



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:24 PM UTC

PDB ID : 4M8O / pdb_00004m8o
Title : TERNARY COMPLEX OF DNA POLYMERASE EPSILON WITH AN IN-COMING dATP
Authors : Sauer-Eriksson, A.E.; Hogg, M.; Osterman, P.; Johansson, E.
Deposited on : 2013-08-13
Resolution : 2.20 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

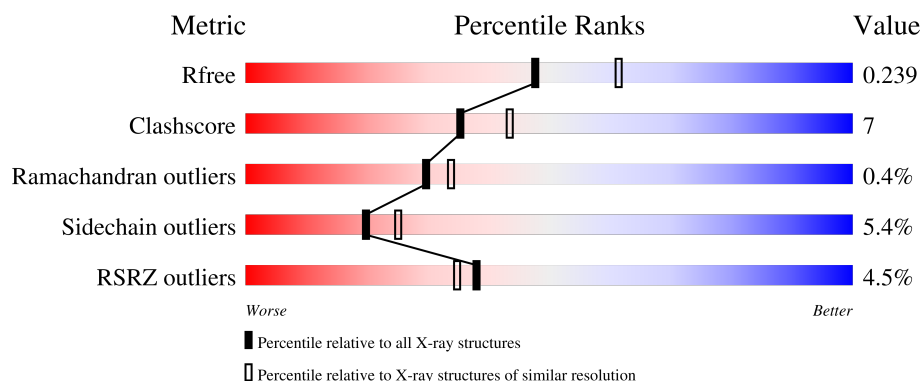
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

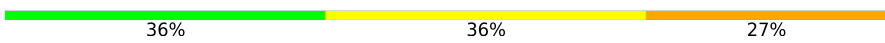
The reported resolution of this entry is 2.20 Å.

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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	1228	
2	P	11	
3	T	16	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	TAU	A	1304	-	X	-	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 10235 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 DNA polymerase epsilon catalytic subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1126	Total	C	N	O	S	0	0	0
			9173	5870	1539	1719	45			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	290	ALA	ASP	engineered mutation	UNP P21951
A	292	ALA	GLU	engineered mutation	UNP P21951

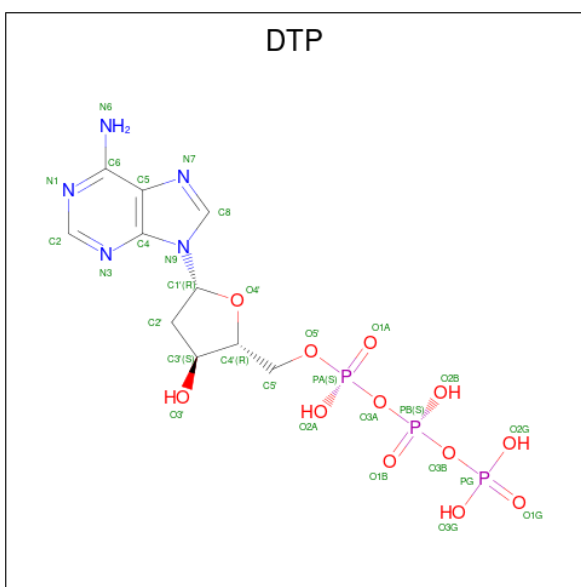
- Molecule 2 is a DNA chain called PRIMER DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	11	Total	C	I	N	O	P	0	0
			224	103	6	38	66	11		

- Molecule 3 is a DNA chain called TEMPLATE DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	T	15	Total	C	I	N	O	P	0	1
			331	152	8	56	99	16		0

- Molecule 4 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (CCD ID: DTP) (formula: C₁₀H₁₆N₅O₁₂P₃)



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 30	C 10	N 5	O 12	P 3	0	0

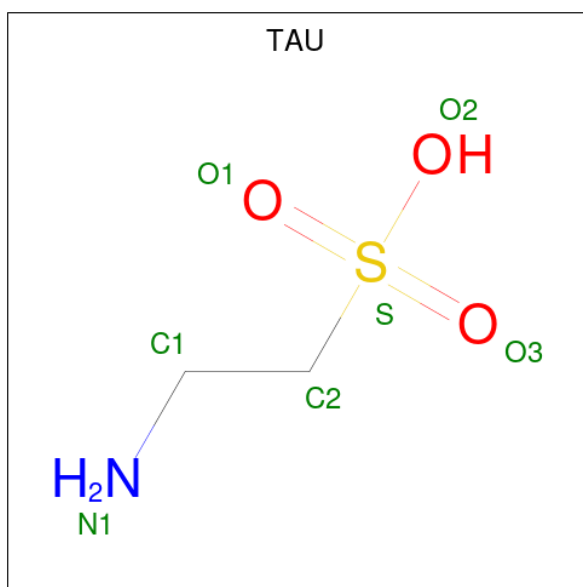
- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Zn 1 1	0	0

- Molecule 7 is 2-AMINOETHANESULFONIC ACID (CCD ID: TAU) (formula: $\text{C}_2\text{H}_7\text{NO}_3\text{S}$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	S	0	0
			7	2	1	3	1		
7	A	1	Total	C	N	O	S	0	0
			7	2	1	3	1		

- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	P	2	Total	Cl	0	0
			2	2		

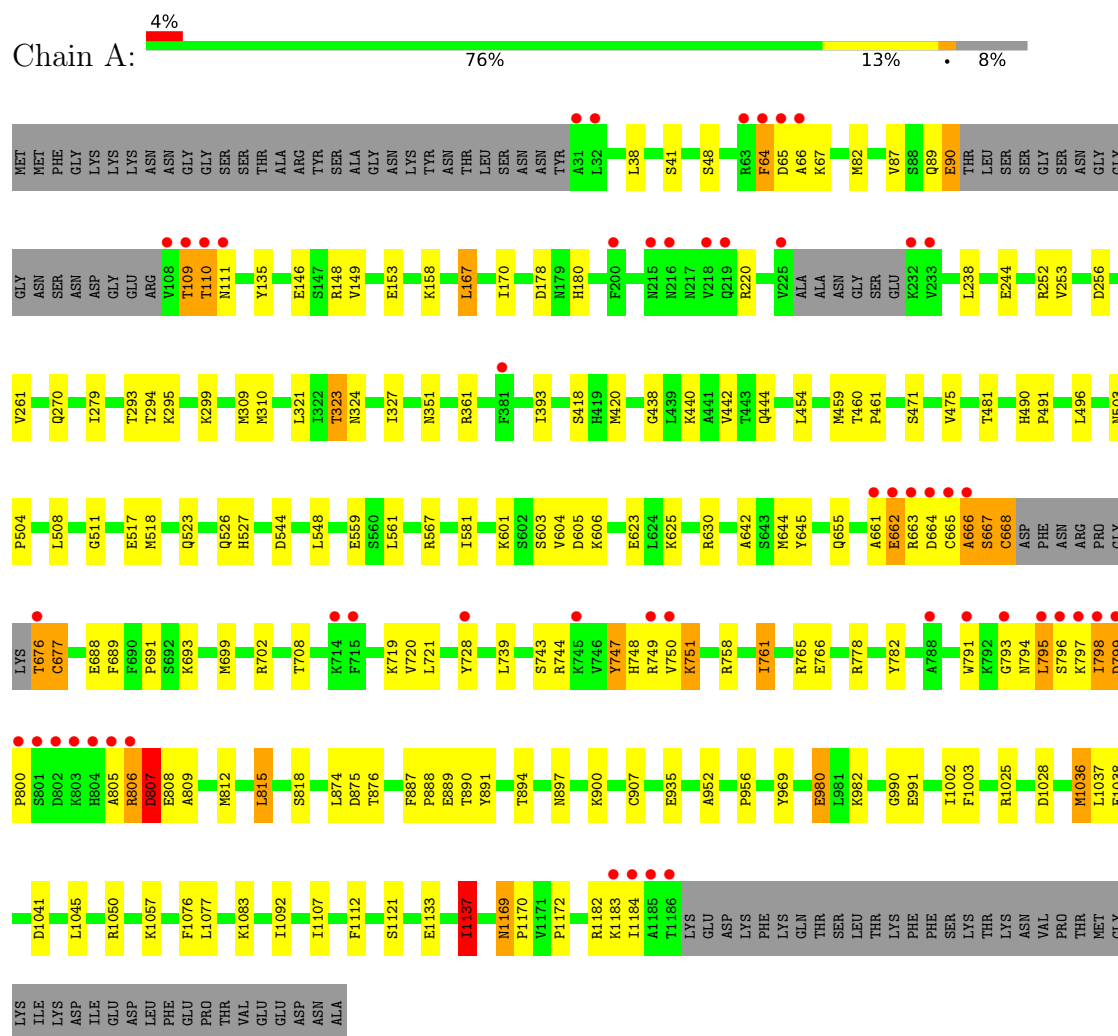
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	407	Total	O	0	0
			407	407		
9	P	22	Total	O	0	0
			22	22		
9	T	30	Total	O	0	0
			30	30		

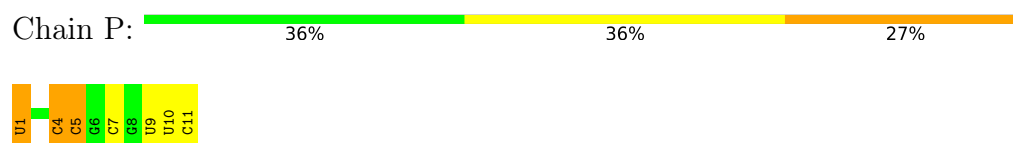
3 Residue-property plots [i](#)

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: DNA polymerase epsilon catalytic subunit A

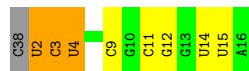


• Molecule 2: PRIMER DNA



- Molecule 3: TEMPLATE DNA

Chain T: 44% 31% 19% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	148.50Å 68.92Å 149.85Å 90.00° 109.50° 90.00°	Depositor
Resolution (Å)	47.05 – 2.20 47.05 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.05-2.20) 99.9 (47.05-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.180 , 0.237 0.187 , 0.239	Depositor DCC
R_{free} test set	3667 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	31.8	Xtriage
Anisotropy	0.310	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 39.8	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	0.95	EDS
Total number of atoms	10235	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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: DTP, TAU, CL, 5IU, ZN, C38, MG, DOC

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	1.11	15/9381 (0.2%)	1.09	16/12676 (0.1%)
2	P	0.39	0/95	0.98	0/140
3	T	0.74	0/190	1.09	1/285 (0.4%)
All	All	1.10	15/9666 (0.2%)	1.09	17/13101 (0.1%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	511	GLY	N-CA	6.26	1.52	1.45
1	A	1107	ILE	N-CA	-5.80	1.40	1.46
1	A	876	THR	C-O	-5.59	1.17	1.24
1	A	481	THR	N-CA	-5.51	1.39	1.46
1	A	1169	ASN	C-N	5.48	1.40	1.34
1	A	526	GLN	C-O	-5.45	1.17	1.24
1	A	361	ARG	CA-C	5.32	1.59	1.52
1	A	1170	PRO	N-CD	5.29	1.55	1.47
1	A	642	ALA	C-O	-5.25	1.17	1.24
1	A	517	GLU	CA-C	5.25	1.59	1.52
1	A	256	ASP	C-O	-5.11	1.17	1.24
1	A	1172	PRO	N-CD	5.11	1.54	1.47
1	A	135	TYR	C-O	-5.08	1.17	1.23
1	A	875	ASP	C-O	-5.07	1.17	1.23
1	A	253	VAL	C-O	-5.06	1.18	1.24

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	747	TYR	N-CA-C	12.95	129.30	112.72
1	A	109	THR	CB-CA-C	-8.38	96.87	113.45
1	A	666	ALA	N-CA-C	7.39	121.25	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	64	PHE	N-CA-C	-6.22	97.55	110.80
3	T	12	DG	C2'-C3'-O3'	-6.08	102.38	111.50
1	A	1169	ASN	CA-C-N	-5.88	113.76	119.87
1	A	1169	ASN	C-N-CA	-5.88	113.76	119.87
1	A	818	SER	N-CA-C	-5.86	104.97	111.36
1	A	677	CYS	N-CA-C	5.50	122.52	110.80
1	A	518	MET	N-CA-C	-5.34	105.53	111.36
1	A	295	LYS	CA-C-N	-5.24	115.89	119.66
1	A	295	LYS	C-N-CA	-5.24	115.89	119.66
1	A	645	TYR	CA-C-N	-5.20	113.28	119.05
1	A	645	TYR	C-N-CA	-5.20	113.28	119.05
1	A	644	MET	N-CA-C	5.18	117.34	111.02
1	A	110	THR	CB-CA-C	-5.15	100.17	110.42
1	A	815	LEU	N-CA-C	5.14	116.57	110.97

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	9173	0	9089	127	0
2	P	224	0	113	3	0
3	T	331	0	165	11	0
4	A	30	0	12	0	0
5	A	1	0	0	0	0
6	A	1	0	0	0	0
7	A	14	0	14	1	0
8	P	2	0	0	0	0
9	A	407	0	0	4	0
9	P	22	0	0	1	0
9	T	30	0	0	0	0
All	All	10235	0	9393	141	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 7.

