



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:36 PM UTC

PDB ID : 1ZET / pdb_00001zet
Title : X-ray data do not support hoogsteen base-pairing during replication by human polymerase iota
Authors : Wang, J.
Deposited on : 2005-04-19
Resolution : 2.30 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

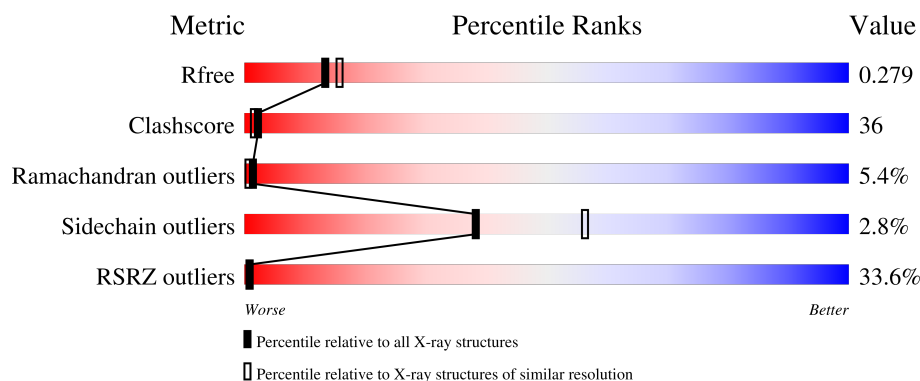
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	T	14	36% 36% 64%
2	P	13	15% 62% 38%
3	A	388	34% 51% 43% 5%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 3816 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 DNA chain called 5'-D(P*AP*GP*GP*GP*(BRU)P*CP*CP*(BRU)P*(BRU)P*CP*CP*CP*CP*C)-3'.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	T	14	Total	Br	C	N	O	P	0	0	0
			280	3	130	47	86	14			

- Molecule 2 is a DNA chain called 5'-D(*GP*GP*GP*GP*GP*AP*AP*GP*GP*AP*CP*CP*(DOC))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	13	Total	C	N	O	P	0	0	0
			270	127	59	72	12			

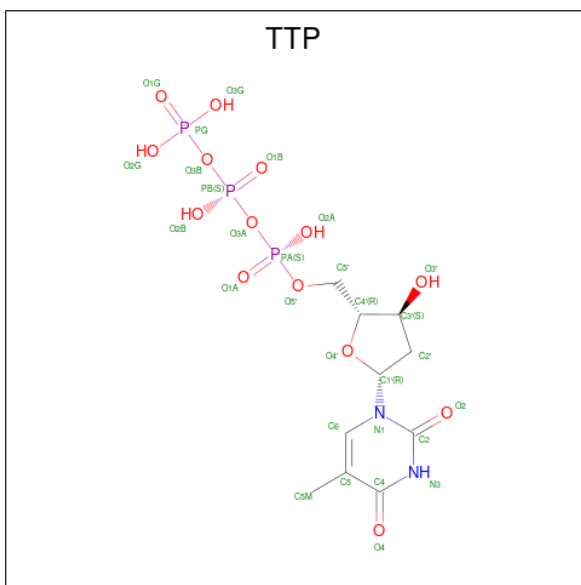
- Molecule 3 is a protein called Polymerase (DNA directed) iota.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	388	Total	C	N	O	S	0	0	0
			3068	1939	534	573	22			

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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



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

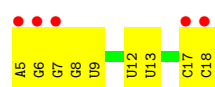
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	T	6	Total O 6 6	0	0
6	P	2	Total O 2 2	0	0
6	A	160	Total O 160 160	0	0

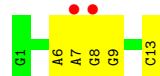
3 Residue-property plots [i](#)

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.

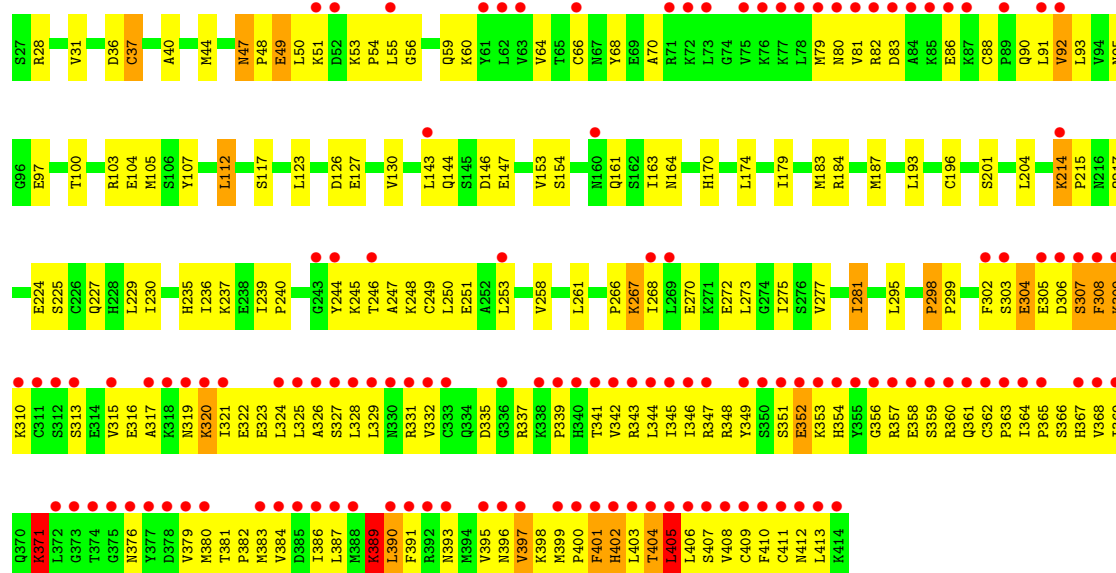
- Molecule 1: 5'-D(P*AP*GP*GP*GP*(BRU)P*CP*CP*(BRU)P*(BRU)P*CP*CP*CP*CP*C)-3'



