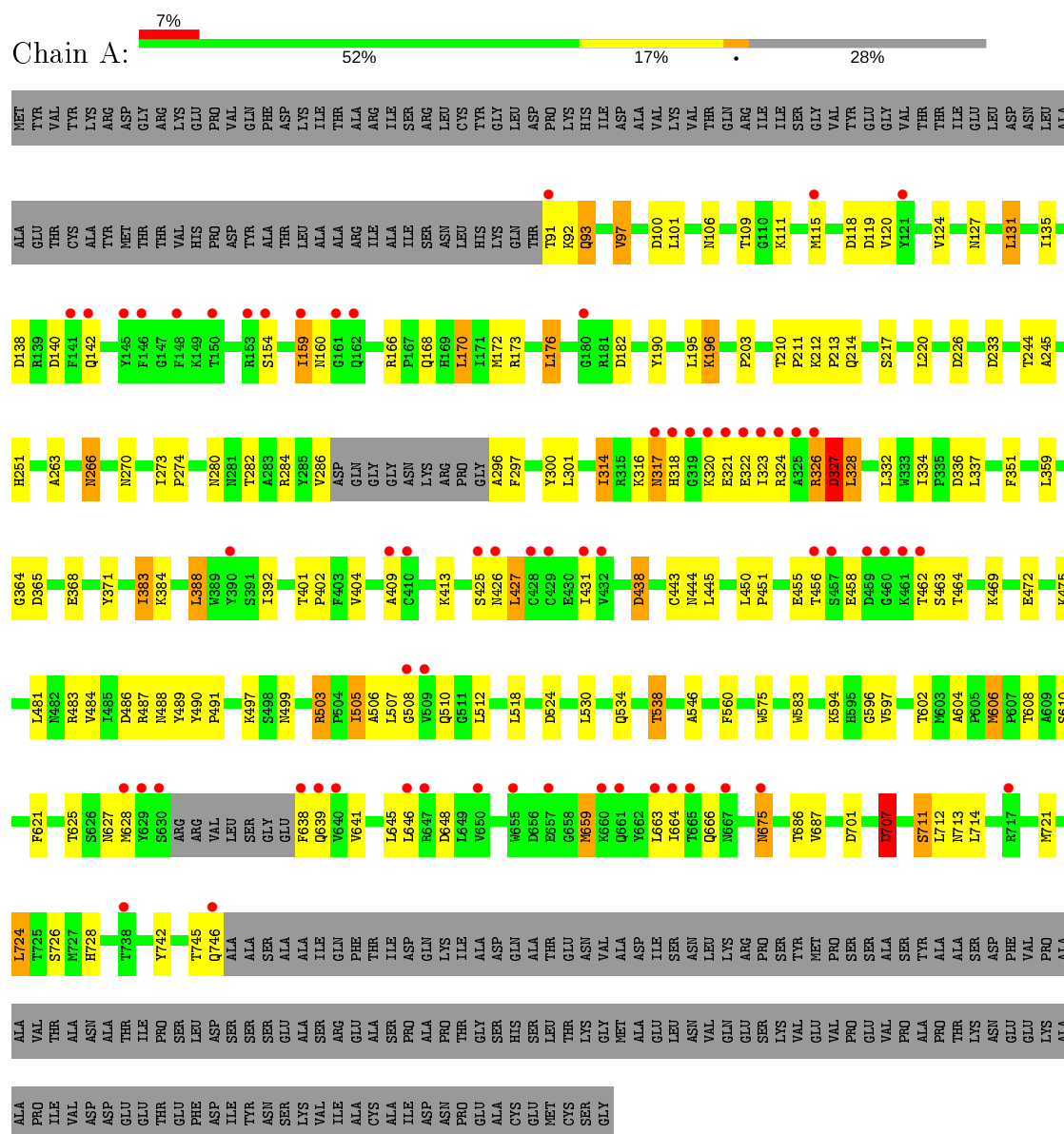
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	74	Total	O	0
			74	74	

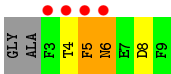
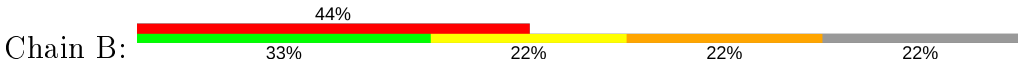
### 3 Residue-property plots

