



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:02 PM UTC

PDB ID : 2C2D / pdb_00002c2d
Title : Efficient and High Fidelity Incorporation of dCTP Opposite 7,8- Dihydro-8-oxodeoxyguanosine by Sulfolobus solfataricus DNA Polymerase Dpo4
Authors : Irimia, A.; Loukachevitch, L.V.; Egli, M.
Deposited on : 2005-09-27
Resolution : 2.57 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)
Xtrriage (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

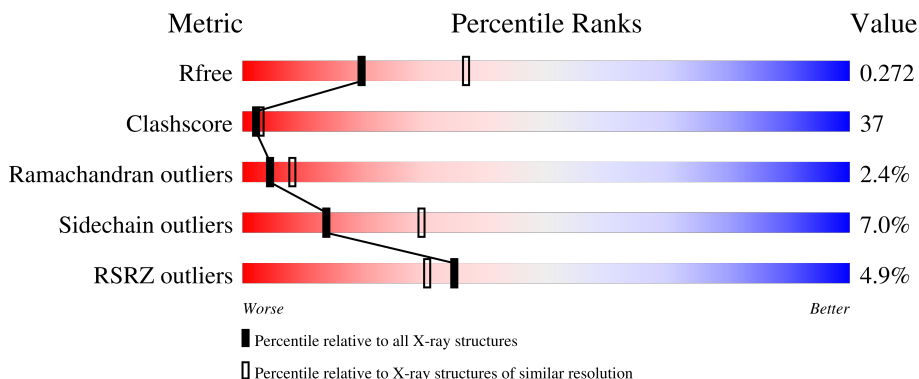
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.57 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	4770 (2.60-2.56)
Clashscore	190562	5124 (2.60-2.56)
Ramachandran outliers	187476	5046 (2.60-2.56)
Sidechain outliers	187428	5046 (2.60-2.56)
RSRZ outliers	180081	4770 (2.60-2.56)

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	358	 5% 39% 50% 6%
2	P	13	 23% 69% 8%
3	T	18	 6% 22% 44% 17% 17%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3474 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 IV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	342	2744	1760	473	504	7	0	0	1

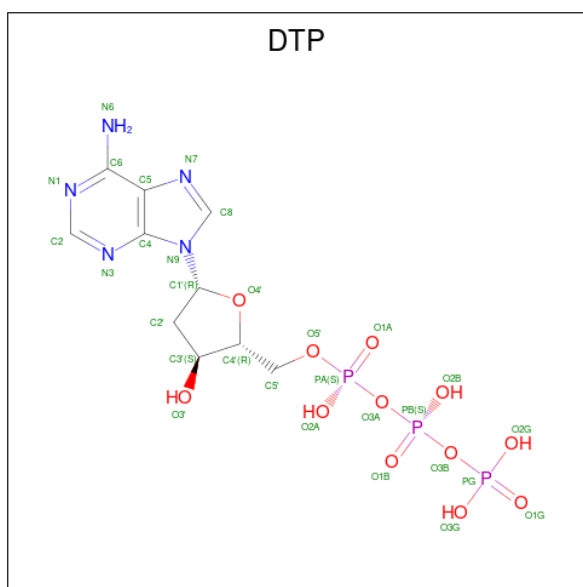
- Molecule 2 is a DNA chain called 5'-D(*GP*GP*GP*GP*GP*AP*AP*GP*GP*AP*TP*TP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	P	13	273	129	57	75	12	0	0	0

- Molecule 3 is a DNA chain called 5'-D(*TP*CP*AP*C 8OGP*GP*AP*AP*TP*CP*CP *TP*TP*CP*CP*CP*CP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	T	15	296	142	50	90	14	0	0	0

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



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

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	5	Total	Ca	0	0
			5	5		

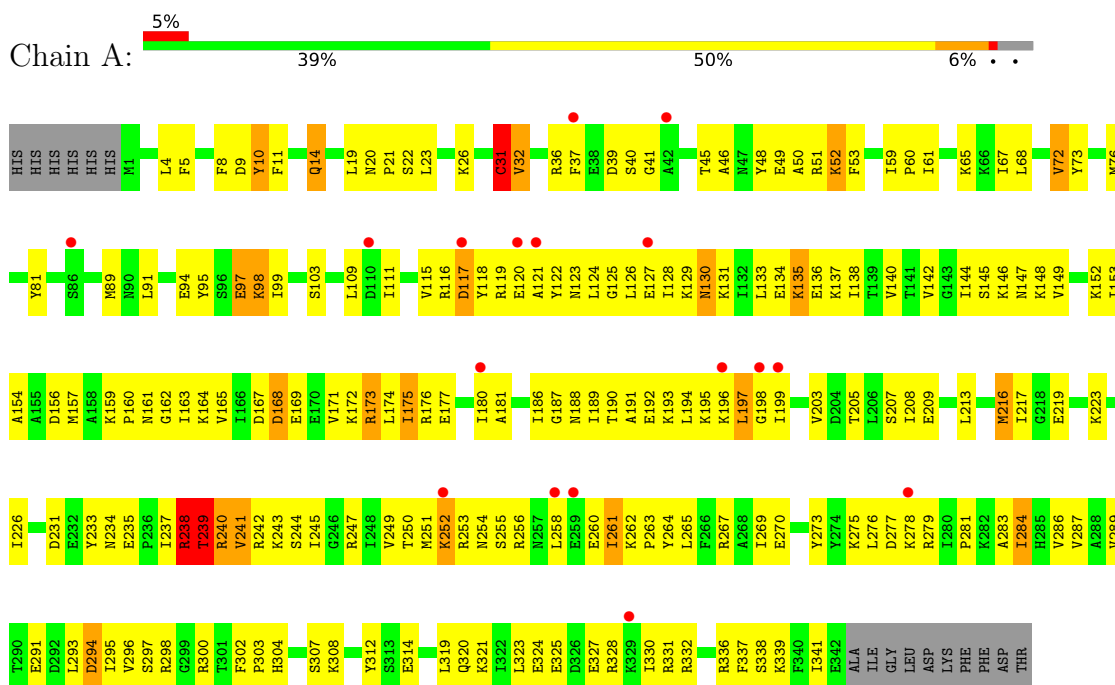
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	60	Total	O	0	0
			60	60		
6	P	18	Total	O	0	0
			18	18		
6	T	18	Total	O	0	0
			18	18		

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.

