



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 08:52 am BST

PDB ID : 2R8K
Title : Structure of the Eukaryotic DNA Polymerase ϵ in complex with 1,2-d(GpG)-cisplatin containing DNA
Authors : Carell, T.; Alt, A.; Lammens, K.
Deposited on : 2007-09-11
Resolution : 3.30 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

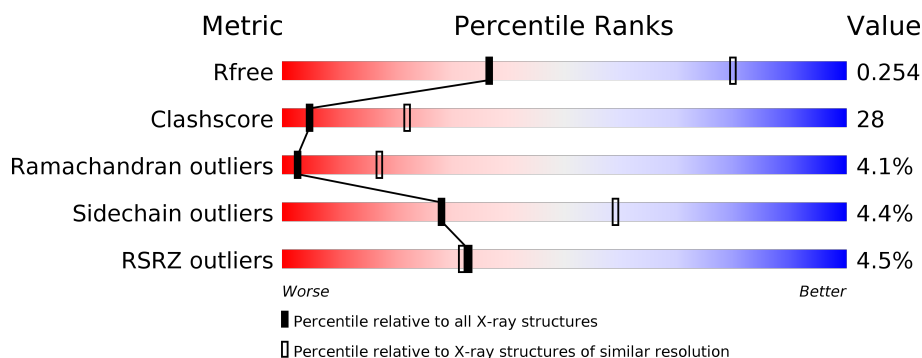
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	P	9	<div> <div>11%</div> <div> <div>33%</div> <div>67%</div> </div> </div>
1	Q	9	<div> <div>44%</div> <div> <div>22%</div> <div>67%</div> <div>11%</div> </div> </div>
2	T	10	<div> <div>30%</div> <div> <div>20%</div> <div>60%</div> <div>20%</div> </div> </div>
2	U	10	<div> <div>30%</div> <div>100%</div> </div>
3	A	554	<div> <div>5%</div> <div> <div>51%</div> <div>38%</div> <div>8%</div> </div> </div>
3	B	554	<div> <div>2%</div> <div> <div>48%</div> <div>38%</div> <div>5%</div> <div>8%</div> </div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8962 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(*DGP*DTP*DGP*DGP*DTP*DGP*DAP*DGP*D C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	9	Total	C	N	O	P	0	0	0
			186	89	37	52	8			
1	P	9	Total	C	N	O	P	0	0	0
			186	89	37	52	8			

- Molecule 2 is a DNA chain called 5'-D(P*DGP*DGP*DCP*DTP*DCP*DAP*DCP*DCP*DAP*DC)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	U	10	Total	C	N	O	P	0	0	0
			201	95	37	59	10			
2	T	10	Total	C	N	O	P	0	0	0
			201	95	37	59	10			

- Molecule 3 is a protein called DNA polymerase eta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	511	Total	C	N	O	S	72	0	0
			4059	2585	684	766	24			
3	B	511	Total	C	N	O	S	79	0	0
			4059	2585	684	766	24			

There are 46 discrepancies between the modelled and reference sequences:

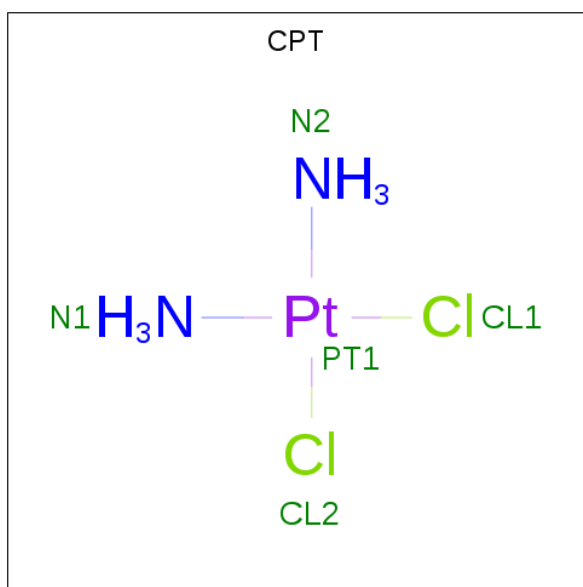
Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	EXPRESSION TAG	UNP Q04049
A	-21	ALA	-	EXPRESSION TAG	UNP Q04049
A	-20	SER	-	EXPRESSION TAG	UNP Q04049
A	-19	TRP	-	EXPRESSION TAG	UNP Q04049
A	-18	SER	-	EXPRESSION TAG	UNP Q04049
A	-17	HIS	-	EXPRESSION TAG	UNP Q04049

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	PRO	-	EXPRESSION TAG	UNP Q04049
A	-15	GLN	-	EXPRESSION TAG	UNP Q04049
A	-14	PHE	-	EXPRESSION TAG	UNP Q04049
A	-13	GLU	-	EXPRESSION TAG	UNP Q04049
A	-12	LYS	-	EXPRESSION TAG	UNP Q04049
A	-11	GLY	-	EXPRESSION TAG	UNP Q04049
A	-10	ALA	-	EXPRESSION TAG	UNP Q04049
A	-9	SER	-	EXPRESSION TAG	UNP Q04049
A	-8	THR	-	EXPRESSION TAG	UNP Q04049
A	-7	SER	-	EXPRESSION TAG	UNP Q04049
A	-6	LEU	-	EXPRESSION TAG	UNP Q04049
A	-5	TYR	-	EXPRESSION TAG	UNP Q04049
A	-4	LYS	-	EXPRESSION TAG	UNP Q04049
A	-3	LYS	-	EXPRESSION TAG	UNP Q04049
A	-2	ALA	-	EXPRESSION TAG	UNP Q04049
A	-1	GLY	-	EXPRESSION TAG	UNP Q04049
A	0	ARG	-	EXPRESSION TAG	UNP Q04049
B	-22	MET	-	EXPRESSION TAG	UNP Q04049
B	-21	ALA	-	EXPRESSION TAG	UNP Q04049
B	-20	SER	-	EXPRESSION TAG	UNP Q04049
B	-19	TRP	-	EXPRESSION TAG	UNP Q04049
B	-18	SER	-	EXPRESSION TAG	UNP Q04049
B	-17	HIS	-	EXPRESSION TAG	UNP Q04049
B	-16	PRO	-	EXPRESSION TAG	UNP Q04049
B	-15	GLN	-	EXPRESSION TAG	UNP Q04049
B	-14	PHE	-	EXPRESSION TAG	UNP Q04049
B	-13	GLU	-	EXPRESSION TAG	UNP Q04049
B	-12	LYS	-	EXPRESSION TAG	UNP Q04049
B	-11	GLY	-	EXPRESSION TAG	UNP Q04049
B	-10	ALA	-	EXPRESSION TAG	UNP Q04049
B	-9	SER	-	EXPRESSION TAG	UNP Q04049
B	-8	THR	-	EXPRESSION TAG	UNP Q04049
B	-7	SER	-	EXPRESSION TAG	UNP Q04049
B	-6	LEU	-	EXPRESSION TAG	UNP Q04049
B	-5	TYR	-	EXPRESSION TAG	UNP Q04049
B	-4	LYS	-	EXPRESSION TAG	UNP Q04049
B	-3	LYS	-	EXPRESSION TAG	UNP Q04049
B	-2	ALA	-	EXPRESSION TAG	UNP Q04049
B	-1	GLY	-	EXPRESSION TAG	UNP Q04049
B	0	ARG	-	EXPRESSION TAG	UNP Q04049

- Molecule 4 is Cisplatin (three-letter code: CPT) (formula: Cl₂H₆N₂Pt).

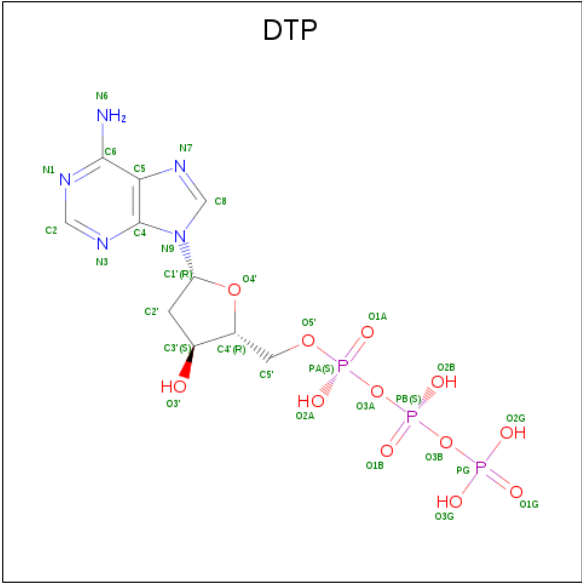


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	U	1	Total	N	Pt	0	0
			3	2	1		
4	T	1	Total	N	Pt	0	0
			3	2	1		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	Ca	0	0
			2	2		
5	A	2	Total	Ca	0	0
			2	2		

- Molecule 6 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (three-letter code: DTP) (formula: C₁₀H₁₆N₅O₁₂P₃).

