



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 08:58 am BST

PDB ID : 3PZP
Title : Human DNA polymerase kappa extending opposite a cis-syn thymine dimer
Authors : Vasquez-Del Carpio, R.; Silverstein, T.D.; Lone, S.; Johnson, R.E.; Prakash, S.; Prakash, L.; Aggarwal, A.K.
Deposited on : 2010-12-14
Resolution : 3.34 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

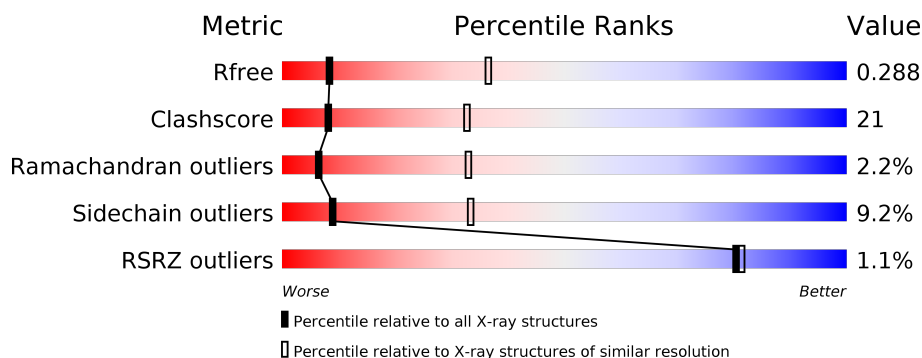
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.34 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	1060 (3.38-3.30)
Clashscore	141614	1111 (3.38-3.30)
Ramachandran outliers	138981	1090 (3.38-3.30)
Sidechain outliers	138945	1089 (3.38-3.30)
RSRZ outliers	127900	1028 (3.38-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	A	517	<div> <div>%</div> <div> <div></div> <div>51%</div> <div>30%</div> <div>•</div> <div>15%</div> </div> </div>
1	B	517	<div> <div>%</div> <div> <div></div> <div>54%</div> <div>27%</div> <div>•</div> <div>14%</div> </div> </div>
2	P	13	<div> <div></div> <div>31%</div> <div>62%</div> <div>8%</div> </div>
2	Q	13	<div> <div></div> <div>38%</div> <div>38%</div> <div>15%</div> <div>8%</div> </div>
3	T	17	<div> <div></div> <div>12%</div> <div>47%</div> <div>29%</div> <div>12%</div> </div>
3	U	17	<div> <div></div> <div>29%</div> <div>35%</div> <div>18%</div> <div>18%</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7743 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 kappa.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	440	Total	C	N	O	S	0	0	0
			3352	2105	577	648	22			
1	B	443	Total	C	N	O	S	0	0	0
			3192	1994	546	631	21			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	GLY	-	EXPRESSION TAG	UNP Q9UBT6
A	13	PRO	-	EXPRESSION TAG	UNP Q9UBT6
A	14	GLY	-	EXPRESSION TAG	UNP Q9UBT6
A	15	GLY	-	EXPRESSION TAG	UNP Q9UBT6
A	16	ASP	-	EXPRESSION TAG	UNP Q9UBT6
A	17	PRO	-	EXPRESSION TAG	UNP Q9UBT6
A	18	HIS	-	EXPRESSION TAG	UNP Q9UBT6
B	12	GLY	-	EXPRESSION TAG	UNP Q9UBT6
B	13	PRO	-	EXPRESSION TAG	UNP Q9UBT6
B	14	GLY	-	EXPRESSION TAG	UNP Q9UBT6
B	15	GLY	-	EXPRESSION TAG	UNP Q9UBT6
B	16	ASP	-	EXPRESSION TAG	UNP Q9UBT6
B	17	PRO	-	EXPRESSION TAG	UNP Q9UBT6
B	18	HIS	-	EXPRESSION TAG	UNP Q9UBT6

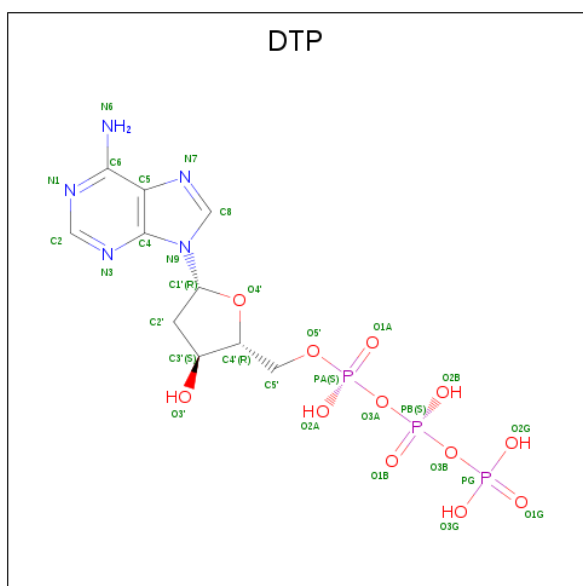
- Molecule 2 is a DNA chain called 5'-D(*GP*GP*GP*GP*GP*AP*AP*GP*GP*AP*CP*CP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	13	Total	C	N	O	P	0	0	0
			272	128	61	71	12			
2	Q	12	Total	C	N	O	P	0	0	0
			250	118	56	65	11			

- Molecule 3 is a DNA chain called 5'-D(*TP*TP*CP*CP*(TTD)P*GP*GP*TP*CP*CP*T
P*TP*CP*CP*CP*CP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	T	15	Total	C	N	O	P	0	0	0
			312	151	47	99	15			
3	U	14	Total	C	N	O	P	0	0	0
			293	142	44	93	14			

- Molecule 4 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (three-letter code: DTP) (formula: $C_{10}H_{16}N_5O_{12}P_3$).



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

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

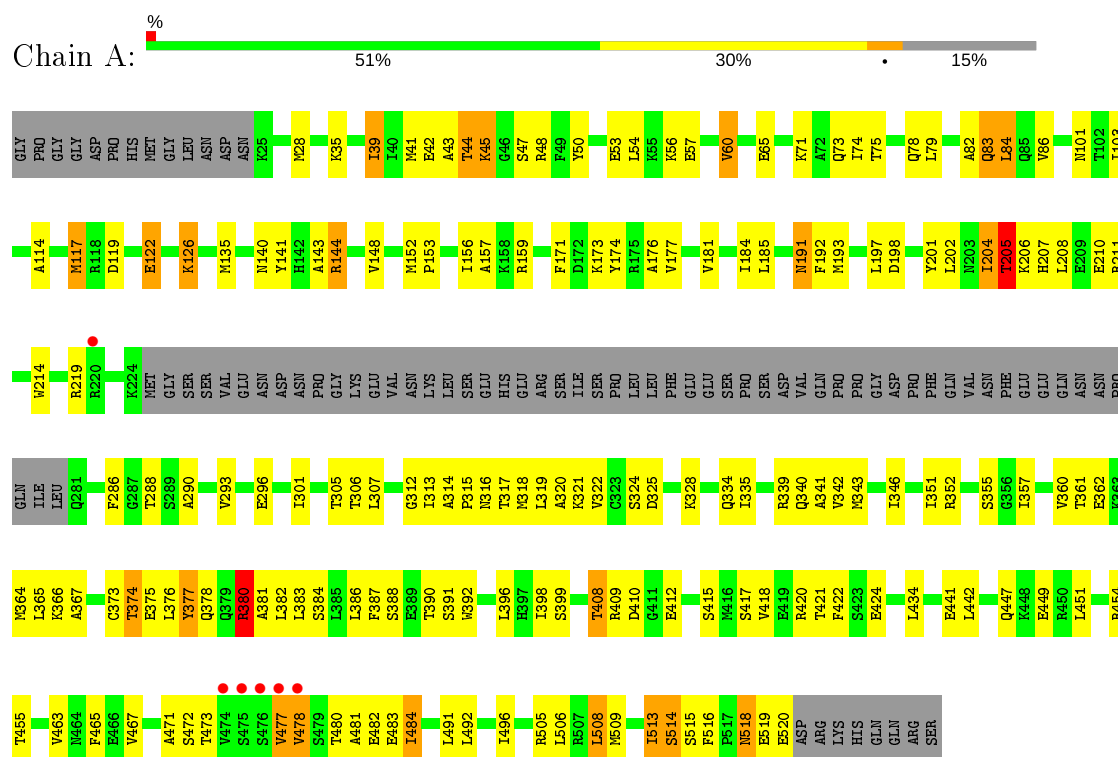
- Molecule 6 is water.