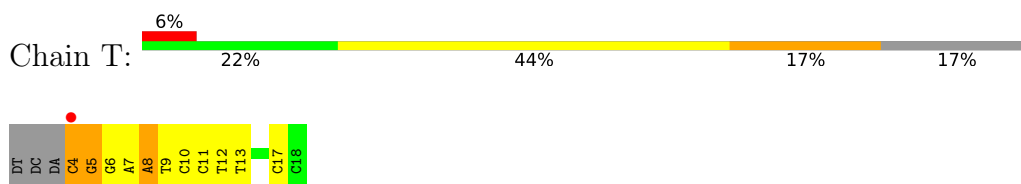
- Molecule 1: DNA POLYMERASE IV



- Molecule 2: 5'-D(*GP*GP*GP*GP*GP*AP*AP*GP*GP*AP *TP*TP*C)-3'



- Molecule 3: 5'-D(*TP*CP*AP*C 8OGP*GP*AP*AP*TP*CP*CP *TP*TP*CP*CP*CP*CP*C)-3'



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	97.51Å 102.02Å 53.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.99 – 2.57 43.99 – 2.57	Depositor EDS
% Data completeness (in resolution range)	97.0 (43.99-2.57) 97.3 (43.99-2.57)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 2.58Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.240 , 0.280 0.235 , 0.272	Depositor DCC
R_{free} test set	828 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	77.0	Xtrriage
Anisotropy	0.148	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 85.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.032 for k,h,-l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3474	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% 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: CA, SOG, DTP

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	0.59	1/2783 (0.0%)	1.07	19/3738 (0.5%)
2	P	0.30	0/308	0.74	1/476 (0.2%)
3	T	0.40	0/302	1.11	2/459 (0.4%)
All	All	0.55	1/3393 (0.0%)	1.05	22/4673 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	T	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	341	ILE	C-N	-5.94	1.25	1.33

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	4	DC	C2'-C3'-O3'	10.29	126.93	111.50
1	A	97	GLU	N-CA-C	-9.53	101.42	113.43
1	A	11	PHE	N-CA-C	7.90	124.33	111.37
1	A	294	ASP	N-CA-C	-7.16	99.86	110.46
2	P	13	DC	C2'-C3'-O3'	-6.26	102.11	111.50
1	A	286	VAL	N-CA-C	-6.14	99.53	108.87
1	A	238	ARG	N-CA-C	6.10	123.78	110.80
1	A	135	LYS	N-CA-C	6.06	118.84	111.82
1	A	134	GLU	N-CA-C	-6.05	104.38	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	4	DC	C5'-C4'-C3'	-6.01	105.89	114.90
1	A	239	THR	N-CA-C	5.77	123.08	110.80
1	A	72	VAL	CB-CA-C	-5.71	104.00	111.25
1	A	239	THR	N-CA-CB	-5.62	100.99	110.49
1	A	338	SER	N-CA-C	5.48	115.52	108.34
1	A	255	SER	N-CA-C	5.48	117.13	108.96
1	A	31	CYS	N-CA-C	5.36	117.13	109.14
1	A	89	MET	N-CA-C	-5.35	105.35	111.07
1	A	48	TYR	N-CA-C	5.26	117.76	111.71
1	A	261	ILE	N-CA-C	5.13	115.35	110.53
1	A	59	ILE	CA-C-N	5.11	124.87	119.76
1	A	59	ILE	C-N-CA	5.11	124.87	119.76
1	A	149	VAL	N-CA-C	5.04	115.19	110.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	T	8	DA	Sidechain

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	2744	0	2889	205	1
2	P	273	0	147	23	0
3	T	296	0	170	21	0
4	A	60	0	24	15	0
5	A	5	0	0	0	0
6	A	60	0	0	27	0
6	P	18	0	0	7	0
6	T	18	0	0	7	0
All	All	3474	0	3230	242	1

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 37.

