Full wwPDB X-ray Structure Validation Report ⓘ

Aug 28, 2023 – 04:48 AM EDT

PDB ID	:	3K5L
Title	:	Crystal structure of E.coli Pol II-abasic DNA-dATP Lt(0, 3) ternary complex
Authors	:	Yang, W.; Wang, F.
Deposited on	:	2009-10-07
Resolution	:	2.70 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:

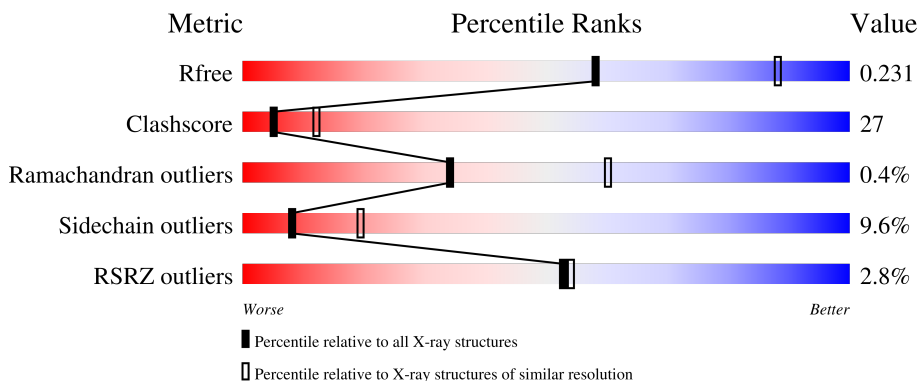|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.70 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	Percentile Ranks	Value
Rfree		0.231
Clashscore		27
Ramachandran outliers		0.4%
Sidechain outliers		9.6%
RSRZ outliers		2.8%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 <=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	786	2% / 55% / 39% / 5% ··
2	T	18	17% / 39% / 56% / 6%
3	P	13	8% / 23% / 62% / 15%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7057 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 II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	781	Total 6331	C 4030	N 1130	O 1147	S 24	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P21189
A	-1	PRO	-	expression tag	UNP P21189
A	0	HIS	-	expression tag	UNP P21189
A	335	ASN	ASP	engineered mutation	UNP P21189

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	18	Total 357	C 171	N 65	O 104	P 17	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	13	Total 262	C 126	N 48	O 76	P 12	0	0	0

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

DTP

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

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

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	64	Total 64	O 64	0	0
6	T	8	Total 8	O 8	0	0
6	P	3	Total 3	O 3	0	0

3 Residue-property plots ⓘ

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.
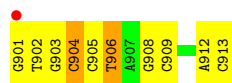
• Molecule 1: DNA polymerase II
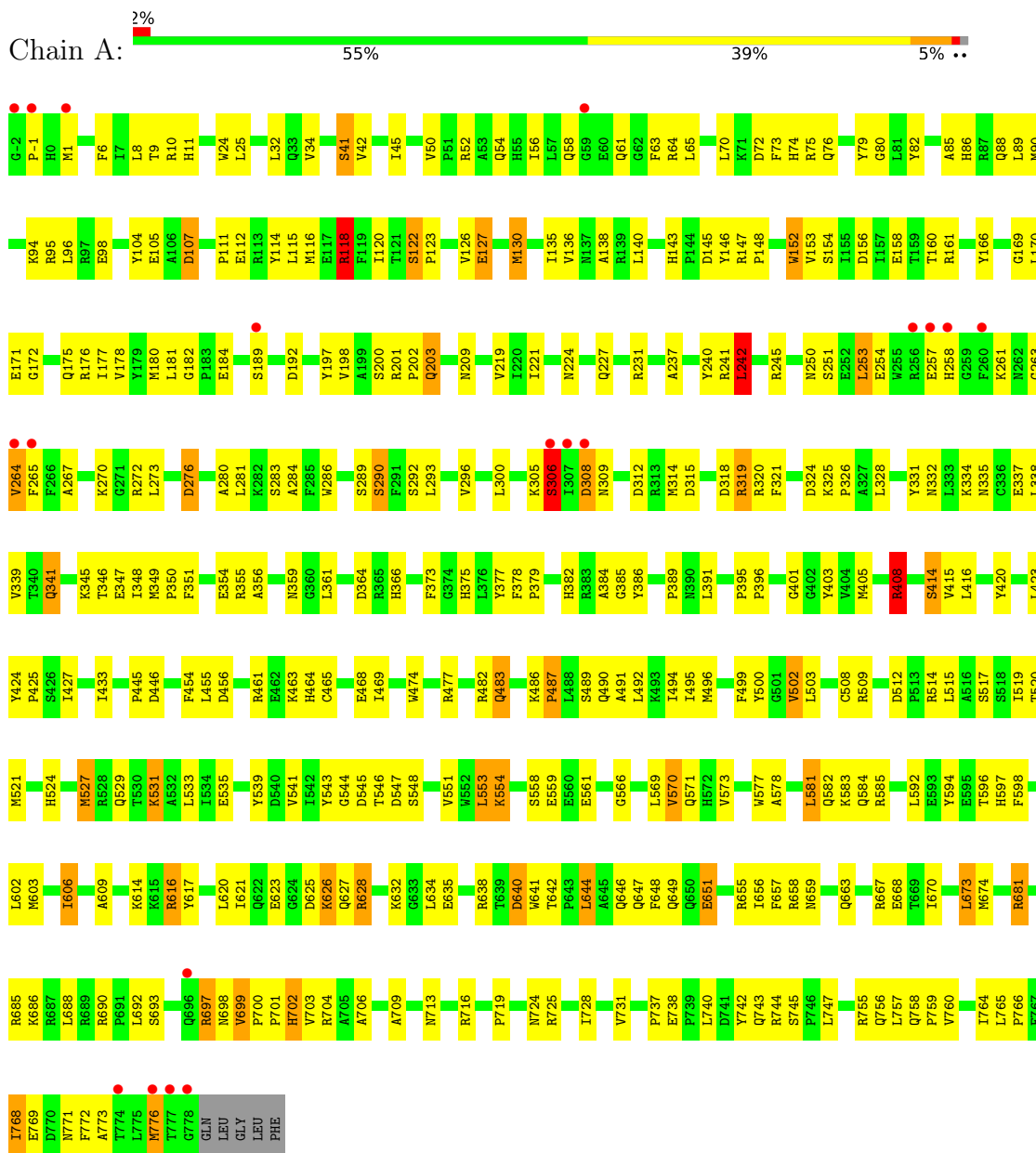
• Molecule 2: DNA (5'-D(*TP*AP*TP*(3DR)P*GP*TP*AP*CP*GP*CP*TP*AP*GP*GP*CP *AP*CP*A)-3')