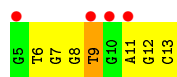


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
6	B	1	Total	C	N	O	P	0	0
			30	10	5	12	3		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

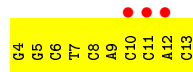
- Molecule 1: 5'-D(*DGP*DTP*DGP*DGP*DTP*DGP*DAP*DGP*DC)-3'



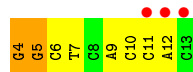
- Molecule 1: 5'-D(*DGP*DTP*DGP*DGP*DTP*DGP*DAP*DGP*DC)-3'



- Molecule 2: 5'-D(P*DGP*DGP*DCP*DTP*DCP*DAP*DCP*DCP*DAP*DC)-3'

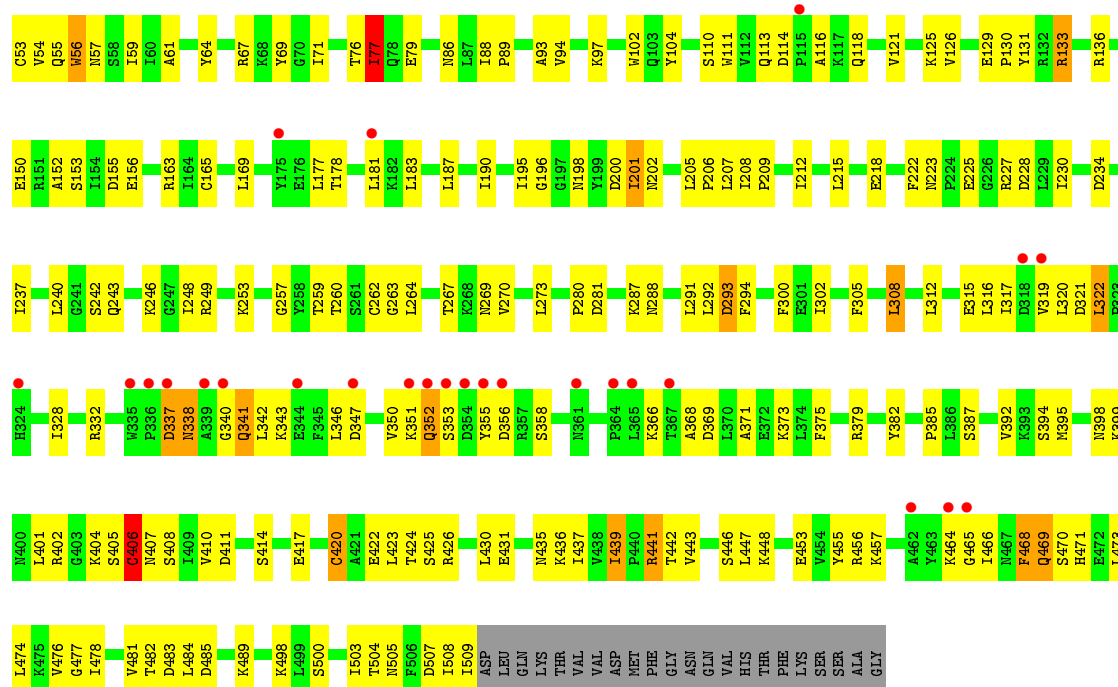


- Molecule 2: 5'-D(P*DGP*DGP*DCP*DTP*DCP*DAP*DCP*DCP*DAP*DC)-3'

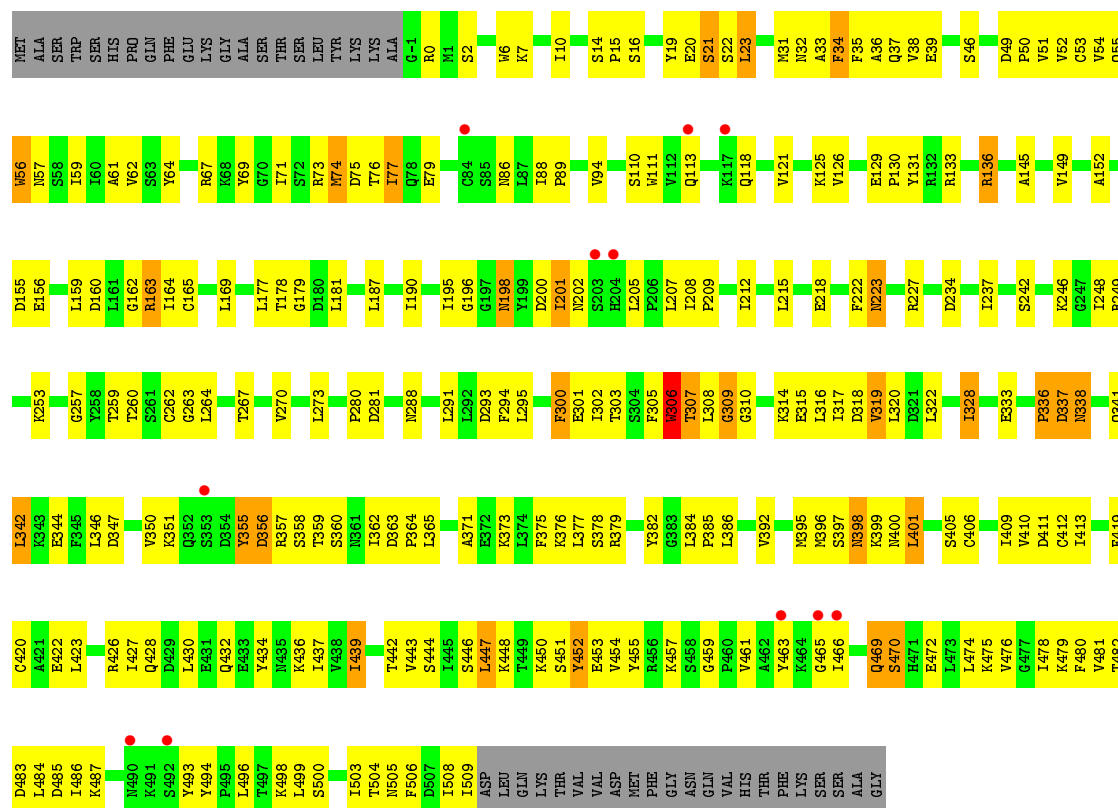


- Molecule 3: DNA polymerase eta





• Molecule 3: DNA polymerase eta



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	103.74Å 103.74Å 292.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 3.30 46.39 – 3.29	Depositor EDS
% Data completeness (in resolution range)	98.8 (25.00-3.30) 98.5 (46.39-3.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.51 (at 3.32Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.230 , 0.267 0.220 , 0.254	Depositor DCC
R_{free} test set	1945 reflections (7.84%)	wwPDB-VP
Wilson B-factor (Å ²)	60.4	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 60.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	8962	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.35% 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, DTP, CPT

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	P	0.48	0/209	0.94	0/322
1	Q	0.69	0/209	1.05	1/322 (0.3%)
2	T	1.46	3/224 (1.3%)	1.53	4/342 (1.2%)
2	U	1.74	6/224 (2.7%)	1.69	5/342 (1.5%)
3	A	0.29	0/4137	0.51	0/5578
3	B	0.29	0/4137	0.53	1/5578 (0.0%)
All	All	0.47	9/9140 (0.1%)	0.66	11/12484 (0.1%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	U	5	DG	C3'-O3'	11.23	1.58	1.44
2	T	4	DG	P-O5'	-7.95	1.51	1.59
2	U	5	DG	N3-C4	6.95	1.40	1.35
2	T	4	DG	C5'-C4'	6.88	1.58	1.51
2	U	4	DG	C8-N7	-6.67	1.26	1.30
2	U	5	DG	O3'-P	6.07	1.68	1.61
2	U	4	DG	N3-C4	6.01	1.39	1.35
2	U	5	DG	C2-N3	5.29	1.36	1.32
2	T	5	DG	C5-C6	5.26	1.47	1.42

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	U	4	DG	O4'-C1'-N9	11.34	115.94	108.00
2	U	5	DG	O4'-C1'-N9	7.98	113.59	108.00
1	Q	9	DT	N1-C1'-C2'	7.75	127.32	112.60
2	U	4	DG	C4'-C3'-C2'	-7.71	96.16	103.10
2	U	5	DG	N3-C2-N2	7.30	125.01	119.90
2	T	5	DG	C8-N9-C4	-5.67	104.13	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	4	DG	O4'-C1'-N9	5.48	111.84	108.00
2	T	4	DG	O4'-C4'-C3'	-5.27	102.39	104.50
2	U	5	DG	C4'-C3'-O3'	5.12	122.53	112.30
2	T	5	DG	N9-C4-C5	5.02	107.41	105.40
3	B	451	SER	N-CA-C	-5.01	97.47	111.00

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	P	186	0	101	7	0
1	Q	186	0	101	14	0
2	T	201	0	112	6	0
2	U	201	0	112	7	0
3	A	4059	0	4105	199	0
3	B	4059	0	4105	250	0
4	T	3	0	0	0	0
4	U	3	0	0	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	30	0	12	3	0
6	B	30	0	12	1	0
All	All	8962	0	8660	477	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 28.