All (242) 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:144:ILE:HB	6:A:2029:HOH:O	1.45	1.17
4:A:1002:DTP:O1B	2:P:13:DC:H3'	1.44	1.15
1:A:123:ASN:HA	6:A:2025:HOH:O	1.47	1.10
1:A:116:ARG:HG2	1:A:117:ASP:H	1.01	1.09
1:A:116:ARG:HG2	1:A:117:ASP:N	1.62	1.05
1:A:303:PRO:HD3	6:A:2049:HOH:O	1.61	0.98
2:P:12:DT:H3'	6:P:2017:HOH:O	1.60	0.98
1:A:165:VAL:HG22	6:A:2029:HOH:O	1.65	0.96
4:A:1001:DTP:O1G	4:A:1001:DTP:PA	2.23	0.96
4:A:1001:DTP:O1G	4:A:1001:DTP:H5'1	1.68	0.94
1:A:4:LEU:HG	1:A:144:ILE:HD11	1.45	0.93
1:A:189:ILE:HD11	1:A:193:LYS:HE3	1.49	0.92
1:A:133:LEU:HD12	1:A:137:LYS:HA	1.52	0.92
1:A:131:LYS:HG2	6:A:2018:HOH:O	1.68	0.91
1:A:115:VAL:HG12	1:A:116:ARG:H	1.35	0.90
2:P:5:DG:H2''	2:P:6:DA:C8	2.11	0.86
1:A:277:ASP:CG	1:A:278:LYS:H	1.81	0.86
1:A:4:LEU:HA	1:A:144:ILE:HG12	1.58	0.84
1:A:122:TYR:HE2	1:A:126:LEU:HD11	1.43	0.84
4:A:1001:DTP:O1G	4:A:1001:DTP:C5'	2.25	0.83
1:A:189:ILE:HG21	2:P:11:DT:H3'	1.60	0.83
1:A:116:ARG:CG	1:A:117:ASP:H	1.90	0.83
2:P:4:DG:H2''	2:P:5:DG:H5''	1.60	0.81
1:A:241:VAL:HG23	6:A:2042:HOH:O	1.80	0.81
1:A:115:VAL:HG12	1:A:116:ARG:N	1.93	0.80
1:A:126:LEU:HD12	6:A:2025:HOH:O	1.82	0.79
1:A:323:LEU:HB2	6:A:2053:HOH:O	1.83	0.78
1:A:300:ARG:HH11	1:A:300:ARG:HG2	1.49	0.78
4:A:1001:DTP:HN62	3:T:5:8OG:H7	1.32	0.76
1:A:199:ILE:HD11	1:A:208:ILE:HG13	1.67	0.75
1:A:116:ARG:O	1:A:117:ASP:O	2.04	0.75
1:A:23:LEU:HA	1:A:26:LYS:HE3	1.69	0.74
4:A:1001:DTP:O2A	4:A:1002:DTP:O2G	2.04	0.74
1:A:95:TYR:HD2	1:A:124:LEU:HD11	1.53	0.74
1:A:31:CYS:HB2	1:A:61:ILE:HD11	1.71	0.73
1:A:239:THR:HG22	1:A:240:ARG:N	2.03	0.72
1:A:115:VAL:HG12	1:A:116:ARG:O	1.90	0.72
1:A:247:ARG:HG3	1:A:247:ARG:HH11	1.55	0.72
1:A:91:LEU:O	1:A:94:GLU:HG2	1.90	0.72
1:A:277:ASP:CG	1:A:278:LYS:N	2.47	0.71
1:A:103:SER:HB3	4:A:1002:DTP:O3'	1.88	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:VAL:CG1	1:A:116:ARG:H	2.03	0.70
1:A:99:ILE:HG13	1:A:109:LEU:HD23	1.72	0.70
2:P:5:DG:H2'	2:P:6:DA:H8	1.56	0.70
3:T:11:DC:H5'	6:T:2013:HOH:O	1.92	0.68
2:P:4:DG:C2'	2:P:5:DG:H5'	2.23	0.68
1:A:180:ILE:HD13	1:A:194:LEU:HD13	1.74	0.68
1:A:300:ARG:HG2	1:A:300:ARG:NH1	2.08	0.68
1:A:23:LEU:HA	1:A:26:LYS:CE	2.23	0.68
1:A:91:LEU:HD11	1:A:135:LYS:HD2	1.76	0.67
1:A:240:ARG:NH1	6:T:2012:HOH:O	2.27	0.67
4:A:1002:DTP:PA	2:P:13:DC:O3'	2.51	0.67
1:A:188:ASN:O	1:A:192:GLU:HG2	1.96	0.66
4:A:1002:DTP:PB	2:P:13:DC:H3'	2.35	0.66
1:A:154:ALA:HA	1:A:157:MET:HE2	1.76	0.66
1:A:189:ILE:CG2	2:P:11:DT:H3'	2.25	0.65
1:A:256:ARG:HH21	1:A:327:GLU:C	2.03	0.65
1:A:122:TYR:CE2	1:A:126:LEU:HD11	2.29	0.65
1:A:273:TYR:HE1	6:A:2051:HOH:O	1.78	0.65
1:A:328:ARG:H	1:A:328:ARG:HD3	1.61	0.65
1:A:111:ILE:O	1:A:111:ILE:HG13	1.97	0.65
1:A:189:ILE:HG22	2:P:12:DT:OP2	1.97	0.64
1:A:76:MET:HG3	1:A:81:TYR:HE2	1.61	0.64
3:T:10:DC:H6	6:T:2011:HOH:O	1.81	0.63
1:A:189:ILE:CD1	1:A:193:LYS:HE3	2.26	0.63
1:A:319:LEU:HD12	1:A:319:LEU:O	1.99	0.63
1:A:186:ILE:C	6:P:2017:HOH:O	2.41	0.62
1:A:52:LYS:NZ	6:A:2012:HOH:O	2.31	0.62
1:A:4:LEU:HG	1:A:144:ILE:CD1	2.25	0.62
1:A:60:PRO:HG3	3:T:4:DC:O2	2.00	0.61
1:A:267:ARG:NE	6:A:2046:HOH:O	2.34	0.61
6:A:2034:HOH:O	3:T:11:DC:H5'	2.01	0.61
1:A:173:ARG:NE	1:A:177:GLU:HG3	2.16	0.61
1:A:270:GLU:HG2	1:A:312:TYR:OH	2.01	0.60
1:A:287:VAL:HA	1:A:297:SER:HB3	1.83	0.60
1:A:95:TYR:CD2	1:A:124:LEU:HD11	2.36	0.60
1:A:45:THR:HG22	1:A:46:ALA:N	2.17	0.60
1:A:152:LYS:NZ	4:A:1002:DTP:O2B	2.34	0.60
1:A:300:ARG:HD3	6:A:2054:HOH:O	2.02	0.60
1:A:129:LYS:NZ	1:A:161:ASN:OD1	2.27	0.59