Chain T:

17%

| 39% | 56% | 6% |

T801 A802 T803 T806 A807 C808 G809 C810 T811 A812 G813 G814 C815 A816 C817 A818

• Molecule 3: DNA (5'-D(*GP*TP*GP*CP*CP*TP*AP*GP*CP*GP*TP*AP*(DOC))-3')

Chain P:

8%

| 23% | 62% | 15% |

G901 T902 G903 C904 C905 T906 A907 G908 C909 A912 C913

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	79.97Å 101.20Å 121.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	22.42 – 2.70 29.14 – 2.71	Depositor EDS
% Data completeness (in resolution range)	78.6 (22.42-2.70) 79.2 (29.14-2.71)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.32 (at 2.72Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.224 , 0.241 0.215 , 0.231	Depositor DCC
R_{free} test set	600 reflections (2.50%)	wwPDB-VP
Wilson B-factor (Å²)	22.3	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.34 , 35.0	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	7057	wwPDB-VP
Average B, all atoms (Å²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 3DR, DTP, DOC, MG

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	0.66	1/6501 (0.0%)	0.94	13/8819 (0.1%)
2	T	0.56	0/387	1.06	1/593 (0.2%)
3	P	0.62	0/273	1.05	1/420 (0.2%)
All	All	0.65	1/7161 (0.0%)	0.95	15/9832 (0.2%)

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
1	A	0	1
3	P	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	152	TRP	CB-CG	-5.67	1.40	1.50

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	118	ARG	NE-CZ-NH2	-13.25	113.67	120.30
1	A	776	MET	N-CA-C	8.95	135.16	111.00
1	A	309	ASN	N-CA-C	-8.56	87.90	111.00
1	A	391	LEU	CA-CB-CG	7.80	133.24	115.30
1	A	122	SER	C-N-CD	-7.02	105.15	120.60
1	A	308	ASP	N-CA-C	6.66	128.98	111.00
1	A	182	GLY	C-N-CD	-6.52	106.26	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	118	ARG	CG-CD-NE	-6.23	98.71	111.80
2	T	815	DC	C1'-O4'-C4'	-5.56	104.54	110.10
1	A	306	SER	N-CA-C	-5.46	96.25	111.00
1	A	242	LEU	CB-CG-CD2	-5.42	101.79	111.00
1	A	408	ARG	N-CA-C	-5.39	96.45	111.00
1	A	688	LEU	N-CA-C	-5.32	96.63	111.00
1	A	553	LEU	N-CA-C	-5.14	97.13	111.00
3	P	906	DT	C3'-C2'-C1'	-5.05	96.43	102.50

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	118	ARG	Sidechain
3	P	904	DC	Sidechain

5.2   Too-close contacts (i)

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	6331	0	6193	336	0
2	T	357	0	201	20	0
3	P	262	0	148	18	0
4	A	30	0	12	3	0
5	A	2	0	0	0	0
6	A	64	0	0	1	0
6	P	3	0	0	1	0
6	T	8	0	0	0	0
All	All	7057	0	6554	363	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 27.