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: Ribonucleoside-diphosphate reductase large chain 1



- Molecule 2: 9-per peptide from Ribonucleoside-diphosphate reductase small chain 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	108.06 Å   117.59 Å   64.22 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	50.00 – 2.40 49.10 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.9 (50.00-2.40) 97.8 (49.10-2.40)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.12 (at 2.39 Å)	Xtriage
Refinement program	REFMAC 5.2.0007	Depositor
R, $R_{free}$	0.218   ,   0.263 0.215   ,   0.260	Depositor DCC
$R_{free}$ test set	3222 reflections (10.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.8	Xtriage
Anisotropy	0.462	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 41.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5298	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% 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

### 5.1 Standard geometry

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

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	0.67	0/5247	0.86	16/7103 (0.2%)
2	B	0.63	0/68	0.93	1/89 (1.1%)
All	All	0.67	0/5315	0.87	17/7192 (0.2%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	503	ARG	NE-CZ-NH2	-9.20	115.70	120.30
1	A	365	ASP	CB-CG-OD2	7.61	125.14	118.30
1	A	233	ASP	CB-CG-OD2	7.20	124.78	118.30
1	A	226	ASP	CB-CG-OD2	7.16	124.74	118.30
1	A	100	ASP	CB-CG-OD2	7.10	124.69	118.30
1	A	336	ASP	CB-CG-OD2	6.62	124.25	118.30
1	A	707	ASP	CB-CG-OD2	6.13	123.82	118.30
1	A	138	ASP	CB-CG-OD2	5.97	123.67	118.30
2	B	8	ASP	CB-CG-OD2	5.92	123.63	118.30
1	A	438	ASP	CB-CG-OD2	5.61	123.35	118.30
1	A	648	ASP	CB-CG-OD2	5.43	123.19	118.30
1	A	140	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	118	ASP	CB-CG-OD2	5.21	122.98	118.30
1	A	182	ASP	CB-CG-OD2	5.16	122.94	118.30
1	A	701	ASP	CB-CG-OD2	5.08	122.87	118.30
1	A	503	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	A	119	ASP	CB-CG-OD2	5.02	122.81	118.30

There are no chirality outliers.

There are no planarity outliers.



## 5.2 Too-close contacts ⓘ

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	5128	0	5057	90	0
2	B	66	0	49	2	0
3	A	1	0	0	0	0
4	A	29	0	13	1	0
5	A	74	0	0	3	0
All	All	5298	0	5119	92	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 9.