- Molecule 2: 5'-D(*GP*GP*GP*GP*GP*AP*AP*GP*GP*AP*CP*CP*(DOC))-3'



- Molecule 3: Polymerase (DNA directed) iota



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	98.83Å 98.83Å 202.75Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.43 – 2.30 39.43 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.5 (39.43-2.30) 98.5 (39.43-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.34 (at 2.29Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.261 , 0.288 0.254 , 0.279	Depositor DCC
R_{free} test set	1529 reflections (5.77%)	wwPDB-VP
Wilson B-factor (Å ²)	44.0	Xtriage
Anisotropy	0.445	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 68.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	3816	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DOC, MG, BRU, 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	T	1.09	2/243 (0.8%)	1.10	3/366 (0.8%)
2	P	0.28	0/285	0.53	0/440
3	A	0.36	0/3116	0.87	10/4201 (0.2%)
All	All	0.44	2/3644 (0.1%)	0.87	13/5007 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	T	18	DC	P-O5'	12.73	1.85	1.60
1	T	18	DC	P-OP2	-9.62	1.29	1.48

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	18	DC	P-O5'-C5'	-11.51	102.74	120.00
1	T	18	DC	O5'-P-OP2	-9.10	80.71	108.00
3	A	214	LYS	CA-C-N	-8.40	109.34	119.84
3	A	214	LYS	C-N-CA	-8.40	109.34	119.84
3	A	117	SER	CA-C-N	6.89	126.41	119.24
3	A	117	SER	C-N-CA	6.89	126.41	119.24
1	T	17	DC	C2'-C3'-O3'	6.76	121.64	111.50
3	A	298	PRO	CA-C-N	5.76	125.69	119.76
3	A	298	PRO	C-N-CA	5.76	125.69	119.76
3	A	390	LEU	N-CA-C	-5.48	106.55	113.18
3	A	214	LYS	N-CA-C	5.44	121.82	109.81
3	A	47	ASN	CA-C-N	5.18	125.22	119.32
3	A	47	ASN	C-N-CA	5.18	125.22	119.32

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	T	280	0	149	5	0
2	P	270	0	145	28	0
3	A	3068	0	3154	259	0
4	A	1	0	0	0	0
5	A	29	0	10	1	0
6	A	160	0	0	3	0
6	P	2	0	0	0	0
6	T	6	0	0	1	0
All	All	3816	0	3458	259	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 36.