All (363) 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:699:VAL:HG23	2:T:814:DG:OP1	1.46	1.13
1:A:245:ARG:HG2	1:A:245:ARG:HH11	1.06	1.09
1:A:673:LEU:O	1:A:673:LEU:HD12	1.56	1.05
1:A:490:GLN:O	1:A:494:ILE:HD13	1.59	1.03
3:P:912:DA:H2"	3:P:913:DOC:H5'	1.44	0.99
1:A:54:GLN:HG2	1:A:54:GLN:O	1.62	0.98
3:P:904:DC:H2"	3:P:905:DC:O5'	1.65	0.96
3:P:901:DG:H2'	3:P:902:DT:H72	1.49	0.94
1:A:258:HIS:HB3	1:A:261:LYS:O	1.68	0.93
1:A:623:GLU:OE2	1:A:628:ARG:HD3	1.69	0.93
1:A:408:ARG:HG3	1:A:408:ARG:HH11	1.34	0.92
1:A:200:SER:HB3	1:A:203:GLN:OE1	1.69	0.92
1:A:58:GLN:HG3	1:A:58:GLN:O	1.68	0.91
3:P:906:DT:H3'	6:P:76:HOH:O	1.70	0.90
1:A:245:ARG:HG2	1:A:245:ARG:NH1	1.70	0.90
1:A:698:ASN:HB3	1:A:700:PRO:HD3	1.54	0.89
1:A:771:ASN:OD1	1:A:773:ALA:HB3	1.71	0.89
3:P:901:DG:H2'	3:P:902:DT:C7	2.03	0.88
1:A:527:MET:HE2	1:A:527:MET:HA	1.56	0.87
1:A:577:TRP:O	1:A:581:LEU:HB2	1.74	0.86
1:A:90:MET:HA	1:A:90:MET:HE2	1.61	0.82
1:A:237:ALA:HB1	1:A:242:LEU:O	1.80	0.82
1:A:169:GLY:O	1:A:170:LEU:HD23	1.79	0.81
1:A:126:VAL:HG23	1:A:140:LEU:HD23	1.61	0.81
1:A:554:LYS:H	1:A:554:LYS:HD2	1.48	0.79
1:A:143:HIS:CD2	1:A:146:TYR:HB2	2.18	0.79
1:A:414:SER:HB3	1:A:597:HIS:HE1	1.48	0.79
1:A:171:GLU:OE1	1:A:337:GLU:HA	1.84	0.77
1:A:126:VAL:HG23	1:A:140:LEU:CD2	2.14	0.77
1:A:627:GLN:NE2	1:A:658:ARG:HE	1.82	0.77
2:T:801:DT:H5"	2:T:803:DT:OP1	1.84	0.76
1:A:647:GLN:HE22	1:A:681:ARG:NH1	1.83	0.76
1:A:566:GLY:O	1:A:570:VAL:HG13	1.86	0.75
1:A:34:VAL:CG1	1:A:138:ALA:CB	2.64	0.75
1:A:647:GLN:HE22	1:A:681:ARG:CZ	1.99	0.75
1:A:198:VAL:HB	1:A:203:GLN:HB3	1.69	0.74
1:A:181:LEU:HD22	1:A:201:ARG:HG3	1.68	0.74
1:A:401:GLY:O	1:A:524:HIS:HE1	1.70	0.74
1:A:627:GLN:HE22	1:A:658:ARG:HE	1.35	0.74
1:A:219:VAL:HG12	1:A:221:ILE:HG23	1.68	0.74
1:A:517:SER:O	1:A:521:MET:HB2	1.87	0.73
1:A:697:ARG:H	1:A:697:ARG:HD2	1.52	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:PHE:O	1:A:325:LYS:HE3	1.89	0.73
1:A:616:ARG:HG2	1:A:634:LEU:HD21	1.71	0.72
2:T:801:DT:C5'	2:T:803:DT:OP1	2.38	0.72
1:A:423:LEU:HD22	1:A:547:ASP:HB3	1.71	0.72
1:A:554:LYS:HD2	1:A:554:LYS:N	2.04	0.72
1:A:616:ARG:HG2	1:A:634:LEU:CD2	2.20	0.72
1:A:483:GLN:HG3	6:A:802:HOH:O	1.88	0.72
1:A:258:HIS:HA	1:A:264:VAL:O	1.90	0.72
1:A:337:GLU:O	1:A:341:GLN:HG3	1.90	0.72
2:T:815:DC:H2"	2:T:816:DA:C8	2.26	0.71
1:A:319:ARG:HH11	1:A:319:ARG:CG	2.03	0.70
1:A:602:LEU:HD22	1:A:764:ILE:HD12	1.74	0.70
1:A:673:LEU:HD12	1:A:673:LEU:C	2.10	0.70
1:A:321:PHE:O	1:A:325:LYS:CE	2.40	0.69
1:A:-1:PRO:O	1:A:130:MET:N	2.23	0.69
1:A:41:SER:HB3	1:A:89:LEU:HD22	1.73	0.69
1:A:647:GLN:NE2	1:A:681:ARG:NH1	2.41	0.69
1:A:258:HIS:NE2	1:A:265:PHE:CZ	2.61	0.69
1:A:355:ARG:HH22	1:A:366:HIS:HD2	1.40	0.68
1:A:616:ARG:HG3	1:A:634:LEU:HD23	1.75	0.68
1:A:702:HIS:HB2	1:A:728:ILE:HG21	1.76	0.68
1:A:111:PRO:HD2	1:A:112:GLU:OE1	1.92	0.68
1:A:408:ARG:HG3	1:A:408:ARG:NH1	2.00	0.68
1:A:616:ARG:CG	1:A:634:LEU:HD23	2.24	0.68
1:A:200:SER:OG	1:A:202:PRO:HD2	1.94	0.67
1:A:697:ARG:HG2	1:A:698:ASN:N	2.10	0.67
1:A:403:TYR:CE2	1:A:405:MET:HG2	2.30	0.66
1:A:731:VAL:HG13	1:A:740:LEU:CD1	2.27	0.65
1:A:544:GLY:HA2	1:A:548:SER:O	1.95	0.65
1:A:34:VAL:HG13	1:A:138:ALA:HB2	1.79	0.65
1:A:416:LEU:CD1	1:A:553:LEU:HD11	2.27	0.65
1:A:503:LEU:HD22	1:A:515:LEU:HD13	1.78	0.64
1:A:10:ARG:HG3	1:A:10:ARG:HH11	1.61	0.64
1:A:90:MET:HA	1:A:90:MET:CE	2.27	0.64
1:A:147:ARG:NH2	1:A:354:GLU:OE1	2.29	0.64
1:A:86:HIS:O	1:A:90:MET:HG2	1.96	0.63
1:A:245:ARG:HH11	1:A:245:ARG:CG	1.90	0.63
1:A:651:GLU:O	1:A:655:ARG:HG3	1.98	0.63
1:A:491:ALA:O	1:A:495:ILE:HG13	1.99	0.63
1:A:656:ILE:HD13	1:A:768:ILE:CD1	2.29	0.62
1:A:403:TYR:HD2	1:A:527:MET:HG2	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:697:ARG:H	1:A:697:ARG:CD	2.11	0.62
1:A:154:SER:HA	1:A:221:ILE:HG13	1.80	0.62
1:A:512:ASP:OD2	1:A:514:ARG:HB2	1.99	0.62
1:A:649:GLN:HG3	1:A:760:VAL:HG13	1.81	0.62
1:A:403:TYR:CD2	1:A:527:MET:HG2	2.35	0.62
1:A:319:ARG:NH1	1:A:319:ARG:HG2	2.14	0.62
1:A:699:VAL:N	1:A:700:PRO:CD	2.62	0.62