All (92) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:ILE:HG23	1:A:160:ASN:H	1.35	0.91
1:A:270:ASN:HB3	1:A:274:PRO:HG2	1.54	0.89
2:B:5:PHE:O	2:B:6:ASN:HB2	1.82	0.78
1:A:251:HIS:HD2	5:A:2014:HOH:O	1.65	0.78
1:A:170:LEU:HD22	1:A:173:ARG:NH2	1.99	0.77
1:A:263:ALA:HB3	4:A:1001:TTP:O1G	1.85	0.74
1:A:213:PRO:HD2	1:A:489:TYR:HB2	1.69	0.74
1:A:109:THR:HG23	1:A:111:LYS:H	1.53	0.73
1:A:334:ILE:HD12	1:A:404:VAL:HG13	1.73	0.71
1:A:210:THR:HB	1:A:211:PRO:HD2	1.75	0.69
1:A:273:ILE:HD12	1:A:314:ILE:HD11	1.76	0.67
1:A:296:ALA:HB3	1:A:427:LEU:HD21	1.79	0.65
1:A:486:ASP:CG	1:A:503:ARG:HH22	2.01	0.64
1:A:318:HIS:O	1:A:324:ARG:NH1	2.30	0.64
1:A:317:ASN:HA	1:A:326:ARG:NH2	2.14	0.63
1:A:445:LEU:HD23	1:A:506:ALA:HB3	1.81	0.61
1:A:486:ASP:OD2	1:A:503:ARG:NH2	2.33	0.61
1:A:127:ASN:HB2	1:A:131:LEU:HD22	1.82	0.61
1:A:481:LEU:HB3	1:A:505:ILE:HD12	1.82	0.61
1:A:606:MET:HE2	5:A:2017:HOH:O	2.00	0.60
1:A:538:THR:HB	1:A:583:TRP:NE1	2.16	0.60
1:A:92:LYS:HB2	1:A:166:ARG:HH22	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:ILE:HG23	1:A:160:ASN:N	2.13	0.59
1:A:280:ASN:HB2	1:A:328:LEU:HD11	1.84	0.58
1:A:438:ASP:OD1	1:A:497:LYS:NZ	2.34	0.58
1:A:560:PHE:CZ	1:A:596:GLY:HA2	2.38	0.58
1:A:92:LYS:HB2	1:A:166:ARG:NH2	2.19	0.57
1:A:332:LEU:HD11	1:A:392:ILE:HD12	1.87	0.57
1:A:456:THR:HA	1:A:463:SER:HA	1.88	0.56
1:A:212:LYS:HD2	1:A:489:TYR:CE1	2.41	0.56
1:A:318:HIS:H	1:A:318:HIS:CD2	2.23	0.56
1:A:317:ASN:HA	1:A:326:ARG:HH21	1.71	0.55
1:A:510:GLN:HB3	1:A:608:THR:HG21	1.87	0.55
1:A:401:THR:HB	1:A:402:PRO:HA	1.90	0.54
1:A:444:ASN:HD21	1:A:499:ASN:HD21	1.56	0.53
1:A:625:THR:HA	1:A:687:VAL:HG12	1.91	0.53
1:A:92:LYS:HD2	1:A:166:ARG:HH12	1.74	0.52
1:A:388:LEU:O	1:A:392:ILE:HG12	2.10	0.52
1:A:484:VAL:O	1:A:488:ASN:HB2	2.10	0.52
1:A:508:GLY:HA3	1:A:606:MET:CE	2.40	0.52
1:A:506:ALA:HB1	1:A:604:ALA:HB3	1.93	0.51
1:A:106:ASN:OD1	1:A:109:THR:HG22	2.11	0.51
1:A:101:LEU:HB3	1:A:115:MET:HB3	1.93	0.51
1:A:383:ILE:CG1	1:A:384:LYS:H	2.23	0.51
1:A:409:ALA:HB2	5:A:2019:HOH:O	2.11	0.51
1:A:316:LYS:HD3	1:A:318:HIS:CE1	2.47	0.50
1:A:508:GLY:HA3	1:A:606:MET:HE1	1.94	0.49
1:A:217:SER:OG	1:A:445:LEU:HD12	2.13	0.48
1:A:455:GLU:O	1:A:464:THR:N	2.39	0.48
1:A:93:GLN:O	1:A:97:VAL:HG13	2.14	0.48
1:A:159:ILE:CG2	1:A:160:ASN:H	2.18	0.48
1:A:602:THR:N	1:A:707:ASP:OD2	2.47	0.47
1:A:745:THR:O	1:A:746:GLN:HB2	2.14	0.46
1:A:266:ASN:H	1:A:266:ASN:ND2	2.12	0.46
1:A:413:LYS:HE3	1:A:575:TRP:CE2	2.50	0.46
1:A:273:ILE:HB	1:A:274:PRO:HD3	1.97	0.46
1:A:220:LEU:HD21	1:A:426:ASN:HB3	1.96	0.46
1:A:217:SER:CB	1:A:445:LEU:HD12	2.46	0.46
1:A:282:THR:O	1:A:286:VAL:HG22	2.16	0.46
1:A:203:PRO:HG2	1:A:217:SER:HA	1.98	0.45
1:A:326:ARG:O	1:A:327:ASP:HB2	2.15	0.45
1:A:170:LEU:HD22	1:A:173:ARG:HH22	1.75	0.45
1:A:713:ASN:ND2	1:A:742:TYR:H	2.14	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:ILE:HG21	1:A:323:ILE:HA	2.00	0.44
1:A:534:GLN:O	1:A:538:THR:HG23	2.16	0.44
1:A:195:LEU:O	1:A:196:LYS:HB2	2.17	0.44
1:A:713:ASN:HD22	1:A:742:TYR:H	1.65	0.44
1:A:675:ASN:ND2	1:A:675:ASN:O	2.47	0.44
1:A:383:ILE:HG13	1:A:384:LYS:H	1.82	0.44
1:A:280:ASN:CB	1:A:328:LEU:HD11	2.48	0.43
1:A:120:VAL:O	1:A:124:VAL:HG23	2.19	0.43
1:A:168:GLN:NE2	1:A:190:TYR:OH	2.46	0.43
1:A:475:LYS:HD2	1:A:546:ALA:HB2	2.00	0.43
1:A:135:ILE:HG23	1:A:168:GLN:HB3	2.00	0.43
1:A:431:ILE:HG13	1:A:443:CYS:SG	2.59	0.43
1:A:351:PHE:HE1	1:A:371:TYR:CE1	2.37	0.42
1:A:472:GLU:O	1:A:475:LYS:HB2	2.19	0.42
1:A:450:LEU:N	1:A:451:PRO:CD	2.82	0.42
2:B:5:PHE:O	2:B:6:ASN:CB	2.59	0.42
1:A:172:MET:O	1:A:176:LEU:HD22	2.20	0.42
1:A:641:VAL:HG13	1:A:646:LEU:HD22	2.02	0.41
1:A:328:LEU:HD12	1:A:328:LEU:H	1.85	0.41
1:A:627:ASN:HB3	1:A:645:LEU:HD22	2.02	0.41
1:A:300:TYR:OH	1:A:425:SER:HB3	2.21	0.41
1:A:621:PHE:HZ	1:A:711:SER:O	2.02	0.41
1:A:724:LEU:HD22	1:A:728:HIS:CD2	2.55	0.41
1:A:481:LEU:CD1	1:A:505:ILE:HG23	2.50	0.41
1:A:109:THR:OG1	1:A:111:LYS:HG3	2.21	0.40
1:A:124:VAL:HA	1:A:131:LEU:HD23	2.02	0.40
1:A:490:TYR:HA	1:A:491:PRO:HD2	1.91	0.40
1:A:483:ARG:NH2	1:A:487:ARG:HD2	2.36	0.40
1:A:364:GLY:O	1:A:368:GLU:HG3	2.21	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	
1	A	634/888 (71%)	589 (93%)	34 (5%)	11 (2%)	9	11
2	B	5/9 (56%)	4 (80%)	0	1 (20%)	0	0
All	All	639/897 (71%)	593 (93%)	34 (5%)	12 (2%)	8	10