All (141) 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:178:ASP:OD1	1:A:664:ASP:HB3	1.50	1.07
1:A:663:ARG:HD3	1:A:664:ASP:CG	1.83	1.03
1:A:110:THR:HG22	1:A:111:ASN:H	1.25	1.01
1:A:64:PHE:CB	1:A:270:GLN:HG2	1.90	1.00
1:A:603:SER:OG	1:A:606:LYS:HE2	1.61	1.00
1:A:64:PHE:CD1	1:A:270:GLN:HB3	1.98	0.97
1:A:64:PHE:HB2	1:A:270:GLN:CG	1.95	0.96
1:A:310:MET:HE2	1:A:321:LEU:HD11	1.43	0.96
1:A:64:PHE:HB2	1:A:270:GLN:HG2	0.99	0.96
1:A:806:ARG:HD3	1:A:809:ALA:HB2	1.44	0.95
1:A:310:MET:CE	1:A:321:LEU:HD11	2.01	0.91
1:A:806:ARG:HG2	1:A:809:ALA:H	1.35	0.89
1:A:798:ILE:C	1:A:800:PRO:HD2	1.98	0.88
1:A:806:ARG:HA	1:A:808:GLU:H	1.35	0.88
1:A:797:LYS:CG	1:A:798:ILE:HD12	2.09	0.81
1:A:64:PHE:CD1	1:A:270:GLN:CB	2.63	0.81
1:A:797:LYS:HG3	1:A:798:ILE:HD12	1.64	0.78
1:A:799:ASP:N	1:A:800:PRO:CD	2.47	0.76
3:T:3:C38:H2'2	3:T:4[B]:5IU:C6	2.17	0.75
1:A:662:GLU:O	1:A:663:ARG:HG2	1.87	0.73
1:A:688:GLU:OE1	1:A:751:LYS:HE3	1.90	0.72
1:A:1002:ILE:HD12	1:A:1003:PHE:N	2.05	0.72
1:A:110:THR:HG22	1:A:111:ASN:N	2.02	0.72
1:A:799:ASP:N	1:A:800:PRO:HD2	2.04	0.71
1:A:796:SER:HA	1:A:800:PRO:HG3	1.73	0.70
1:A:797:LYS:O	1:A:798:ILE:HG13	1.91	0.70
1:A:663:ARG:HD3	1:A:664:ASP:OD1	1.91	0.69
1:A:665:CYS:HB3	1:A:668:CYS:HB2	1.74	0.69
1:A:170:ILE:HD12	1:A:170:ILE:C	2.18	0.68
1:A:310:MET:HE2	1:A:321:LEU:CD1	2.23	0.68
1:A:791:TRP:CE2	1:A:812:MET:HG3	2.29	0.68
1:A:795:LEU:O	1:A:800:PRO:HB3	1.94	0.67
2:P:5:C38:I	9:P:214:HOH:O	2.81	0.67
1:A:794:ASN:O	1:A:799:ASP:HB2	1.94	0.67
1:A:797:LYS:HG2	1:A:798:ILE:HD12	1.78	0.64
1:A:310:MET:CE	1:A:321:LEU:HD21	2.28	0.63
1:A:806:ARG:HG2	1:A:809:ALA:N	2.11	0.62
1:A:806:ARG:HA	1:A:808:GLU:N	2.11	0.62
1:A:1112:PHE:CE2	1:A:1137:ILE:HD12	2.34	0.62
1:A:744:ARG:O	1:A:748:HIS:HB3	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:GLU:O	1:A:149:VAL:HG23	2.01	0.61
1:A:1112:PHE:CZ	1:A:1137:ILE:HD12	2.35	0.61
1:A:418:SER:HB3	1:A:420:MET:HE3	1.84	0.60
1:A:294:THR:HG22	1:A:309:MET:HE1	1.85	0.59
3:T:2:5IU:H6	3:T:2:5IU:H3'	1.85	0.59
1:A:743:SER:O	1:A:747:TYR:HB2	2.03	0.58
3:T:3:C38:H2'1	3:T:4[A]:5IU:H5''	1.86	0.57
1:A:460:THR:HB	1:A:461:PRO:HD3	1.86	0.57
1:A:294:THR:N	1:A:309:MET:HE3	2.19	0.57
1:A:815:LEU:HD11	9:A:1597:HOH:O	2.04	0.57
3:T:3:C38:H2'2	3:T:4[B]:5IU:H6	1.88	0.56
1:A:294:THR:CG2	1:A:309:MET:HE1	2.37	0.55
1:A:661:ALA:O	1:A:662:GLU:HB2	2.06	0.55
1:A:791:TRP:CD1	1:A:812:MET:HB3	2.42	0.55
3:T:3:C38:O1P	3:T:3:C38:I	2.94	0.55
1:A:603:SER:HG	1:A:606:LYS:HE2	1.69	0.55
1:A:744:ARG:O	1:A:748:HIS:HA	2.06	0.54
1:A:623:GLU:OE1	1:A:630:ARG:NH2	2.40	0.54
1:A:82:MET:HE3	1:A:261:VAL:HG23	1.90	0.54
1:A:663:ARG:CD	1:A:664:ASP:CG	2.71	0.53
1:A:806:ARG:CD	1:A:809:ALA:HB2	2.30	0.53
1:A:805:ALA:O	1:A:807:ASP:HB3	2.09	0.53
1:A:523:GLN:O	1:A:527:HIS:HD2	1.92	0.53
3:T:4[A]:5IU:C2'	3:T:4[A]:5IU:O2	2.54	0.53
1:A:454:LEU:HD23	1:A:459:MET:HG2	1.89	0.53
1:A:666:ALA:N	1:A:667:SER:HA	2.23	0.53
1:A:299:LYS:HE2	1:A:1077:LEU:O	2.09	0.53
1:A:324:ASN:OD1	1:A:324:ASN:C	2.52	0.52
1:A:548:LEU:HD23	1:A:689:PHE:HB3	1.92	0.52
1:A:420:MET:HE1	1:A:504:PRO:C	2.34	0.52
1:A:1050:ARG:NH1	9:A:1527:HOH:O	2.43	0.52
1:A:310:MET:HE3	1:A:321:LEU:HD21	1.90	0.51
1:A:688:GLU:HB3	1:A:751:LYS:HG2	1.92	0.51
1:A:805:ALA:C	1:A:807:ASP:HB3	2.36	0.51
1:A:676:THR:OG1	1:A:677:CYS:N	2.43	0.51
1:A:323:THR:HG21	1:A:351:ASN:OD1	2.10	0.51
1:A:969:TYR:CZ	1:A:982:LYS:HG3	2.46	0.51
1:A:310:MET:HE3	1:A:321:LEU:HD11	1.89	0.50
1:A:310:MET:HE1	1:A:471:SER:HA	1.93	0.50
3:T:2:5IU:H6	3:T:2:5IU:C3'	2.41	0.50
1:A:440:LYS:NZ	1:A:444:GLN:OE1	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:THR:CG2	1:A:309:MET:CE	2.91	0.49
1:A:761:ILE:N	1:A:761:ILE:CD1	2.75	0.49
1:A:604:VAL:HG23	1:A:605:ASP:N	2.27	0.49
1:A:980:GLU:HG3	7:A:1305:TAU:H1C2	1.94	0.49
1:A:65:ASP:OD1	1:A:66:ALA:N	2.45	0.49
3:T:3:C38:H2'1	3:T:4[A]:5IU:C5'	2.42	0.48
1:A:64:PHE:HD1	1:A:270:GLN:CB	2.22	0.48
1:A:293:THR:C	1:A:309:MET:HE3	2.38	0.48
1:A:310:MET:CE	1:A:321:LEU:CD1	2.84	0.48
1:A:805:ALA:C	1:A:807:ASP:CB	2.87	0.48
1:A:812:MET:HE2	1:A:812:MET:HA	1.95	0.48
1:A:309:MET:HB3	1:A:309:MET:HE2	1.57	0.48
1:A:744:ARG:O	1:A:748:HIS:CA	2.62	0.48
1:A:1037:LEU:HD21	1:A:1045:LEU:HD12	1.96	0.47
1:A:1182:ARG:O	1:A:1183:LYS:C	2.57	0.47
1:A:887:PHE:CG	1:A:888:PRO:HD2	2.50	0.47
2:P:1:5IU:H5'	2:P:1:5IU:H6	1.96	0.46
1:A:490:HIS:HB3	1:A:491:PRO:HD3	1.98	0.46
1:A:148:ARG:CZ	1:A:238:LEU:HD11	2.45	0.46
1:A:990:GLY:O	1:A:991:GLU:HB2	2.14	0.46
1:A:180:HIS:NE2	1:A:766:GLU:OE2	2.49	0.46
1:A:699:MET:HE3	1:A:699:MET:HB2	1.91	0.46
1:A:567:ARG:HG3	1:A:952:ALA:HB2	1.97	0.46
1:A:980:GLU:HG2	1:A:982:LYS:HE2	1.97	0.45
1:A:508:LEU:HD12	9:A:1693:HOH:O	2.16	0.45
1:A:956:PRO:HD2	9:A:1692:HOH:O	2.16	0.45
1:A:677:CYS:SG	1:A:765:ARG:HD3	2.57	0.45
1:A:167:LEU:C	1:A:167:LEU:HD23	2.42	0.45
3:T:3:C38:H2'1	3:T:4[B]:5IU:H5''	1.98	0.45
1:A:244:GLU:OE1	1:A:252:ARG:NH2	2.49	0.45
1:A:691:PRO:HD3	1:A:750:VAL:O	2.17	0.45
1:A:294:THR:N	1:A:309:MET:CE	2.80	0.44
1:A:178:ASP:OD1	1:A:664:ASP:CB	2.42	0.44
1:A:744:ARG:O	1:A:748:HIS:CB	2.65	0.43
1:A:791:TRP:CZ2	1:A:812:MET:HG3	2.53	0.43
1:A:471:SER:O	1:A:475:VAL:HG13	2.18	0.43
1:A:153:GLU:HG3	1:A:167:LEU:HD21	2.01	0.43
1:A:559:GLU:OE1	1:A:561:LEU:HD21	2.19	0.42
1:A:665:CYS:CB	1:A:668:CYS:HB2	2.45	0.42
1:A:663:ARG:CD	1:A:664:ASP:OD1	2.65	0.42
1:A:889:GLU:HB3	1:A:890:THR:H	1.65	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:581:ILE:HG21	1:A:625:LYS:HB2	2.02	0.42
1:A:310:MET:HE1	1:A:321:LEU:HD21	2.01	0.41
2:P:4:C38:H2'	2:P:5:C38:I	2.90	0.41
1:A:623:GLU:HG3	1:A:630:ARG:NH2	2.36	0.41
1:A:89:GLN:O	1:A:90:GLU:HB2	2.20	0.41
1:A:438:GLY:O	1:A:442:VAL:HG23	2.21	0.41
1:A:743:SER:O	1:A:744:ARG:C	2.62	0.41
1:A:794:ASN:HD22	1:A:797:LYS:HE2	1.85	0.41
1:A:793:GLY:O	1:A:797:LYS:N	2.52	0.41
1:A:1028:ASP:HB3	1:A:1036:MET:HE1	2.03	0.41
1:A:170:ILE:C	1:A:170:ILE:CD1	2.89	0.40
1:A:891:TYR:CD1	1:A:891:TYR:N	2.89	0.40
3:T:4[A]:5IU:O2	3:T:4[A]:5IU:C3'	2.70	0.40
1:A:294:THR:HA	1:A:309:MET:HE1	2.04	0.40
1:A:503:ASN:HB2	1:A:504:PRO:CD	2.52	0.40
1:A:739:LEU:HD23	1:A:739:LEU:HA	1.91	0.40
1:A:294:THR:CA	1:A:309:MET:HE1	2.51	0.40
1:A:778:ARG:HD3	1:A:782:TYR:CE2	2.56	0.40
3:T:4[A]:5IU:O2	3:T:4[A]:5IU:H3'	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1118/1228 (91%)	1066 (95%)	47 (4%)	5 (0%)	30 34