All (477) 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:B:328:ILE:HD12	3:B:328:ILE:H	1.03	1.13
3:B:223:ASN:HD21	3:B:227:ARG:H	1.12	0.95
3:B:136:ARG:HB2	3:B:136:ARG:HH11	1.30	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:328:ILE:H	3:B:328:ILE:CD1	1.83	0.91
3:B:413:ILE:HG13	3:B:478:ILE:HD12	1.52	0.91
2:U:9:DA:H2''	2:U:10:DC:H5''	1.52	0.89
3:B:328:ILE:HD12	3:B:328:ILE:N	1.87	0.89
3:A:169:LEU:HD22	3:A:237:ILE:HD11	1.53	0.87
3:B:169:LEU:HD22	3:B:237:ILE:HD11	1.54	0.87
3:A:223:ASN:HD21	3:A:227:ARG:H	1.21	0.86
3:A:448:LYS:HD2	3:A:498:LYS:HE2	1.56	0.85
3:A:136:ARG:HB2	3:A:136:ARG:HH11	1.43	0.84
3:B:136:ARG:HB2	3:B:136:ARG:NH1	1.94	0.83
3:A:375:PHE:HE1	3:A:379:ARG:HH21	1.22	0.81
3:B:412:CYS:HB3	3:B:481:VAL:HG21	1.60	0.81
1:P:7:DG:H2''	1:P:8:DG:H5''	1.62	0.81
3:B:409:ILE:O	3:B:413:ILE:HD13	1.81	0.80
3:B:457:LYS:HB2	3:B:484:LEU:HD21	1.64	0.79
3:A:55:GLN:HE21	3:A:126:VAL:HG11	1.46	0.79
3:A:31:MET:HG2	3:A:260:THR:HG22	1.64	0.79
3:B:338:ASN:H	3:B:341:GLN:HE21	1.32	0.78
3:B:253:LYS:O	3:B:257:GLY:HA2	1.84	0.78
1:P:6:DT:H2''	1:P:7:DG:C8	2.19	0.77
3:B:169:LEU:HD12	3:B:187:LEU:HD13	1.66	0.77
3:B:338:ASN:ND2	3:B:341:GLN:HG3	2.00	0.77
3:B:337:ASP:HB2	3:B:341:GLN:NE2	2.00	0.76
3:B:362:ILE:HG22	3:B:363:ASP:H	1.51	0.76
1:Q:6:DT:H2''	1:Q:7:DG:N7	2.00	0.76
3:A:94:VAL:HG12	3:A:126:VAL:HA	1.68	0.75
3:B:447:LEU:HD11	3:B:455:TYR:HB2	1.69	0.75
3:B:94:VAL:HG12	3:B:126:VAL:HA	1.69	0.75
3:B:504:THR:HG22	3:B:505:ASN:H	1.51	0.75
3:A:136:ARG:NH1	3:A:136:ARG:HB2	2.02	0.75
3:A:133:ARG:NH2	3:A:133:ARG:HB3	2.01	0.74
1:Q:6:DT:H2''	1:Q:7:DG:C5	2.22	0.74
3:B:209:PRO:O	3:B:212:ILE:HG22	1.88	0.72
3:B:31:MET:HG2	3:B:260:THR:HG22	1.71	0.72
3:A:332:ARG:HG3	3:A:379:ARG:NH1	2.04	0.72
3:A:292:LEU:HD22	3:A:332:ARG:CZ	2.19	0.72
3:A:209:PRO:O	3:A:212:ILE:HG22	1.89	0.71
3:B:55:GLN:HE21	3:B:126:VAL:HG11	1.56	0.69
3:B:301:GLU:HA	3:B:328:ILE:HD11	1.73	0.69
3:A:317:ILE:HA	3:A:322:LEU:HD12	1.74	0.69
2:U:9:DA:C2'	2:U:10:DC:H5''	2.21	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:300:PHE:O	3:B:328:ILE:HD11	1.93	0.68
3:B:338:ASN:H	3:B:341:GLN:NE2	1.90	0.68
3:B:55:GLN:NE2	3:B:126:VAL:HG11	2.09	0.67
3:B:396:MET:HG2	3:B:397:SER:N	2.10	0.67
3:B:406:CYS:SG	3:B:496:LEU:HD12	2.34	0.67
3:B:457:LYS:CB	3:B:484:LEU:HD21	2.25	0.67
3:A:408:SER:OG	3:A:410:VAL:HG22	1.95	0.66
3:A:447:LEU:HA	3:A:498:LYS:O	1.96	0.66
3:A:21:SER:O	3:A:22:SER:HB3	1.97	0.65
3:A:398:ASN:CG	3:A:399:LYS:N	2.50	0.65
3:B:21:SER:O	3:B:22:SER:HB3	1.97	0.65
3:B:455:TYR:HB3	3:B:484:LEU:HD12	1.79	0.65
1:Q:8:DG:H1'	1:Q:9:DT:H5'	1.77	0.65
3:B:395:MET:CE	3:B:426:ARG:HB3	2.28	0.64
3:B:333:GLU:O	3:B:336:PRO:HD3	1.98	0.64
3:B:160:ASP:HB2	3:B:386:LEU:HD22	1.78	0.64
3:B:33:ALA:HB1	3:B:36:ALA:HB3	1.80	0.64
2:U:6:DC:H2''	2:U:7:DT:OP2	1.98	0.64
3:B:392:VAL:HG11	3:B:430:LEU:HD13	1.80	0.64
3:B:113:GLN:HE21	3:B:113:GLN:HA	1.62	0.64
3:A:169:LEU:HD12	3:A:187:LEU:HD13	1.80	0.64
3:B:86:ASN:O	3:B:88:ILE:HD12	1.98	0.63
3:A:253:LYS:O	3:A:257:GLY:HA2	1.98	0.63
3:B:208:ILE:O	3:B:208:ILE:HD12	1.98	0.63
3:B:307:THR:HG21	3:B:373:LYS:NZ	2.13	0.63
3:B:508:ILE:HD12	3:B:508:ILE:N	2.13	0.63
1:Q:12:DG:H2''	1:Q:13:DC:OP2	1.97	0.63
3:B:320:LEU:HB2	3:B:322:LEU:HG	1.79	0.63
3:B:447:LEU:HD12	3:B:447:LEU:O	1.98	0.63
3:B:319:VAL:O	3:B:319:VAL:HG12	1.99	0.63
3:B:342:LEU:HD13	3:B:371:ALA:HA	1.80	0.63
3:A:404:LYS:HG2	3:A:407:ASN:HD21	1.61	0.63
3:B:64:TYR:CD2	3:B:280:PRO:HD3	2.34	0.63
3:A:366:LYS:HB3	3:A:369:ASP:OD2	1.97	0.63
3:B:442:THR:HG21	3:B:505:ASN:HD22	1.64	0.62
1:Q:6:DT:H5'	3:A:456:ARG:NH1	2.14	0.62
3:A:55:GLN:NE2	3:A:126:VAL:HG11	2.15	0.62
3:B:267:THR:HB	3:B:270:VAL:HG23	1.81	0.62
3:B:453:GLU:HG2	3:B:454:VAL:N	2.14	0.62
3:A:31:MET:HG2	3:A:260:THR:CG2	2.30	0.62
1:Q:7:DG:H4'	1:Q:8:DG:OP1	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:11:DC:H1'	2:T:12:DA:C5	2.35	0.62
3:B:442:THR:HG22	3:B:505:ASN:HB2	1.81	0.61
3:B:315:GLU:O	3:B:319:VAL:HG23	1.99	0.61
3:B:398:ASN:HB2	3:B:499:LEU:O	2.00	0.61
3:B:439:ILE:HD13	3:B:439:ILE:N	2.15	0.61
1:Q:13:DC:H5''	3:A:153:SER:HB2	1.82	0.61
3:A:169:LEU:HD22	3:A:237:ILE:CD1	2.30	0.61
3:A:69:TYR:HB2	3:A:71:ILE:HD13	1.82	0.61
3:A:208:ILE:O	3:A:208:ILE:HD12	2.01	0.61
3:A:474:LEU:O	3:A:478:ILE:HG13	2.01	0.61
3:A:424:THR:O	3:A:424:THR:HG22	2.01	0.61
3:B:308:LEU:HD23	3:B:316:LEU:HD13	1.83	0.60
3:A:350:VAL:HA	3:A:355:TYR:HE1	1.67	0.60
3:B:447:LEU:CD1	3:B:455:TYR:HB2	2.32	0.60
3:A:302:ILE:HA	3:A:328:ILE:HD11	1.82	0.60
3:B:362:ILE:HG22	3:B:363:ASP:N	2.17	0.60
3:A:341:GLN:HE21	3:A:341:GLN:C	2.05	0.59
3:A:437:ILE:HD11	3:B:202:ASN:ND2	2.17	0.59
3:A:308:LEU:HD11	3:A:316:LEU:HD11	1.84	0.59
3:B:149:VAL:HG22	3:B:159:LEU:CD2	2.32	0.59
3:B:0:ARG:HA	3:B:207:LEU:HD11	1.84	0.59
3:B:337:ASP:N	3:B:341:GLN:HE22	1.99	0.59
3:B:23:LEU:HD23	3:B:234:ASP:HA	1.84	0.59
3:B:152:ALA:HB3	3:B:156:GLU:HB2	1.85	0.59
3:B:480:PHE:O	3:B:484:LEU:HD23	2.03	0.59
3:A:457:LYS:HE2	3:A:483:ASP:OD1	2.03	0.58
3:B:32:ASN:HD21	3:B:281:ASP:H	1.51	0.58
3:A:56:TRP:CZ2	3:A:126:VAL:HG23	2.39	0.58
3:B:69:TYR:HB2	3:B:71:ILE:HD13	1.85	0.58
3:A:54:VAL:HG21	3:A:111:TRP:CZ3	2.39	0.57
3:A:379:ARG:HG2	3:A:379:ARG:HH11	1.68	0.57
3:B:377:LEU:HD23	3:B:382:TYR:CD2	2.39	0.57
3:B:423:LEU:O	3:B:427:ILE:HG12	2.05	0.57
3:B:355:TYR:O	3:B:356:ASP:CB	2.52	0.57
3:B:448:LYS:HG2	3:B:454:VAL:HG22	1.85	0.57
3:A:177:LEU:O	3:A:178:THR:HG23	2.05	0.57
3:A:340:GLY:O	3:A:343:LYS:HB3	2.04	0.57
3:B:177:LEU:O	3:B:178:THR:HG23	2.04	0.57
3:B:249:ARG:HD2	3:B:262:CYS:HB2	1.86	0.56
3:B:35:PHE:O	3:B:39:GLU:HG2	2.05	0.56
3:A:121:VAL:O	3:A:121:VAL:HG22	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:376:LYS:HB2	3:B:376:LYS:NZ	2.20	0.56
3:A:509:ILE:C	3:A:509:ILE:HD12	2.26	0.56
3:B:200:ASP:C	3:B:202:ASN:H	2.09	0.56
3:A:38:VAL:HG21	3:A:131:TYR:CD2	2.40	0.56
3:A:437:ILE:HB	3:A:509:ILE:HD11	1.87	0.56
3:B:200:ASP:O	3:B:202:ASN:N	2.39	0.56
3:A:21:SER:C	3:A:23:LEU:H	2.09	0.56
3:A:342:LEU:O	3:A:342:LEU:HD23	2.05	0.56
3:A:398:ASN:HA	3:A:500:SER:HB3	1.87	0.56
3:B:165:CYS:HB3	3:B:237:ILE:HG23	1.87	0.56
3:A:228:ASP:O	3:A:287:LYS:NZ	2.35	0.56
3:A:446:SER:OG	3:A:456:ARG:HD3	2.05	0.56
3:A:508:ILE:HG13	3:A:508:ILE:O	2.06	0.56
3:B:474:LEU:O	3:B:478:ILE:HG12	2.06	0.56
3:B:338:ASN:HD21	3:B:341:GLN:HG3	1.71	0.55
3:B:52:VAL:HG12	3:B:89:PRO:HA	1.88	0.55
3:A:312:LEU:O	3:A:316:LEU:HG	2.06	0.55
3:B:382:TYR:CZ	3:B:384:LEU:HD21	2.42	0.55
3:A:32:ASN:HD21	3:A:281:ASP:H	1.54	0.55
3:B:413:ILE:HG13	3:B:478:ILE:CD1	2.32	0.55
3:B:437:ILE:HB	3:B:509:ILE:HG13	1.88	0.55
3:A:341:GLN:NE2	3:A:341:GLN:C	2.60	0.55
3:A:346:LEU:O	3:A:350:VAL:HG13	2.06	0.55
3:A:64:TYR:CD2	3:A:280:PRO:HD3	2.41	0.55
3:B:303:THR:O	3:B:309:GLY:HA2	2.07	0.55
3:A:442:THR:HG21	3:A:505:ASN:ND2	2.22	0.55
3:A:20:GLU:O	3:A:22:SER:N	2.40	0.55
3:B:305:PHE:CG	3:B:377:LEU:HD11	2.43	0.54
3:B:53:CYS:HB3	3:B:61:ALA:HB3	1.89	0.54
3:B:395:MET:HE2	3:B:426:ARG:HB3	1.88	0.54
1:Q:7:DG:H1'	1:Q:8:DG:C8	2.43	0.54
3:A:442:THR:HG21	3:A:505:ASN:HD22	1.69	0.54
3:A:86:ASN:O	3:A:88:ILE:HD12	2.06	0.54
3:A:469:GLN:O	3:A:471:HIS:N	2.41	0.54
3:B:355:TYR:OH	3:B:362:ILE:HB	2.08	0.54
3:B:76:THR:OG1	3:B:79:GLU:HG3	2.08	0.54
3:A:35:PHE:O	3:A:39:GLU:HG2	2.07	0.54
3:A:392:VAL:HG11	3:A:430:LEU:HD11	1.90	0.54
3:B:56:TRP:CZ2	3:B:126:VAL:HG23	2.42	0.54
3:B:149:VAL:HG22	3:B:159:LEU:HD22	1.89	0.54
3:B:315:GLU:OE2	3:B:362:ILE:HG12	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:35:PHE:CD1	6:A:2001:DTP:O3'	2.61	0.53
3:B:308:LEU:HD12	3:B:308:LEU:N	2.23	0.53
3:A:249:ARG:HD2	3:A:262:CYS:HB2	1.90	0.53
3:A:350:VAL:HB	3:A:355:TYR:OH	2.09	0.53
3:A:394:SER:HB3	3:A:504:THR:HG22	1.90	0.53
3:B:347:ASP:O	3:B:351:LYS:HG3	2.08	0.53
1:Q:6:DT:H5'	3:A:456:ARG:HH11	1.73	0.53
3:B:155:ASP:OD2	3:B:156:GLU:HG3	2.09	0.53
3:B:54:VAL:HG21	3:B:111:TRP:CZ3	2.43	0.53
3:B:398:ASN:C	3:B:398:ASN:ND2	2.60	0.53
3:A:33:ALA:O	3:A:36:ALA:HB3	2.09	0.53
3:B:169:LEU:HD22	3:B:237:ILE:CD1	2.32	0.53
3:A:52:VAL:HG12	3:A:89:PRO:HA	1.90	0.53
3:B:2:SER:HB3	3:B:205:LEU:O	2.09	0.53
3:A:56:TRP:C	3:A:57:ASN:HD22	2.12	0.52
1:Q:8:DG:H2''	1:Q:9:DT:O5'	2.09	0.52
3:B:452:TYR:N	3:B:452:TYR:CD2	2.76	0.52
3:A:133:ARG:HB3	3:A:133:ARG:CZ	2.39	0.52
3:B:21:SER:C	3:B:23:LEU:H	2.11	0.52
3:A:401:LEU:HD13	3:A:406:CYS:HB2	1.91	0.52
3:A:200:ASP:C	3:A:202:ASN:H	2.13	0.52
3:A:332:ARG:HG3	3:A:379:ARG:HH12	1.73	0.52
3:A:398:ASN:CG	3:A:399:LYS:H	2.13	0.52
3:B:35:PHE:CD1	6:B:4001:DTP:O3'	2.63	0.52
3:A:338:ASN:HD22	3:A:338:ASN:N	2.07	0.52
3:A:33:ALA:HB1	3:A:36:ALA:HB3	1.92	0.51
3:B:223:ASN:ND2	3:B:227:ARG:H	1.94	0.51
3:B:56:TRP:C	3:B:57:ASN:HD22	2.14	0.51
3:B:508:ILE:HD12	3:B:508:ILE:H	1.74	0.51
3:A:6:TRP:O	3:A:10:ILE:HG12	2.10	0.51
3:B:504:THR:HG22	3:B:505:ASN:N	2.22	0.51
3:B:452:TYR:N	3:B:452:TYR:HD2	2.09	0.51
3:B:434:TYR:O	3:B:436:LYS:HG3	2.11	0.51
3:B:453:GLU:HG2	3:B:454:VAL:H	1.74	0.51
3:B:478:ILE:O	3:B:481:VAL:HG12	2.11	0.51
3:B:55:GLN:HG3	3:B:126:VAL:HG21	1.93	0.51
3:B:38:VAL:HG21	3:B:131:TYR:CD2	2.46	0.51
3:B:406:CYS:HA	3:B:411:ASP:HB3	1.93	0.51
1:P:7:DG:C2'	1:P:8:DG:H5''	2.38	0.51
3:A:125:LYS:HE3	3:A:422:GLU:OE1	2.11	0.51
1:Q:13:DC:H5''	3:A:153:SER:CB	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:152:ALA:HB3	3:A:156:GLU:HB2	1.92	0.51
3:A:273:LEU:HD11	3:A:305:PHE:HE2	1.75	0.51
3:A:76:THR:O	3:A:79:GLU:N	2.44	0.51
1:Q:8:DG:H1'	1:Q:9:DT:C5'	2.41	0.51
3:B:398:ASN:CB	3:B:500:SER:HB3	2.41	0.51
3:B:20:GLU:O	3:B:22:SER:N	2.44	0.50
3:B:222:PHE:CE2	3:B:294:PHE:HA	2.46	0.50
3:B:398:ASN:HB2	3:B:500:SER:HB3	1.93	0.50
3:A:288:ASN:HA	3:A:291:LEU:HG	1.92	0.50
3:A:55:GLN:HG3	3:A:126:VAL:HG21	1.94	0.50
3:B:338:ASN:H	3:B:338:ASN:HD22	1.59	0.50
3:A:292:LEU:HD22	3:A:332:ARG:NH2	2.26	0.50
3:A:437:ILE:HD11	3:B:202:ASN:HD22	1.77	0.50
3:B:338:ASN:HD22	3:B:338:ASN:N	2.10	0.50
3:B:342:LEU:CD1	3:B:371:ALA:HA	2.40	0.50
3:B:373:LYS:HE3	3:B:382:TYR:CE2	2.46	0.50
3:B:248:ILE:HD12	3:B:248:ILE:H	1.77	0.50
3:B:196:GLY:C	3:B:198:ASN:H	2.14	0.49
3:B:264:LEU:N	3:B:264:LEU:HD12	2.27	0.49
3:B:145:ALA:O	3:B:164:ILE:HD11	2.13	0.49
3:B:306:TRP:HE3	3:B:306:TRP:HA	1.76	0.49
3:B:195:ILE:N	3:B:195:ILE:HD12	2.28	0.49
3:B:110:SER:HA	3:B:118:GLN:OE1	2.12	0.49
3:A:259:THR:HB	3:A:281:ASP:HB2	1.94	0.49
3:A:395:MET:HE2	3:A:430:LEU:CD1	2.41	0.49
3:B:113:GLN:NE2	3:B:113:GLN:HA	2.25	0.49
3:B:19:TYR:CE2	3:B:385:PRO:HD3	2.47	0.49
3:B:439:ILE:HG12	3:B:439:ILE:O	2.11	0.49
3:B:73:ARG:C	3:B:75:ASP:H	2.16	0.49
3:A:373:LYS:HE3	3:A:382:TYR:OH	2.11	0.49
3:A:402:ARG:HH11	3:A:402:ARG:HB3	1.76	0.49