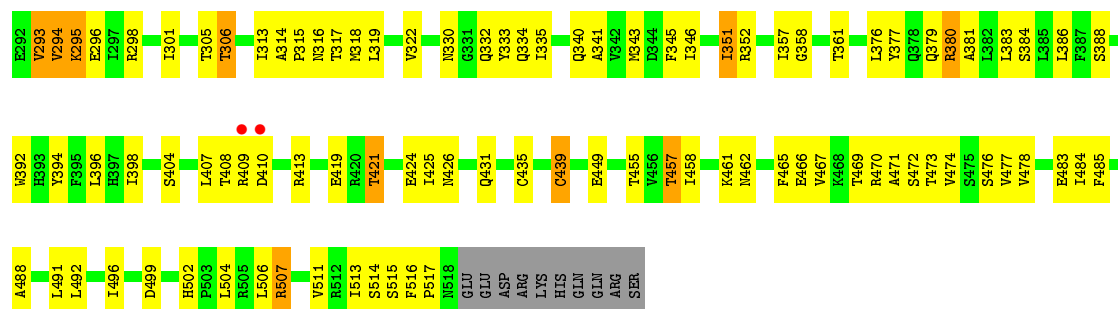
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	5	Total 5	O 5	0	0
6	B	3	Total 3	O 3	0	0

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: DNA polymerase kappa

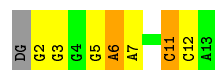




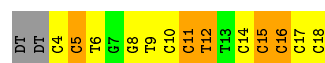
• Molecule 2: 5'-D(*GP*GP*GP*GP*GP*AP*AP*GP*GP*AP*CP*CP*A)-3'



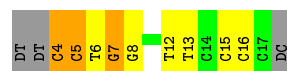
• Molecule 2: 5'-D(*GP*GP*GP*GP*GP*AP*AP*GP*GP*AP*CP*CP*A)-3'



• Molecule 3: 5'-D(*TP*TP*CP*CP*(TTD)P*GP*GP*TP*CP*CP*TP*TP*CP*CP*CP*CP*C)-3'



• Molecule 3: 5'-D(*TP*TP*CP*CP*(TTD)P*GP*GP*TP*CP*CP*TP*TP*CP*CP*CP*CP*C)-3'



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	117.14Å 154.48Å 217.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.67 – 3.34 45.63 – 3.34	Depositor EDS
% Data completeness (in resolution range)	99.2 (46.67-3.34) 99.2 (45.63-3.34)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.53 (at 3.32Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.242 , 0.288 0.244 , 0.288	Depositor DCC
R_{free} test set	1452 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	98.9	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 95.2	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	0.92	EDS
Total number of atoms	7743	wwPDB-VP
Average B, all atoms (Å ²)	118.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% 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: MG, DTP, TTD

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	0.56	0/3403	0.71	1/4607 (0.0%)
1	B	0.47	0/3240	0.63	0/4406
2	P	1.19	0/308	1.63	11/475 (2.3%)
2	Q	0.99	1/283 (0.4%)	1.55	5/436 (1.1%)
3	T	1.17	1/300 (0.3%)	2.13	17/456 (3.7%)
3	U	1.12	1/279 (0.4%)	1.86	10/424 (2.4%)
All	All	0.65	3/7813 (0.0%)	0.96	44/10804 (0.4%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	T	4	DC	C3'-O3'	5.37	1.50	1.44
3	U	12	DT	C1'-N1	5.05	1.55	1.49
2	Q	11	DC	C3'-O3'	-5.03	1.37	1.44

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	U	5	DC	O4'-C4'-C3'	-10.84	99.50	106.00
3	T	15	DC	O4'-C4'-C3'	-10.57	99.66	106.00
3	T	16	DC	O4'-C1'-N1	9.58	114.70	108.00
2	P	4	DG	O4'-C1'-N9	9.08	114.36	108.00
3	T	11	DC	O4'-C1'-N1	9.07	114.35	108.00
3	U	12	DT	O4'-C1'-N1	9.01	114.31	108.00
3	T	5	DC	O5'-P-OP2	-9.01	97.59	105.70
2	Q	2	DG	P-O3'-C3'	7.22	128.37	119.70
2	P	1	DG	P-O3'-C3'	6.95	128.03	119.70
3	T	12	DT	O4'-C1'-C2'	-6.82	100.45	105.90
3	U	7	DG	O4'-C1'-N9	6.72	112.70	108.00
3	T	4	DC	P-O3'-C3'	6.60	127.62	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	380	ARG	NE-CZ-NH1	6.59	123.60	120.30
2	P	8	DG	O4'-C1'-N9	-6.48	103.46	108.00
2	P	1	DG	O4'-C1'-N9	6.46	112.52	108.00
3	T	4	DC	O4'-C1'-N1	6.46	112.52	108.00
2	Q	11	DC	O4'-C1'-N1	6.35	112.44	108.00
3	U	12	DT	N3-C4-O4	6.35	123.71	119.90
3	T	8	DG	N1-C6-O6	6.15	123.59	119.90
3	U	4	DC	P-O3'-C3'	6.12	127.04	119.70
2	P	8	DG	C1'-O4'-C4'	-6.10	104.00	110.10
2	P	5	DG	O4'-C1'-C2'	-6.04	101.06	105.90
3	T	10	DC	O4'-C1'-N1	5.96	112.17	108.00
3	U	5	DC	C6-N1-C2	-5.94	117.93	120.30
3	T	11	DC	P-O3'-C3'	-5.84	112.69	119.70
3	T	15	DC	P-O3'-C3'	5.79	126.64	119.70
3	T	14	DC	O4'-C1'-N1	5.70	111.99	108.00
3	T	9	DT	O4'-C1'-N1	-5.69	104.01	108.00
3	U	13	DT	N3-C4-O4	5.69	123.31	119.90
2	P	8	DG	O4'-C1'-C2'	-5.59	101.42	105.90
2	P	5	DG	O4'-C1'-N9	5.59	111.91	108.00
2	P	5	DG	C1'-O4'-C4'	-5.57	104.53	110.10
3	U	8	DG	N1-C6-O6	5.54	123.22	119.90
3	U	12	DT	C5-C4-O4	-5.50	121.05	124.90
3	U	13	DT	C5-C4-O4	-5.50	121.05	124.90
2	Q	12	DC	O4'-C1'-N1	5.46	111.83	108.00
2	Q	12	DC	O4'-C4'-C3'	-5.43	102.33	104.50
3	T	4	DC	N1-C2-O2	5.42	122.15	118.90
3	T	12	DT	P-O3'-C3'	5.32	126.08	119.70
3	T	8	DG	C5-C6-O6	-5.25	125.45	128.60
2	Q	6	DA	P-O3'-C3'	-5.16	113.51	119.70
2	P	4	DG	O4'-C1'-C2'	-5.13	101.79	105.90
2	P	12	DC	O4'-C4'-C3'	-5.10	102.46	104.50
3	T	18	DC	O4'-C1'-N1	5.04	111.53	108.00

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	A	3352	0	3229	157	0
1	B	3192	0	2896	141	0
2	P	272	0	143	6	0
2	Q	250	0	132	6	0
3	T	312	0	183	6	0
3	U	293	0	172	5	0
4	A	30	0	12	1	0
4	B	30	0	12	1	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	5	0	0	0	0
6	B	3	0	0	1	0
All	All	7743	0	6779	307	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 21.

