



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 08:01 AM UTC

PDB ID : 2CVY / pdb_00002cvy
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

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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

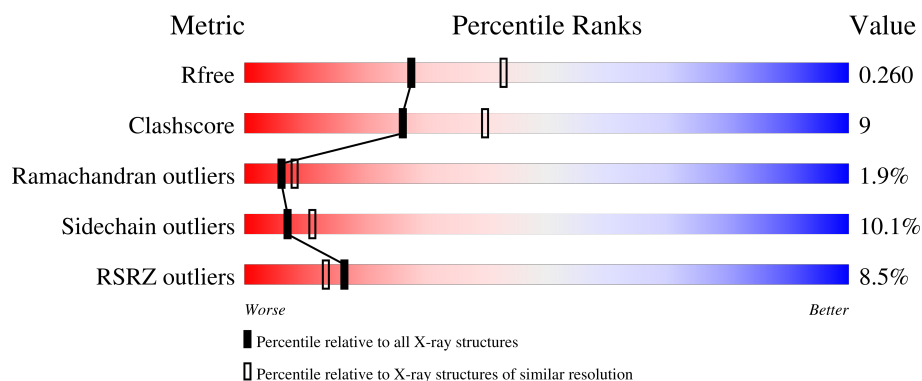
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

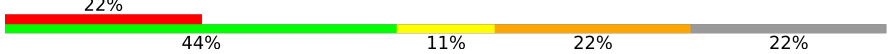
The reported resolution of this entry is 2.40 Å.

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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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 [i](#)

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			

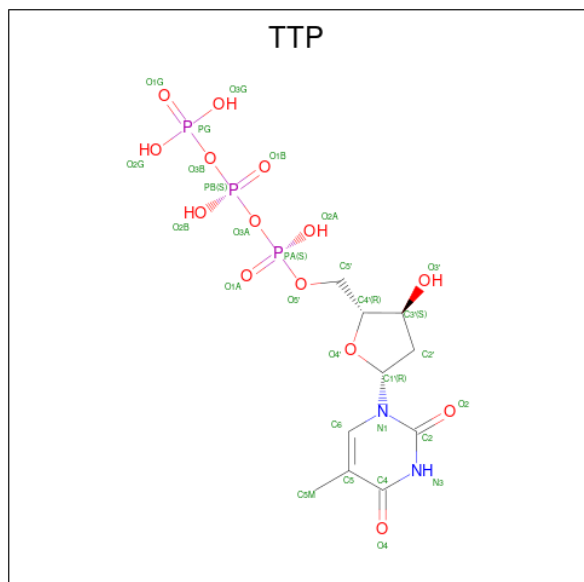
- Molecule 2 is a protein called 9-per peptide from Ribonucleoside-diphosphate reductase small chain 1.

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 (CCD ID: MG) (formula: Mg).

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

- Molecule 4 is THYMIDINE-5'-TRIPHOSPHATE (CCD ID: TTP) (formula: C₁₀H₁₇N₂O₁₄P₃).



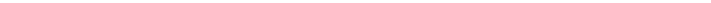
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			29	10	2	14	3		

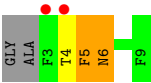
- Molecule 5 is water.

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

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.

- [illegible]

- Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	108.06Å 117.59Å 64.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 50.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.9 (50.00-2.40) 98.1 (50.00-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.12 (at 2.39Å)	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 (9.79%)	wwPDB-VP
Wilson B-factor (Å ²)	42.8	Xtriage
Anisotropy	0.462	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 33.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: TTP, 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	0.84	2/5247 (0.0%)	1.08	4/7103 (0.1%)
2	B	0.71	0/68	0.93	0/89
All	All	0.84	2/5315 (0.0%)	1.07	4/7192 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	273	ILE	CA-CB	5.09	1.57	1.54
1	A	383	ILE	CG1-CD1	5.06	1.71	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	334	ILE	N-CA-C	8.66	116.51	107.76
1	A	352	SER	N-CA-C	-8.22	99.71	110.07
1	A	308	ILE	N-CA-C	6.49	117.24	110.62
1	A	457	SER	N-CA-C	5.97	118.14	108.41