1:A:160:THR:HG22	1:A:166:TYR:CZ	2.36	0.61
1:A:638:ARG:O	1:A:646:GLN:NE2	2.33	0.61
1:A:143:HIS:HD2	1:A:146:TYR:H	1.47	0.61
1:A:765:LEU:N	1:A:766:PRO:HD2	2.16	0.61
1:A:176:ARG:HH22	1:A:192:ASP:HB2	1.64	0.61
1:A:702:HIS:H	1:A:702:HIS:CD2	2.19	0.60
1:A:306:SER:CB	1:A:331:TYR:HD1	2.14	0.60
1:A:658:ARG:O	1:A:659:ASN:HB2	2.00	0.60
1:A:414:SER:HA	1:A:598:PHE:O	2.00	0.60
3:P:903:DG:H2"	3:P:904:DC:OP2	2.01	0.60
1:A:227:GLN:O	1:A:231:ARG:HD3	2.02	0.60
1:A:180:MET:HE1	1:A:328:LEU:HD23	1.84	0.60
2:T:815:DC:H42	3:P:903:DG:H1	1.49	0.60
1:A:698:ASN:CB	1:A:700:PRO:HD3	2.29	0.59
1:A:219:VAL:HG12	1:A:221:ILE:CG2	2.32	0.59
1:A:697:ARG:HG2	1:A:698:ASN:H	1.67	0.59
1:A:319:ARG:HH11	1:A:319:ARG:HG2	1.66	0.59
1:A:616:ARG:CG	1:A:634:LEU:CD2	2.80	0.58
1:A:647:GLN:O	1:A:651:GLU:HB2	2.03	0.58
1:A:161:ARG:HG2	1:A:719:PRO:HG3	1.85	0.58
1:A:90:MET:CE	1:A:90:MET:CA	2.81	0.58
1:A:240:TYR:HB3	1:A:242:LEU:HD22	1.86	0.58
1:A:424:TYR:CD2	4:A:914:DTP:H2'1	2.38	0.58
1:A:520:THR:O	1:A:524:HIS:ND1	2.37	0.58
1:A:547:ASP:CG	4:A:914:DTP:H5'1	2.24	0.58
1:A:606:ILE:HG12	1:A:609:ALA:HB3	1.86	0.58
1:A:482:ARG:NH1	1:A:482:ARG:HG2	2.18	0.58
1:A:772:PHE:O	1:A:776:MET:N	2.24	0.57
1:A:116:MET:O	1:A:379:PRO:HB3	2.03	0.57
1:A:486:LYS:HB3	1:A:487:PRO:HD3	1.87	0.57
1:A:569:LEU:O	1:A:573:VAL:HG23	2.04	0.57
1:A:290:SER:HB2	1:A:685:ARG:HH22	1.70	0.57
1:A:424:TYR:CG	4:A:914:DTP:H2'1	2.39	0.57
1:A:334:LYS:O	1:A:338:LEU:HG	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:527:MET:HE1	1:A:547:ASP:HA	1.86	0.57
1:A:699:VAL:N	1:A:700:PRO:HD3	2.20	0.57
1:A:34:VAL:CG1	1:A:138:ALA:HB2	2.33	0.56
1:A:261:LYS:HB3	1:A:264:VAL:HG21	1.88	0.56
1:A:74:HIS:O	1:A:75:ARG:HB2	2.05	0.56
1:A:245:ARG:NH1	1:A:245:ARG:CG	2.51	0.56
1:A:115:LEU:HD22	1:A:120:ILE:HG21	1.87	0.56
1:A:502:VAL:O	1:A:508:CYS:HB3	2.06	0.56
1:A:697:ARG:HD2	1:A:697:ARG:N	2.20	0.56
2:T:815:DC:N4	3:P:903:DG:H1	2.03	0.56
1:A:314:MET:O	1:A:314:MET:CE	2.54	0.55
1:A:713:ASN:ND2	1:A:742:TYR:OH	2.39	0.55
1:A:-1:PRO:HA	1:A:130:MET:HB2	1.89	0.55
1:A:531:LYS:O	1:A:535:GLU:HG3	2.06	0.55
1:A:306:SER:HB2	1:A:331:TYR:CD1	2.42	0.55
1:A:221:ILE:HD12	1:A:339:VAL:HG12	1.88	0.54
2:T:816:DA:O5'	2:T:816:DA:H2'	2.07	0.54
1:A:529:GLN:O	1:A:533:LEU:HG	2.08	0.54
1:A:122:SER:H	1:A:123:PRO:HD2	1.72	0.54
1:A:319:ARG:CG	1:A:319:ARG:NH1	2.65	0.54
1:A:384:ALA:O	1:A:463:LYS:NZ	2.40	0.54
1:A:454:PHE:CE1	1:A:521:MET:HB3	2.43	0.54
1:A:558:SER:OG	1:A:561:GLU:HB3	2.08	0.53
1:A:531:LYS:HD2	1:A:541:VAL:HB	1.90	0.53
1:A:640:ASP:HB3	1:A:641:TRP:HD1	1.73	0.53
1:A:640:ASP:HB3	1:A:641:TRP:CD1	2.44	0.53
1:A:359:ASN:HB3	1:A:361:LEU:H	1.72	0.53
1:A:626:LYS:HD2	1:A:626:LYS:N	2.23	0.53
1:A:6:PHE:CB	1:A:148:PRO:HG3	2.39	0.53
2:T:811:DT:H2''	2:T:812:DA:C8	2.44	0.53
1:A:416:LEU:HD13	1:A:553:LEU:HD11	1.90	0.53
1:A:72:ASP:HB2	1:A:104:TYR:CE2	2.43	0.53
1:A:227:GLN:HE22	1:A:265:PHE:H	1.56	0.53
1:A:527:MET:HA	1:A:527:MET:CE	2.35	0.53
1:A:698:ASN:HB3	1:A:700:PRO:CD	2.33	0.53
1:A:70:LEU:HD23	1:A:385:GLY:HA2	1.91	0.52
1:A:644:LEU:HA	1:A:681:ARG:HG2	1.91	0.52
1:A:702:HIS:HB2	1:A:728:ILE:CG2	2.39	0.52
1:A:416:LEU:HD11	1:A:553:LEU:HD11	1.90	0.52
1:A:702:HIS:HE1	3:P:909:DC:OP1	1.91	0.52
1:A:321:PHE:O	1:A:325:LYS:HE2	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:ILE:CG1	1:A:178:VAL:N	2.72	0.52
3:P:902:DT:H2"	3:P:903:DG:OP2	2.09	0.52
1:A:254:GLU:O	1:A:267:ALA:HA	2.10	0.52
1:A:34:VAL:HG21	1:A:126:VAL:HG21	1.90	0.52
1:A:120:ILE:O	1:A:375:HIS:HE1	1.93	0.52
1:A:305:LYS:O	1:A:334:LYS:HG2	2.10	0.52
1:A:482:ARG:HG2	1:A:482:ARG:HH11	1.74	0.52
1:A:702:HIS:H	1:A:702:HIS:HD2	1.58	0.52
1:A:11:HIS:CE1	1:A:24:TRP:HD1	2.27	0.52
1:A:635:GLU:HG2	1:A:641:TRP:CE3	2.44	0.52
1:A:656:ILE:HD13	1:A:768:ILE:HD13	1.91	0.51
3:P:905:DC:H2"	3:P:906:DT:O5'	2.10	0.51
1:A:755:ARG:NH1	2:T:812:DA:OP2	2.41	0.51
1:A:10:ARG:HG3	1:A:10:ARG:NH1	2.26	0.51
1:A:32:LEU:HD21	1:A:135:ILE:HG13	1.93	0.51
1:A:270:LYS:O	1:A:270:LYS:HG3	2.10	0.51