All (307) 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:B:457:THR:HG23	1:B:471:ALA:HB2	1.34	1.05
1:B:455:THR:HG22	1:B:473:THR:HB	1.47	0.96
1:A:455:THR:HG23	1:A:515:SER:OG	1.64	0.95
1:B:193:MET:HE2	1:B:408:THR:HG23	1.54	0.90
1:A:83:GLN:HE22	1:A:380:ARG:HH21	1.23	0.87
1:A:382:LEU:HD21	1:A:386:LEU:HD12	1.57	0.86
1:A:143:ALA:HB1	1:A:148:VAL:HG11	1.56	0.86
1:A:378:GLN:HG2	1:B:343:MET:HG2	1.59	0.85
1:B:457:THR:HG23	1:B:471:ALA:CB	2.06	0.84
1:B:473:THR:HG21	2:Q:5:DG:H3'	1.60	0.84
1:B:457:THR:CG2	1:B:471:ALA:HB2	2.07	0.83
1:B:478:VAL:HG13	1:B:483:GLU:HB3	1.60	0.82
1:A:35:LYS:O	1:A:39:ILE:HD13	1.79	0.81
1:B:30:GLY:HA3	1:B:31:LEU:HG	1.61	0.81
1:B:288:THR:O	1:B:288:THR:HG22	1.80	0.80
1:A:382:LEU:CD2	1:A:386:LEU:HD12	2.12	0.79
1:B:455:THR:HG22	1:B:473:THR:CB	2.12	0.79
1:B:193:MET:HE2	1:B:408:THR:CG2	2.13	0.78
1:A:117:MET:CE	1:A:140:ASN:HD22	1.98	0.76
1:B:127:PRO:HA	1:B:140:ASN:HD21	1.50	0.76
1:B:24:ASN:HD21	1:B:33:LYS:NZ	1.83	0.76
1:B:408:THR:HG23	1:B:410:ASP:HB3	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:519:GLU:O	1:A:520:GLU:HB2	1.87	0.75
1:A:82:ALA:O	1:A:86:VAL:HG23	1.87	0.74
1:B:57:GLU:O	1:B:60:VAL:HG12	1.86	0.74
1:B:496:ILE:HD13	1:B:504:LEU:HD22	1.69	0.74
1:A:319:LEU:HD11	1:A:342:VAL:HG13	1.70	0.74
1:B:20:GLY:HA2	1:B:41:MET:CE	2.19	0.72
1:B:317:THR:HG23	1:B:404:SER:O	1.89	0.72
1:A:382:LEU:HD21	1:A:386:LEU:CD1	2.20	0.72
1:A:516:PHE:HE1	1:A:518:ASN:HB3	1.54	0.72
1:A:201:TYR:C	1:A:202:LEU:HD12	2.11	0.71
1:A:57:GLU:HA	1:A:60:VAL:HG23	1.71	0.71
1:B:408:THR:HG23	1:B:410:ASP:CB	2.21	0.70
1:B:478:VAL:HG13	1:B:483:GLU:CB	2.22	0.70
1:A:318:MET:SD	1:A:398:ILE:HG23	2.31	0.70
1:A:380:ARG:HD2	1:A:381:ALA:N	2.06	0.69
1:A:114:ALA:HB1	1:A:307:LEU:HD22	1.74	0.69
1:A:384:SER:HA	1:A:392:TRP:CG	2.27	0.69
1:B:473:THR:O	1:B:473:THR:HG23	1.91	0.69
1:A:117:MET:HE3	1:A:140:ASN:HD22	1.58	0.69
1:B:425:ILE:O	1:B:431:GLN:NE2	2.25	0.68
1:B:170:ASN:HB3	1:B:173:LYS:HD3	1.75	0.68
1:B:496:ILE:HD13	1:B:504:LEU:HD13	1.75	0.67
1:A:351:ILE:HD12	1:A:376:LEU:HD13	1.77	0.67
1:A:351:ILE:HD13	1:A:365:LEU:HD12	1.78	0.66
1:B:24:ASN:HD22	1:B:24:ASN:N	1.91	0.66
1:A:50:TYR:CE2	1:A:54:LEU:HD22	2.31	0.66
1:B:496:ILE:CD1	1:B:504:LEU:HD22	2.26	0.65
1:A:173:LYS:O	1:A:176:ALA:HB3	1.96	0.65
3:T:6:TTD:H2'	3:T:6:TTD:O4R	1.97	0.65
1:B:211:ARG:HB3	1:B:288:THR:HG23	1.78	0.65
1:A:351:ILE:CD1	1:A:365:LEU:HD12	2.27	0.65
1:A:83:GLN:HE22	1:A:380:ARG:NH2	1.94	0.65
1:B:318:MET:O	1:B:322:VAL:HG23	1.97	0.64
1:A:422:PHE:CE2	1:A:434:LEU:HD21	2.33	0.64
1:B:89:PHE:CE2	1:B:93:LEU:HD12	2.33	0.63
1:B:294:VAL:O	1:B:294:VAL:HG12	1.99	0.63
1:A:210:GLU:OE1	1:A:214:TRP:CD1	2.51	0.63
1:B:193:MET:CE	1:B:407:LEU:HD12	2.29	0.63
1:B:396:LEU:O	1:B:396:LEU:HD12	1.99	0.62
3:T:15:DC:H2'	3:T:16:DC:C6	2.33	0.62
1:A:318:MET:O	1:A:322:VAL:HG23	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:GLY:HA2	1:B:41:MET:HE1	1.81	0.61
1:B:431:GLN:NE2	1:B:504:LEU:O	2.32	0.61
1:A:473:THR:HG22	2:P:6:DA:P	2.41	0.61
1:B:380:ARG:HA	1:B:383:LEU:HD12	1.83	0.61
1:B:20:GLY:HA2	1:B:41:MET:HE3	1.82	0.60
1:A:204:ILE:HD12	1:A:293:VAL:HG21	1.82	0.60
1:B:492:LEU:O	1:B:492:LEU:HD23	2.01	0.60
1:B:288:THR:CG2	1:B:288:THR:O	2.49	0.60
1:A:473:THR:HG22	2:P:6:DA:OP1	2.00	0.60
1:A:378:GLN:HG2	1:B:343:MET:CG	2.31	0.60
1:B:143:ALA:HB1	1:B:148:VAL:HG11	1.83	0.59
1:B:343:MET:O	1:B:346:ILE:HG22	2.02	0.59
1:A:197:LEU:H	1:A:197:LEU:HD12	1.66	0.59
1:A:191:ASN:OD1	1:A:191:ASN:N	2.36	0.59
1:B:283:SER:O	1:B:284:VAL:HG13	2.02	0.59
2:P:8:DG:H2''	2:P:9:DG:H5'	1.83	0.59
3:U:15:DC:H4'	3:U:16:DC:OP1	2.02	0.59
1:A:210:GLU:OE1	1:A:210:GLU:C	2.42	0.58
1:A:377:TYR:O	1:A:380:ARG:HG3	2.04	0.57
1:B:170:ASN:HB3	1:B:173:LYS:CD	2.35	0.57
1:A:472:SER:HB2	1:A:491:LEU:HD21	1.86	0.57
1:A:184:ILE:HD12	1:A:301:ILE:HG12	1.87	0.57
1:A:210:GLU:OE1	1:A:214:TRP:NE1	2.37	0.57
1:A:202:LEU:HD12	1:A:202:LEU:N	2.20	0.57
1:B:516:PHE:HB3	1:B:517:PRO:HD2	1.86	0.57
1:A:117:MET:HE1	1:A:140:ASN:HD22	1.68	0.57
1:B:351:ILE:HG23	1:B:352:ARG:N	2.20	0.57
1:A:204:ILE:HG13	1:A:208:LEU:HD12	1.86	0.56
1:A:41:MET:O	1:A:42:GLU:C	2.43	0.56
1:B:492:LEU:C	1:B:492:LEU:HD23	2.26	0.56
1:A:455:THR:HG23	1:A:515:SER:HG	1.69	0.56
2:P:8:DG:H2''	2:P:9:DG:C5'	2.36	0.56
1:A:417:SER:O	1:A:418:VAL:HG23	2.06	0.55
1:A:463:VAL:HG12	1:A:463:VAL:O	2.07	0.55
1:A:83:GLN:OE1	1:A:381:ALA:HB2	2.05	0.55
1:B:458:ILE:HG22	1:B:511:VAL:HG22	1.87	0.55
1:A:207:HIS:NE2	1:A:211:ARG:HD2	2.21	0.55
1:B:193:MET:HE1	1:B:407:LEU:HD12	1.88	0.55
1:B:478:VAL:CG1	1:B:483:GLU:HB3	2.35	0.55