All (259) 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:A:309:LYS:HD3	3:A:406:LEU:HB2	1.34	1.05
2:P:7:DA:H5'	3:A:360:ARG:HD3	1.42	1.02
3:A:321:ILE:HD13	3:A:384:VAL:HA	1.43	1.00
2:P:9:DG:H5''	3:A:357:ARG:HB2	1.42	0.98
3:A:371:LYS:H	3:A:371:LYS:HD3	1.30	0.96
2:P:8:DG:H5'	3:A:359:SER:N	1.88	0.89
2:P:6:DA:H5''	3:A:361:GLN:HG3	1.52	0.89
2:P:6:DA:H3'	3:A:361:GLN:O	1.74	0.87
3:A:267:LYS:H	3:A:267:LYS:HD2	1.39	0.87
3:A:47:ASN:ND2	3:A:49:GLU:HG2	1.89	0.86
3:A:346:ILE:HD12	3:A:405:LEU:HD12	1.57	0.86
3:A:47:ASN:HD21	3:A:49:GLU:HG2	1.43	0.84
2:P:8:DG:H5'	3:A:359:SER:H	1.46	0.81
3:A:371:LYS:HD3	3:A:371:LYS:N	1.96	0.80
3:A:310:LYS:HA	3:A:404:THR:HA	1.65	0.79
3:A:316:GLU:HB2	3:A:320:LYS:HE3	1.64	0.79
3:A:325:LEU:HD21	3:A:408:VAL:HG11	1.65	0.79
2:P:7:DA:H5'	3:A:360:ARG:CD	2.15	0.76
3:A:164:ASN:H	3:A:170:HIS:HD2	1.33	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:329:LEU:O	3:A:332:VAL:HG12	1.88	0.74
2:P:8:DG:H3'	3:A:358:GLU:HA	1.69	0.73
3:A:349:TYR:HB2	3:A:403:LEU:HD22	1.72	0.72
3:A:396:ASN:HA	3:A:400:PRO:HG3	1.72	0.72
3:A:368:VAL:HG23	3:A:369:ILE:HD12	1.72	0.72
3:A:247:ALA:O	3:A:251:GLU:HG3	1.90	0.71
3:A:342:VAL:HG21	3:A:386:ILE:HD12	1.73	0.71
3:A:381:THR:HB	3:A:382:PRO:HD3	1.73	0.70
3:A:107:TYR:OH	3:A:299:PRO:HG3	1.91	0.70
3:A:324:LEU:HD11	3:A:406:LEU:HD11	1.73	0.70
3:A:383:MET:HA	3:A:386:ILE:HD11	1.74	0.69
3:A:309:LYS:HZ1	3:A:391:PHE:HE2	1.40	0.69
3:A:359:SER:O	3:A:360:ARG:HG2	1.92	0.68
3:A:369:ILE:HD12	3:A:369:ILE:H	1.59	0.68
3:A:244:TYR:HE2	3:A:352:GLU:HG3	1.59	0.68
3:A:270:GLU:HG3	3:A:275:ILE:HA	1.78	0.66
3:A:365:PRO:HB2	3:A:369:ILE:HG12	1.78	0.66
3:A:324:LEU:HD13	3:A:408:VAL:HG23	1.77	0.66
2:P:6:DA:OP1	3:A:363:PRO:HD3	1.96	0.65
3:A:53:LYS:NZ	3:A:92:VAL:HG21	2.10	0.64
3:A:214:LYS:HZ3	3:A:214:LYS:HB3	1.61	0.64
1:T:7:DG:OP2	3:A:304:GLU:HG3	1.96	0.64
3:A:348:ARG:NH2	3:A:399:MET:HB2	2.13	0.64
3:A:112:LEU:C	3:A:112:LEU:HD23	2.22	0.64
3:A:95:ASN:HD21	3:A:97:GLU:HB2	1.63	0.63
2:P:9:DG:C5'	3:A:357:ARG:HB2	2.25	0.63
3:A:343:ARG:HA	3:A:360:ARG:O	1.98	0.63
3:A:267:LYS:HD2	3:A:267:LYS:N	2.11	0.63
3:A:214:LYS:HB3	3:A:214:LYS:NZ	2.15	0.62
3:A:360:ARG:HB3	3:A:390:LEU:HD13	1.79	0.62
3:A:319:ASN:C	3:A:321:ILE:H	2.08	0.62
2:P:8:DG:OP2	3:A:360:ARG:HG2	2.00	0.61
3:A:367:HIS:CD2	3:A:368:VAL:HG22	2.36	0.61
3:A:342:VAL:O	3:A:361:GLN:HA	2.00	0.61
3:A:345:ILE:HA	3:A:359:SER:HA	1.83	0.61
3:A:395:VAL:HG13	3:A:400:PRO:HB3	1.83	0.60
3:A:161:GLN:NE2	3:A:225:SER:OG	2.34	0.60
3:A:196:CYS:SG	3:A:214:LYS:O	2.59	0.60
3:A:244:TYR:CE2	3:A:353:LYS:HB2	2.36	0.60
3:A:315:VAL:HG22	3:A:401:PHE:HE2	1.66	0.60
3:A:59:GLN:NE2	3:A:64:VAL:HG11	2.15	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:365:PRO:O	3:A:369:ILE:HB	2.01	0.60
2:P:6:DA:OP2	3:A:363:PRO:HG3	2.00	0.60
3:A:81:VAL:HG13	3:A:93:LEU:CD1	2.31	0.60
3:A:309:LYS:CD	3:A:406:LEU:HB2	2.21	0.59
3:A:36:ASP:O	3:A:37:CYS:C	2.45	0.59
3:A:343:ARG:HE	3:A:359:SER:CB	2.16	0.59
3:A:324:LEU:HD11	3:A:406:LEU:CD1	2.32	0.58
3:A:54:PRO:HA	3:A:70:ALA:HB2	1.86	0.58
3:A:386:ILE:HG13	3:A:387:LEU:H	1.68	0.58
3:A:389:LYS:NZ	3:A:389:LYS:HB3	2.19	0.58
3:A:245:LYS:HD3	3:A:245:LYS:C	2.29	0.57
3:A:376:ASN:O	3:A:379:VAL:HG12	2.03	0.57
3:A:245:LYS:HD3	3:A:246:THR:N	2.19	0.57
2:P:8:DG:C8	3:A:359:SER:HB2	2.40	0.57
3:A:345:ILE:HG12	3:A:359:SER:OG	2.05	0.57
3:A:53:LYS:HD2	3:A:90:GLN:HG2	1.86	0.57
3:A:100:THR:O	3:A:104:GLU:HG3	2.05	0.56
1:T:6:DG:OP1	3:A:97:GLU:HG2	2.05	0.56
3:A:309:LYS:HD3	3:A:406:LEU:CB	2.23	0.56
3:A:405:LEU:N	3:A:405:LEU:HD23	2.21	0.56
3:A:389:LYS:HD2	3:A:389:LYS:O	2.05	0.56
2:P:8:DG:H8	3:A:359:SER:HB2	1.71	0.55
3:A:215:PRO:O	3:A:217:GLN:HG3	2.05	0.55
3:A:146:ASP:OD1	3:A:147:GLU:HG2	2.05	0.55
3:A:163:ILE:HG21	3:A:174:LEU:HD11	1.89	0.55