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	798	ILE
1	A	807	ASP

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Mol	Chain	Res	Type
1	A	799	ASP
1	A	1169	ASN
1	A	1137	ILE

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	1017/1102 (92%)	962 (95%)	55 (5%)	20	25

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	LEU
1	A	41	SER
1	A	48	SER
1	A	67	LYS
1	A	87	VAL
1	A	90	GLU
1	A	109	THR
1	A	158	LYS
1	A	167	LEU
1	A	220	ARG
1	A	279	ILE
1	A	323	THR
1	A	327	ILE
1	A	393	ILE
1	A	496	LEU
1	A	544	ASP
1	A	601	LYS
1	A	655	GLN
1	A	662	GLU
1	A	667	SER
1	A	668	CYS
1	A	676	THR
1	A	693	LYS

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Mol	Chain	Res	Type
1	A	702	ARG
1	A	708	THR
1	A	719	LYS
1	A	720	VAL
1	A	721	LEU
1	A	728	TYR
1	A	749	ARG
1	A	751	LYS
1	A	758	ARG
1	A	761	ILE
1	A	795	LEU
1	A	806	ARG
1	A	807	ASP
1	A	874	LEU
1	A	894	THR
1	A	897	ASN
1	A	900	LYS
1	A	907	CYS
1	A	935	GLU
1	A	980	GLU
1	A	1025	ARG
1	A	1036	MET
1	A	1038	GLU
1	A	1041	ASP
1	A	1057	LYS
1	A	1076	PHE
1	A	1083	LYS
1	A	1092	ILE
1	A	1121	SER
1	A	1133	GLU
1	A	1137	ILE
1	A	1184	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	36	GLN
1	A	83	HIS
1	A	197	ASN
1	A	216	ASN
1	A	224	ASN

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Mol	Chain	Res	Type
1	A	389	ASN
1	A	469	HIS
1	A	526	GLN
1	A	527	HIS
1	A	572	ASN
1	A	748	HIS
1	A	794	ASN
1	A	804	HIS
1	A	973	ASN
1	A	993	GLN
1	A	997	ASN
1	A	1062	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