3:T:10:DC:H2'	6:T:2011:HOH:O	2.01	0.59
1:A:189:ILE:O	1:A:193:LYS:HG3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:ARG:HD2	1:A:260:GLU:OE2	2.03	0.59
4:A:1001:DTP:O1G	4:A:1001:DTP:O5'	2.21	0.59
4:A:1002:DTP:O1B	2:P:13:DC:C3'	2.36	0.58
1:A:174:LEU:C	1:A:176:ARG:H	2.11	0.58
1:A:205:THR:HG22	1:A:226:ILE:HG12	1.84	0.58
1:A:265:LEU:HD12	1:A:319:LEU:HD22	1.84	0.58
3:T:12:DT:H2''	3:T:13:DT:H71	1.86	0.58
1:A:174:LEU:C	1:A:176:ARG:N	2.60	0.58
1:A:126:LEU:CG	6:A:2025:HOH:O	2.52	0.57
1:A:174:LEU:O	1:A:176:ARG:N	2.36	0.57
1:A:332:ARG:HH12	3:T:5:8OG:H2''	1.70	0.57
4:A:1002:DTP:PA	2:P:13:DC:HO3'	2.27	0.57
1:A:60:PRO:HG3	3:T:4:DC:H1'	1.86	0.57
1:A:254:ASN:HA	1:A:330:ILE:O	2.05	0.57
1:A:193:LYS:HG2	1:A:216:MET:HE1	1.86	0.57
1:A:37:PHE:CD1	1:A:40:SER:HB3	2.40	0.56
1:A:239:THR:HA	6:A:2040:HOH:O	2.05	0.56
3:T:12:DT:C2'	3:T:13:DT:H71	2.35	0.56
1:A:244:SER:HG	1:A:336:ARG:HH11	1.54	0.56
2:P:9:DG:C5'	6:P:2011:HOH:O	2.53	0.56
1:A:4:LEU:HD12	1:A:111:ILE:HD13	1.88	0.55
1:A:195:LYS:C	1:A:197:LEU:H	2.15	0.55
4:A:1001:DTP:PA	4:A:1001:DTP:PG	3.04	0.55
3:T:17:DC:H1'	6:T:2018:HOH:O	2.07	0.55
1:A:115:VAL:HG13	1:A:120:GLU:HB3	1.90	0.54
1:A:296:VAL:HG12	6:A:2048:HOH:O	2.07	0.54
1:A:241:VAL:O	1:A:242:ARG:C	2.50	0.54
1:A:20:ASN:C	1:A:20:ASN:HD22	2.16	0.54
1:A:37:PHE:CE1	1:A:40:SER:HB3	2.42	0.54
1:A:123:ASN:CA	6:A:2025:HOH:O	2.25	0.54
1:A:127:GLU:CD	1:A:127:GLU:C	2.76	0.54
1:A:265:LEU:CD1	1:A:319:LEU:HD22	2.37	0.54
1:A:293:LEU:N	1:A:293:LEU:HD22	2.23	0.54
1:A:270:GLU:OE2	1:A:308:LYS:HD3	2.09	0.53
1:A:298:ARG:CZ	2:P:8:DG:H3'	2.38	0.53
2:P:9:DG:H5''	6:P:2011:HOH:O	2.07	0.53
1:A:295:ILE:HG23	1:A:295:ILE:O	2.08	0.53
1:A:118:TYR:CE2	1:A:167:ASP:HA	2.44	0.53
1:A:247:ARG:HH12	1:A:249:VAL:HG12	1.73	0.53
2:P:3:DG:H2''	2:P:4:DG:H5'	1.91	0.53
1:A:95:TYR:OH	1:A:127:GLU:OE2	2.18	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:GLU:C	1:A:127:GLU:OE2	2.52	0.52
1:A:289:VAL:HA	1:A:294:ASP:O	2.10	0.52
1:A:49:GLU:H	1:A:49:GLU:CD	2.18	0.52
1:A:32:VAL:O	1:A:32:VAL:HG23	2.10	0.52
1:A:302:PHE:HZ	1:A:314:GLU:OE1	1.93	0.51
1:A:262:LYS:N	1:A:263:PRO:HD2	2.26	0.51
1:A:39:ASP:OD2	1:A:65:LYS:CE	2.58	0.51
1:A:173:ARG:CZ	1:A:177:GLU:HG3	2.39	0.51
1:A:36:ARG:NH1	1:A:251:MET:O	2.43	0.51
1:A:256:ARG:O	1:A:256:ARG:HG2	2.11	0.51
1:A:265:LEU:O	1:A:269:ILE:HG13	2.10	0.51
1:A:191:ALA:C	1:A:193:LYS:H	2.18	0.51
3:T:9:DT:H2''	6:T:2011:HOH:O	2.11	0.51
1:A:251:MET:HG2	1:A:264:TYR:CD2	2.46	0.50
3:T:6:DG:N7	6:T:2003:HOH:O	2.34	0.50
1:A:252:LYS:HE3	1:A:252:LYS:HA	1.94	0.50
1:A:67:ILE:O	1:A:68:LEU:HD23	2.11	0.50
1:A:46:ALA:HB1	1:A:50:ALA:HB3	1.93	0.50
1:A:324:GLU:HG3	6:A:2053:HOH:O	2.12	0.49
1:A:261:ILE:C	1:A:263:PRO:HD2	2.38	0.49
1:A:4:LEU:HD23	1:A:5:PHE:N	2.28	0.49
1:A:136:GLU:O	1:A:137:LYS:HB2	2.13	0.49
1:A:154:ALA:HA	1:A:157:MET:CE	2.40	0.49
1:A:126:LEU:CD1	6:A:2025:HOH:O	2.48	0.49
1:A:291:GLU:OE2	1:A:331:ARG:NH1	2.45	0.49
1:A:320:GLN:O	1:A:321:LYS:C	2.56	0.48
1:A:189:ILE:CG2	2:P:12:DT:OP2	2.60	0.48
1:A:121:ALA:O	1:A:124:LEU:HB3	2.14	0.48
1:A:241:VAL:O	1:A:243:LYS:HG3	2.13	0.48
1:A:10:TYR:CZ	1:A:14:GLN:NE2	2.82	0.48
1:A:237:ILE:O	1:A:238:ARG:HB3	2.15	0.47
1:A:121:ALA:O	1:A:122:TYR:C	2.57	0.47
1:A:296:VAL:N	6:A:2048:HOH:O	2.47	0.47
1:A:304:HIS:NE2	6:A:2050:HOH:O	2.36	0.47
4:A:1001:DTP:C6	3:T:5:8OG:H7	2.28	0.47
1:A:49:GLU:CD	1:A:49:GLU:N	2.73	0.47
3:T:11:DC:H2'	3:T:12:DT:H72	1.97	0.47
1:A:133:LEU:CD1	1:A:137:LYS:HA	2.34	0.47
1:A:320:GLN:O	1:A:324:GLU:HG3	2.15	0.47