3:A:308:PHE:HD1	3:A:308:PHE:O	1.90	0.55
3:A:68:TYR:C	3:A:70:ALA:H	2.15	0.55
3:A:82:ARG:HD2	3:A:86:GLU:OE1	2.07	0.55
3:A:383:MET:O	3:A:387:LEU:HD13	2.07	0.55
3:A:105:MET:CG	3:A:193:LEU:HD11	2.38	0.55
3:A:369:ILE:HD12	3:A:369:ILE:N	2.22	0.55
3:A:344:LEU:O	3:A:359:SER:HA	2.07	0.54
3:A:204:LEU:CD1	3:A:240:PRO:HD2	2.37	0.54
3:A:320:LYS:O	3:A:324:LEU:HD12	2.07	0.54
3:A:48:PRO:C	3:A:50:LEU:H	2.15	0.54
3:A:347:ARG:HD3	3:A:347:ARG:N	2.22	0.54
3:A:268:ILE:O	3:A:272:GLU:HG2	2.08	0.54
3:A:315:VAL:HG22	3:A:402:HIS:HE1	1.73	0.54
3:A:360:ARG:HB3	3:A:390:LEU:HB3	1.89	0.54
3:A:389:LYS:HD2	3:A:389:LYS:C	2.32	0.54
3:A:349:TYR:CB	3:A:403:LEU:HD22	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:49:GLU:O	3:A:53:LYS:HE2	2.07	0.54
3:A:319:ASN:HB3	3:A:323:GLU:OE2	2.08	0.54
3:A:325:LEU:HD23	3:A:328:LEU:HD23	1.89	0.53
3:A:236:ILE:HD12	3:A:250:LEU:CD1	2.38	0.53
3:A:342:VAL:HG13	3:A:364:ILE:HD11	1.91	0.53
3:A:164:ASN:H	3:A:170:HIS:CD2	2.20	0.53
3:A:170:HIS:O	3:A:174:LEU:HG	2.09	0.53
3:A:184:ARG:HA	3:A:187:MET:HE3	1.91	0.53
3:A:368:VAL:CG2	3:A:369:ILE:HD12	2.39	0.53
2:P:6:DA:H5'	3:A:362:CYS:HA	1.91	0.52
3:A:236:ILE:HD12	3:A:250:LEU:HD13	1.90	0.52
6:T:78:HOH:O	3:A:103:ARG:HD3	2.09	0.52
3:A:306:ASP:OD1	3:A:307:SER:N	2.42	0.52
3:A:348:ARG:HH21	3:A:399:MET:HB2	1.71	0.52
3:A:379:VAL:C	3:A:382:PRO:HD2	2.34	0.52
2:P:7:DA:N7	3:A:361:GLN:CD	2.68	0.52
1:T:5:DA:H2'	3:A:310:LYS:HZ3	1.74	0.52
3:A:412:ASN:C	3:A:413:LEU:HD12	2.35	0.52
3:A:365:PRO:HB2	3:A:369:ILE:CG1	2.39	0.52
3:A:267:LYS:H	3:A:267:LYS:CD	2.09	0.51
3:A:306:ASP:HB3	3:A:406:LEU:CD2	2.41	0.51
3:A:54:PRO:HB3	3:A:70:ALA:HB2	1.93	0.51
3:A:161:GLN:OE1	3:A:224:GLU:HB2	2.11	0.51
3:A:55:LEU:HD12	3:A:56:GLY:H	1.76	0.51
3:A:60:LYS:NZ	3:A:307:SER:HB3	2.26	0.51
2:P:7:DA:C8	3:A:361:GLN:HG2	2.46	0.51
3:A:31:VAL:HG12	3:A:130:VAL:HB	1.93	0.50
3:A:399:MET:HB3	3:A:403:LEU:CD1	2.41	0.50
3:A:380:MET:O	3:A:384:VAL:HG23	2.12	0.50
3:A:360:ARG:CZ	3:A:393:ASN:HD22	2.24	0.50
3:A:371:LYS:HE2	3:A:376:ASN:CG	2.37	0.50
3:A:308:PHE:O	3:A:313:SER:HB3	2.12	0.50
3:A:86:GLU:C	3:A:88:CYS:H	2.19	0.49
3:A:153:VAL:HG22	3:A:154:SER:N	2.27	0.49
3:A:239:ILE:HD11	3:A:258:VAL:HG22	1.95	0.49
2:P:6:DA:P	3:A:363:PRO:HG3	2.52	0.49
3:A:48:PRO:O	3:A:51:LYS:HG2	2.11	0.49
2:P:7:DA:H3'	3:A:360:ARG:HG2	1.94	0.49
3:A:31:VAL:CG1	3:A:130:VAL:HB	2.42	0.49
3:A:60:LYS:HZ3	3:A:307:SER:CB	2.26	0.49
3:A:309:LYS:HE2	3:A:405:LEU:HG	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:398:LYS:C	3:A:400:PRO:HD3	2.37	0.49
3:A:37:CYS:HA	5:A:451:TTP:O1B	2.12	0.49
3:A:327:SER:C	3:A:329:LEU:H	2.21	0.49
3:A:347:ARG:HG2	3:A:404:THR:O	2.13	0.49
3:A:339:PRO:HA	3:A:413:LEU:HG	1.94	0.48
3:A:362:CYS:SG	3:A:390:LEU:HD11	2.53	0.48
3:A:54:PRO:CA	3:A:70:ALA:HB2	2.44	0.48
3:A:235:HIS:ND1	3:A:237:LYS:HG2	2.28	0.48
3:A:399:MET:O	3:A:403:LEU:HD12	2.13	0.48
3:A:413:LEU:HD12	3:A:413:LEU:N	2.27	0.48
3:A:371:LYS:HE2	3:A:376:ASN:HA	1.95	0.48
3:A:309:LYS:HE2	3:A:405:LEU:CD1	2.43	0.48
3:A:341:THR:HB	3:A:412:ASN:HD22	1.78	0.48
3:A:360:ARG:NH2	3:A:393:ASN:ND2	2.62	0.48
3:A:126:ASP:HA	6:A:557:HOH:O	2.13	0.48
3:A:316:GLU:CB	3:A:320:LYS:HE3	2.41	0.48
3:A:325:LEU:O	3:A:329:LEU:HG	2.13	0.47
3:A:341:THR:CB	3:A:412:ASN:HD22	2.28	0.47
3:A:389:LYS:HB3	3:A:389:LYS:HZ2	1.80	0.47
3:A:310:LYS:HE2	3:A:347:ARG:HH11	1.80	0.47
3:A:315:VAL:HG13	3:A:401:PHE:CZ	2.50	0.47
3:A:315:VAL:HG12	3:A:315:VAL:O	2.14	0.47
3:A:55:LEU:O	3:A:66:CYS:HB2	2.16	0.46
3:A:307:SER:O	3:A:308:PHE:C	2.58	0.46
3:A:399:MET:N	3:A:400:PRO:CD	2.79	0.46
2:P:7:DA:N7	3:A:361:GLN:OE1	2.48	0.46
3:A:343:ARG:HE	3:A:359:SER:HB3	1.81	0.46
3:A:143:LEU:HD11	3:A:147:GLU:HB2	1.96	0.46
3:A:307:SER:O	3:A:309:LYS:N	2.48	0.46
2:P:8:DG:OP2	3:A:360:ARG:CZ	2.64	0.46
3:A:360:ARG:CD	3:A:390:LEU:HD22	2.46	0.46