3:B:306:TRP:CE3	3:B:306:TRP:HA	2.46	0.49
3:B:32:ASN:ND2	3:B:281:ASP:H	2.10	0.49
3:A:55:GLN:CG	3:A:126:VAL:HG21	2.43	0.49
3:A:196:GLY:C	3:A:198:ASN:H	2.14	0.49
3:A:2:SER:HB3	3:A:205:LEU:O	2.13	0.49
3:A:347:ASP:O	3:A:350:VAL:HG22	2.12	0.49
3:B:169:LEU:HD12	3:B:187:LEU:CD1	2.40	0.49
3:B:355:TYR:O	3:B:356:ASP:HB2	2.13	0.49
3:B:392:VAL:HG11	3:B:430:LEU:CD1	2.42	0.49
3:B:49:ASP:O	3:B:51:VAL:HG12	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:21:SER:O	3:A:22:SER:CB	2.61	0.48
3:A:52:VAL:HG21	3:A:59:ILE:HD13	1.93	0.48
3:B:461:VAL:HG23	3:B:476:VAL:HG21	1.94	0.48
3:B:482:THR:O	3:B:486:ILE:HG12	2.12	0.48
3:B:218:GLU:HG2	3:B:246:LYS:HB2	1.94	0.48
3:B:446:SER:HB3	3:B:500:SER:OG	2.12	0.48
3:B:31:MET:HG2	3:B:260:THR:CG2	2.40	0.48
3:B:89:PRO:HG2	3:B:111:TRP:CE2	2.48	0.48
3:A:23:LEU:HD23	3:A:234:ASP:HA	1.94	0.48
3:A:49:ASP:O	3:A:51:VAL:HG12	2.13	0.48
3:B:376:LYS:NZ	3:B:376:LYS:CB	2.77	0.48
3:B:14:SER:C	3:B:16:SER:H	2.17	0.48
3:B:493:TYR:HD2	3:B:494:TYR:CE2	2.31	0.48
3:B:71:ILE:HD12	3:B:71:ILE:N	2.29	0.48
3:A:442:THR:CG2	3:A:505:ASN:HD22	2.27	0.48
3:B:358:SER:OG	3:B:359:THR:N	2.45	0.48
3:B:315:GLU:OE1	3:B:360:SER:HA	2.14	0.48
3:A:14:SER:C	3:A:16:SER:H	2.17	0.48
3:A:76:THR:O	3:A:77:ILE:C	2.52	0.48
3:B:7:LYS:HB2	3:B:201:ILE:O	2.14	0.48
3:A:69:TYR:HB2	3:A:71:ILE:CD1	2.43	0.47
3:B:342:LEU:O	3:B:342:LEU:HD22	2.14	0.47
3:B:459:GLY:HA3	3:B:480:PHE:HZ	1.79	0.47
3:A:150:GLU:HG3	3:A:387:SER:O	2.15	0.47
3:B:129:GLU:N	3:B:130:PRO:CD	2.78	0.47
3:B:314:LYS:O	3:B:317:ILE:HB	2.14	0.47
3:A:32:ASN:ND2	3:A:281:ASP:H	2.11	0.47
3:B:273:LEU:HB3	3:B:300:PHE:CE2	2.49	0.47
3:A:26:ILE:HG22	3:A:27:ALA:N	2.28	0.47
3:B:397:SER:HG	3:B:419:PHE:HD1	1.63	0.47
3:A:379:ARG:HG2	3:A:379:ARG:NH1	2.29	0.47
3:A:7:LYS:HB2	3:A:201:ILE:O	2.14	0.47
3:B:346:LEU:O	3:B:350:VAL:HG22	2.14	0.47
3:B:307:THR:HG21	3:B:373:LYS:CE	2.45	0.47
3:A:53:CYS:HB3	3:A:61:ALA:HB3	1.97	0.47
3:B:443:VAL:HG12	3:B:444:SER:N	2.28	0.47
3:B:475:LYS:C	3:B:475:LYS:HD3	2.35	0.47
2:T:6:DC:H2"	2:T:7:DT:OP2	2.13	0.47
6:A:2001:DTP:H5'2	6:A:2001:DTP:O2B	2.15	0.47
3:A:225:GLU:HG2	3:A:293:ASP:OD2	2.14	0.47
3:A:242:SER:HA	3:A:264:LEU:HD21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:71:ILE:HD12	3:A:71:ILE:N	2.30	0.47
3:B:300:PHE:N	3:B:300:PHE:CD1	2.83	0.47
1:Q:6:DT:H2"	1:Q:7:DG:C8	2.50	0.47
3:A:165:CYS:HB3	3:A:237:ILE:HG23	1.96	0.47
3:A:394:SER:CB	3:A:504:THR:HG22	2.45	0.47
3:B:336:PRO:HG2	3:B:337:ASP:H	1.80	0.47
3:B:480:PHE:C	3:B:482:THR:H	2.17	0.47
2:U:12:DA:H2"	2:U:13:DC:C6	2.50	0.46
3:A:49:ASP:O	3:A:51:VAL:N	2.48	0.46
3:B:479:LYS:HE2	3:B:483:ASP:OD1	2.15	0.46
3:A:129:GLU:N	3:A:130:PRO:CD	2.78	0.46
3:A:402:ARG:NH1	3:A:402:ARG:HB3	2.31	0.46
3:A:443:VAL:HG22	3:A:503:ILE:HG22	1.97	0.46
3:B:442:THR:CG2	3:B:505:ASN:HD22	2.27	0.46
3:B:52:VAL:HG22	3:B:59:ILE:HG23	1.97	0.46
3:B:337:ASP:HB2	3:B:341:GLN:CD	2.36	0.46
3:A:129:GLU:HB3	3:A:130:PRO:HD3	1.97	0.46
3:B:35:PHE:CE1	3:B:131:TYR:HB3	2.50	0.46
3:B:378:SER:C	3:B:379:ARG:HG3	2.36	0.46
3:B:125:LYS:HE3	3:B:422:GLU:OE1	2.15	0.46
3:A:71:ILE:HD12	3:A:71:ILE:H	1.82	0.45
3:B:163:ARG:HD3	3:B:163:ARG:N	2.31	0.45
3:A:248:ILE:HD12	3:A:248:ILE:H	1.80	0.45
3:B:121:VAL:HG22	3:B:121:VAL:O	2.16	0.45
3:B:242:SER:HA	3:B:264:LEU:HD21	1.99	0.45
3:B:302:ILE:HD12	3:B:305:PHE:CE1	2.51	0.45
3:B:69:TYR:HB2	3:B:71:ILE:CD1	2.46	0.45
3:A:97:LYS:HG2	3:A:414:SER:HB3	1.97	0.45
3:B:32:ASN:O	3:B:33:ALA:C	2.55	0.45
3:A:417:GLU:HG2	3:A:474:LEU:HD21	1.98	0.45
3:B:223:ASN:HD21	3:B:227:ARG:N	1.95	0.45
3:B:447:LEU:HA	3:B:498:LYS:O	2.16	0.45
3:A:113:GLN:HE21	3:A:113:GLN:HA	1.81	0.45
3:A:200:ASP:O	3:A:202:ASN:N	2.49	0.45
3:A:222:PHE:CE2	3:A:294:PHE:HA	2.50	0.45
3:A:273:LEU:HB3	3:A:300:PHE:CE2	2.51	0.45
3:A:442:THR:HG22	3:A:505:ASN:HB2	1.97	0.45
3:B:212:ILE:HD11	3:B:215:LEU:HD22	1.97	0.45
3:B:398:ASN:C	3:B:398:ASN:HD22	2.19	0.45
3:B:480:PHE:C	3:B:482:THR:N	2.69	0.45
3:A:195:ILE:HD12	3:A:195:ILE:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:291:LEU:O	3:B:295:LEU:HD13	2.16	0.45
1:P:11:DA:OP1	3:B:310:GLY:HA3	2.16	0.45
1:P:5:DG:H2''	1:P:6:DT:O5'	2.17	0.45
3:A:89:PRO:HG2	3:A:111:TRP:CE2	2.52	0.45
3:B:300:PHE:O	3:B:328:ILE:CD1	2.63	0.45
3:B:52:VAL:HG23	3:B:62:VAL:HG22	1.99	0.45
3:A:264:LEU:HD12	3:A:264:LEU:N	2.31	0.44
3:A:332:ARG:CG	3:A:379:ARG:HH12	2.30	0.44
3:A:133:ARG:HB3	3:A:133:ARG:HH21	1.78	0.44
3:A:350:VAL:HG23	3:A:351:LYS:HG3	1.99	0.44
3:A:441:ARG:HG3	3:A:441:ARG:HH11	1.81	0.44
3:B:136:ARG:HD3	3:B:432:GLN:HB3	1.99	0.44
3:A:31:MET:HA	3:A:260:THR:HG22	1.97	0.44
3:A:32:ASN:O	3:A:33:ALA:C	2.56	0.44
3:B:443:VAL:HG22	3:B:503:ILE:HG22	1.98	0.44
3:B:506:PHE:N	3:B:506:PHE:CD2	2.85	0.44
3:A:352:GLN:HG3	3:A:353:SER:H	1.83	0.44
3:A:352:GLN:HG3	3:A:353:SER:N	2.33	0.44
3:B:267:THR:HB	3:B:270:VAL:CG2	2.46	0.44
3:B:6:TRP:O	3:B:10:ILE:HG12	2.18	0.44
3:A:110:SER:HA	3:A:118:GLN:OE1	2.17	0.44
3:A:338:ASN:ND2	3:A:338:ASN:N	2.65	0.44
3:B:88:ILE:O	3:B:88:ILE:HG22	2.17	0.44
3:A:431:GLU:OE2	3:A:437:ILE:HA	2.18	0.44
3:B:38:VAL:HG21	3:B:131:TYR:CE2	2.53	0.44
3:A:129:GLU:HG2	3:A:133:ARG:CG	2.48	0.44
3:A:263:GLY:C	3:A:264:LEU:HD12	2.38	0.44
3:B:263:GLY:C	3:B:264:LEU:HD12	2.38	0.44
3:B:301:GLU:CA	3:B:328:ILE:HD11	2.44	0.44
3:B:479:LYS:O	3:B:482:THR:HB	2.18	0.44
3:B:49:ASP:O	3:B:51:VAL:N	2.49	0.44
3:A:341:GLN:HE21	3:A:342:LEU:N	2.16	0.43
3:A:411:ASP:O	3:A:414:SER:HB2	2.18	0.43
3:B:46:SER:HB3	3:B:49:ASP:OD2	2.17	0.43
3:A:223:ASN:HD21	3:A:227:ARG:N	2.02	0.43
3:B:347:ASP:O	3:B:350:VAL:HG22	2.17	0.43
3:A:356:ASP:C	3:A:358:SER:H	2.21	0.43
3:B:273:LEU:HD22	3:B:300:PHE:CD2	2.53	0.43
3:B:288:ASN:HA	3:B:291:LEU:HG	2.01	0.43
3:B:19:TYR:CD1	3:B:385:PRO:HB3	2.53	0.43
3:A:129:GLU:HG2	3:A:133:ARG:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:422:GLU:O	3:A:425:SER:HB3	2.19	0.43
3:B:56:TRP:CZ2	3:B:121:VAL:HG23	2.54	0.43
3:B:21:SER:O	3:B:22:SER:CB	2.65	0.43
3:B:350:VAL:HB	3:B:355:TYR:CD1	2.53	0.43
1:P:6:DT:H4'	1:P:6:DT:OP1	2.19	0.43
2:T:11:DC:H2''	2:T:12:DA:N7	2.34	0.43
3:A:113:GLN:HA	3:A:113:GLN:NE2	2.34	0.43
3:A:155:ASP:OD2	3:A:156:GLU:HG3	2.18	0.43
3:B:363:ASP:O	3:B:365:LEU:N	2.52	0.43
3:A:114:ASP:OD1	3:A:116:ALA:HB3	2.19	0.43
6:A:2001:DTP:H5'2	6:A:2001:DTP:PB	2.59	0.43
3:A:288:ASN:HA	3:A:291:LEU:CD1	2.49	0.43
3:A:320:LEU:C	3:A:322:LEU:H	2.22	0.43
3:A:448:LYS:HA	3:A:453:GLU:O	2.18	0.43
3:B:377:LEU:HD23	3:B:382:TYR:HD2	1.83	0.43
3:B:375:PHE:CE1	3:B:379:ARG:NH2	2.87	0.43
3:A:93:ALA:HB1	3:A:102:TRP:CE3	2.53	0.43
3:A:423:LEU:C	3:A:425:SER:H	2.22	0.42
3:B:318:ASP:C	3:B:320:LEU:H	2.21	0.42
2:U:10:DC:H2''	2:U:11:DC:C6	2.54	0.42
3:A:267:THR:HB	3:A:270:VAL:HG23	2.01	0.42
3:A:317:ILE:CA	3:A:322:LEU:HD12	2.45	0.42
3:A:88:ILE:HG22	3:A:88:ILE:O	2.18	0.42
3:B:506:PHE:HD2	3:B:506:PHE:N	2.16	0.42
3:A:368:ALA:O	3:A:371:ALA:HB3	2.19	0.42
3:B:508:ILE:CD1	3:B:508:ILE:N	2.82	0.42
3:A:183:LEU:HD22	3:A:187:LEU:CD1	2.50	0.42
3:A:205:LEU:HB3	3:A:206:PRO:HD2	2.00	0.42
3:B:55:GLN:CG	3:B:126:VAL:HG21	2.48	0.42
2:U:9:DA:H2''	2:U:10:DC:C5'	2.35	0.42
2:T:4:DG:H3'	2:T:5:DG:H5'	2.02	0.42
3:B:169:LEU:CD1	3:B:187:LEU:HD13	2.45	0.42
3:A:19:TYR:CE2	3:A:385:PRO:HD3	2.54	0.42
3:A:430:LEU:HA	3:A:430:LEU:HD23	1.87	0.42
3:A:482:THR:O	3:A:485:ASP:HB3	2.20	0.42
3:B:302:ILE:HD12	3:B:305:PHE:CD1	2.54	0.42
1:P:8:DG:H2''	1:P:9:DT:C6	2.55	0.42
3:A:422:GLU:O	3:A:426:ARG:HG3	2.20	0.42
2:U:8:DC:OP1	3:A:426:ARG:NH2	2.53	0.42
3:A:489:LYS:HD3	3:A:489:LYS:HA	1.87	0.42
3:A:64:TYR:CZ	3:A:67:ARG:NH1	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:34:PHE:O	3:B:37:GLN:N	2.53	0.42
3:B:88:ILE:HD12	3:B:88:ILE:N	2.34	0.42
3:A:230:ILE:O	3:A:230:ILE:HG22	2.20	0.42
3:A:52:VAL:HG22	3:A:59:ILE:HG23	2.01	0.42
3:B:439:ILE:H	3:B:439:ILE:HD13	1.82	0.42
3:B:307:THR:OG1	3:B:308:LEU:HD12	2.20	0.41
3:A:35:PHE:CE1	3:A:131:TYR:HB3	2.55	0.41
3:A:337:ASP:CG	3:A:341:GLN:HG3	2.41	0.41
3:A:375:PHE:CE1	3:A:379:ARG:NH2	2.80	0.41
3:A:431:GLU:O	3:A:435:ASN:N	2.53	0.41
3:B:64:TYR:CZ	3:B:67:ARG:NH1	2.88	0.41
3:B:73:ARG:O	3:B:74:MET:HB2	2.20	0.41
3:A:56:TRP:HB2	3:A:57:ASN:H	1.73	0.41
3:B:338:ASN:HD22	3:B:341:GLN:HG3	1.78	0.41
3:B:399:LYS:HG3	3:B:401:LEU:H	1.84	0.41
3:B:463:TYR:HD1	3:B:472:GLU:HG3	1.85	0.41
3:A:315:GLU:O	3:A:319:VAL:HG23	2.20	0.41
3:A:46:SER:HB3	3:A:49:ASP:OD2	2.21	0.41
3:A:476:VAL:O	3:A:477:GLY:C	2.58	0.41
3:B:129:GLU:HB3	3:B:130:PRO:HD3	2.02	0.41
3:B:396:MET:CG	3:B:397:SER:N	2.81	0.41
3:B:450:LYS:HB2	3:B:493:TYR:O	2.20	0.41
2:T:6:DC:H2"	2:T:7:DT:H71	2.03	0.41
3:B:200:ASP:C	3:B:202:ASN:N	2.71	0.41
3:B:318:ASP:O	3:B:320:LEU:N	2.54	0.41
3:B:469:GLN:O	3:B:470:SER:C	2.58	0.41
3:A:337:ASP:HB2	3:A:338:ASN:H	1.73	0.41
3:B:259:THR:HB	3:B:281:ASP:HB2	2.03	0.41
3:B:308:LEU:HD23	3:B:316:LEU:CD1	2.48	0.41
3:A:200:ASP:C	3:A:202:ASN:N	2.74	0.41
3:A:320:LEU:O	3:A:321:ASP:HB2	2.21	0.41
3:A:468:PHE:HA	3:A:468:PHE:HD2	1.67	0.41
3:B:113:GLN:HE21	3:B:113:GLN:CA	2.27	0.41
3:B:420:CYS:SG	3:B:474:LEU:HD13	2.61	0.41
3:A:338:ASN:ND2	3:A:341:GLN:H	2.19	0.41
3:A:439:ILE:H	3:A:439:ILE:HD13	1.85	0.41
3:A:218:GLU:HG2	3:A:246:LYS:HB2	2.02	0.41
3:A:455:TYR:HB3	3:A:484:LEU:HD22	2.03	0.41
3:B:160:ASP:C	3:B:162:GLY:H	2.24	0.41
3:B:376:LYS:HZ2	3:B:376:LYS:HB2	1.86	0.41
3:B:76:THR:O	3:B:77:ILE:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:215:LEU:HB3	3:A:230:ILE:HD13	2.02	0.41
3:A:240:LEU:O	3:A:243:GLN:HB2	2.21	0.41
3:A:338:ASN:HD22	3:A:338:ASN:C	2.24	0.41
3:A:39:GLU:OE2	3:A:104:TYR:OH	2.35	0.41
3:A:395:MET:HE2	3:A:430:LEU:HD11	2.03	0.40
3:B:400:ASN:HA	3:B:400:ASN:HD22	1.69	0.40
3:A:1:MET:N	3:A:207:LEU:HD21	2.36	0.40
3:B:178:THR:HB	3:B:179:GLY:H	1.65	0.40
3:B:23:LEU:CD2	3:B:234:ASP:HA	2.51	0.40
3:B:398:ASN:HB3	3:B:500:SER:CB	2.52	0.40
3:A:267:THR:HG22	3:A:269:ASN:H	1.87	0.40
3:B:376:LYS:HZ3	3:B:376:LYS:CB	2.34	0.40
3:B:71:ILE:H	3:B:71:ILE:HD12	1.86	0.40
2:T:9:DA:H2"	2:T:10:DC:C6	2.56	0.40
3:A:420:CYS:SG	3:A:474:LEU:HB2	2.61	0.40
3:B:273:LEU:HD22	3:B:300:PHE:HD2	1.87	0.40
3:B:336:PRO:O	3:B:337:ASP:C	2.60	0.40
3:B:377:LEU:HD13	3:B:377:LEU:O	2.22	0.40
3:B:410:VAL:HG23	3:B:411:ASP:N	2.35	0.40
3:B:478:ILE:HA	3:B:481:VAL:HG12	2.04	0.40
3:B:480:PHE:O	3:B:482:THR:N	2.55	0.40
3:B:484:LEU:HD22	3:B:484:LEU:N	2.36	0.40
1:Q:11:DA:H1'	1:Q:12:DG:H5'	2.02	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	
3	A	509/554 (92%)	422 (83%)	70 (14%)	17 (3%)	4	22
3	B	509/554 (92%)	412 (81%)	72 (14%)	25 (5%)	2	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1018/1108 (92%)	834 (82%)	142 (14%)	42 (4%)	3	17