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	6	ASN
1	A	245	ALA
1	A	327	ASP
1	A	458	GLU
1	A	659	MET
1	A	664	ILE
1	A	93	GLN
1	A	159	ILE
1	A	320	LYS
1	A	639	GLN
1	A	666	GLN
1	A	196	LYS

### 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	557/761 (73%)	506 (91%)	51 (9%)	9	13
2	B	7/7 (100%)	5 (71%)	2 (29%)	0	0
All	All	564/768 (73%)	511 (91%)	53 (9%)	8	13

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91	THR
1	A	97	VAL
1	A	131	LEU
1	A	142	GLN

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Mol	Chain	Res	Type
1	A	154	SER
1	A	170	LEU
1	A	176	LEU
1	A	214	GLN
1	A	244	THR
1	A	266	ASN
1	A	284	ARG
1	A	297	PHE
1	A	301	LEU
1	A	314	ILE
1	A	317	ASN
1	A	321	GLU
1	A	322	GLU
1	A	326	ARG
1	A	327	ASP
1	A	328	LEU
1	A	337	LEU
1	A	359	LEU
1	A	383	ILE
1	A	388	LEU
1	A	427	LEU
1	A	462	THR
1	A	469	LYS
1	A	505	ILE
1	A	507	LEU
1	A	512	LEU
1	A	518	LEU
1	A	524	ASP
1	A	530	LEU
1	A	538	THR
1	A	594	LYS
1	A	597	VAL
1	A	606	MET
1	A	610	SER
1	A	628	MET
1	A	638	PHE
1	A	659	MET
1	A	663	LEU
1	A	675	ASN
1	A	686	THR
1	A	707	ASP
1	A	711	SER

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Mol	Chain	Res	Type
1	A	712	LEU
1	A	714	LEU
1	A	721	MET
1	A	724	LEU
1	A	726	SER
2	B	4	THR
2	B	5	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	127	ASN
1	A	142	GLN
1	A	168	GLN
1	A	251	HIS
1	A	266	ASN
1	A	317	ASN
1	A	444	ASN
1	A	613	GLN
1	A	618	ASN
1	A	692	GLN
1	A	713	ASN