3:A:395:VAL:HG13	3:A:395:VAL:O	2.15	0.46
3:A:371:LYS:HE2	3:A:376:ASN:CB	2.46	0.46
3:A:324:LEU:HD13	3:A:408:VAL:CG2	2.45	0.45
3:A:349:TYR:H	3:A:403:LEU:HB3	1.80	0.45
3:A:40:ALA:O	3:A:44:MET:HG3	2.16	0.45
3:A:395:VAL:O	3:A:395:VAL:HG22	2.14	0.45
2:P:8:DG:N7	3:A:343:ARG:NH2	2.65	0.45
3:A:327:SER:C	3:A:329:LEU:N	2.72	0.45
3:A:325:LEU:CD2	3:A:328:LEU:HD23	2.47	0.45
3:A:322:GLU:HG2	3:A:380:MET:SD	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:360:ARG:CB	3:A:390:LEU:HB3	2.47	0.45
3:A:409:CYS:SG	3:A:410:PHE:N	2.90	0.45
1:T:8:DG:OP1	3:A:103:ARG:NE	2.49	0.45
3:A:306:ASP:HB2	3:A:324:LEU:CD2	2.47	0.45
3:A:347:ARG:HD3	3:A:347:ARG:H	1.81	0.45
3:A:360:ARG:NH1	3:A:390:LEU:O	2.43	0.45
3:A:360:ARG:HH12	3:A:393:ASN:C	2.25	0.45
3:A:244:TYR:O	3:A:248:LYS:HG2	2.17	0.44
3:A:306:ASP:HB2	3:A:324:LEU:HD23	1.99	0.44
3:A:179:ILE:O	3:A:183:MET:HG3	2.17	0.44
3:A:55:LEU:HD12	3:A:56:GLY:N	2.32	0.44
3:A:53:LYS:HZ2	3:A:92:VAL:HG21	1.81	0.44
3:A:249:CYS:SG	3:A:273:LEU:HD21	2.58	0.44
3:A:347:ARG:HH22	3:A:407:SER:HB2	1.83	0.44
3:A:353:LYS:HE3	3:A:354:HIS:CD2	2.52	0.44
1:T:5:DA:H4'	3:A:60:LYS:HB2	1.99	0.44
3:A:345:ILE:O	3:A:346:ILE:HD13	2.17	0.44
3:A:302:PHE:O	3:A:328:LEU:HD11	2.18	0.43
3:A:411:CYS:SG	3:A:412:ASN:N	2.91	0.43
3:A:103:ARG:HD2	6:A:561:HOH:O	2.18	0.43
3:A:309:LYS:HG2	3:A:405:LEU:CD2	2.49	0.43
3:A:371:LYS:HE2	3:A:376:ASN:ND2	2.33	0.43
3:A:382:PRO:O	3:A:386:ILE:HG12	2.18	0.43
3:A:321:ILE:O	3:A:325:LEU:HB2	2.18	0.43
3:A:346:ILE:HG23	3:A:405:LEU:CB	2.48	0.43
3:A:344:LEU:HD12	3:A:407:SER:O	2.19	0.43
3:A:345:ILE:HB	3:A:407:SER:HB3	2.00	0.43
3:A:28:ARG:O	3:A:201:SER:HA	2.18	0.43
3:A:277:VAL:O	3:A:281:ILE:HB	2.18	0.43
3:A:308:PHE:O	3:A:308:PHE:CD1	2.69	0.43
3:A:369:ILE:H	3:A:369:ILE:CD1	2.29	0.43
2:P:6:DA:H2'	3:A:361:GLN:CG	2.49	0.43
3:A:53:LYS:CE	3:A:92:VAL:HG21	2.49	0.43
3:A:395:VAL:O	3:A:400:PRO:HB3	2.18	0.43
3:A:302:PHE:HE1	3:A:413:LEU:HD22	1.83	0.43
3:A:317:ALA:C	3:A:319:ASN:N	2.75	0.43
3:A:335:ASP:OD2	3:A:337:ARG:HD3	2.18	0.43
3:A:346:ILE:O	3:A:358:GLU:HB2	2.19	0.43
2:P:8:DG:N7	3:A:343:ARG:CZ	2.82	0.43
3:A:303:SER:O	3:A:304:GLU:HB2	2.18	0.43
3:A:306:ASP:HB3	3:A:406:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:360:ARG:HD2	3:A:390:LEU:HB3	2.01	0.42
2:P:8:DG:H5'	3:A:358:GLU:C	2.44	0.42
3:A:360:ARG:HD2	3:A:390:LEU:HD22	2.00	0.42
3:A:383:MET:O	3:A:386:ILE:HG13	2.19	0.42
3:A:147:GLU:HA	3:A:147:GLU:OE1	2.19	0.42
3:A:251:GLU:C	3:A:253:LEU:H	2.28	0.42
3:A:54:PRO:HB2	3:A:88:CYS:SG	2.59	0.42
3:A:346:ILE:HD12	3:A:405:LEU:HB2	2.02	0.42
3:A:266:PRO:HD2	3:A:267:LYS:CE	2.50	0.42
3:A:123:LEU:O	3:A:127:GLU:HB2	2.20	0.42
3:A:295:LEU:HD22	6:A:535:HOH:O	2.19	0.42
3:A:251:GLU:C	3:A:253:LEU:N	2.77	0.41
3:A:366:SER:C	3:A:367:HIS:ND1	2.78	0.41
3:A:397:VAL:O	3:A:398:LYS:HD3	2.20	0.41
2:P:8:DG:H5'	3:A:358:GLU:HA	2.03	0.41
3:A:371:LYS:NZ	3:A:376:ASN:ND2	2.68	0.41
2:P:7:DA:H5'	3:A:360:ARG:NE	2.34	0.41
3:A:91:LEU:O	3:A:92:VAL:C	2.62	0.41
3:A:342:VAL:HG11	3:A:383:MET:SD	2.60	0.41
3:A:298:PRO:HA	3:A:299:PRO:HD3	1.86	0.41
3:A:316:GLU:O	3:A:320:LYS:HD2	2.20	0.41
3:A:319:ASN:C	3:A:321:ILE:N	2.74	0.41
3:A:351:SER:O	3:A:353:LYS:N	2.53	0.41
3:A:386:ILE:HG13	3:A:387:LEU:N	2.34	0.41
3:A:227:GLN:O	3:A:230:ILE:HG22	2.21	0.41
3:A:329:LEU:C	3:A:331:ARG:H	2.28	0.41
3:A:341:THR:N	3:A:364:ILE:HD12	2.35	0.41
3:A:353:LYS:HG3	3:A:354:HIS:N	2.36	0.41
3:A:54:PRO:HB3	3:A:70:ALA:CB	2.51	0.41
3:A:309:LYS:HE2	3:A:405:LEU:HD11	2.02	0.41
3:A:346:ILE:HG23	3:A:405:LEU:HB2	2.03	0.40
3:A:60:LYS:NZ	3:A:307:SER:CB	2.84	0.40
3:A:401:PHE:O	3:A:402:HIS:C	2.64	0.40
3:A:309:LYS:HE2	3:A:405:LEU:CG	2.51	0.40
2:P:7:DA:H3'	3:A:360:ARG:NE	2.36	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	A	386/388 (100%)	302 (78%)	63 (16%)	21 (5%)	1 1