1:A:380:ARG:HH11	1:A:380:ARG:HG3	1.71	0.55
1:A:516:PHE:CE1	1:A:518:ASN:HB3	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:ILE:CD1	1:A:376:LEU:HD13	2.37	0.55
1:A:340:GLN:O	1:A:343:MET:N	2.40	0.55
1:A:346:ILE:O	1:A:373:CYS:HB2	2.07	0.55
1:B:30:GLY:CA	1:B:31:LEU:HG	2.36	0.55
1:B:136:LEU:HD22	1:B:166:ILE:HD12	1.88	0.54
1:A:357:ILE:HG23	1:A:361:THR:CG2	2.37	0.54
1:A:480:THR:O	1:A:484:ILE:HG23	2.07	0.54
1:A:177:VAL:O	1:A:181:VAL:HG13	2.07	0.54
1:B:193:MET:CE	1:B:407:LEU:CD1	2.86	0.54
1:B:132:SER:CA	1:B:166:ILE:HD11	2.38	0.53
1:B:143:ALA:HB1	1:B:148:VAL:CG1	2.38	0.53
1:B:135:MET:HA	1:B:153:PRO:HA	1.91	0.53
1:A:141:TYR:HA	1:A:144:ARG:HD3	1.90	0.53
1:A:471:ALA:HB3	2:P:6:DA:C2'	2.38	0.53
1:A:79:LEU:HD23	1:A:83:GLN:HG2	1.90	0.53
1:A:321:LYS:HD2	1:A:355:SER:HB2	1.90	0.53
1:B:384:SER:HA	1:B:392:TRP:CD1	2.44	0.53
1:A:380:ARG:HH11	1:A:380:ARG:CG	2.22	0.53
1:B:516:PHE:HB3	1:B:517:PRO:CD	2.39	0.52
1:B:473:THR:CG2	2:Q:5:DG:H3'	2.37	0.52
1:A:513:ILE:HD12	1:A:514:SER:N	2.24	0.52
1:B:103:ILE:HD13	1:B:203:ASN:HA	1.92	0.52
1:B:409:ARG:N	1:B:410:ASP:HA	2.23	0.52
1:A:208:LEU:HD11	1:A:290:ALA:HB2	1.90	0.52
1:B:351:ILE:CD1	1:B:376:LEU:HD13	2.39	0.52
1:B:439:CYS:SG	1:B:484:ILE:HG22	2.50	0.52
1:B:419:GLU:HG2	3:U:7:DG:OP2	2.08	0.52
1:B:21:LEU:H	1:B:41:MET:CE	2.22	0.52
1:B:193:MET:HE3	1:B:407:LEU:HD12	1.92	0.52
1:A:103:ILE:HD12	1:A:316:ASN:C	2.31	0.52
1:A:454:ARG:H	1:A:515:SER:HB2	1.75	0.52
1:B:21:LEU:H	1:B:41:MET:HE2	1.75	0.51
1:A:114:ALA:CB	1:A:307:LEU:HD22	2.39	0.51
1:B:113:ALA:H	1:B:138:THR:HG21	1.76	0.51
1:B:413:ARG:NH2	1:B:449:GLU:OE2	2.43	0.51
1:A:101:ASN:HA	1:A:205:THR:OG1	2.11	0.51
1:A:321:LYS:CD	1:A:355:SER:HB2	2.41	0.51
1:A:44:THR:HG22	1:A:50:TYR:HB2	1.91	0.51
1:A:478:VAL:CG1	1:A:484:ILE:HG22	2.40	0.51
1:A:516:PHE:HE1	1:A:518:ASN:CB	2.22	0.50
1:A:508:LEU:HD13	1:A:509:MET:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:ILE:HG21	1:B:160:LEU:HD12	1.94	0.50
1:A:84:LEU:HD11	1:B:95:GLN:CB	2.42	0.50
1:B:357:ILE:HG23	1:B:361:THR:CG2	2.42	0.50
1:B:71:LYS:HA	1:B:74:ILE:HD12	1.94	0.50
1:A:214:TRP:O	1:A:219:ARG:NH1	2.44	0.49
1:B:193:MET:CE	1:B:408:THR:HG22	2.42	0.49
1:B:24:ASN:ND2	1:B:24:ASN:N	2.57	0.49
3:T:5:DC:H5'	3:T:5:DC:H6	1.77	0.49
1:B:458:ILE:O	1:B:469:THR:HA	2.13	0.49
1:A:143:ALA:HB1	1:A:148:VAL:CG1	2.35	0.49
1:B:335:ILE:HD11	1:B:345:PHE:CE2	2.47	0.49
1:A:480:THR:CG2	1:A:483:GLU:HG2	2.43	0.49
1:B:499:ASP:O	1:B:502:HIS:N	2.33	0.49
1:B:193:MET:HE2	1:B:410:ASP:HB3	1.94	0.49
1:B:472:SER:H	1:B:491:LEU:HD11	1.78	0.48
1:A:192:PHE:CD1	1:A:192:PHE:C	2.86	0.48
1:A:364:MET:O	1:A:367:ALA:HB3	2.14	0.48
1:A:204:ILE:HD12	1:A:293:VAL:CG2	2.44	0.48
1:A:319:LEU:HD13	1:A:335:ILE:HD13	1.96	0.48
1:A:290:ALA:HA	1:A:293:VAL:HG22	1.94	0.48
1:B:129:ALA:HB1	1:B:136:LEU:HD13	1.96	0.48
1:B:298:ARG:NH2	1:B:330:ASN:O	2.47	0.48
1:B:193:MET:CE	1:B:408:THR:CG2	2.86	0.48
1:B:129:ALA:CB	1:B:136:LEU:HD13	2.44	0.48
1:A:492:LEU:CD2	1:A:496:ILE:HG13	2.44	0.48
1:B:67:MET:CG	1:B:386:LEU:HD13	2.44	0.48
1:B:504:LEU:HB3	1:B:506:LEU:HD13	1.95	0.48
1:B:305:THR:O	1:B:306:THR:CB	2.61	0.48
1:B:340:GLN:O	1:B:343:MET:N	2.47	0.48
1:B:39:ILE:CG2	1:B:160:LEU:HD12	2.44	0.48
1:A:374:THR:HG22	1:A:375:GLU:N	2.29	0.47
1:A:43:ALA:HB2	1:A:159:ARG:CZ	2.44	0.47
1:A:205:THR:HG22	1:A:206:LYS:N	2.29	0.47
1:A:342:VAL:HG12	1:A:343:MET:CE	2.44	0.47
1:B:435:CYS:SG	1:B:488:ALA:HB1	2.54	0.47
1:A:202:LEU:CD1	1:A:202:LEU:N	2.77	0.47
1:B:379:GLN:O	1:B:381:ALA:N	2.48	0.47
1:A:122:GLU:O	1:A:126:LYS:NZ	2.47	0.47
1:A:513:ILE:HD12	1:A:514:SER:CA	2.44	0.47
1:A:421:THR:HB	3:T:6:TTD:PB	2.55	0.47
1:A:480:THR:HG23	1:A:483:GLU:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:SER:O	1:B:150:ALA:HB1	2.15	0.47
1:B:212:GLN:HA	1:B:288:THR:HG21	1.97	0.47
1:A:79:LEU:CD2	1:A:381:ALA:HB1	2.44	0.47
1:B:455:THR:CG2	1:B:473:THR:OG1	2.63	0.46
1:B:90:ALA:O	1:B:91:MET:C	2.54	0.46
1:A:152:MET:CE	1:A:156:ILE:HG22	2.45	0.46
1:A:383:LEU:HD22	1:A:387:PHE:CE2	2.50	0.46
1:B:314:ALA:HB1	1:B:315:PRO:CD	2.46	0.46
1:B:461:LYS:HG3	1:B:467:VAL:HG23	1.98	0.46
1:A:513:ILE:C	1:A:513:ILE:HD12	2.35	0.46
1:A:339:ARG:O	1:A:343:MET:HG2	2.15	0.46
1:A:39:ILE:CD1	1:A:39:ILE:N	2.79	0.46
1:A:325:ASP:HA	1:A:328:LYS:HG3	1.97	0.46
1:B:290:ALA:O	1:B:293:VAL:HG13	2.15	0.46
1:A:83:GLN:NE2	1:A:380:ARG:HH21	2.03	0.46
1:A:478:VAL:HG12	1:A:483:GLU:HG3	1.98	0.46
2:Q:6:DA:H2''	2:Q:7:DA:H5'	1.98	0.46
1:A:286:PHE:CD1	1:A:296:GLU:HG3	2.51	0.45
1:A:463:VAL:HG23	1:A:505:ARG:O	2.16	0.45
1:B:474:VAL:HG23	1:B:476:SER:O	2.16	0.45