3:T:11:DC:H2''	3:T:12:DT:C6	2.50	0.47
1:A:32:VAL:O	1:A:41:GLY:HA3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:VAL:CG2	6:A:2029:HOH:O	2.42	0.46
1:A:247:ARG:HG3	1:A:247:ARG:NH1	2.24	0.46
1:A:303:PRO:CD	6:A:2049:HOH:O	2.38	0.46
1:A:119:ARG:N	6:A:2024:HOH:O	2.48	0.46
1:A:195:LYS:C	1:A:197:LEU:N	2.74	0.46
1:A:332:ARG:NH1	3:T:5:8OG:H2''	2.30	0.46
1:A:14:GLN:HG2	1:A:138:ILE:HD12	1.97	0.46
1:A:20:ASN:C	1:A:20:ASN:ND2	2.73	0.46
1:A:127:GLU:OE2	1:A:128:ILE:N	2.48	0.46
1:A:129:LYS:HZ3	1:A:162:GLY:N	2.14	0.46
1:A:51:ARG:C	1:A:53:PHE:H	2.24	0.46
1:A:146:LYS:NZ	1:A:231:ASP:OD2	2.49	0.45
1:A:115:VAL:CG1	1:A:120:GLU:HB3	2.45	0.45
1:A:156:ASP:O	1:A:159:LYS:HG2	2.15	0.45
1:A:233:TYR:CZ	1:A:235:GLU:HG2	2.51	0.45
1:A:65:LYS:HG2	1:A:73:TYR:CZ	2.51	0.45
1:A:9:ASP:O	1:A:10:TYR:C	2.60	0.45
1:A:128:ILE:C	1:A:130:ASN:H	2.25	0.45
1:A:133:LEU:HD12	1:A:133:LEU:O	2.17	0.45
1:A:32:VAL:O	1:A:32:VAL:CG2	2.65	0.45
1:A:160:PRO:O	1:A:161:ASN:C	2.59	0.44
1:A:190:THR:HG23	1:A:217:ILE:HG22	1.98	0.44
1:A:68:LEU:C	6:A:2014:HOH:O	2.60	0.44
1:A:190:THR:HA	1:A:193:LYS:HD2	1.99	0.44
1:A:250:THR:OG1	1:A:332:ARG:HD3	2.18	0.44
1:A:276:LEU:O	1:A:277:ASP:HB3	2.17	0.44
1:A:242:ARG:NE	3:T:8:DA:H5''	2.33	0.44
1:A:245:ILE:HG13	1:A:279:ARG:HH21	1.83	0.44
2:P:11:DT:C6	2:P:12:DT:H72	2.53	0.44
1:A:129:LYS:HZ3	1:A:161:ASN:C	2.25	0.44
1:A:39:ASP:OD2	1:A:65:LYS:HE3	2.19	0.43
1:A:242:ARG:CZ	3:T:8:DA:H5''	2.48	0.43
1:A:238:ARG:O	1:A:238:ARG:HG3	2.18	0.43
1:A:247:ARG:HD2	3:T:7:DA:OP1	2.17	0.43
1:A:8:PHE:HA	1:A:140:VAL:HG12	2.00	0.43
1:A:157:MET:CE	1:A:164:LYS:HE3	2.48	0.43
1:A:168:ASP:O	1:A:172:LYS:HG2	2.17	0.43
1:A:219:GLU:HG2	1:A:223:LYS:HZ2	1.84	0.43
1:A:275:LYS:NZ	6:A:2047:HOH:O	2.51	0.43
1:A:195:LYS:O	1:A:198:GLY:N	2.51	0.43
1:A:237:ILE:N	1:A:237:ILE:HD12	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:GLU:HG3	1:A:95:TYR:CE1	2.54	0.43
1:A:193:LYS:HG2	1:A:216:MET:CE	2.48	0.42
1:A:258:LEU:HD12	1:A:258:LEU:O	2.19	0.42
1:A:169:GLU:CD	1:A:169:GLU:C	2.86	0.42
1:A:146:LYS:HD3	1:A:171:VAL:HG21	2.00	0.42
1:A:175:ILE:O	1:A:175:ILE:HG22	2.20	0.42
1:A:242:ARG:NH2	3:T:8:DA:H5''	2.35	0.42
1:A:247:ARG:NH1	1:A:247:ARG:CG	2.80	0.42
1:A:307:SER:O	1:A:308:LYS:C	2.61	0.42
1:A:293:LEU:N	1:A:293:LEU:CD2	2.82	0.42
2:P:10:DA:H1'	2:P:11:DT:H5''	2.02	0.42
1:A:208:ILE:HG22	1:A:209:GLU:N	2.34	0.42
2:P:11:DT:OP2	6:P:2014:HOH:O	2.21	0.42
1:A:194:LEU:HB3	1:A:199:ILE:HB	2.01	0.42
1:A:284:ILE:HD12	1:A:337:PHE:HE1	1.83	0.42
1:A:300:ARG:HH11	1:A:300:ARG:CG	2.24	0.42
1:A:142:VAL:HB	1:A:163:ILE:HG13	2.02	0.42
1:A:180:ILE:CG2	1:A:181:ALA:N	2.83	0.42
1:A:297:SER:N	6:P:2012:HOH:O	2.52	0.42
1:A:98:LYS:NZ	6:A:2022:HOH:O	2.52	0.41
2:P:4:DG:C6	2:P:5:DG:C6	3.08	0.41
1:A:23:LEU:HD22	1:A:72:VAL:HG21	2.02	0.41
1:A:147:ASN:ND2	1:A:233:TYR:HD2	2.19	0.41
1:A:128:ILE:C	1:A:130:ASN:N	2.79	0.41
1:A:21:PRO:O	1:A:22:SER:C	2.61	0.41
2:P:10:DA:H2''	2:P:11:DT:C5'	2.51	0.41
1:A:260:GLU:O	1:A:263:PRO:HD2	2.20	0.41
1:A:283:ALA:HB2	1:A:339:LYS:HD2	2.03	0.41
1:A:45:THR:CG2	1:A:46:ALA:N	2.82	0.41
1:A:195:LYS:O	1:A:197:LEU:N	2.53	0.41
1:A:147:ASN:HD22	1:A:233:TYR:HD2	1.68	0.41
1:A:265:LEU:O	1:A:265:LEU:HD23	2.21	0.41
1:A:8:PHE:CD1	1:A:8:PHE:N	2.86	0.40
1:A:187:GLY:N	6:P:2017:HOH:O	2.54	0.40
1:A:190:THR:O	1:A:193:LYS:HB2	2.21	0.40
1:A:125:GLY:C	1:A:127:GLU:N	2.79	0.40
1:A:152:LYS:O	1:A:153:ILE:C	2.63	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:ASN:OD1	1:A:324:GLU:OE2[4_446]	2.11	0.09