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	308	PHE
3	A	326	ALA
3	A	80	ASN
3	A	83	ASP
3	A	304	GLU
3	A	309	LYS
3	A	371	LYS
3	A	397	VAL
3	A	37	CYS
3	A	79	MET
3	A	307	SER
3	A	320	LYS
3	A	352	GLU
3	A	402	HIS
3	A	49	GLU
3	A	305	GLU
3	A	404	THR
3	A	92	VAL
3	A	389	LYS
3	A	405	LEU
3	A	356	GLY

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	A	353/353 (100%)	343 (97%)	10 (3%)	38 56

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	112	LEU
3	A	144	GLN
3	A	229	LEU
3	A	261	LEU
3	A	267	LYS
3	A	281	ILE
3	A	371	LYS
3	A	389	LYS
3	A	401	PHE
3	A	405	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	47	ASN
3	A	59	GLN
3	A	95	ASN
3	A	161	GLN
3	A	170	HIS
3	A	227	GLN
3	A	262	GLN
3	A	340	HIS
3	A	370	GLN
3	A	376	ASN
3	A	393	ASN
3	A	412	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	BRU	T	12	1,2	18,21,22	2.83	1 (5%)	25,30,33	0.86	1 (4%)
2	DOC	P	13	1,2	16,19,20	0.37	0	20,26,29	0.71	1 (5%)
1	BRU	T	9	1,2	18,21,22	2.82	1 (5%)	25,30,33	0.87	1 (4%)
1	BRU	T	13	1,2	18,21,22	2.82	1 (5%)	25,30,33	0.85	1 (4%)

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
1	BRU	T	12	1,2	-	1/7/21/22	0/2/2/2
2	DOC	P	13	1,2	-	0/7/18/19	0/2/2/2
1	BRU	T	9	1,2	-	0/7/21/22	0/2/2/2
1	BRU	T	13	1,2	-	2/7/21/22	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	T	12	BRU	BR-C5	-11.96	1.60	1.88
1	T	13	BRU	BR-C5	-11.93	1.60	1.88
1	T	9	BRU	BR-C5	-11.90	1.61	1.88

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	12	BRU	C6-C5-C4	-2.88	117.74	120.67
1	T	9	BRU	C6-C5-C4	-2.81	117.82	120.67
1	T	13	BRU	C6-C5-C4	-2.69	117.94	120.67
2	P	13	DOC	O4'-C4'-C5'	-2.43	104.97	109.34

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	T	13	BRU	C4'-C5'-O5'-P
1	T	13	BRU	C3'-C4'-C5'-O5'
1	T	12	BRU	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	$\# Z > 2$
5	TTP	A	451	4	29,30,30	5.45	13 (44%)	43,47,47	2.60	19 (44%)

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
5	TTP	A	451	4	-	2/22/34/34	0/2/2/2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	451	TTP	C5M-C5	-21.15	0.99	1.50
5	A	451	TTP	PA-O3A	9.30	1.69	1.59
5	A	451	TTP	PB-O3B	8.34	1.68	1.59
5	A	451	TTP	PB-O3A	7.80	1.67	1.59
5	A	451	TTP	O4-C4	5.60	1.34	1.23
5	A	451	TTP	C6-C5	5.41	1.43	1.34
5	A	451	TTP	C1'-N1	5.08	1.60	1.48
5	A	451	TTP	PA-O1A	-4.99	1.33	1.50
5	A	451	TTP	PA-O5'	-4.74	1.40	1.59
5	A	451	TTP	O5'-C5'	4.67	1.62	1.44
5	A	451	TTP	C2-N1	4.42	1.45	1.38
5	A	451	TTP	C4-C5	2.80	1.49	1.44
5	A	451	TTP	PG-O1G	2.24	1.57	1.50

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	451	TTP	C5-C4-N3	6.24	120.75	115.32
5	A	451	TTP	N3-C2-N1	5.74	122.36	114.89
5	A	451	TTP	C6-N1-C2	-5.31	116.01	121.30
5	A	451	TTP	C1'-N1-C6	4.61	128.49	120.74
5	A	451	TTP	C4-N3-C2	-4.58	121.33	127.34
5	A	451	TTP	O2-C2-N3	-4.13	113.87	121.49
5	A	451	TTP	C5M-C5-C4	4.05	123.10	118.78
5	A	451	TTP	C6-C5-C4	-3.91	114.80	118.02
5	A	451	TTP	C2'-C1'-N1	-3.35	105.45	113.81
5	A	451	TTP	O2A-PA-O5'	3.29	122.46	107.57
5	A	451	TTP	O5'-C5'-C4'	3.03	119.32	108.99
5	A	451	TTP	O4-C4-N3	-2.99	114.50	120.11
5	A	451	TTP	O4'-C1'-N1	2.93	113.07	107.86
5	A	451	TTP	O2A-PA-O1A	-2.47	100.96	112.44
5	A	451	TTP	O3A-PB-O1B	-2.45	103.34	110.70
5	A	451	TTP	O4'-C1'-C2'	2.23	110.42	106.25
5	A	451	TTP	O2B-PB-O3A	2.16	113.11	107.27
5	A	451	TTP	O3G-PG-O3B	2.12	111.73	104.64
5	A	451	TTP	C2'-C3'-C4'	2.02	106.90	102.80

There are no chirality outliers.