1:A:317:THR:O	1:A:320:ALA:N	2.50	0.45
1:B:196:SER:OG	1:B:197:LEU:N	2.49	0.45
1:A:396:LEU:O	1:A:399:SER:HB2	2.17	0.45
1:A:424:GLU:HA	1:A:506:LEU:O	2.16	0.45
1:A:47:SER:O	1:A:48:ARG:C	2.52	0.45
1:B:358:GLY:HA3	2:Q:11:DC:P	2.56	0.45
1:A:71:LYS:O	1:A:74:ILE:N	2.40	0.45
1:B:118:ARG:NH2	1:B:119:ASP:OD1	2.48	0.45
1:A:340:GLN:O	1:A:341:ALA:C	2.54	0.45
1:B:193:MET:HE3	1:B:407:LEU:CD1	2.47	0.45
1:B:351:ILE:CG2	1:B:352:ARG:N	2.80	0.45
1:B:193:MET:HE1	1:B:407:LEU:HB2	1.98	0.45
1:A:314:ALA:HB1	1:A:315:PRO:CD	2.46	0.45
2:Q:3:DG:O6	3:U:16:DC:N3	2.50	0.45
1:A:377:TYR:C	1:A:377:TYR:CD2	2.90	0.45
1:A:152:MET:HE2	1:A:156:ILE:HG22	1.99	0.44
1:A:204:ILE:O	1:A:205:THR:C	2.55	0.44
1:A:516:PHE:C	1:A:516:PHE:CD1	2.89	0.44
1:B:470:ARG:HA	2:Q:7:DA:OP2	2.17	0.44
1:B:340:GLN:O	1:B:341:ALA:C	2.55	0.44
1:A:185:LEU:HD22	1:A:202:LEU:HD21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:ARG:HD2	1:A:380:ARG:C	2.38	0.44
1:B:485:PHE:CD1	1:B:485:PHE:O	2.70	0.44
1:A:360:VAL:O	1:A:361:THR:C	2.56	0.44
1:B:294:VAL:O	1:B:294:VAL:CG1	2.65	0.44
1:A:463:VAL:HG23	1:A:505:ARG:C	2.36	0.44
1:B:496:ILE:HD13	1:B:504:LEU:CD2	2.44	0.44
1:B:313:ILE:O	1:B:334:GLN:HA	2.18	0.44
1:A:79:LEU:HD21	1:A:381:ALA:HB1	2.00	0.44
1:A:43:ALA:HB2	1:A:159:ARG:NH2	2.33	0.44
1:A:75:THR:HG23	1:A:78:GLN:OE1	2.18	0.44
1:B:23:ASP:C	1:B:24:ASN:HD22	2.19	0.44
1:B:473:THR:O	1:B:473:THR:CG2	2.62	0.44
1:A:420:ARG:NH2	1:A:441:GLU:OE1	2.50	0.44
1:B:408:THR:HG23	1:B:410:ASP:HB2	1.98	0.44
3:U:4:DC:H2''	3:U:5:DC:OP1	2.16	0.43
3:U:6:TTD:H2''	3:U:6:TTD:H6	1.46	0.43
1:A:492:LEU:CD2	1:A:496:ILE:CG1	2.97	0.43
1:B:132:SER:N	1:B:166:ILE:HD11	2.32	0.43
1:A:44:THR:O	1:A:45:LYS:C	2.56	0.43
1:B:394:TYR:O	1:B:398:ILE:HD12	2.19	0.43
1:A:352:ARG:HD3	1:A:362:GLU:OE2	2.19	0.43
1:A:328:LYS:HE2	4:A:1:DTP:PG	2.58	0.43
1:A:422:PHE:CE2	1:A:434:LEU:CD2	3.00	0.43
1:A:449:GLU:CB	1:A:451:LEU:HG	2.49	0.43
1:B:424:GLU:HA	1:B:506:LEU:O	2.19	0.43
1:A:143:ALA:O	1:A:148:VAL:HG12	2.19	0.43
1:A:313:ILE:HG21	1:A:334:GLN:NE2	2.34	0.43
1:B:291:GLN:O	1:B:295:LYS:HG3	2.19	0.43
1:A:211:ARG:HD2	1:A:293:VAL:CG1	2.48	0.43
1:B:87:ASP:CG	1:B:380:ARG:HH12	2.18	0.43
1:B:193:MET:HE1	1:B:407:LEU:CD1	2.47	0.43
1:A:386:LEU:HA	1:A:386:LEU:HD23	1.88	0.43
1:B:294:VAL:O	1:B:332:GLN:NE2	2.52	0.43
1:A:312:GLY:HA3	1:A:324:SER:N	2.34	0.42
1:A:114:ALA:HB1	1:A:307:LEU:CD2	2.45	0.42
1:A:152:MET:CE	1:A:157:ALA:HA	2.48	0.42
1:A:153:PRO:HG2	1:A:156:ILE:HD12	2.02	0.42
2:P:2:DG:H2'	2:P:3:DG:C8	2.54	0.42
1:A:465:PHE:O	1:A:467:VAL:HG23	2.19	0.42
1:A:508:LEU:CD1	1:A:509:MET:N	2.82	0.42
1:A:408:THR:HG22	1:A:409:ARG:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:480:THR:HG22	1:A:483:GLU:CD	2.40	0.42
3:T:11:DC:H2"	3:T:12:DT:C6	2.55	0.42
1:A:305:THR:O	1:A:306:THR:CB	2.68	0.42
1:A:204:ILE:O	1:A:207:HIS:N	2.53	0.42
1:A:378:GLN:CG	1:B:343:MET:HG2	2.42	0.41
1:A:478:VAL:HG12	1:A:484:ILE:HG22	2.01	0.41
1:B:181:VAL:HG13	1:B:301:ILE:HD11	2.02	0.41
1:B:421:THR:HA	1:B:507:ARG:O	2.20	0.41
1:B:461:LYS:HG3	1:B:466:GLU:O	2.19	0.41
1:A:184:ILE:HD12	1:A:301:ILE:CG1	2.49	0.41
1:B:173:LYS:O	1:B:176:ALA:HB3	2.20	0.41
1:B:286:PHE:CD2	1:B:296:GLU:HB2	2.55	0.41
1:A:114:ALA:O	1:A:307:LEU:HD21	2.20	0.41
1:A:318:MET:CE	1:A:398:ILE:HG23	2.51	0.41
1:A:41:MET:O	1:A:44:THR:N	2.53	0.41
1:B:181:VAL:HG13	1:B:301:ILE:CD1	2.50	0.41
1:B:316:ASN:ND2	1:B:319:LEU:HD12	2.36	0.41
1:B:107:ASP:OD1	1:B:108:MET:N	2.54	0.41
1:B:333:TYR:HA	6:B:5:HOH:O	2.20	0.41
1:B:138:THR:HG23	1:B:139:SER:N	2.35	0.41
1:A:342:VAL:HG12	1:A:343:MET:HE1	2.03	0.41
1:A:357:ILE:HG23	1:A:361:THR:HG21	2.02	0.41
1:B:193:MET:HE3	1:B:193:MET:HB2	1.94	0.41
1:A:171:PHE:HA	1:A:174:TYR:CD1	2.56	0.41
1:A:210:GLU:O	1:A:210:GLU:OE1	2.38	0.41
1:B:137:SER:O	4:B:2:DTP:H2'2	2.21	0.41
1:B:37:ASN:O	1:B:41:MET:HG2	2.21	0.41
1:A:86:VAL:HG11	1:A:380:ARG:HD3	2.02	0.40
1:A:480:THR:OG1	1:A:481:ALA:N	2.54	0.40
1:A:53:GLU:O	1:A:56:LYS:N	2.54	0.40
1:B:202:LEU:N	1:B:202:LEU:HD12	2.36	0.40
1:A:152:MET:HE1	1:A:157:ALA:HA	2.03	0.40
1:B:111:PHE:CD2	1:B:198:ASP:HB3	2.56	0.40
1:B:319:LEU:HB3	1:B:335:ILE:HD13	2.04	0.40
1:B:455:THR:HG22	1:B:473:THR:OG1	2.22	0.40
1:A:135:MET:HA	1:A:153:PRO:HA	2.03	0.40
1:B:104:VAL:HG12	1:B:105:HIS:N	2.36	0.40
3:T:16:DC:H2"	3:T:17:DC:C5	2.57	0.40
1:B:24:ASN:HD21	1:B:33:LYS:HZ2	1.67	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	436/517 (84%)	367 (84%)	61 (14%)	8 (2%)	8	37
1	B	439/517 (85%)	367 (84%)	61 (14%)	11 (2%)	5	30
All	All	875/1034 (85%)	734 (84%)	122 (14%)	19 (2%)	6	33