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	340/358 (95%)	294 (86%)	38 (11%)	8 (2%)	4 8

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	117	ASP
1	A	239	THR
1	A	175	ILE
1	A	10	TYR
1	A	196	LYS
1	A	240	ARG
1	A	52	LYS
1	A	325	GLU

5.3.2 Protein sidechains [i](#)

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	300/315 (95%)	279 (93%)	21 (7%)	14 29

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	19	LEU
1	A	31	CYS
1	A	32	VAL
1	A	97	GLU
1	A	98	LYS
1	A	130	ASN
1	A	145	SER
1	A	148	LYS
1	A	168	ASP
1	A	173	ARG
1	A	197	LEU
1	A	203	VAL
1	A	207	SER
1	A	213	LEU
1	A	216	MET
1	A	238	ARG
1	A	241	VAL
1	A	252	LYS
1	A	281	PRO
1	A	284	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	234	ASN
1	A	285	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

1 non-standard protein/DNA/RNA residue is 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	8OG	T	5	3	22,25,26	1.44	5 (22%)	26,37,40	2.09	6 (23%)

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	8OG	T	5	3	-	1/7/21/22	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	T	5	8OG	C4-N9	-3.33	1.33	1.39
3	T	5	8OG	C8-N9	-3.27	1.35	1.40
3	T	5	8OG	C5-N7	-2.36	1.33	1.37
3	T	5	8OG	C5-C4	2.23	1.40	1.37
3	T	5	8OG	C8-N7	-2.01	1.34	1.38

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	5	8OG	C2-N3-C4	5.69	122.10	112.30
3	T	5	8OG	N9-C4-N3	5.11	132.51	126.13
3	T	5	8OG	C2-N1-C6	-3.45	118.86	125.11
3	T	5	8OG	N7-C8-N9	3.01	109.97	106.61
3	T	5	8OG	O6-C6-C5	-2.82	120.47	127.26
3	T	5	8OG	C5-C6-N1	2.70	119.55	112.13

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	T	5	8OG	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	T	5	8OG	4	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 5 are monoatomic - leaving 2 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	DTP	A	1002	5	31,32,32	2.84	5 (16%)	46,50,50	2.80	10 (21%)
4	DTP	A	1001	5	31,32,32	3.62	7 (22%)	46,50,50	1.34	6 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	DTP	A	1002	5	-	10/22/34/34	0/3/3/3
4	DTP	A	1001	5	-	6/22/34/34	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1001	DTP	PA-O3A	15.25	1.76	1.59
4	A	1001	DTP	PB-O3A	11.07	1.71	1.59
4	A	1002	DTP	PB-O3B	10.23	1.70	1.59
4	A	1002	DTP	PB-O3A	-8.66	1.50	1.59
4	A	1002	DTP	PA-O1A	-6.68	1.27	1.50
4	A	1001	DTP	PB-O3B	3.52	1.63	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1001	DTP	O5'-C5'	2.44	1.53	1.44
4	A	1001	DTP	C4-N3	2.41	1.38	1.34
4	A	1002	DTP	PB-O2B	-2.27	1.44	1.55
4	A	1002	DTP	PG-O3G	-2.24	1.46	1.54
4	A	1001	DTP	C2-N1	2.08	1.37	1.33
4	A	1001	DTP	PG-O2G	-2.03	1.47	1.54

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1002	DTP	O3A-PA-O1A	-9.82	81.16	110.70
4	A	1002	DTP	O2A-PA-O3A	8.99	131.58	107.27
4	A	1002	DTP	O2B-PB-O3A	-8.40	84.57	107.27
4	A	1002	DTP	O2B-PB-O3B	5.62	122.46	107.27
4	A	1002	DTP	O5'-C5'-C4'	4.55	124.50	108.99
4	A	1001	DTP	O5'-PA-O1A	-4.18	92.38	108.94
4	A	1001	DTP	O3A-PA-O1A	-4.11	98.35	110.70
4	A	1002	DTP	O3B-PB-O1B	-3.97	98.76	110.70
4	A	1001	DTP	O3G-PG-O3B	3.10	115.04	104.64
4	A	1002	DTP	O5'-PA-O1A	-2.85	97.64	108.94
4	A	1001	DTP	O3A-PB-O1B	2.52	118.28	110.70
4	A	1002	DTP	O2G-PG-O3B	2.41	112.71	104.64
4	A	1001	DTP	O4'-C4'-C5'	2.40	117.02	109.33
4	A	1002	DTP	O4'-C1'-N9	2.18	111.87	107.96
4	A	1002	DTP	O2G-PG-O1G	-2.01	102.99	110.83
4	A	1001	DTP	PA-O5'-C5'	2.00	132.83	121.35

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1001	DTP	O4'-C4'-C5'-O5'
4	A	1002	DTP	PB-O3B-PG-O2G
4	A	1001	DTP	C3'-C4'-C5'-O5'
4	A	1002	DTP	O4'-C4'-C5'-O5'
4	A	1002	DTP	C3'-C4'-C5'-O5'
4	A	1001	DTP	PG-O3B-PB-O3A
4	A	1002	DTP	PB-O3A-PA-O5'
4	A	1002	DTP	C5'-O5'-PA-O1A
4	A	1002	DTP	C5'-O5'-PA-O3A
4	A	1001	DTP	O4'-C1'-N9-C4
4	A	1001	DTP	O4'-C1'-N9-C8