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	5128	0	5057	95	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	97	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 (97) 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:486:ASP:CG	1:A:503:ARG:HH22	2.01	0.68
1:A:273:ILE:HD12	1:A:314:ILE:HD11	1.76	0.67
1:A:508:GLY:HA3	1:A:606:MET:HE1	1.75	0.66
1:A:296:ALA:HB3	1:A:427:LEU:HD21	1.79	0.65
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:606:MET:HE2	5:A:2017:HOH:O	2.11	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:217:SER:OG	1:A:445:LEU:HD12	2.13	0.48
1:A:93:GLN:O	1:A:97:VAL:HG13	2.14	0.48
1:A:455:GLU:O	1:A:464:THR:N	2.39	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:417:LYS:HE3	1:A:574:MET:HE1	1.97	0.47
1:A:745:THR:O	1:A:746:GLN:HB2	2.14	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
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:713:ASN:HD22	1:A:742:TYR:H	1.65	0.44
1:A:266:ASN:ND2	1:A:266:ASN:H	2.12	0.44
1:A:675:ASN:O	1:A:675:ASN:ND2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:195:LEU:O	1:A:196:LYS:HB2	2.17	0.43
1:A:520:ARG:HH22	1:A:648:ASP:CG	2.27	0.43
1:A:351:PHE:HE1	1:A:371:TYR:CE1	2.37	0.42
1:A:602:THR:H	1:A:707:ASP:CG	2.26	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:481:LEU:CD1	1:A:505:ILE:HG23	2.50	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:675:ASN:HD22	1:A:675:ASN:C	2.27	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:319:GLY:C	1:A:321:GLU:H	2.30	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%)	7	10
2	B	5/9 (56%)	4 (80%)	0	1 (20%)	0	0
All	All	639/897 (71%)	593 (93%)	34 (5%)	12 (2%)	6	8

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%)	502 (90%)	55 (10%)	7	11
2	B	7/7 (100%)	5 (71%)	2 (29%)	0	0
All	All	564/768 (73%)	507 (90%)	57 (10%)	7	11

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91	THR
1	A	97	VAL
1	A	115	MET
1	A	131	LEU

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Mol	Chain	Res	Type
1	A	142	GLN
1	A	154	SER
1	A	170	LEU
1	A	176	LEU
1	A	183	ILE
1	A	214	GLN
1	A	220	LEU
1	A	244	THR
1	A	266	ASN
1	A	282	THR
1	A	284	ARG
1	A	301	LEU
1	A	314	ILE
1	A	317	ASN
1	A	318	HIS
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	443	CYS
1	A	461	LYS
1	A	462	THR
1	A	469	LYS
1	A	473	ILE
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

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Mol	Chain	Res	Type
1	A	638	PHE
1	A	641	VAL
1	A	663	LEU
1	A	686	THR
1	A	711	SER
1	A	712	LEU
1	A	714	LEU
1	A	721	MET
1	A	724	LEU
2	B	4	THR
2	B	5	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	GLN
1	A	168	GLN
1	A	251	HIS
1	A	266	ASN
1	A	270	ASN
1	A	317	ASN
1	A	444	ASN
1	A	561	GLN
1	A	567	GLN
1	A	613	GLN
1	A	618	ASN
1	A	692	GLN
1	A	713	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 oligosaccharides in this entry.

5.6 Ligand geometry

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	29,30,30	1.47	7 (24%)	43,47,47	1.98	11 (25%)

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 Torsions and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	TTP	A	1001	3	-	1/22/34/34	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1001	TTP	C4-C5	3.30	1.50	1.44
4	A	1001	TTP	C6-C5	2.74	1.39	1.34
4	A	1001	TTP	PA-O3A	2.44	1.62	1.59
4	A	1001	TTP	C2-N1	2.41	1.42	1.38
4	A	1001	TTP	PB-O3B	2.18	1.61	1.59
4	A	1001	TTP	PB-O3A	2.17	1.61	1.59
4	A	1001	TTP	O2-C2	2.01	1.26	1.23

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1001	TTP	C5-C4-N3	5.15	119.80	115.32
4	A	1001	TTP	C4-N3-C2	-5.05	120.72	127.34
4	A	1001	TTP	O4-C4-C5	-4.49	119.78	124.92
4	A	1001	TTP	N3-C2-N1	4.13	120.26	114.89
4	A	1001	TTP	C5M-C5-C4	3.97	123.02	118.78
4	A	1001	TTP	C5-C6-N1	-3.33	119.70	123.31
4	A	1001	TTP	O2B-PB-O3A	2.72	114.62	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1001	TTP	C5M-C5-C6	-2.49	119.47	122.85
4	A	1001	TTP	O2-C2-N1	-2.39	119.69	122.80
4	A	1001	TTP	O2G-PG-O3B	2.36	112.55	104.64
4	A	1001	TTP	O3B-PB-O1B	2.09	117.01	110.70

There are no chirality outliers.