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	477	VAL
1	B	351	ILE
1	B	465	PHE
1	A	410	ASP
1	B	306	THR
1	B	380	ARG
1	A	45	LYS
1	A	83	GLN
1	A	205	THR
1	B	111	PHE
1	A	44	THR
1	A	412	GLU
1	B	148	VAL
1	B	171	PHE
1	B	515	SER
1	A	122	GLU
1	B	211	ARG
1	B	204	ILE
1	B	294	VAL

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	349/460 (76%)	314 (90%)	35 (10%)	7	29
1	B	306/460 (66%)	281 (92%)	25 (8%)	11	39
All	All	655/920 (71%)	595 (91%)	60 (9%)	9	33

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	MET
1	A	39	ILE
1	A	60	VAL
1	A	65	GLU
1	A	73	GLN
1	A	84	LEU
1	A	117	MET
1	A	119	ASP
1	A	126	LYS
1	A	144	ARG
1	A	191	ASN
1	A	193	MET
1	A	198	ASP
1	A	204	ILE
1	A	205	THR
1	A	288	THR
1	A	366	LYS
1	A	374	THR
1	A	377	TYR
1	A	380	ARG
1	A	388	SER
1	A	390	THR
1	A	391	SER
1	A	408	THR
1	A	415	SER
1	A	442	LEU
1	A	447	GLN
1	A	477	VAL
1	A	478	VAL
1	A	482	GLU
1	A	484	ILE
1	A	508	LEU
1	A	513	ILE

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Mol	Chain	Res	Type
1	A	514	SER
1	A	518	ASN
1	B	23	ASP
1	B	24	ASN
1	B	28	MET
1	B	31	LEU
1	B	75	THR
1	B	118	ARG
1	B	135	MET
1	B	138	THR
1	B	166	ILE
1	B	178	SER
1	B	198	ASP
1	B	211	ARG
1	B	293	VAL
1	B	295	LYS
1	B	377	TYR
1	B	388	SER
1	B	421	THR
1	B	426	ASN
1	B	439	CYS
1	B	457	THR
1	B	462	ASN
1	B	477	VAL
1	B	507	ARG
1	B	513	ILE
1	B	514	SER

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

Mol	Chain	Res	Type
1	A	83	GLN
1	A	95	GLN
1	A	212	GLN
1	A	332	GLN
1	A	334	GLN
1	A	518	ASN
1	B	24	ASN
1	B	83	GLN
1	B	120	ASN
1	B	291	GLN
1	B	332	GLN

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Mol	Chain	Res	Type
1	B	334	GLN
1	B	378	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	TTD	U	6	3	42,45,46	1.44	7 (16%)	62,74,77	2.56	13 (20%)
3	TTD	T	6	3	42,45,46	1.48	9 (21%)	62,74,77	2.34	12 (19%)

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	TTD	U	6	3	-	8/22/109/110	0/5/6/6
3	TTD	T	6	3	-	7/22/109/110	0/5/6/6

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	U	6	TTD	C5-C6	-3.82	1.50	1.55
3	U	6	TTD	C1R-N1T	3.60	1.50	1.45
3	T	6	TTD	C2T-N3T	-3.53	1.31	1.38
3	T	6	TTD	C4-N3	-3.36	1.32	1.37
3	U	6	TTD	C2T-N3T	-3.33	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	T	6	TTD	C4T-N3T	-3.19	1.32	1.37
3	T	6	TTD	C5-C6	-3.09	1.51	1.55
3	U	6	TTD	C4T-N3T	-3.08	1.32	1.37
3	U	6	TTD	C2-N3	-2.85	1.32	1.38
3	T	6	TTD	C2-N3	-2.85	1.32	1.38
3	U	6	TTD	C2T-N1T	2.60	1.41	1.36
3	T	6	TTD	C2T-N1T	2.50	1.41	1.36
3	T	6	TTD	C1R-N1T	2.17	1.48	1.45
3	T	6	TTD	C6T-N1T	2.15	1.49	1.46
3	T	6	TTD	O3R-C3R	-2.15	1.41	1.46
3	U	6	TTD	C4-N3	-2.08	1.34	1.37

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	6	TTD	O4R-C1R-N1T	8.89	119.19	108.65
3	U	6	TTD	O4T-C4T-C5T	-7.86	116.60	122.88
3	U	6	TTD	O4R-C1R-N1T	7.37	117.39	108.65
3	U	6	TTD	C2R-C1R-N1T	-7.23	105.82	115.59
3	T	6	TTD	C2'-C1'-N1	-5.96	107.53	115.59
3	U	6	TTD	C5-C4-N3	5.91	121.20	116.06
3	U	6	TTD	O4'-C1'-N1	5.83	115.56	108.65
3	T	6	TTD	O4T-C4T-C5T	-5.75	118.28	122.88
3	U	6	TTD	N3T-C2T-N1T	5.70	122.61	116.69
3	T	6	TTD	C2R-C1R-N1T	-5.53	108.12	115.59
3	T	6	TTD	C5T-C4T-N3T	5.13	120.53	116.06
3	T	6	TTD	N3T-C2T-N1T	4.95	121.83	116.69
3	U	6	TTD	C2'-C1'-N1	-4.55	109.44	115.59
3	T	6	TTD	O4'-C1'-N1	4.42	113.89	108.65
3	T	6	TTD	C4-N3-C2	-4.20	120.22	126.67
3	U	6	TTD	C5T-C4T-N3T	4.17	119.69	116.06
3	U	6	TTD	O4-C4-C5	-3.85	119.80	122.88
3	T	6	TTD	C5-C6-N1	-3.59	110.58	115.61
3	U	6	TTD	O2T-C2T-N1T	-3.39	118.23	123.49
3	T	6	TTD	C5-C4-N3	2.97	118.64	116.06
3	T	6	TTD	O2T-C2T-N1T	-2.84	119.08	123.49
3	U	6	TTD	C5-C5T-C6T	2.35	91.31	88.38
3	T	6	TTD	C5-C5T-C6T	2.26	91.19	88.38
3	U	6	TTD	C5-C6-C6T	2.02	92.61	89.28
3	U	6	TTD	O4T-C4T-N3T	2.01	123.70	120.50