All (2) torsion outliers are listed below:

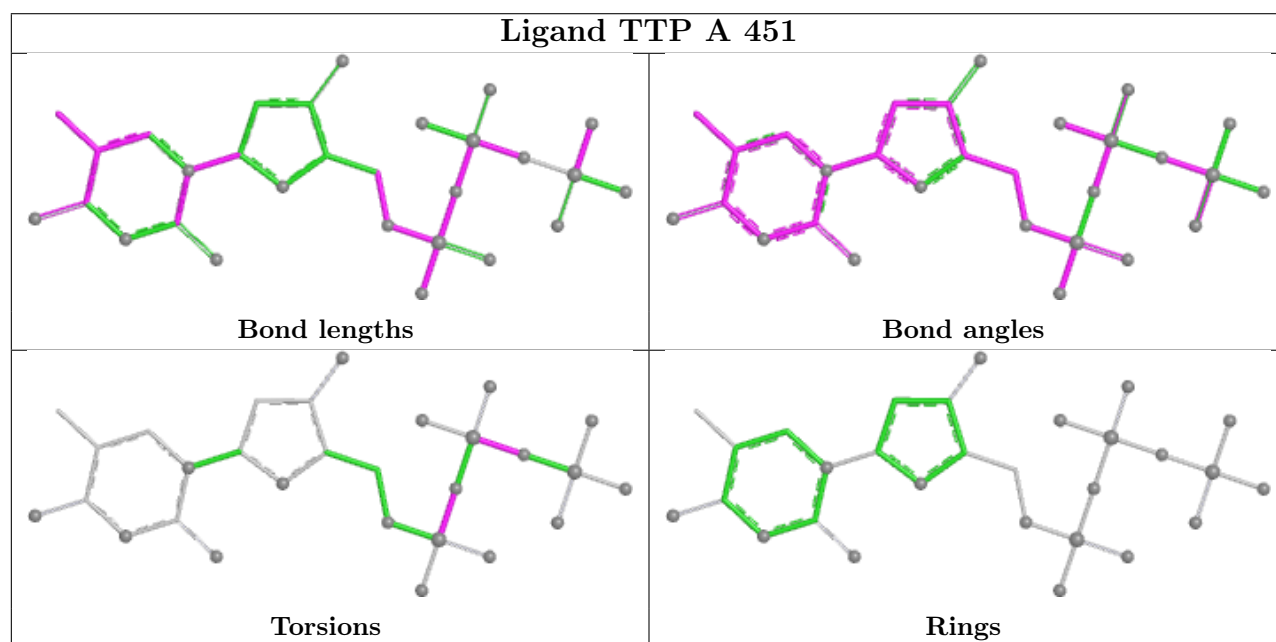
Mol	Chain	Res	Type	Atoms
5	A	451	TTP	PB-O3A-PA-O1A
5	A	451	TTP	PG-O3B-PB-O2B

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	451	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	T	11/14 (78%)	1.91	5 (45%) 0 0	21, 27, 38, 41	11 (100%)
2	P	12/13 (92%)	1.04	2 (16%) 4 5	23, 27, 35, 37	12 (100%)
3	A	388/388 (100%)	1.42	131 (33%) 1 1	28, 61, 136, 147	0
All	All	411/415 (99%)	1.42	138 (33%) 1 1	21, 57, 135, 147	23 (5%)

All (138) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	344	LEU	9.3
3	A	368	VAL	7.5
3	A	359	SER	7.0
3	A	324	LEU	6.9
3	A	345	ILE	6.6
3	A	317	ALA	6.3
3	A	315	VAL	6.1
3	A	405	LEU	6.0
3	A	401	PHE	5.8
3	A	81	VAL	5.7
3	A	321	ILE	5.3
3	A	343	ARG	5.2
1	T	5	DA	5.1
3	A	387	LEU	5.0
3	A	408	VAL	4.9
3	A	326	ALA	4.9
3	A	395	VAL	4.8
3	A	407	SER	4.8
3	A	325	LEU	4.8
3	A	388	MET	4.8
3	A	84	ALA	4.7
3	A	354	HIS	4.6
3	A	309	LYS	4.6