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	21	SER
3	A	352	GLN
3	A	466	ILE
3	A	470	SER
3	B	21	SER
3	B	201	ILE
3	B	306	TRP
3	B	356	ASP
3	B	405	SER
3	B	465	GLY
3	B	466	ILE
3	A	322	LEU
3	A	405	SER
3	B	34	PHE
3	B	181	LEU
3	B	319	VAL
3	B	336	PRO
3	B	401	LEU
3	B	469	GLN
3	A	181	LEU
3	A	201	ILE
3	A	469	GLN
3	B	337	ASP
3	B	355	TYR
3	B	470	SER
3	A	34	PHE
3	B	198	ASN
3	A	56	TRP
3	A	406	CYS
3	B	357	ARG
3	A	308	LEU
3	B	56	TRP
3	B	344	GLU
3	B	364	PRO
3	B	487	LYS
3	A	15	PRO
3	A	77	ILE

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Mol	Chain	Res	Type
3	A	50	PRO
3	B	15	PRO
3	B	50	PRO
3	B	309	GLY
3	A	465	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	457/493 (93%)	438 (96%)	19 (4%)	30	60
3	B	457/493 (93%)	436 (95%)	21 (5%)	27	58
All	All	914/986 (93%)	874 (96%)	40 (4%)	28	59