1:A:649:GLN:HB2	1:A:760:VAL:HG11	1.92	0.51
1:A:738:GLU:OE2	1:A:745:SER:HB2	2.11	0.51
1:A:698:ASN:C	1:A:700:PRO:HD3	2.31	0.51
1:A:543:TYR:CG	1:A:603:MET:HE3	2.46	0.51
2:T:801:DT:H5'	2:T:803:DT:OP1	2.09	0.51
2:T:810:DC:C2'	2:T:811:DT:H71	2.41	0.51
1:A:378:PHE:N	1:A:379:PRO:HD2	2.25	0.51
1:A:692:LEU:HD11	1:A:703:VAL:HG13	1.92	0.51
1:A:85:ALA:O	1:A:88:GLN:HB3	2.10	0.50
1:A:258:HIS:NE2	1:A:265:PHE:CE1	2.79	0.50
1:A:314:MET:O	1:A:314:MET:HE3	2.12	0.50
1:A:72:ASP:OD1	1:A:76:GLN:HB3	2.12	0.50
1:A:384:ALA:O	1:A:463:LYS:CE	2.60	0.50
1:A:758:GLN:N	1:A:759:PRO:CD	2.74	0.50
1:A:9:THR:OG1	1:A:11:HIS:CE1	2.64	0.50
1:A:65:LEU:HA	1:A:80:GLY:O	2.12	0.49
1:A:171:GLU:OE1	1:A:337:GLU:CA	2.59	0.49
1:A:200:SER:O	1:A:203:GLN:HB2	2.12	0.49
1:A:107:ASP:OD2	1:A:509:ARG:NH2	2.42	0.49
1:A:308:ASP:CG	1:A:308:ASP:O	2.50	0.49
1:A:45:ILE:O	1:A:79:TYR:N	2.45	0.49
1:A:263:GLY:HA3	1:A:724:ASN:HD21	1.76	0.49
1:A:308:ASP:O	1:A:308:ASP:OD1	2.29	0.49
1:A:389:PRO:O	1:A:509:ARG:HB2	2.12	0.49
1:A:408:ARG:HH11	1:A:408:ARG:CG	2.15	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:807:DA:C2	3:P:912:DA:C2	3.01	0.49
1:A:420:TYR:HB2	1:A:547:ASP:HB2	1.93	0.49
1:A:627:GLN:HE22	1:A:658:ARG:NE	2.07	0.49
1:A:347:GLU:O	1:A:350:PRO:HG2	2.11	0.49
1:A:494:ILE:N	1:A:494:ILE:HD12	2.28	0.49
1:A:45:ILE:HD11	1:A:96:LEU:HD13	1.94	0.49
1:A:90:MET:HE3	1:A:90:MET:N	2.27	0.49
1:A:161:ARG:CG	1:A:719:PRO:HG3	2.43	0.49
1:A:284:ALA:HB3	1:A:286:TRP:HD1	1.78	0.49
1:A:649:GLN:HB2	1:A:760:VAL:CG1	2.43	0.48
1:A:11:HIS:HE1	1:A:24:TRP:HD1	1.61	0.48
1:A:261:LYS:HB3	1:A:264:VAL:CG2	2.43	0.48
1:A:731:VAL:HG13	1:A:740:LEU:HD13	1.93	0.48
1:A:347:GLU:HA	1:A:347:GLU:OE2	2.14	0.48
1:A:56:ILE:HD12	1:A:96:LEU:HD23	1.96	0.48
1:A:483:GLN:HE21	1:A:483:GLN:HA	1.78	0.48
1:A:559:GLU:OE1	1:A:597:HIS:HD2	1.96	0.48
1:A:176:ARG:HH22	1:A:192:ASP:CB	2.27	0.48
1:A:724:ASN:O	1:A:725:ARG:HB2	2.12	0.48
1:A:346:THR:O	1:A:347:GLU:HB2	2.14	0.48
1:A:180:MET:O	1:A:197:TYR:HA	2.13	0.47
1:A:706:ALA:HA	1:A:728:ILE:HD13	1.96	0.47
1:A:127:GLU:O	1:A:138:ALA:HA	2.13	0.47
1:A:349:MET:N	1:A:350:PRO:HD2	2.29	0.47
1:A:433:ILE:HG21	1:A:519:ILE:HG13	1.96	0.47
1:A:280:ALA:O	1:A:283:SER:HB3	2.15	0.47
1:A:332:ASN:O	1:A:335:ASN:HB2	2.14	0.47
1:A:614:LYS:HD3	2:T:808:DC:H5"	1.96	0.47
1:A:704:ARG:CD	1:A:737:PRO:HG2	2.45	0.47
1:A:63:PHE:HA	1:A:82:TYR:O	2.15	0.47
1:A:95:ARG:O	1:A:98:GLU:HB2	2.15	0.47
1:A:401:GLY:O	1:A:524:HIS:CE1	2.58	0.47
1:A:219:VAL:HG22	1:A:273:LEU:HD12	1.97	0.47
1:A:649:GLN:CG	1:A:760:VAL:HG13	2.45	0.47
1:A:765:LEU:N	1:A:766:PRO:CD	2.77	0.47
1:A:169:GLY:C	1:A:170:LEU:HD23	2.35	0.47
1:A:594:TYR:OH	1:A:597:HIS:HB2	2.15	0.47
1:A:153:VAL:HG13	1:A:153:VAL:O	2.15	0.47
1:A:154:SER:HB2	1:A:221:ILE:HD11	1.97	0.47
1:A:201:ARG:N	1:A:202:PRO:CD	2.79	0.46
1:A:240:TYR:N	1:A:240:TYR:CD1	2.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:644:LEU:HB2	1:A:681:ARG:HB3	1.97	0.46
2:T:816:DA:O5'	2:T:816:DA:C2'	2.63	0.46
1:A:114:TYR:CE1	1:A:118:ARG:NH1	2.84	0.46
1:A:617:TYR:CZ	1:A:632:LYS:HG3	2.50	0.46
1:A:638:ARG:HB3	1:A:640:ASP:HB2	1.97	0.46
1:A:115:LEU:HD22	1:A:120:ILE:CG2	2.46	0.46
1:A:143:HIS:CD2	1:A:146:TYR:CB	2.94	0.46
1:A:377:TYR:CE1	1:A:465:CYS:HB2	2.50	0.46
1:A:283:SER:OG	1:A:355:ARG:NH1	2.48	0.46
1:A:52:ARG:O	1:A:56:ILE:HG13	2.16	0.46
1:A:152:TRP:O	1:A:172:GLY:HA3	2.14	0.46
1:A:474:TRP:CD1	1:A:474:TRP:C	2.89	0.46
1:A:554:LYS:H	1:A:554:LYS:CD	2.23	0.46
1:A:642:THR:H	1:A:756:GLN:NE2	2.14	0.46
1:A:496:MET:O	1:A:499:PHE:HB2	2.16	0.46
1:A:348:ILE:HD12	1:A:351:PHE:HB3	1.98	0.46
1:A:306:SER:CB	1:A:331:TYR:CD1	2.95	0.46
1:A:461:ARG:O	1:A:464:HIS:NE2	2.49	0.46
1:A:673:LEU:C	1:A:673:LEU:CD1	2.79	0.46
1:A:105:GLU:OE2	1:A:382:HIS:NE2	2.40	0.45
1:A:454:PHE:CD1	1:A:521:MET:HB3	2.51	0.45
1:A:455:LEU:O	1:A:456:ASP:HB2	2.16	0.45
1:A:160:THR:HG22	1:A:166:TYR:CE1	2.51	0.45
1:A:209:ASN:HD21	1:A:245:ARG:H	1.64	0.45
1:A:395:PRO:HA	1:A:396:PRO:HD2	1.80	0.45
1:A:663:GLN:O	1:A:667:ARG:HG3	2.16	0.45