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	U	6	TTD	C3R-O3R-PB-O4P
3	T	6	TTD	C5R-O5R-PB-O5P
3	T	6	TTD	C5R-O5R-PB-O4P
3	T	6	TTD	O4'-C4R-C5'-O5'
3	U	6	TTD	C2'-C1'-N1-C6
3	T	6	TTD	C5R-O5R-PB-O3R
3	T	6	TTD	C3R-C4R-C5'-O5'
3	U	6	TTD	C2'-C1'-N1-C2
3	U	6	TTD	O4'-C1'-N1-C2
3	T	6	TTD	C3'-C4'-C5R-O5R
3	U	6	TTD	O4'-C1'-N1-C6
3	U	6	TTD	C3R-O3R-PB-O5P
3	U	6	TTD	C3R-O3R-PB-O5R
3	U	6	TTD	O4R-C4'-C5R-O5R
3	T	6	TTD	O4R-C4'-C5R-O5R

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	U	6	TTD	1	0
3	T	6	TTD	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 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	1	5	26,32,32	0.95	0	30,50,50	1.39	4 (13%)
4	DTP	B	2	5	26,32,32	0.90	2 (7%)	30,50,50	1.39	4 (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	1	5	-	4/18/34/34	0/3/3/3
4	DTP	B	2	5	-	2/18/34/34	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2	DTP	C5-C4	2.52	1.47	1.40
4	B	2	DTP	C2-N3	2.14	1.35	1.32

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2	DTP	N3-C2-N1	-3.75	122.81	128.68
4	A	1	DTP	C2'-C1'-N9	-3.65	105.86	114.27
4	A	1	DTP	PB-O3B-PG	-3.05	122.35	132.83
4	A	1	DTP	N3-C2-N1	-2.95	124.06	128.68
4	A	1	DTP	C4-C5-N7	-2.30	107.01	109.40
4	B	2	DTP	PB-O3B-PG	-2.23	125.18	132.83
4	B	2	DTP	C4-C5-N7	-2.19	107.12	109.40
4	B	2	DTP	C2-N1-C6	2.12	122.38	118.75

There are no chirality outliers.

All (6) torsion outliers are listed below:

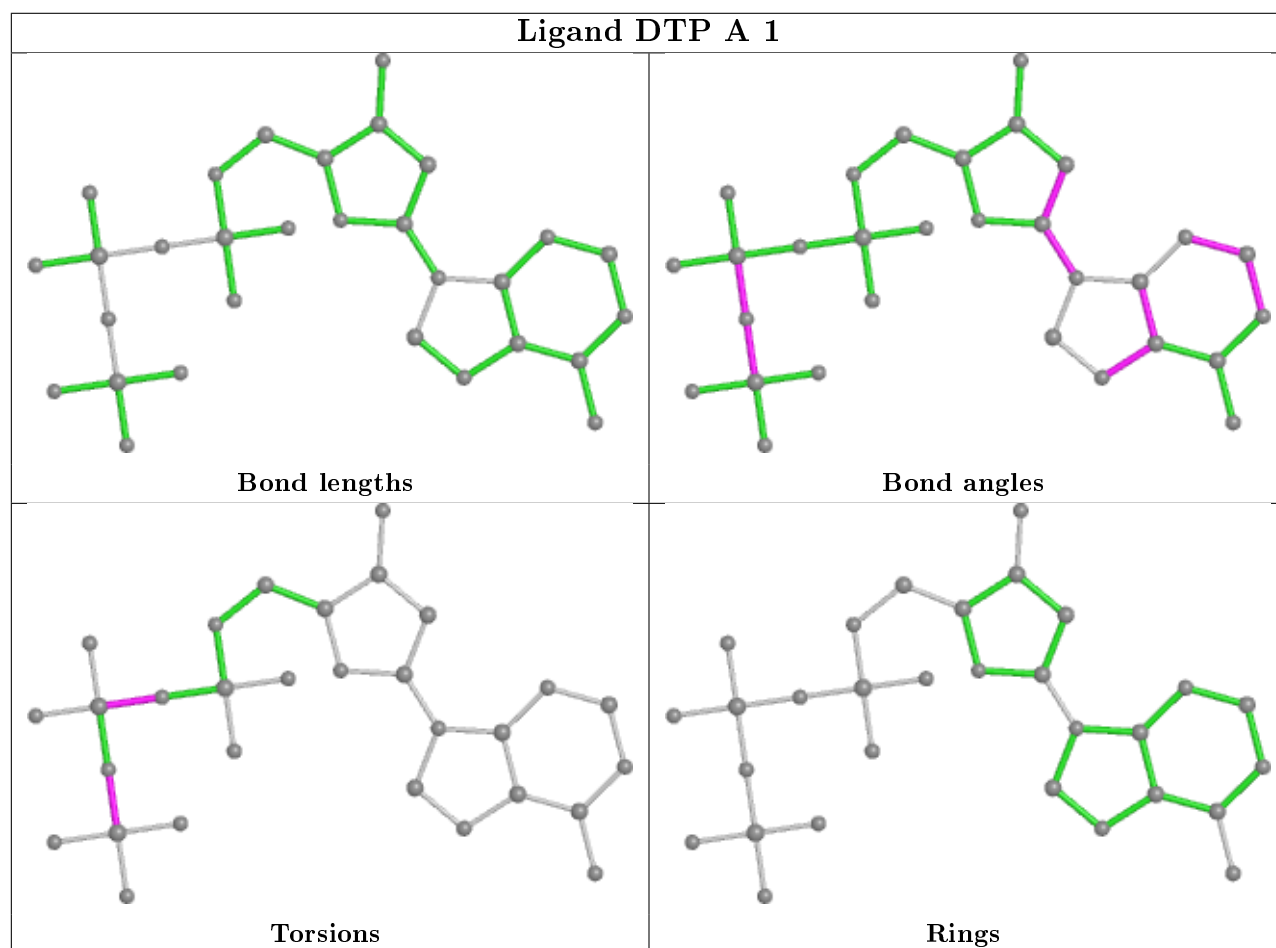
Mol	Chain	Res	Type	Atoms
4	A	1	DTP	PA-O3A-PB-O1B
4	B	2	DTP	PA-O3A-PB-O2B
4	A	1	DTP	PB-O3B-PG-O2G
4	A	1	DTP	PB-O3B-PG-O3G
4	B	2	DTP	PA-O3A-PB-O1B
4	A	1	DTP	PB-O3B-PG-O1G