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	23	LEU
3	A	77	ILE
3	A	133	ARG
3	A	163	ARG
3	A	190	ILE
3	A	293	ASP
3	A	337	ASP
3	A	338	ASN
3	A	341	GLN
3	A	406	CYS
3	A	420	CYS
3	A	436	LYS
3	A	439	ILE
3	A	441	ARG
3	A	464	LYS
3	A	468	PHE
3	A	473	LEU
3	A	481	VAL

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Mol	Chain	Res	Type
3	A	507	ASP
3	B	23	LEU
3	B	74	MET
3	B	77	ILE
3	B	133	ARG
3	B	136	ARG
3	B	163	ARG
3	B	190	ILE
3	B	223	ASN
3	B	293	ASP
3	B	300	PHE
3	B	306	TRP
3	B	307	THR
3	B	328	ILE
3	B	338	ASN
3	B	342	LEU
3	B	398	ASN
3	B	428	GLN
3	B	439	ILE
3	B	447	LEU
3	B	452	TYR
3	B	485	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	28	HIS
3	A	32	ASN
3	A	40	GLN
3	A	55	GLN
3	A	57	ASN
3	A	113	GLN
3	A	198	ASN
3	A	202	ASN
3	A	223	ASN
3	A	269	ASN
3	A	288	ASN
3	A	338	ASN
3	A	341	GLN
3	A	352	GLN
3	A	407	ASN
3	A	505	ASN