All (1) torsion outliers are listed below:

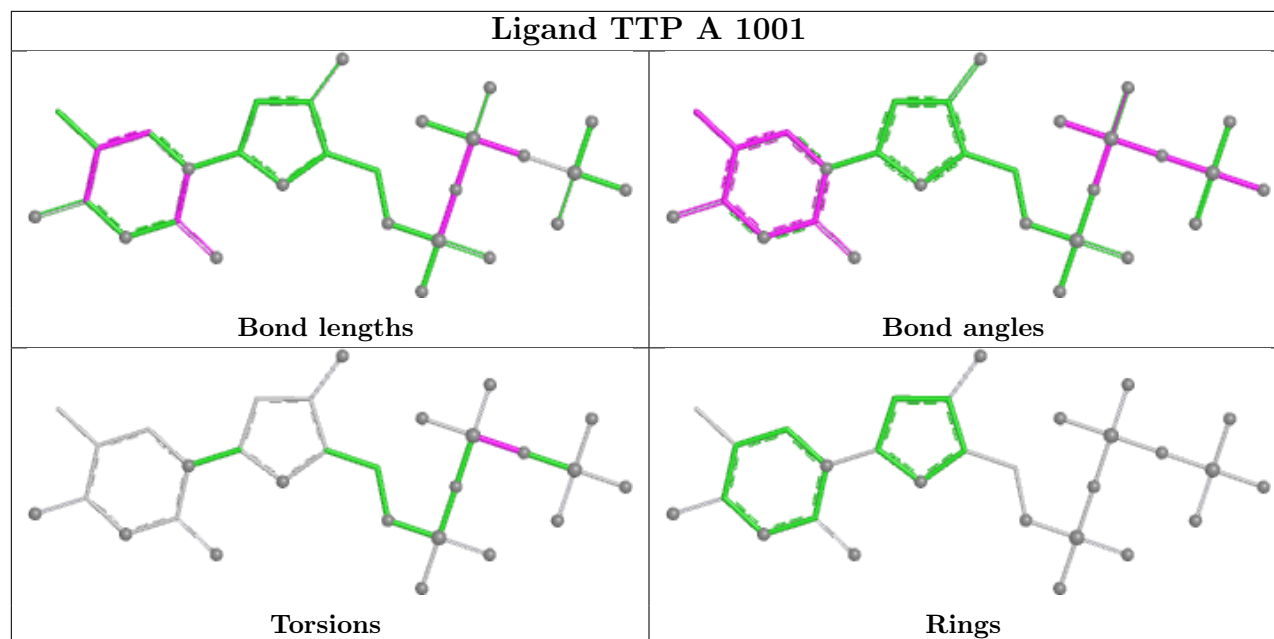
Mol	Chain	Res	Type	Atoms
4	A	1001	TTP	PG-O3B-PB-O1B

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	640/888 (72%)	0.51	53 (8%) 17 14	28, 43, 82, 93	0
2	B	7/9 (77%)	1.75	2 (28%) 1 1	75, 84, 86, 87	0
All	All	647/897 (72%)	0.52	55 (8%) 16 13	28, 43, 84, 93	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	323	ILE	6.9
1	A	460	GLY	5.0
1	A	606	MET	4.9
1	A	664	ILE	4.6
1	A	383	ILE	4.3
1	A	143	TYR	4.0
1	A	457	SER	3.8
2	B	4	THR	3.6
1	A	270	ASN	3.6
1	A	456	THR	3.5
1	A	245	ALA	3.3
1	A	154	SER	3.3
1	A	159	ILE	3.3
1	A	458	GLU	3.2
1	A	630	SER	3.1
1	A	91	THR	3.1
1	A	640	VAL	2.9
1	A	454	ILE	2.8
1	A	638	PHE	2.8
2	B	3	PHE	2.8
1	A	675	ASN	2.8
1	A	217	SER	2.8
1	A	629	TYR	2.7
1	A	319	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	621	PHE	2.7
1	A	318	HIS	2.6
1	A	146	PHE	2.6
1	A	195	LEU	2.6
1	A	390	TYR	2.5
1	A	93	GLN	2.5
1	A	718	ALA	2.5
1	A	265	THR	2.5
1	A	459	ASP	2.5
1	A	647	ARG	2.4
1	A	321	GLU	2.4
1	A	461	LYS	2.4
1	A	663	LEU	2.4
1	A	148	PHE	2.4
1	A	92	LYS	2.4
1	A	607	PRO	2.3
1	A	625	THR	2.3
1	A	665	THR	2.3
1	A	142	GLN	2.3
1	A	136	VAL	2.3
1	A	314	ILE	2.3
1	A	667	ASN	2.2
1	A	746	GLN	2.2
1	A	264	GLY	2.1
1	A	409	ALA	2.1
1	A	615	LEU	2.1
1	A	151	LEU	2.1
1	A	655	TRP	2.1
1	A	609	ALA	2.0
1	A	180	GLY	2.0
1	A	610	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](#)