### 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 carbohydrates in this entry.

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

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	TTP	A	1001	3	23,30,30	1.19	1 (4%)	29,47,47	1.71	5 (17%)

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	TTP	A	1001	3	-	3/19/34/34	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1001	TTP	C4-C5	4.08	1.50	1.41

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1001	TTP	C4-N3-C2	6.61	120.72	115.14
4	A	1001	TTP	PB-O3A-PA	-3.18	121.92	132.83
4	A	1001	TTP	PB-O3B-PG	-2.76	123.35	132.83
4	A	1001	TTP	O2G-PG-O3B	2.36	112.55	104.64
4	A	1001	TTP	C5-C6-N1	-2.31	119.70	122.19

There are no chirality outliers.

All (3) torsion outliers are listed below:

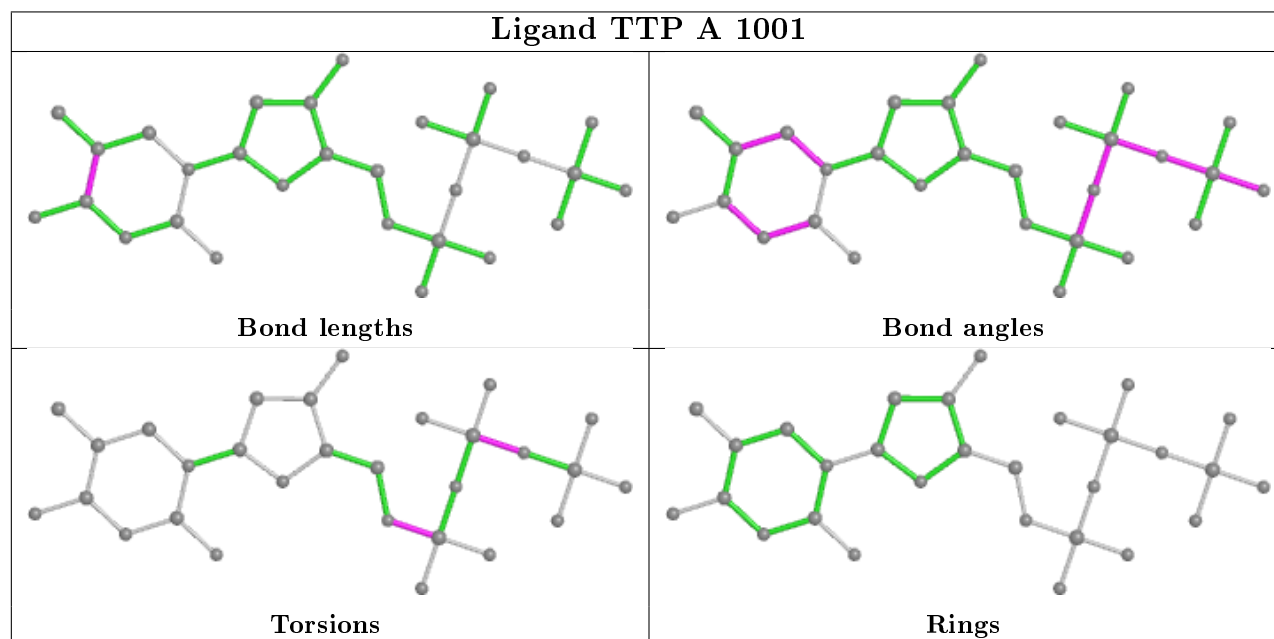
Mol	Chain	Res	Type	Atoms
4	A	1001	TTP	C5'-O5'-PA-O3A
4	A	1001	TTP	PG-O3B-PB-O1B
4	A	1001	TTP	C5'-O5'-PA-O1A