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Mol	Chain	Res	Type
3	B	32	ASN
3	B	40	GLN
3	B	55	GLN
3	B	57	ASN
3	B	113	GLN
3	B	198	ASN
3	B	202	ASN
3	B	223	ASN
3	B	288	ASN
3	B	330	HIS
3	B	338	ASN
3	B	341	GLN
3	B	361	ASN
3	B	400	ASN
3	B	432	GLN
3	B	505	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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
6	DTP	B	4001	5	26,32,32	1.33	5 (19%)	30,50,50	1.24	3 (10%)
4	CPT	T	45	2	0,2,4	0.00	-	-		
4	CPT	U	45	2	0,2,4	0.00	-	-		
6	DTP	A	2001	5	26,32,32	1.23	3 (11%)	30,50,50	1.21	3 (10%)

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
6	DTP	A	2001	5	-	5/18/34/34	0/3/3/3
6	DTP	B	4001	5	-	3/18/34/34	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	4001	DTP	O3'-C3'	-2.84	1.37	1.43
6	A	2001	DTP	C2-N3	2.81	1.36	1.32
6	B	4001	DTP	C2-N3	2.71	1.36	1.32
6	A	2001	DTP	O3'-C3'	-2.51	1.38	1.43
6	B	4001	DTP	C2-N1	2.45	1.38	1.33
6	A	2001	DTP	C2-N1	2.39	1.38	1.33
6	B	4001	DTP	PG-O2G	-2.11	1.46	1.54
6	B	4001	DTP	PG-O3G	2.04	1.62	1.54

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	4001	DTP	N3-C2-N1	-3.52	123.18	128.68
6	A	2001	DTP	N3-C2-N1	-3.43	123.31	128.68
6	A	2001	DTP	O2G-PG-O1G	2.69	121.23	110.68
6	B	4001	DTP	O2G-PG-O1G	2.49	120.42	110.68
6	B	4001	DTP	C5-C6-N6	2.15	123.63	120.35
6	A	2001	DTP	C5-C6-N6	2.11	123.56	120.35

There are no chirality outliers.

All (8) torsion outliers are listed below:

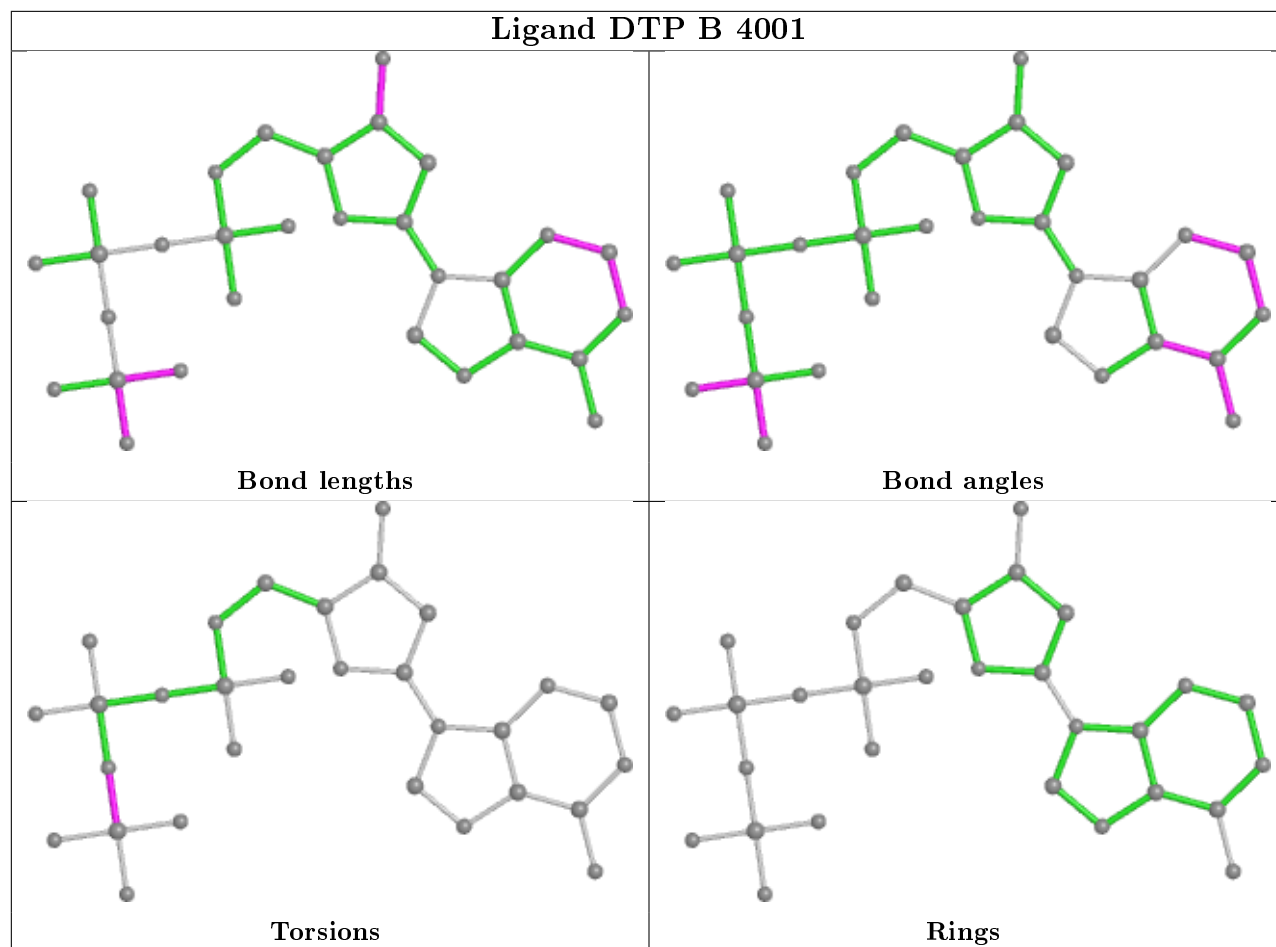
Mol	Chain	Res	Type	Atoms
6	A	2001	DTP	PB-O3B-PG-O2G
6	A	2001	DTP	PB-O3A-PA-O5'
6	B	4001	DTP	PB-O3B-PG-O1G
6	A	2001	DTP	PB-O3B-PG-O1G
6	B	4001	DTP	PB-O3B-PG-O2G
6	A	2001	DTP	PB-O3A-PA-O1A
6	A	2001	DTP	C4'-C5'-O5'-PA
6	B	4001	DTP	PB-O3B-PG-O3G

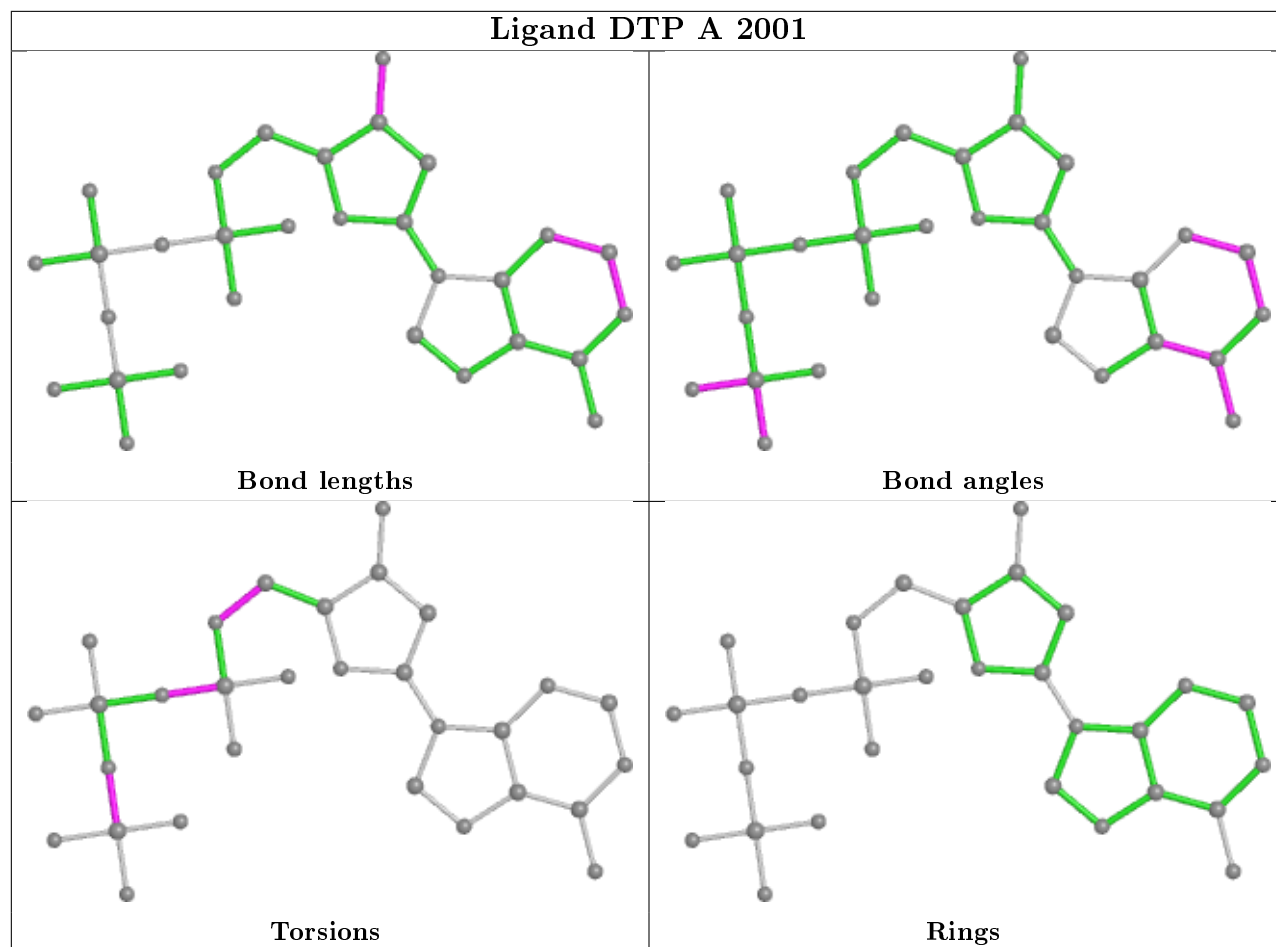
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	4001	DTP	1	0
6	A	2001	DTP	3	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	P	9/9 (100%)	1.19	1 (11%) 5 5	53, 71, 86, 86	0
1	Q	9/9 (100%)	1.99	4 (44%) 0 0	78, 87, 100, 101	0
2	T	10/10 (100%)	1.69	3 (30%) 0 0	66, 79, 101, 105	0
2	U	10/10 (100%)	1.79	3 (30%) 0 0	74, 88, 92, 95	0
3	A	511/554 (92%)	0.19	26 (5%) 28 26	21, 48, 105, 129	19 (3%)
3	B	511/554 (92%)	0.09	11 (2%) 62 60	18, 45, 84, 104	20 (3%)
All	All	1060/1146 (92%)	0.20	48 (4%) 33 32	18, 47, 98, 129	39 (3%)