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Mol	Chain	Res	Type	RSRZ
3	A	310	LYS	4.5
3	A	61	TYR	4.5
3	A	397	VAL	4.5
3	A	358	GLU	4.5
3	A	369	ILE	4.4
3	A	329	LEU	4.4
3	A	386	ILE	4.3
3	A	328	LEU	4.3
3	A	383	MET	4.3
3	A	243	GLY	4.3
3	A	346	ILE	4.2
3	A	391	PHE	4.2
3	A	403	LEU	4.2
3	A	410	PHE	4.1
3	A	360	ARG	4.1
3	A	333	CYS	4.1
3	A	363	PRO	4.1
3	A	377	TYR	4.0
3	A	364	ILE	4.0
3	A	332	VAL	3.9
3	A	380	MET	3.9
3	A	356	GLY	3.9
3	A	409	CYS	3.9
3	A	355	TYR	3.8
3	A	320	LYS	3.8
3	A	406	LEU	3.8
3	A	413	LEU	3.8
3	A	400	PRO	3.8
3	A	92	VAL	3.8
3	A	73	LEU	3.7
3	A	414	LYS	3.7
1	T	6	DG	3.7
3	A	308	PHE	3.7
3	A	311	CYS	3.7
3	A	342	VAL	3.6
3	A	62	LEU	3.6
3	A	372	LEU	3.6
3	A	75	VAL	3.6
3	A	244	TYR	3.5
3	A	390	LEU	3.5
3	A	362	CYS	3.3
3	A	72	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
3	A	404	THR	3.3
3	A	336	GLY	3.2
3	A	327	SER	3.1
3	A	411	CYS	3.1
3	A	86	GLU	3.1
3	A	78	LEU	3.0
3	A	330	ASN	3.0
3	A	51	LYS	3.0
3	A	392	ARG	2.9
3	A	83	ASP	2.9
3	A	357	ARG	2.8
3	A	361	GLN	2.8
3	A	246	THR	2.8
1	T	17	DC	2.8
3	A	85	LYS	2.8
3	A	306	ASP	2.7
3	A	143	LEU	2.7
3	A	399	MET	2.7
3	A	63	VAL	2.7
3	A	313	SER	2.7
3	A	378	ASP	2.6
3	A	384	VAL	2.6
3	A	385	ASP	2.6
3	A	66	CYS	2.6
3	A	341	THR	2.6
1	T	18	DC	2.6
3	A	269	LEU	2.6
3	A	253	LEU	2.6
3	A	80	ASN	2.6
3	A	396	ASN	2.6
3	A	375	GLY	2.5
3	A	307	SER	2.5
3	A	82	ARG	2.5
3	A	52	ASP	2.5
3	A	89	PRO	2.5
3	A	365	PRO	2.5
3	A	373	GLY	2.5
3	A	302	PHE	2.5
3	A	350	SER	2.5
3	A	318	LYS	2.5
3	A	319	ASN	2.5
3	A	340	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
3	A	367	HIS	2.5
3	A	339	PRO	2.5
3	A	379	VAL	2.4
3	A	76	LYS	2.4
3	A	347	ARG	2.4
3	A	353	LYS	2.4
3	A	374	THR	2.4
3	A	77	LYS	2.3
3	A	312	SER	2.3
3	A	351	SER	2.3
3	A	412	ASN	2.3
3	A	55	LEU	2.3
3	A	349	TYR	2.3
3	A	91	LEU	2.2
3	A	338	LYS	2.2
3	A	268	ILE	2.2
2	P	7	DA	2.2
3	A	214	LYS	2.2
3	A	79	MET	2.2
3	A	87	LYS	2.2
3	A	305	GLU	2.1
3	A	402	HIS	2.1
3	A	303	SER	2.1
1	T	7	DG	2.1
2	P	8	DG	2.1
3	A	71	ARG	2.1
3	A	160	ASN	2.1
3	A	393	ASN	2.1
3	A	352	GLU	2.0
3	A	376	ASN	2.0
3	A	331	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
1	BRU	T	13	20/21	0.90	0.15	32,55,70,75	20
1	BRU	T	12	20/21	0.91	0.11	27,46,58,64	20

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	DOC	P	13	18/19	0.91	0.28	19,35,45,49	18
1	BRU	T	9	20/21	0.94	0.11	28,46,60,73	20

6.3 Carbohydrates [i](#)

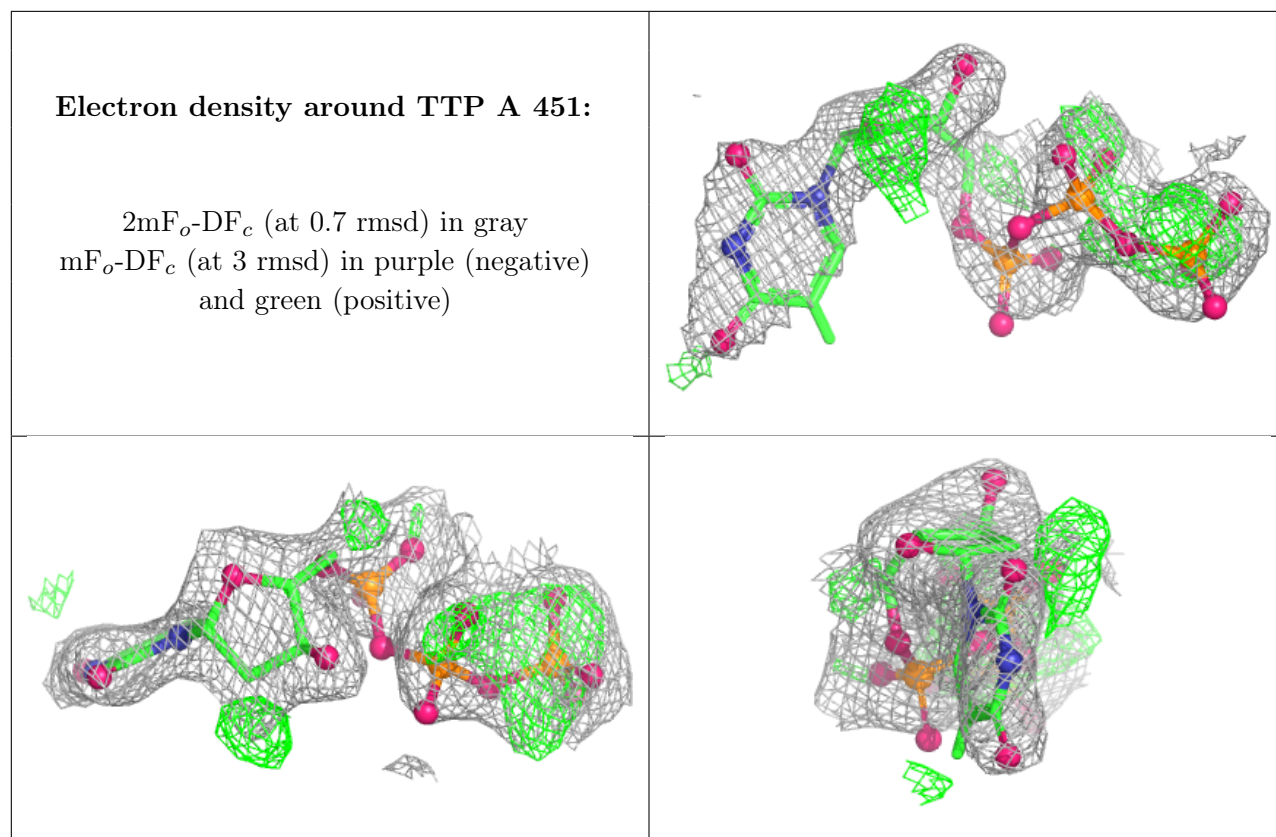
There are no oligosaccharides in this entry.

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
4	MG	A	461	1/1	0.83	0.09	26,26,26,26	1
5	TTP	A	451	29/29	0.86	0.25	27,43,60,65	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.