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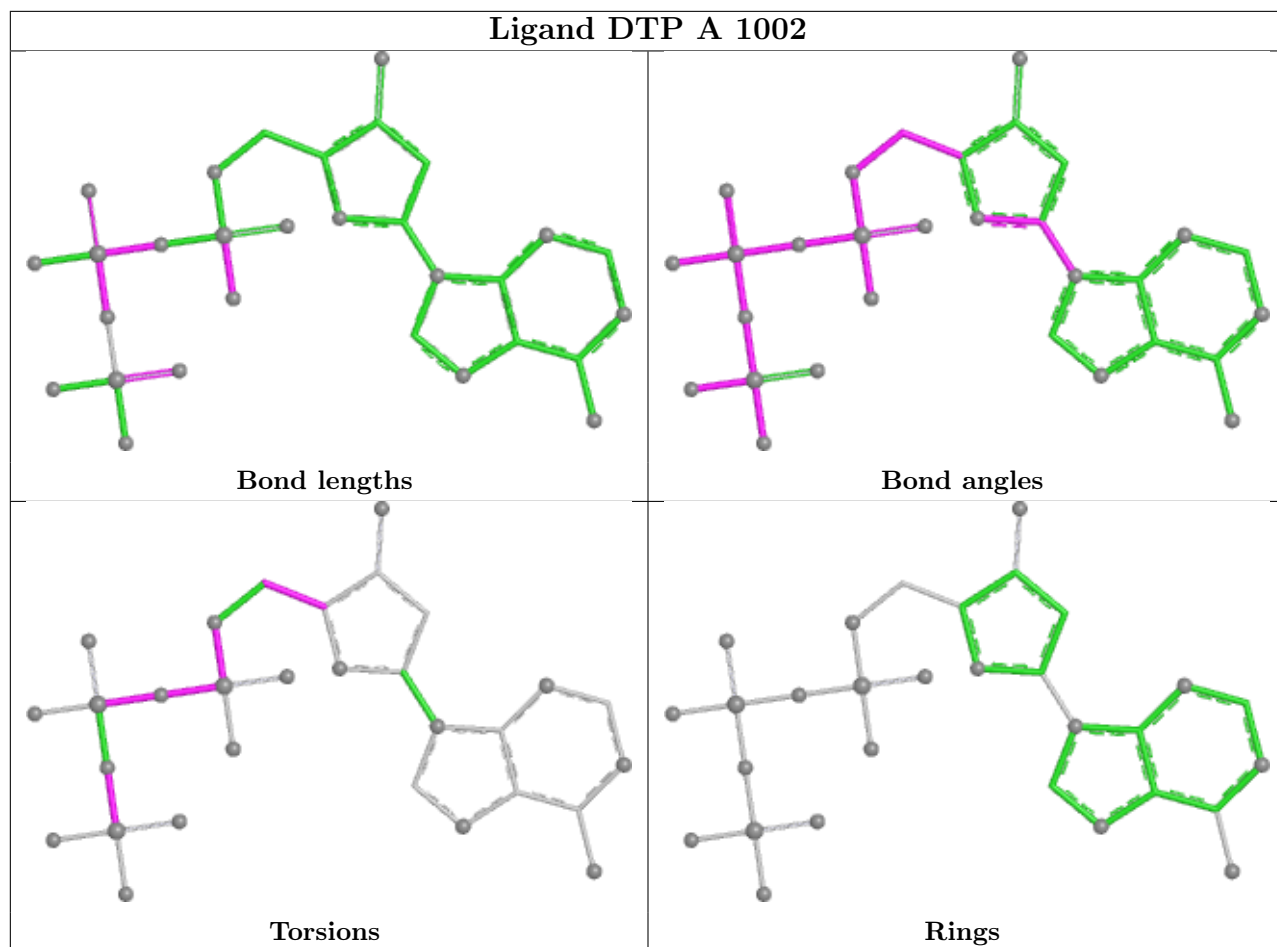
Mol	Chain	Res	Type	Atoms
4	A	1002	DTP	PB-O3A-PA-O1A
4	A	1002	DTP	PB-O3B-PG-O1G
4	A	1001	DTP	PG-O3B-PB-O1B
4	A	1002	DTP	PA-O3A-PB-O1B
4	A	1002	DTP	PA-O3A-PB-O2B

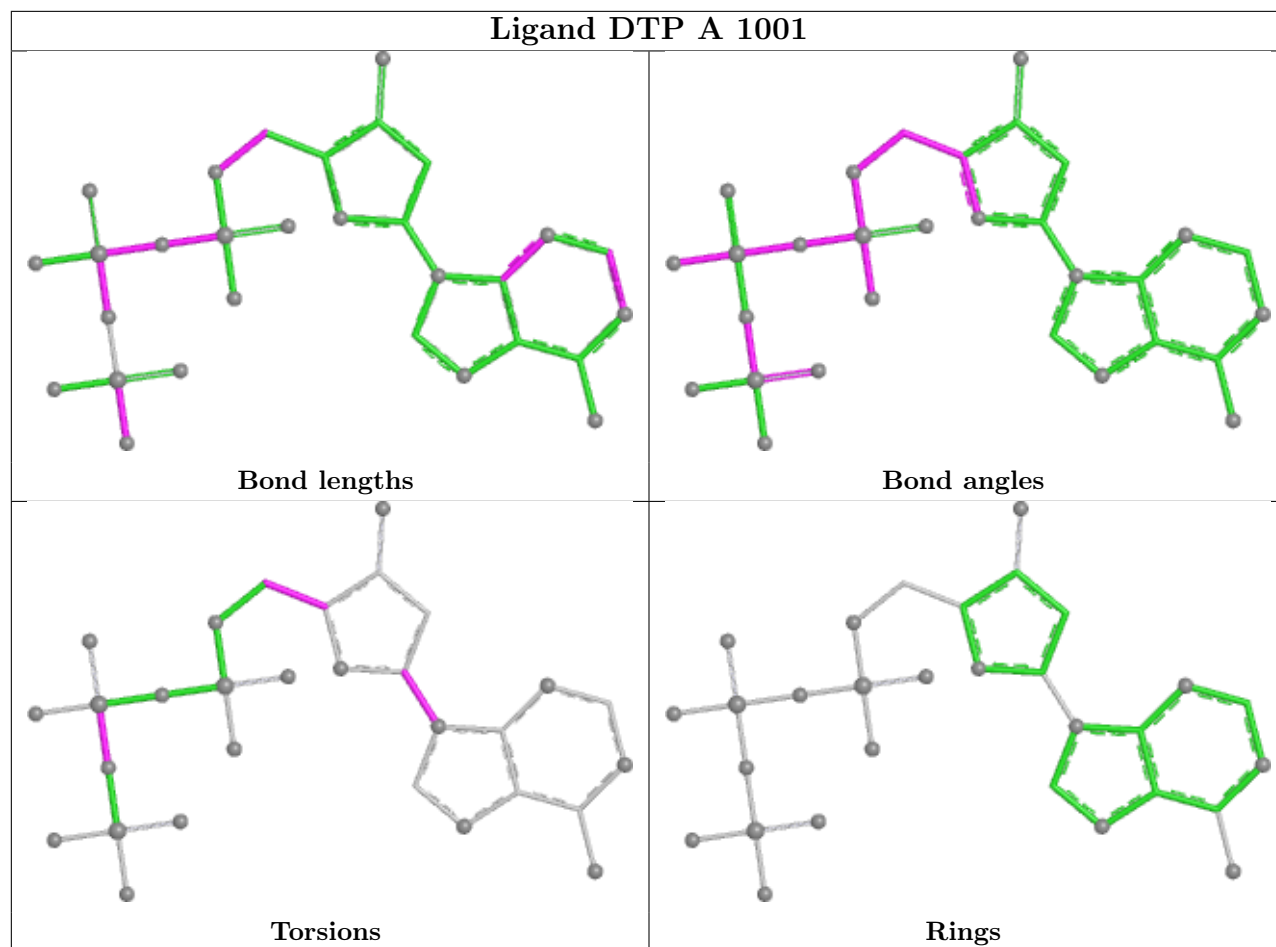
There are no ring outliers.