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	355	TYR	5.5
3	A	354	ASP	4.8
3	A	465	GLY	4.8
3	A	356	ASP	4.3
2	T	13	DC	4.3
3	A	339	ALA	4.1
3	A	364	PRO	4.0
3	A	464	LYS	3.9
2	T	12	DA	3.4
2	U	12	DA	3.4
1	Q	10	DG	3.3
3	B	465	GLY	3.3
3	A	352	GLN	3.2
3	B	466	ILE	3.2
3	A	340	GLY	3.2
1	Q	5	DG	3.1
3	A	353	SER	3.1
2	U	10	DC	3.1
3	A	361	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
3	A	367	THR	3.0
2	U	11	DC	3.0
3	A	336	PRO	3.0
3	A	181	LEU	2.9
2	T	11	DC	2.9
3	A	319	VAL	2.8
3	A	365	LEU	2.8
1	Q	11	DA	2.7
3	B	353	SER	2.7
3	B	84	CYS	2.6
3	A	344	GLU	2.6
3	B	113	GLN	2.6
3	B	204	HIS	2.6
3	B	490	ASN	2.5
3	B	203	SER	2.4
3	A	115	PRO	2.4
3	A	462	ALA	2.3
1	Q	9	DT	2.2
3	A	335	TRP	2.2
1	P	5	DG	2.2
3	A	175	TYR	2.2
3	A	324	HIS	2.2
3	A	337	ASP	2.1
3	A	347	ASP	2.1
3	A	351	LYS	2.1
3	B	117	LYS	2.1
3	A	318	ASP	2.1
3	B	492	SER	2.0
3	B	463	TYR	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

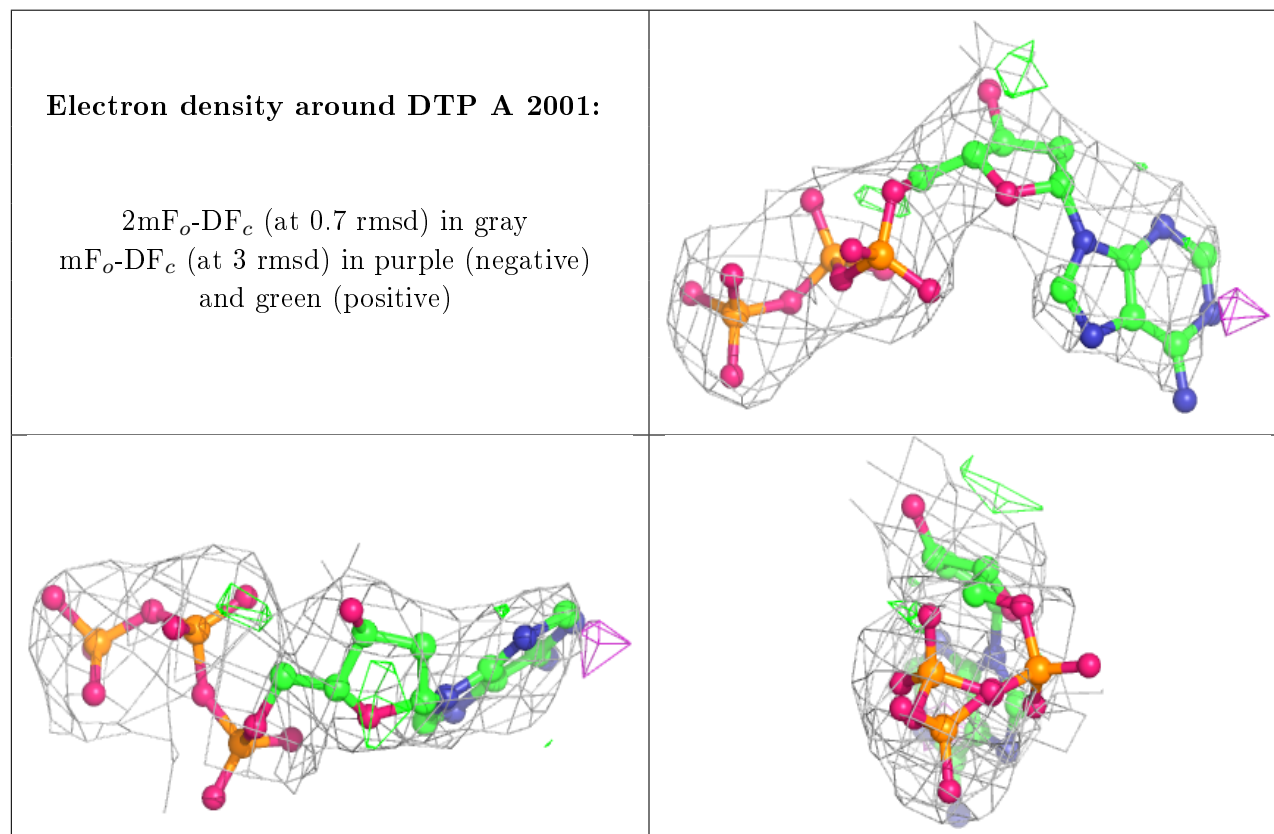
There are no carbohydrates in this entry.

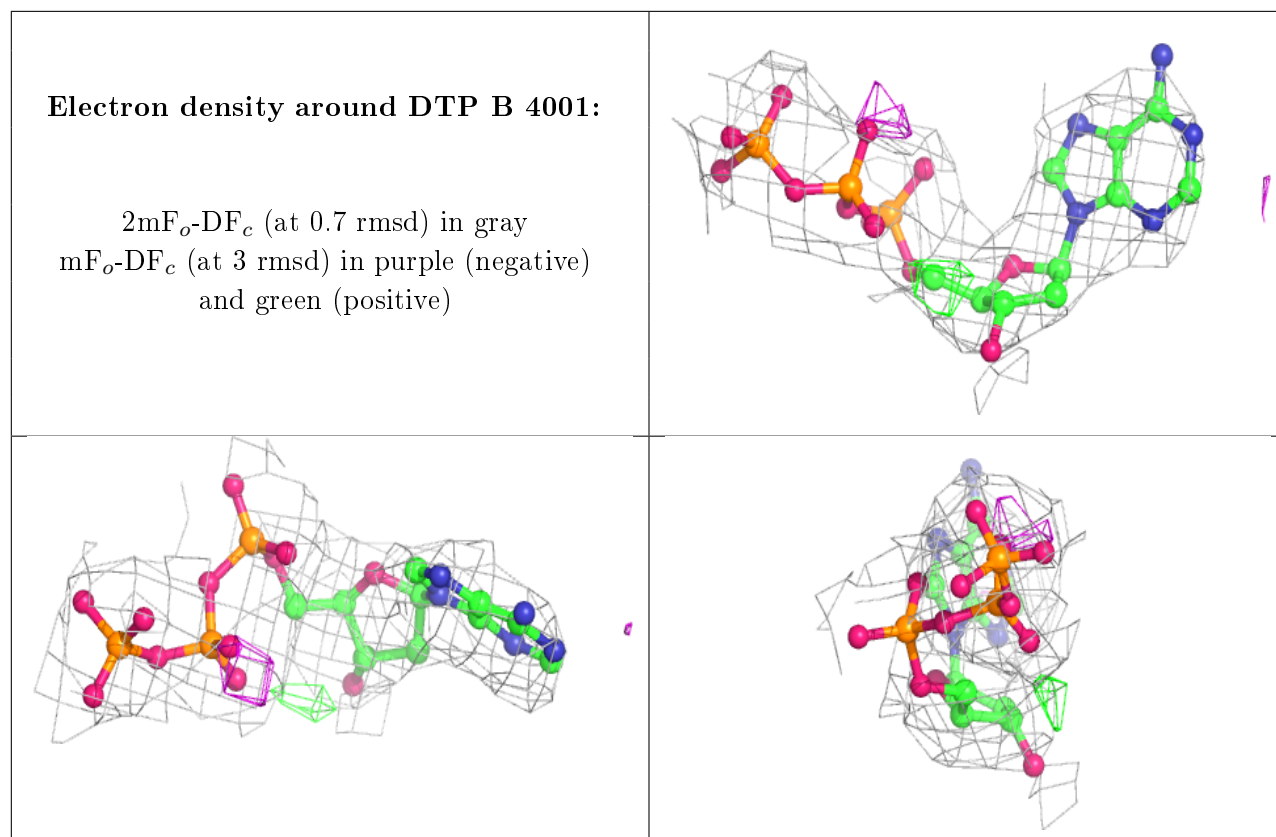
6.4 Ligands ⓘ

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	1001	1/1	0.60	0.17	82,82,82,82	0
5	CA	B	3001	1/1	0.82	0.12	52,52,52,52	0
6	DTP	A	2001	30/30	0.94	0.22	42,46,49,50	0
6	DTP	B	4001	30/30	0.96	0.21	39,41,43,44	0
5	CA	A	1002	1/1	0.97	0.10	36,36,36,36	0
4	CPT	U	45	3/5	0.97	0.22	76,76,78,79	0
5	CA	B	3002	1/1	0.97	0.11	33,33,33,33	0
4	CPT	T	45	3/5	0.99	0.24	62,62,65,65	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.