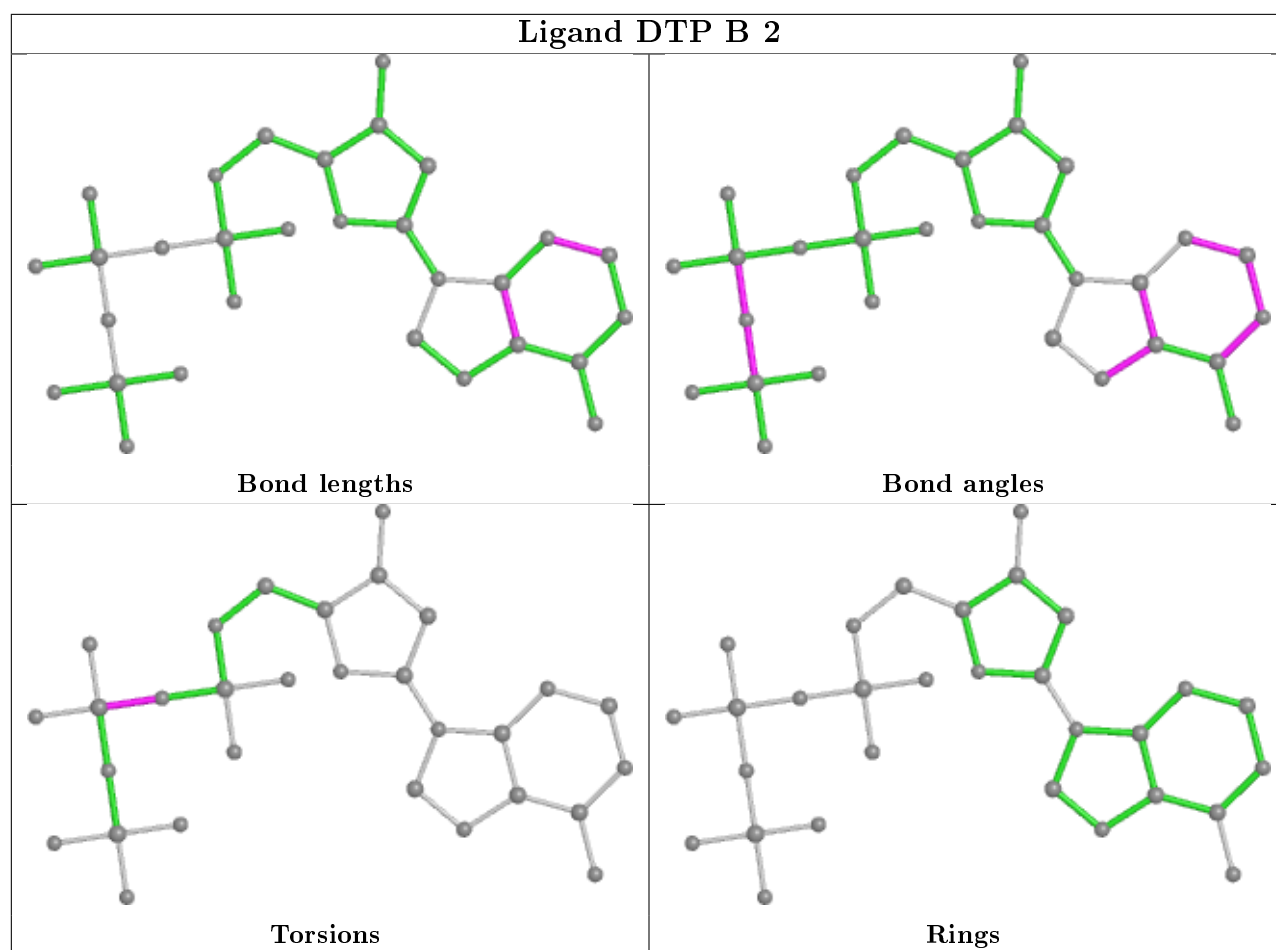
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1	DTP	1	0
4	B	2	DTP	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	440/517 (85%)	-0.08	6 (1%)	75	75	51, 107, 160, 223	0
1	B	443/517 (85%)	-0.19	4 (0%)	84	85	81, 129, 180, 234	0
2	P	13/13 (100%)	-0.04	0	100	100	77, 111, 135, 136	0
2	Q	12/13 (92%)	-0.01	0	100	100	101, 121, 146, 153	0
3	T	14/17 (82%)	-0.08	0	100	100	86, 111, 133, 135	0
3	U	13/17 (76%)	-0.05	0	100	100	104, 122, 147, 147	0
All	All	935/1094 (85%)	-0.13	10 (1%)	80	81	51, 120, 173, 234	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	410	ASP	3.1
1	B	130	VAL	2.6
1	B	409	ARG	2.6
1	A	220	ARG	2.4
1	A	476	SER	2.4
1	A	475	SER	2.4
1	A	477	VAL	2.3
1	A	474	VAL	2.1
1	A	478	VAL	2.1
1	B	22	ASN	2.0

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

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(\AA^2)	Q<0.9
3	TTD	U	6	40/41	0.93	0.23	98,107,111,112	0
3	TTD	T	6	40/41	0.96	0.22	79,85,89,91	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

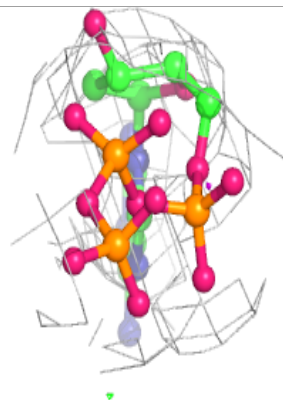
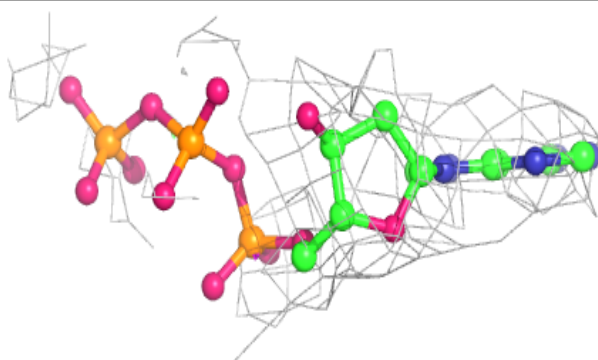
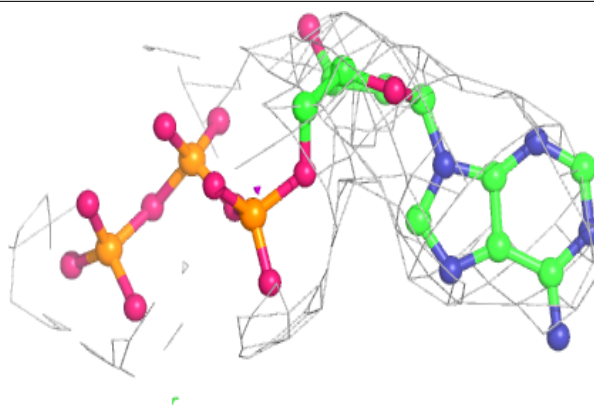
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	MG	B	4	1/1	0.69	0.29	81,81,81,81	0
5	MG	B	1	1/1	0.92	0.13	86,86,86,86	0
5	MG	A	3	1/1	0.94	0.30	76,76,76,76	0
4	DTP	B	2	30/30	0.94	0.18	112,116,121,121	0
4	DTP	A	1	30/30	0.98	0.21	72,75,77,77	0
5	MG	A	2	1/1	0.99	0.17	70,70,70,70	0

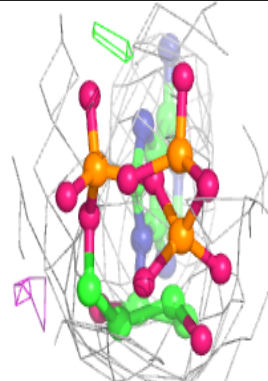
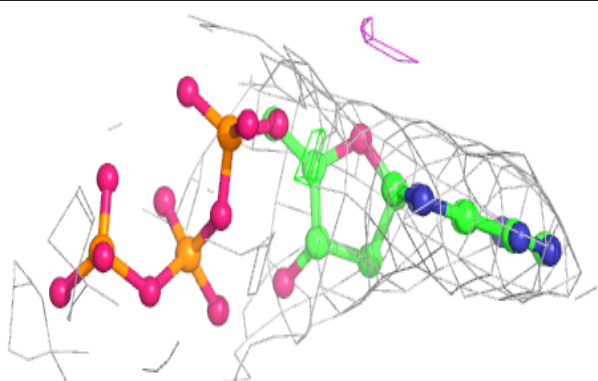
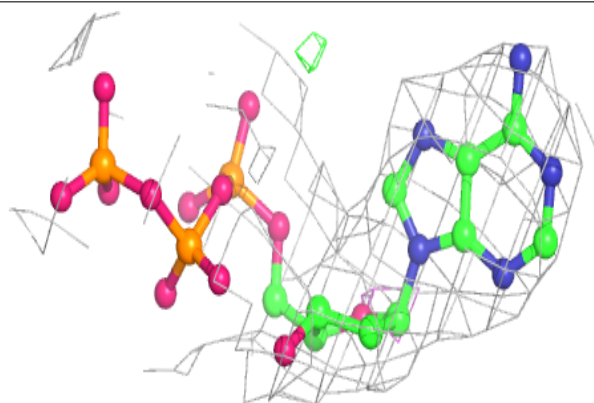
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DTP B 2:

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

**Electron density around DTP A 1:**

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



6.5 Other polymers

There are no such residues in this entry.