15 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
3	5IU	T	14	2,3	18,21,22	1.57	4 (22%)	25,30,33	1.97	7 (28%)
2	C38	P	4	2,3	18,21,22	1.06	2 (11%)	25,30,33	1.41	4 (16%)
2	DOC	P	11	2,3	16,19,20	1.08	1 (6%)	20,26,29	1.68	4 (20%)
2	5IU	P	9	2,3	18,21,22	1.49	2 (11%)	25,30,33	2.01	10 (40%)
2	C38	P	7	2,3	18,21,22	1.15	2 (11%)	25,30,33	1.76	9 (36%)
3	5IU	T	2	3	18,21,22	1.15	1 (5%)	25,30,33	2.16	9 (36%)
3	5IU	T	4[A]	3	18,21,22	1.54	2 (11%)	25,30,33	2.89	13 (52%)
3	5IU	T	15	2,3	18,21,22	1.21	1 (5%)	25,30,33	2.19	6 (24%)
2	5IU	P	1	2,3	18,21,22	1.52	4 (22%)	25,30,33	1.95	5 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	C38	T	3	3	18,21,22	1.25	2 (11%)	25,30,33	2.35	6 (24%)
3	5IU	T	4[B]	3	18,21,22	1.11	1 (5%)	25,30,33	2.38	8 (32%)
3	C38	T	9	2,3	18,21,22	0.93	1 (5%)	25,30,33	1.47	4 (16%)
2	5IU	P	10	2,3	18,21,22	1.35	2 (11%)	25,30,33	1.85	7 (28%)
2	C38	P	5	2,3	18,21,22	1.11	1 (5%)	25,30,33	1.21	2 (8%)
3	C38	T	11	2,3	18,21,22	1.12	1 (5%)	25,30,33	1.60	5 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	5IU	T	14	2,3	-	0/7/21/22	0/2/2/2
2	C38	P	4	2,3	-	2/7/21/22	0/2/2/2
2	DOC	P	11	2,3	-	2/7/18/19	0/2/2/2
2	5IU	P	9	2,3	-	1/7/21/22	0/2/2/2
2	C38	P	7	2,3	-	0/7/21/22	0/2/2/2
3	5IU	T	2	3	-	1/7/21/22	0/2/2/2
3	5IU	T	4[A]	3	-	4/7/21/22	0/2/2/2
3	5IU	T	15	2,3	-	0/7/21/22	0/2/2/2
2	5IU	P	1	2,3	-	3/7/21/22	0/2/2/2
3	C38	T	3	3	-	0/7/21/22	0/2/2/2
3	5IU	T	4[B]	3	-	0/7/21/22	0/2/2/2
3	C38	T	9	2,3	-	0/7/21/22	0/2/2/2
2	5IU	P	10	2,3	-	0/7/21/22	0/2/2/2
2	C38	P	5	2,3	-	0/7/21/22	0/2/2/2
3	C38	T	11	2,3	-	0/7/21/22	0/2/2/2

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	9	5IU	C2-N3	-4.54	1.30	1.38
3	T	14	5IU	C4-N3	-3.88	1.31	1.38
2	P	1	5IU	C4-N3	-3.49	1.32	1.38
2	P	5	C38	C6-N1	-3.37	1.32	1.38
3	T	4[A]	5IU	C4-N3	-3.19	1.32	1.38
2	P	10	5IU	C4-N3	-3.07	1.33	1.38
2	P	1	5IU	C6-N1	-2.98	1.32	1.38
2	P	7	C38	C6-N1	-2.93	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	T	14	5IU	C6-N1	-2.92	1.33	1.38
3	T	11	C38	C6-N1	-2.89	1.33	1.38
3	T	4[A]	5IU	C6-C5	2.85	1.43	1.35
3	T	9	C38	C4-C5	2.68	1.51	1.43
3	T	3	C38	C4-C5	2.61	1.51	1.43
3	T	14	5IU	C2-N3	-2.53	1.33	1.38
2	P	1	5IU	C2-N3	-2.52	1.33	1.38
2	P	1	5IU	C2-N1	2.47	1.42	1.38
3	T	15	5IU	C2-N3	-2.46	1.33	1.38
2	P	10	5IU	C2-N3	-2.46	1.33	1.38
2	P	4	C38	C4-C5	2.45	1.50	1.43
3	T	3	C38	C6-N1	-2.34	1.34	1.38
2	P	9	5IU	O2-C2	2.28	1.27	1.23
3	T	2	5IU	C2-N1	2.22	1.41	1.38
3	T	14	5IU	O4'-C1'	2.20	1.47	1.42
3	T	4[B]	5IU	C6-C5	2.15	1.41	1.35
2	P	7	C38	C6-C5	2.15	1.41	1.35
2	P	4	C38	C6-N1	-2.11	1.34	1.38
2	P	11	DOC	C6-C5	2.06	1.39	1.35