1:A:6:PHE:HB2	1:A:148:PRO:HG3	1.98	0.45
1:A:253:LEU:HD11	1:A:267:ALA:HB1	1.99	0.45
1:A:166:TYR:OH	1:A:318:ASP:OD1	2.32	0.45
2:T:810:DC:H2'	2:T:811:DT:H71	1.98	0.45
1:A:34:VAL:CG1	1:A:138:ALA:HB1	2.47	0.45
1:A:468:GLU:OE1	1:A:468:GLU:N	2.50	0.45
1:A:698:ASN:C	1:A:700:PRO:CD	2.85	0.45
1:A:50:VAL:HG21	1:A:79:TYR:CG	2.51	0.45
1:A:373:PHE:O	1:A:377:TYR:HB2	2.16	0.45
2:T:815:DC:H2"	2:T:816:DA:H8	1.75	0.45
1:A:32:LEU:HD21	1:A:135:ILE:CG1	2.47	0.45
1:A:122:SER:CB	1:A:123:PRO:HD3	2.47	0.45
1:A:293:LEU:HD12	1:A:293:LEU:HA	1.75	0.45
1:A:315:ASP:O	1:A:318:ASP:HB2	2.17	0.45
1:A:492:LEU:HD23	1:A:492:LEU:N	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:668:GLU:HA	1:A:668:GLU:OE1	2.17	0.44
1:A:414:SER:HB3	1:A:597:HIS:CE1	2.39	0.44
1:A:482:ARG:HH11	1:A:482:ARG:CG	2.29	0.44
1:A:224:ASN:N	1:A:276:ASP:OD1	2.44	0.44
1:A:490:GLN:O	1:A:494:ILE:CD1	2.48	0.44
1:A:670:ILE:O	1:A:674:MET:HG2	2.17	0.44
1:A:690:ARG:NH1	3:P:908:DG:OP1	2.51	0.44
1:A:8:LEU:HD22	1:A:273:LEU:HG	2.00	0.44
1:A:126:VAL:HG23	1:A:140:LEU:HD21	1.99	0.44
1:A:621:ILE:HG22	1:A:623:GLU:HG3	2.00	0.44
1:A:743:GLN:HG2	1:A:744:ARG:N	2.32	0.44
1:A:446:ASP:O	1:A:446:ASP:OD1	2.35	0.44
1:A:465:CYS:O	1:A:469:ILE:HG13	2.18	0.44
1:A:527:MET:CE	1:A:527:MET:CA	2.94	0.44
3:P:904:DC:H2"	3:P:905:DC:H6	1.83	0.44
1:A:701:PRO:HG3	2:T:812:DA:H4'	1.98	0.44
1:A:122:SER:N	1:A:123:PRO:HD2	2.33	0.44
1:A:314:MET:O	1:A:314:MET:HE2	2.18	0.44
3:P:904:DC:H2"	3:P:905:DC:C6	2.53	0.43
1:A:240:TYR:CB	1:A:242:LEU:HD22	2.47	0.43
1:A:697:ARG:CG	1:A:698:ASN:N	2.78	0.43
1:A:415:VAL:HA	1:A:551:VAL:O	2.19	0.43
1:A:635:GLU:OE1	1:A:649:GLN:NE2	2.49	0.43
1:A:704:ARG:HD2	1:A:737:PRO:HG2	2.00	0.43
2:T:810:DC:H2"	2:T:811:DT:H71	2.00	0.43
1:A:702:HIS:CD2	1:A:702:HIS:N	2.87	0.43
1:A:738:GLU:OE2	1:A:745:SER:CB	2.67	0.43
1:A:486:LYS:O	1:A:489:SER:HB3	2.18	0.43
2:T:806:DT:H2"	2:T:807:DA:C8	2.53	0.43
1:A:177:ILE:HG12	1:A:178:VAL:N	2.34	0.43
1:A:527:MET:HE2	1:A:527:MET:CA	2.35	0.43
1:A:6:PHE:O	1:A:25:LEU:HA	2.19	0.42
1:A:286:TRP:CZ2	1:A:346:THR:HG22	2.53	0.42
1:A:494:ILE:N	1:A:494:ILE:CD1	2.83	0.42
1:A:423:LEU:HG	1:A:427:ILE:HD12	2.00	0.42
3:P:904:DC:H2'	3:P:905:DC:C5	2.54	0.42
1:A:34:VAL:HG11	1:A:138:ALA:HB1	2.01	0.42
1:A:584:GLN:O	1:A:585:ARG:HB2	2.19	0.42
1:A:156:ASP:OD2	1:A:158:GLU:OE2	2.38	0.42
1:A:686:LYS:HD3	3:P:909:DC:H4'	2.01	0.42
1:A:578:ALA:O	1:A:582:GLN:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:596:THR:HG22	1:A:597:HIS:N	2.35	0.42
3:P:902:DT:C2'	3:P:903:DG:OP2	2.66	0.42
1:A:11:HIS:NE2	1:A:270:LYS:HB2	2.35	0.42
1:A:403:TYR:CZ	1:A:405:MET:HG2	2.55	0.42
1:A:420:TYR:CE2	1:A:592:LEU:HD13	2.54	0.42
1:A:606:ILE:CG1	1:A:609:ALA:HB3	2.49	0.42
1:A:706:ALA:O	1:A:709:ALA:HB3	2.20	0.41
1:A:73:PHE:HE1	1:A:386:TYR:HB3	1.86	0.41
1:A:477:ARG:HG3	1:A:492:LEU:HB2	2.02	0.41
1:A:581:LEU:HD12	1:A:581:LEU:HA	1.67	0.41
1:A:292:SER:O	1:A:296:VAL:HG23	2.20	0.41
1:A:356:ALA:HA	1:A:359:ASN:HB2	2.01	0.41
1:A:620:LEU:HD22	1:A:657:PHE:HB3	2.02	0.41
1:A:716:ARG:NE	1:A:742:TYR:HE1	2.19	0.41
1:A:644:LEU:CA	1:A:681:ARG:HG2	2.50	0.41
1:A:716:ARG:CZ	1:A:742:TYR:HE1	2.33	0.41
1:A:320:ARG:O	1:A:324:ASP:N	2.42	0.41
1:A:700:PRO:HA	1:A:701:PRO:HD2	1.89	0.41
1:A:74:HIS:O	1:A:75:ARG:CB	2.69	0.41
1:A:90:MET:CE	1:A:90:MET:N	2.84	0.41
1:A:490:GLN:HE21	1:A:490:GLN:HB3	1.62	0.41
1:A:403:TYR:CZ	1:A:405:MET:HA	2.55	0.41
1:A:146:TYR:CD2	1:A:146:TYR:C	2.94	0.41
1:A:539:TYR:CD1	1:A:553:LEU:HD23	2.56	0.41
1:A:697:ARG:CG	1:A:698:ASN:H	2.33	0.41
1:A:545:ASP:O	1:A:546:THR:HB	2.20	0.40
1:A:602:LEU:HD12	1:A:603:MET:N	2.36	0.40
1:A:171:GLU:OE1	1:A:337:GLU:CG	2.69	0.40
1:A:405:MET:HE3	1:A:405:MET:HB3	1.85	0.40
1:A:112:GLU:OE1	1:A:112:GLU:N	2.53	0.40
1:A:319:ARG:HH11	1:A:319:ARG:HG3	1.85	0.40
1:A:583:LYS:HB2	1:A:583:LYS:HE3	1.95	0.40
1:A:614:LYS:CD	2:T:808:DC:H5"	2.52	0.40
1:A:648:PHE:CD2	1:A:757:LEU:HD22	2.57	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	779/786 (99%)	755 (97%)	21 (3%)	3 (0%)	34	60