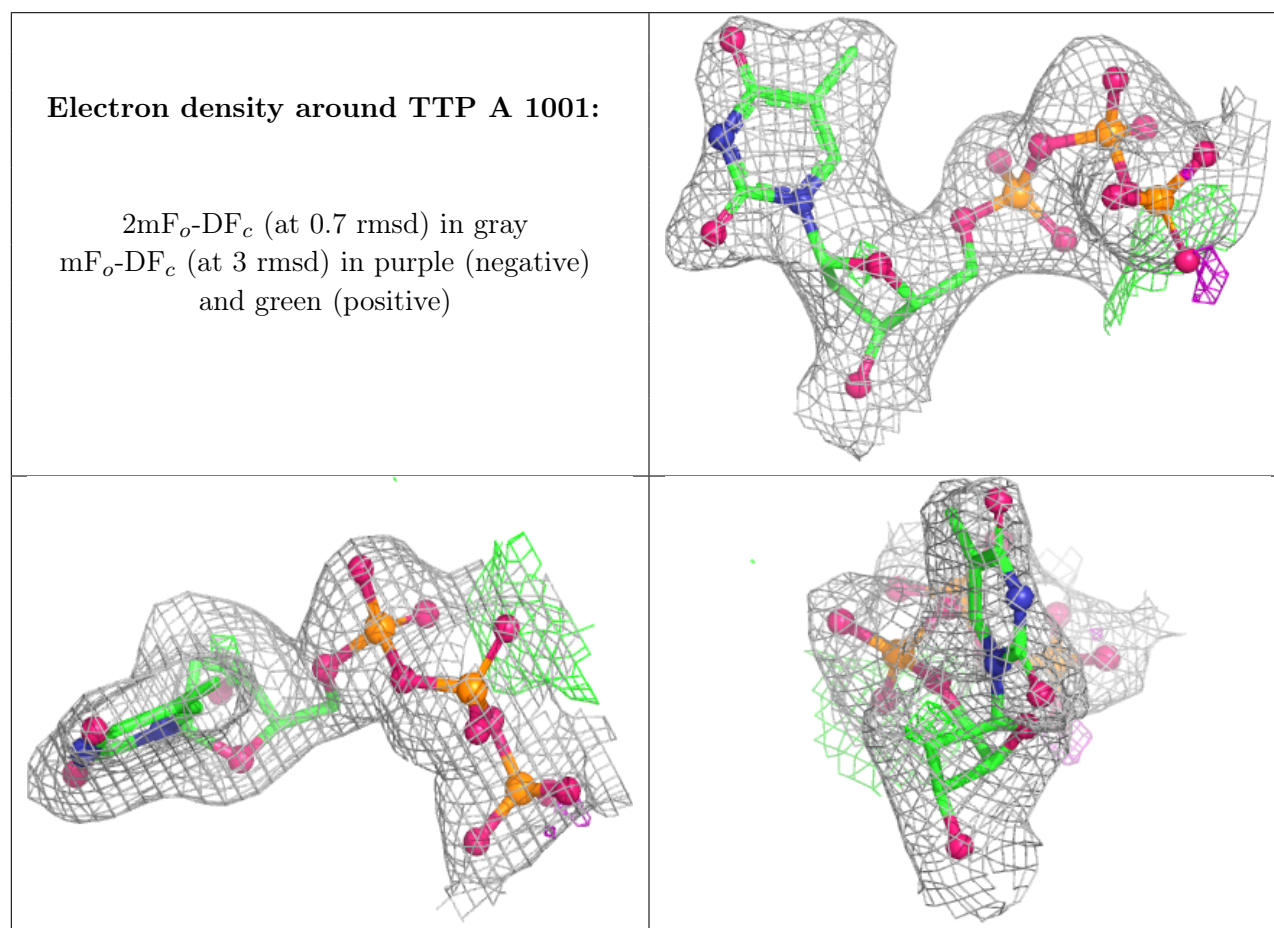
There are no oligosaccharides in this entry.

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, 95th 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	0.87	0.26	48,48,48,48	0
4	TTP	A	1001	29/29	0.90	0.10	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.