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	4[A]	5IU	N3-C2-N1	6.76	123.69	114.89
3	T	3	C38	C4-C5-I	5.87	131.14	122.09
3	T	14	5IU	N3-C2-N1	5.39	121.91	114.89
3	T	15	5IU	C4-N3-C2	-5.26	120.45	127.34
3	T	4[B]	5IU	O4-C4-C5	-5.24	116.43	125.69
3	T	15	5IU	N3-C2-N1	5.22	121.69	114.89
3	T	4[B]	5IU	C4-N3-C2	-5.12	120.62	127.34
2	P	1	5IU	N3-C2-N1	5.07	121.49	114.89
2	P	1	5IU	C4-N3-C2	-5.04	120.73	127.34
3	T	3	C38	C6-C5-I	-5.03	112.57	120.99
3	T	3	C38	C1'-N1-C2	4.86	126.17	117.83
3	T	4[B]	5IU	N3-C2-N1	4.84	121.19	114.89
3	T	2	5IU	C4-C5-I5	4.83	126.47	118.54
3	T	4[A]	5IU	C4-N3-C2	-4.71	121.16	127.34
3	T	4[A]	5IU	C6-C5-I5	4.51	128.54	120.99
3	T	15	5IU	O2-C2-N1	-4.36	117.12	122.80
3	T	11	C38	O2-C2-N3	-4.24	115.64	122.33
3	T	4[A]	5IU	O4'-C1'-N1	4.20	115.32	107.86
3	T	4[A]	5IU	O2-C2-N1	-4.15	117.40	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	2	5IU	N3-C2-N1	4.10	120.22	114.89
2	P	10	5IU	N3-C2-N1	4.06	120.18	114.89
3	T	4[A]	5IU	C1'-N1-C6	4.05	127.54	120.74
3	T	2	5IU	C4-N3-C2	-4.03	122.06	127.34
2	P	7	C38	C5-C4-N3	-3.93	115.66	120.57
3	T	4[B]	5IU	C5-C4-N3	3.88	120.29	113.86
3	T	14	5IU	C4-N3-C2	-3.87	122.26	127.34
3	T	3	C38	C1'-N1-C6	-3.87	114.25	120.74
2	P	9	5IU	C5-C4-N3	3.83	120.20	113.86
2	P	11	DOC	O2-C2-N3	-3.81	116.32	122.33
2	P	10	5IU	C4-C5-I5	3.77	124.73	118.54
3	T	9	C38	O4'-C1'-C2'	-3.74	99.25	106.25
3	T	4[B]	5IU	O2-C2-N1	-3.68	118.01	122.80
3	T	4[A]	5IU	C5-C4-N3	3.60	119.83	113.86
2	P	10	5IU	C5-C4-N3	3.59	119.81	113.86
2	P	9	5IU	C4-C5-I5	3.48	124.25	118.54
3	T	4[A]	5IU	C6-N1-C2	-3.48	117.84	121.30
2	P	9	5IU	C4-N3-C2	-3.45	122.81	127.34
3	T	15	5IU	C5-C4-N3	3.42	119.53	113.86
2	P	9	5IU	O2-C2-N1	-3.41	118.36	122.80
3	T	15	5IU	O4-C4-C5	-3.31	119.84	125.69
3	T	2	5IU	C5-C4-N3	3.30	119.32	113.86
2	P	11	DOC	C3'-C2'-C1'	3.29	106.66	102.87
3	T	11	C38	C5-C6-N1	-3.29	117.10	121.85
3	T	2	5IU	O4-C4-C5	-3.24	119.97	125.69
2	P	9	5IU	C2'-C1'-N1	3.23	121.88	113.81
3	T	9	C38	O4'-C1'-N1	-3.16	102.25	107.86
2	P	9	5IU	N3-C2-N1	3.14	118.98	114.89
3	T	4[B]	5IU	C6-C5-I5	3.06	126.11	120.99
3	T	14	5IU	O4'-C1'-N1	3.00	113.18	107.86
2	P	1	5IU	C5-C4-N3	2.99	118.81	113.86
3	T	4[B]	5IU	C2'-C1'-N1	-2.99	106.34	113.81
2	P	10	5IU	C4-N3-C2	-2.95	123.47	127.34
3	T	9	C38	O2-C2-N3	-2.91	117.74	122.33
2	P	7	C38	O4'-C1'-C2'	-2.90	100.83	106.25
2	P	7	C38	C6-N1-C2	-2.84	117.17	120.95
2	P	7	C38	O2-C2-N3	-2.83	117.86	122.33
2	P	9	5IU	C1'-N1-C6	2.79	125.43	120.74
2	P	5	C38	C2'-C3'-C4'	2.79	108.46	102.80
3	T	4[A]	5IU	O3'-C3'-C2'	2.75	120.45	110.88
2	P	4	C38	O4'-C1'-N1	2.74	112.73	107.86
2	P	7	C38	N1-C2-N3	2.68	123.45	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	14	5IU	C6-N1-C2	-2.67	118.64	121.30
3	T	14	5IU	O4-C4-C5	-2.62	121.05	125.69
3	T	4[B]	5IU	O4'-C1'-N1	2.61	112.49	107.86
2	P	1	5IU	C4-C5-I5	2.58	122.77	118.54
2	P	7	C38	C1'-N1-C2	2.56	122.22	117.83
3	T	3	C38	C3'-C2'-C1'	2.54	108.82	102.60
2	P	5	C38	O2-C2-N3	-2.52	118.35	122.33
3	T	14	5IU	O2-C2-N1	-2.51	119.53	122.80
3	T	4[A]	5IU	O4-C4-C5	-2.42	121.42	125.69
2	P	4	C38	O4'-C1'-C2'	2.39	110.70	106.25
3	T	4[A]	5IU	C4-C5-I5	-2.37	114.64	118.54
2	P	10	5IU	C6-C5-C4	-2.35	114.37	119.81
2	P	7	C38	C2'-C1'-N1	2.33	119.64	113.81
3	T	4[A]	5IU	C3'-C2'-C1'	2.32	108.27	102.60
3	T	11	C38	N1-C2-N3	2.31	122.80	118.80
3	T	4[A]	5IU	O4'-C4'-C5'	2.29	116.67	109.33
2	P	10	5IU	O2-C2-N1	-2.29	119.82	122.80
3	T	11	C38	O3'-C3'-C4'	-2.27	101.45	110.07
3	T	3	C38	O2-C2-N3	-2.26	118.76	122.33
2	P	1	5IU	O2-C2-N3	-2.26	117.32	121.49
3	T	14	5IU	C5-C4-N3	2.26	117.60	113.86
2	P	9	5IU	O4-C4-C5	-2.25	121.71	125.69
2	P	9	5IU	C6-C5-C4	-2.24	114.61	119.81
3	T	2	5IU	O2-C2-N1	-2.23	119.89	122.80
2	P	4	C38	C4-C5-I	-2.23	118.66	122.09
3	T	2	5IU	C1'-N1-C2	2.20	121.95	117.66
3	T	2	5IU	C2'-C1'-N1	-2.19	108.33	113.81
2	P	11	DOC	N1-C2-N3	2.14	122.51	118.80
3	T	9	C38	N1-C2-N3	2.13	122.51	118.80
3	T	11	C38	O3'-C3'-C2'	2.09	118.13	110.88
2	P	10	5IU	O4-C4-C5	-2.09	122.00	125.69
2	P	4	C38	C1'-N1-C2	-2.08	114.27	117.83
3	T	2	5IU	O4'-C1'-N1	2.07	111.53	107.86
3	T	15	5IU	O4'-C4'-C5'	2.06	115.95	109.33
2	P	7	C38	O3'-C3'-C2'	2.06	118.04	110.88
2	P	11	DOC	C5-C4-N4	2.06	124.23	120.63
2	P	7	C38	O3'-C3'-C4'	-2.03	102.38	110.07
2	P	9	5IU	C1'-N1-C2	-2.00	113.74	117.66

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	P	1	5IU	C3'-C4'-C5'-O5'
2	P	1	5IU	C4'-C5'-O5'-P
2	P	11	DOC	C3'-C4'-C5'-O5'
2	P	1	5IU	O4'-C4'-C5'-O5'
2	P	4	C38	C3'-C4'-C5'-O5'
2	P	11	DOC	O4'-C4'-C5'-O5'
3	T	4[A]	5IU	C2'-C1'-N1-C2
2	P	4	C38	O4'-C4'-C5'-O5'
3	T	4[A]	5IU	O4'-C1'-N1-C6
3	T	4[A]	5IU	C2'-C1'-N1-C6
3	T	4[A]	5IU	O4'-C1'-N1-C2
3	T	2	5IU	C4'-C5'-O5'-P
2	P	9	5IU	C4'-C5'-O5'-P

There are no ring outliers.