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1001	TTP	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	640/888 (72%)	0.47	63 (9%) 7 7	28, 43, 82, 93	0
2	B	7/9 (77%)	2.26	4 (57%) 0 0	75, 84, 86, 87	0
All	All	647/897 (72%)	0.49	67 (10%) 6 6	28, 43, 84, 93	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	460	GLY	7.8
1	A	638	PHE	7.1
1	A	91	THR	6.9
1	A	630	SER	6.5
1	A	639	GLN	6.5
1	A	321	GLU	6.4
1	A	323	ILE	6.2
1	A	664	ILE	6.1
1	A	325	ALA	5.7
1	A	320	LYS	5.5
1	A	457	SER	5.2
1	A	145	TYR	5.2
1	A	459	ASP	5.1
1	A	318	HIS	5.0
1	A	319	GLY	5.0
2	B	4	THR	4.9
1	A	461	LYS	4.5
1	A	661	GLN	4.4
1	A	456	THR	4.4
1	A	462	THR	4.4
1	A	667	ASN	4.1
1	A	322	GLU	4.0
1	A	317	ASN	3.9
1	A	146	PHE	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	675	ASN	3.7
1	A	326	ARG	3.6
1	A	650	VAL	3.6
1	A	432	VAL	3.5
1	A	629	TYR	3.5
2	B	5	PHE	3.5
1	A	647	ARG	3.5
1	A	141	PHE	3.4
1	A	628	MET	3.4
2	B	6	ASN	3.3
1	A	324	ARG	3.3
1	A	746	GLN	3.2
1	A	431	ILE	3.1
1	A	429	CYS	3.1
1	A	142	GLN	3.0
1	A	428	CYS	2.9
1	A	657	GLU	2.9
1	A	148	PHE	2.9
1	A	153	ARG	2.9
1	A	655	TRP	2.8
1	A	509	VAL	2.8
1	A	390	TYR	2.8
1	A	162	GLN	2.7
1	A	159	ILE	2.7
1	A	717	ARG	2.6
1	A	663	LEU	2.6
2	B	3	PHE	2.5
1	A	508	GLY	2.4
1	A	646	LEU	2.4
1	A	409	ALA	2.4
1	A	150	THR	2.4
1	A	738	THR	2.4
1	A	410	CYS	2.4
1	A	154	SER	2.3
1	A	121	TYR	2.3
1	A	161	GLY	2.3
1	A	665	THR	2.3
1	A	660	LYS	2.2
1	A	640	VAL	2.2
1	A	426	ASN	2.2
1	A	180	GLY	2.1
1	A	115	MET	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	425	SER	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

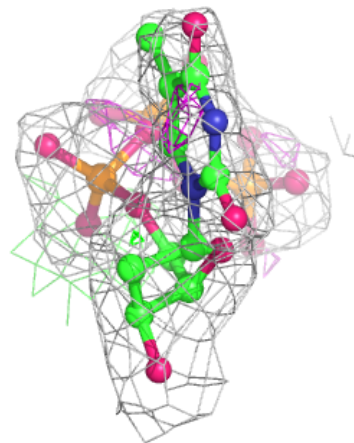
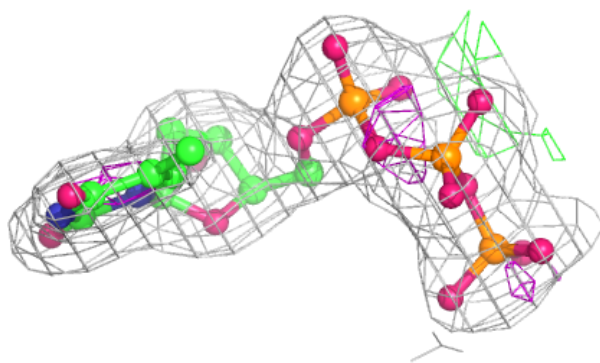
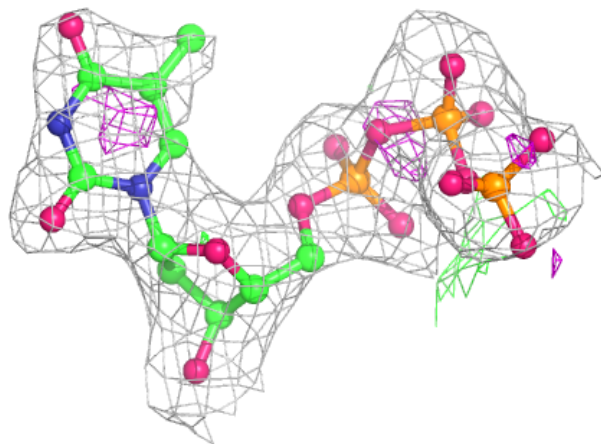
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MG	A	2001	1/1	0.85	0.25	48,48,48,48	0
4	TTP	A	1001	29/29	0.93	0.15	43,50,59,63	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 TTP A 1001:**

$2mF_o-DF_c$  (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.