2 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1002	DTP	8	0
4	A	1001	DTP	8	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	342/358 (95%)	0.46	17 (4%) 34 29	36, 72, 99, 114	50 (14%)
2	P	13/13 (100%)	0.28	0 100 100	65, 89, 104, 109	0
3	T	14/18 (77%)	0.34	1 (7%) 22 18	54, 87, 117, 122	1 (7%)
All	All	369/389 (94%)	0.45	18 (4%) 35 30	36, 72, 102, 122	51 (13%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	198	GLY	5.7
1	A	329	LYS	4.2
1	A	117	ASP	3.2
1	A	37	PHE	3.0
1	A	252	LYS	2.9
1	A	259	GLU	2.9
1	A	278	LYS	2.8
1	A	127	GLU	2.8
1	A	258	LEU	2.5
1	A	120	GLU	2.4
1	A	199	ILE	2.2
1	A	42	ALA	2.2
3	T	4	DC	2.2
1	A	121	ALA	2.1
1	A	196	LYS	2.0
1	A	180	ILE	2.0
1	A	110	ASP	2.0
1	A	86	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	8OG	T	5	23/24	0.91	0.14	71,79,91,95	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

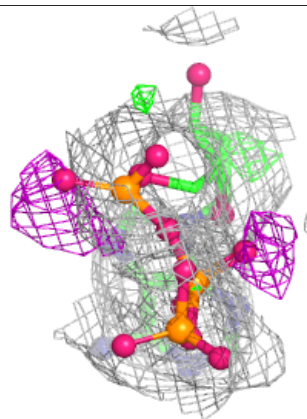
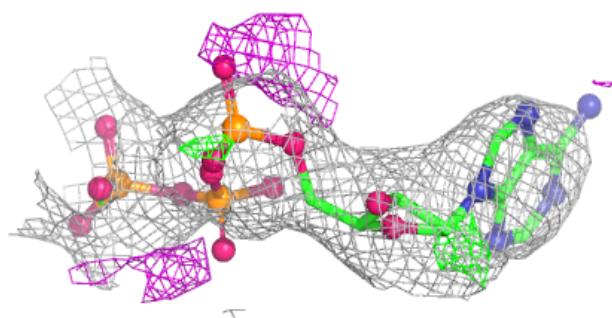
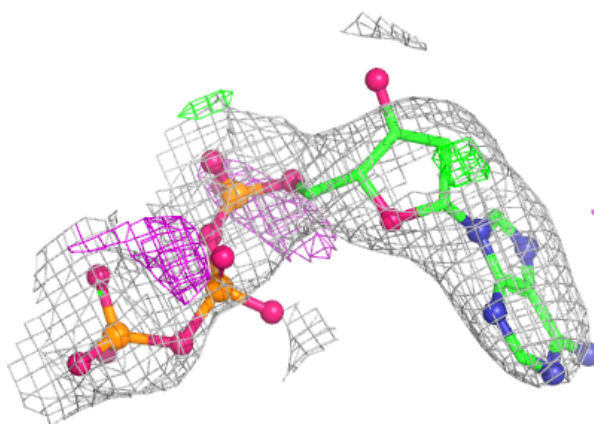
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	CA	A	2003	1/1	0.86	0.09	88,88,88,88	1
5	CA	A	2005	1/1	0.88	0.11	110,110,110,110	1
4	DTP	A	1002	30/30	0.90	0.16	103,105,112,113	8
5	CA	A	2004	1/1	0.91	0.06	114,114,114,114	1
4	DTP	A	1001	30/30	0.91	0.15	82,90,92,94	0
5	CA	A	2001	1/1	0.98	0.07	60,60,60,60	0
5	CA	A	2002	1/1	0.99	0.06	53,53,53,53	0

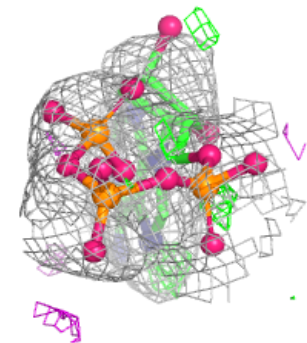
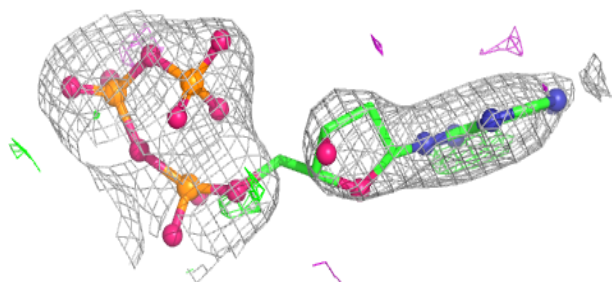
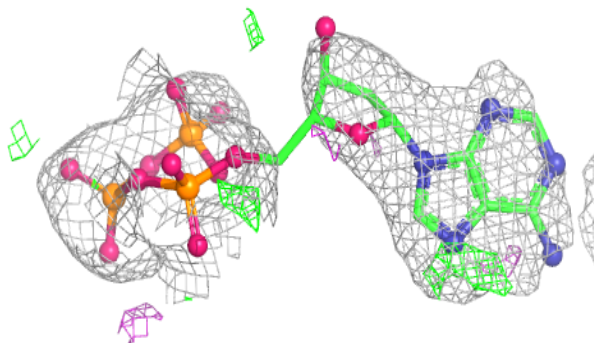
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around DTP A 1002:

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

**Electron density around DTP A 1001:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.