7 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	P	4	C38	1	0
3	T	2	5IU	2	0
3	T	4[A]	5IU	5	0
2	P	1	5IU	1	0
3	T	3	C38	6	0
3	T	4[B]	5IU	3	0
2	P	5	C38	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 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
7	TAU	A	1305	-	6,6,6	2.74	2 (33%)	7,8,8	1.89	3 (42%)
7	TAU	A	1304	-	6,6,6	3.08	2 (33%)	7,8,8	2.18	2 (28%)
4	DTP	A	1301	5	31,32,32	1.61	6 (19%)	46,50,50	2.14	10 (21%)

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
7	TAU	A	1305	-	-	1/4/4/4	-
7	TAU	A	1304	-	-	4/4/4/4	-
4	DTP	A	1301	5	-	5/22/34/34	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1304	TAU	C2-S	-6.06	1.69	1.77
7	A	1305	TAU	C2-S	-5.49	1.69	1.77
4	A	1301	DTP	C5-C4	4.44	1.47	1.39
7	A	1304	TAU	O2-S	4.38	1.63	1.47
7	A	1305	TAU	O2-S	3.69	1.61	1.47
4	A	1301	DTP	C8-N7	3.53	1.38	1.31
4	A	1301	DTP	PB-O2B	-2.59	1.43	1.55
4	A	1301	DTP	C5-N7	-2.52	1.34	1.39
4	A	1301	DTP	C5-C6	2.50	1.48	1.41
4	A	1301	DTP	PA-O2A	-2.30	1.44	1.55

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1301	DTP	C5-C4-N3	-6.95	117.15	126.72
4	A	1301	DTP	N3-C4-N9	5.28	136.14	127.17
4	A	1301	DTP	C2-N3-C4	4.80	123.55	111.83
4	A	1301	DTP	C2'-C1'-N9	-4.71	103.56	114.63
7	A	1304	TAU	O3-S-C2	4.36	113.31	106.73
4	A	1301	DTP	O4'-C1'-N9	3.86	114.89	107.96
4	A	1301	DTP	C5-C6-N6	-3.43	114.79	123.29
7	A	1305	TAU	O1-S-C2	3.06	111.36	106.73
4	A	1301	DTP	N3-C2-N1	-2.98	124.08	128.58
7	A	1304	TAU	O3-S-O1	-2.92	104.31	113.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1305	TAU	O2-S-O3	-2.63	104.83	111.40
7	A	1305	TAU	O2-S-C2	2.31	110.52	106.00
4	A	1301	DTP	O3B-PG-O1G	-2.30	98.91	111.04
4	A	1301	DTP	O3G-PG-O1G	2.29	119.76	110.83
4	A	1301	DTP	N6-C6-N1	2.10	123.06	118.38

There are no chirality outliers.

All (10) torsion outliers are listed below:

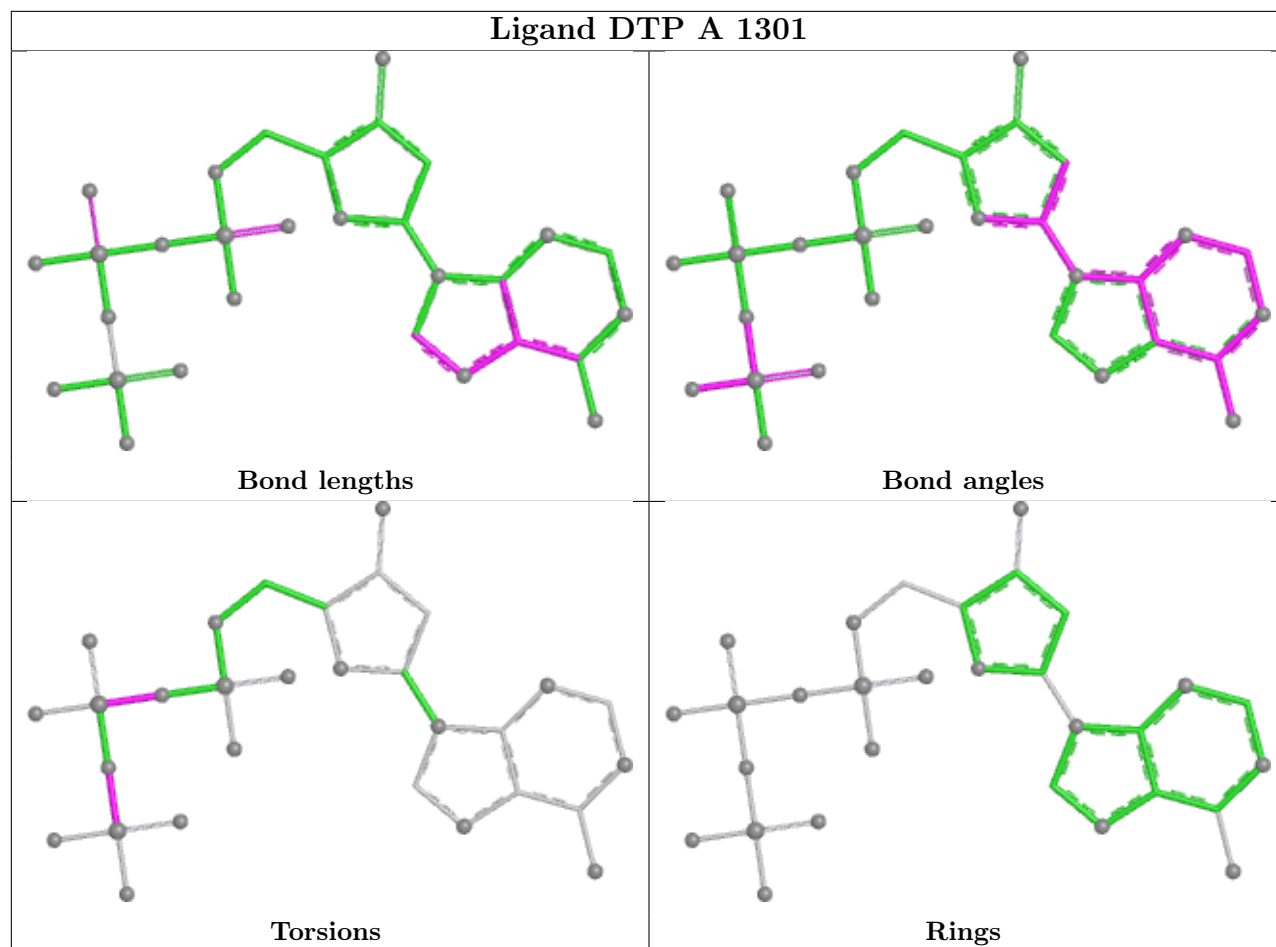
Mol	Chain	Res	Type	Atoms
4	A	1301	DTP	PB-O3B-PG-O3G
7	A	1304	TAU	N1-C1-C2-S
7	A	1304	TAU	C1-C2-S-O1
7	A	1304	TAU	C1-C2-S-O2
7	A	1304	TAU	C1-C2-S-O3
4	A	1301	DTP	PB-O3B-PG-O2G
4	A	1301	DTP	PA-O3A-PB-O1B
7	A	1305	TAU	N1-C1-C2-S
4	A	1301	DTP	PB-O3B-PG-O1G
4	A	1301	DTP	PA-O3A-PB-O2B