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	306	SER
1	A	414	SER
1	A	445	PRO

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	665/672 (99%)	601 (90%)	64 (10%)	8	19

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	41	SER
1	A	42	VAL
1	A	61	GLN
1	A	64	ARG
1	A	94	LYS
1	A	107	ASP
1	A	127	GLU

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Mol	Chain	Res	Type
1	A	130	MET
1	A	136	VAL
1	A	145	ASP
1	A	175	GLN
1	A	184	GLU
1	A	189	SER
1	A	203	GLN
1	A	241	ARG
1	A	242	LEU
1	A	250	ASN
1	A	251	SER
1	A	253	LEU
1	A	257	GLU
1	A	264	VAL
1	A	272	ARG
1	A	276	ASP
1	A	281	LEU
1	A	289	SER
1	A	290	SER
1	A	300	LEU
1	A	306	SER
1	A	312	ASP
1	A	319	ARG
1	A	326	PRO
1	A	341	GLN
1	A	345	LYS
1	A	364	ASP
1	A	408	ARG
1	A	425	PRO
1	A	483	GLN
1	A	487	PRO
1	A	500	TYR
1	A	502	VAL
1	A	527	MET
1	A	531	LYS
1	A	554	LYS
1	A	570	VAL
1	A	571	GLN
1	A	581	LEU
1	A	606	ILE
1	A	616	ARG
1	A	625	ASP

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Mol	Chain	Res	Type
1	A	626	LYS
1	A	628	ARG
1	A	640	ASP
1	A	644	LEU
1	A	651	GLU
1	A	673	LEU
1	A	681	ARG
1	A	693	SER
1	A	697	ARG
1	A	699	VAL
1	A	702	HIS
1	A	747	LEU
1	A	768	ILE
1	A	769	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	HIS
1	A	29	ASN
1	A	143	HIS
1	A	209	ASN
1	A	227	GLN
1	A	250	ASN
1	A	341	GLN
1	A	344	HIS
1	A	366	HIS
1	A	375	HIS
1	A	390	ASN
1	A	483	GLN
1	A	490	GLN
1	A	524	HIS
1	A	571	GLN
1	A	597	HIS
1	A	627	GLN
1	A	647	GLN
1	A	702	HIS
1	A	713	ASN
1	A	751	HIS
1	A	756	GLN

5.3.3   RNA (i)

There are no RNA molecules in this entry.