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1305	TAU	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	1126/1228 (91%)	0.01	51 (4%) 38 35	15, 33, 73, 146	0
2	P	4/11 (36%)	-0.75	0 100 100	20, 31, 46, 48	0
3	T	8/16 (50%)	-1.11	0 100 100	16, 19, 34, 41	0
All	All	1138/1255 (90%)	0.00	51 (4%) 38 35	15, 33, 73, 146	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	225	VAL	5.9
1	A	798	ILE	5.5
1	A	108	VAL	5.5
1	A	64	PHE	5.3
1	A	661	ALA	5.2
1	A	31	ALA	5.2
1	A	800	PRO	5.1
1	A	1186	THR	5.0
1	A	805	ALA	4.6
1	A	1185	ALA	4.3
1	A	233	VAL	4.1
1	A	66	ALA	4.0
1	A	799	ASP	4.0
1	A	664	ASP	3.8
1	A	795	LEU	3.8
1	A	715	PHE	3.7
1	A	802	ASP	3.6
1	A	788	ALA	3.6
1	A	750	VAL	3.6
1	A	791	TRP	3.5
1	A	109	THR	3.3
1	A	728	TYR	3.3
1	A	110	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	666	ALA	3.2
1	A	665	CYS	3.0
1	A	381	PHE	3.0
1	A	801	SER	2.8
1	A	65	ASP	2.7
1	A	663	ARG	2.7
1	A	662	GLU	2.7
1	A	714	LYS	2.6
1	A	749	ARG	2.6
1	A	63	ARG	2.6
1	A	111	ASN	2.6
1	A	806	ARG	2.5
1	A	803	LYS	2.5
1	A	32	LEU	2.5
1	A	793	GLY	2.5
1	A	676	THR	2.4
1	A	219	GLN	2.4
1	A	1184	ILE	2.4
1	A	745	LYS	2.3
1	A	218	VAL	2.3
1	A	804	HIS	2.3
1	A	215	ASN	2.3
1	A	200	PHE	2.3
1	A	216	ASN	2.3
1	A	797	LYS	2.2
1	A	1183	LYS	2.1
1	A	232	LYS	2.0
1	A	796	SER	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
3	5IU	T	2	20/21	0.63	0.15	98,115,123,126	1
3	C38	T	3	20/21	0.69	0.14	37,68,94,110	1
3	5IU	T	4[A]	20/21	0.87	0.12	26,37,58,87	20
3	5IU	T	4[B]	20/21	0.87	0.12	26,37,56,73	20
2	5IU	P	1	20/21	0.89	0.11	43,56,140,144	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	C38	P	4	20/21	0.95	0.09	29,47,65,72	1
3	5IU	T	15	20/21	0.96	0.07	32,39,43,52	1
2	C38	P	5	20/21	0.97	0.07	25,44,56,66	1
2	DOC	P	11	18/19	0.98	0.04	17,19,24,24	0
2	C38	P	7	20/21	0.98	0.05	19,24,29,35	1
3	C38	T	11	20/21	0.98	0.05	22,26,30,32	1
3	5IU	T	14	20/21	0.98	0.06	30,35,38,39	1
2	5IU	P	10	20/21	0.98	0.05	13,18,20,25	1
3	C38	T	9	20/21	0.99	0.05	16,21,25,28	1
2	5IU	P	9	20/21	0.99	0.04	16,18,23,23	1

6.3 Carbohydrates [i](#)

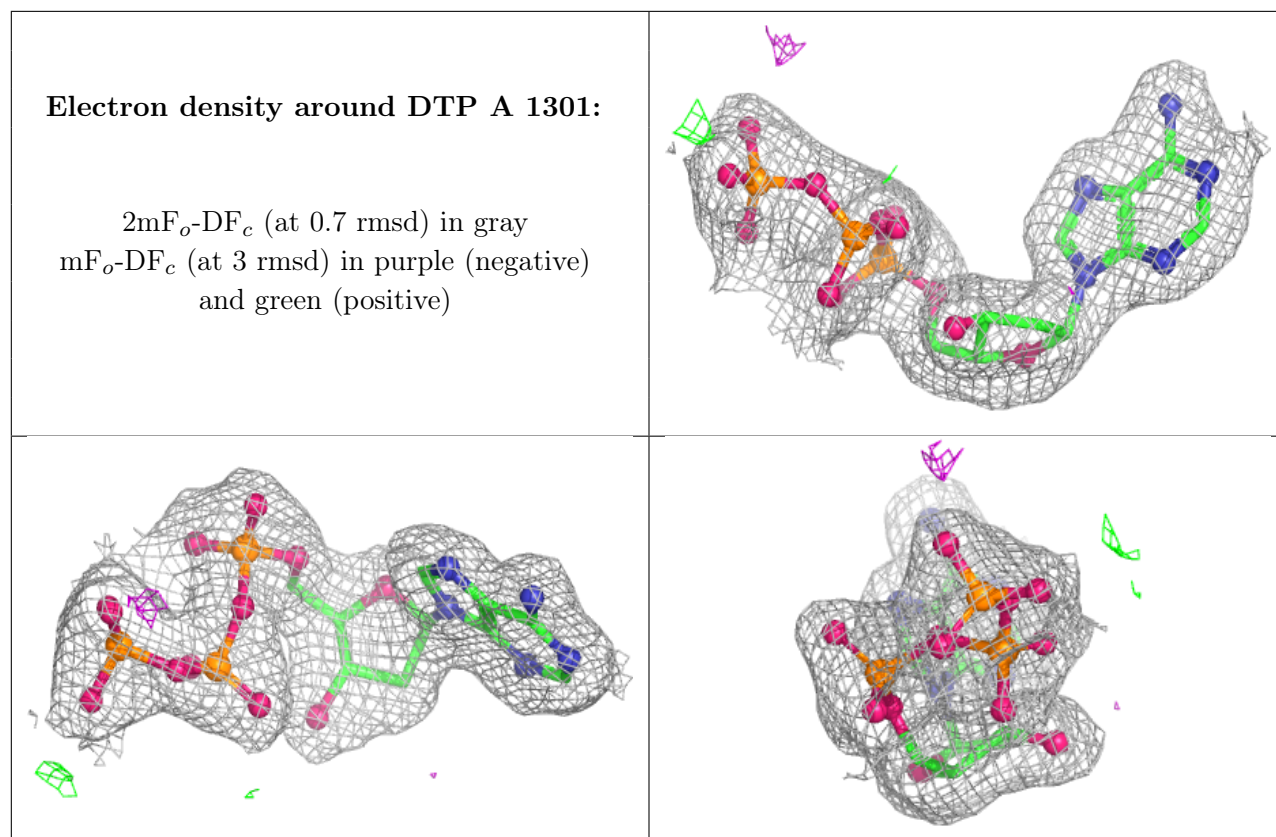
There are no oligosaccharides in this entry.

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
7	TAU	A	1305	7/7	0.82	0.20	50,59,67,68	7
7	TAU	A	1304	7/7	0.84	0.19	66,79,82,88	0
8	CL	P	102	1/1	0.97	0.21	24,24,24,24	1
5	MG	A	1302	1/1	0.98	0.03	21,21,21,21	0
8	CL	P	101	1/1	0.99	0.05	9,9,9,9	0
4	DTP	A	1301	30/30	0.99	0.04	13,14,23,24	0
6	ZN	A	1303	1/1	1.00	0.03	41,41,41,41	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.