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

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	DOC	P	913	3,2	16,19,20	0.58	0	20,26,29	0.66	0
2	3DR	T	804	2	8,11,12	0.33	0	9,14,17	0.62	0

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	DOC	P	913	3,2	-	2/7/18/19	0/2/2/2
2	3DR	T	804	2	-	1/3/15/16	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	P	913	DOC	C3'-C4'-C5'-O5'
3	P	913	DOC	O4'-C4'-C5'-O5'
2	T	804	3DR	C4'-C5'-O5'-P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	P	913	DOC	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
4	DTP	A	914	5	26,32,32	0.95	1 (3%)	30,50,50	1.68	6 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	DTP	A	914	5	-	6/18/34/34	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	914	DTP	C8-N7	-2.33	1.30	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	914	DTP	N3-C2-N1	-4.66	121.39	128.68
4	A	914	DTP	PB-O3B-PG	-4.26	118.19	132.83
4	A	914	DTP	PA-O3A-PB	-3.88	119.51	132.83
4	A	914	DTP	C2'-C1'-N9	-2.58	108.33	114.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	914	DTP	PA-O5'-C5'	-2.57	106.61	121.68
4	A	914	DTP	C4-C5-N7	-2.01	107.30	109.40

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	914	DTP	O4'-C4'-C5'-O5'
4	A	914	DTP	C3'-C4'-C5'-O5'
4	A	914	DTP	PB-O3B-PG-O1G
4	A	914	DTP	PB-O3B-PG-O2G
4	A	914	DTP	PB-O3B-PG-O3G
4	A	914	DTP	PB-O3A-PA-O2A

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	914	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 then 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.

Ligand DTP A 914

Bond lengths

Bond angles

Torsions

Rings
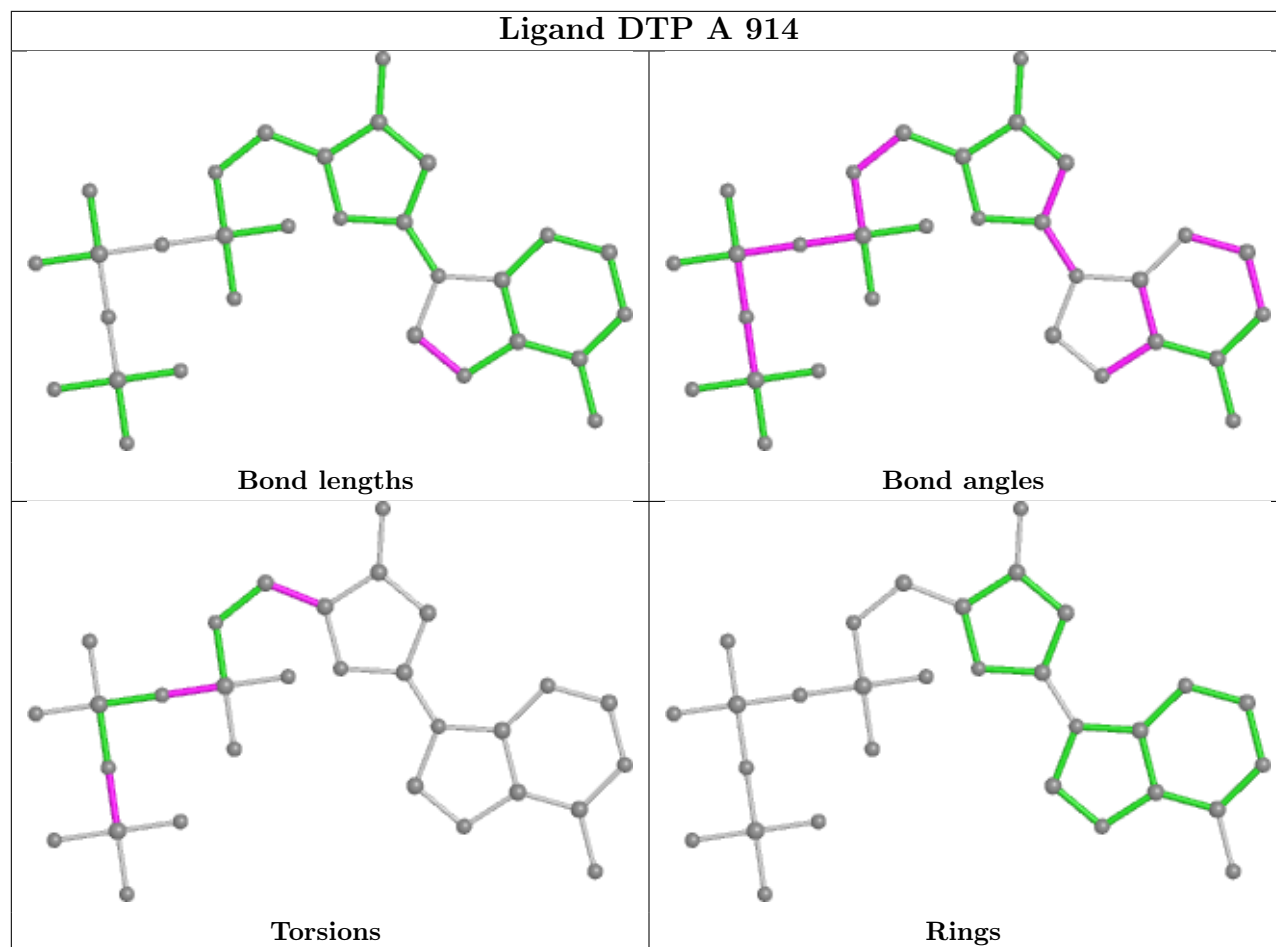
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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(Å²)	Q<0.9
1	A	781/786 (99%)	-0.10	19 (2%)	59	60	5, 19, 35, 55	0
2	T	17/18 (94%)	0.54	3 (17%)	1	1	15, 29, 77, 85	0
3	P	12/13 (92%)	0.32	1 (8%)	11	9	17, 35, 59, 62	0
All	All	810/817 (99%)	-0.08	23 (2%)	53	54	5, 20, 39, 85	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	777	THR	4.9
1	A	-2	GLY	4.5
2	T	818	DA	4.4
1	A	260	PHE	4.4
1	A	308	ASP	4.1
1	A	257	GLU	3.5
1	A	-1	PRO	3.0
2	T	817	DC	3.0
1	A	307	ILE	3.0
1	A	189	SER	2.7
3	P	901	DG	2.7
1	A	776	MET	2.6
1	A	264	VAL	2.6
1	A	306	SER	2.6
2	T	816	DA	2.6
1	A	265	PHE	2.4
1	A	258	HIS	2.4
1	A	696	GLN	2.3
1	A	256	ARG	2.3
1	A	1	MET	2.3
1	A	774	THR	2.1
1	A	778	GLY	2.1
1	A	59	GLY	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.

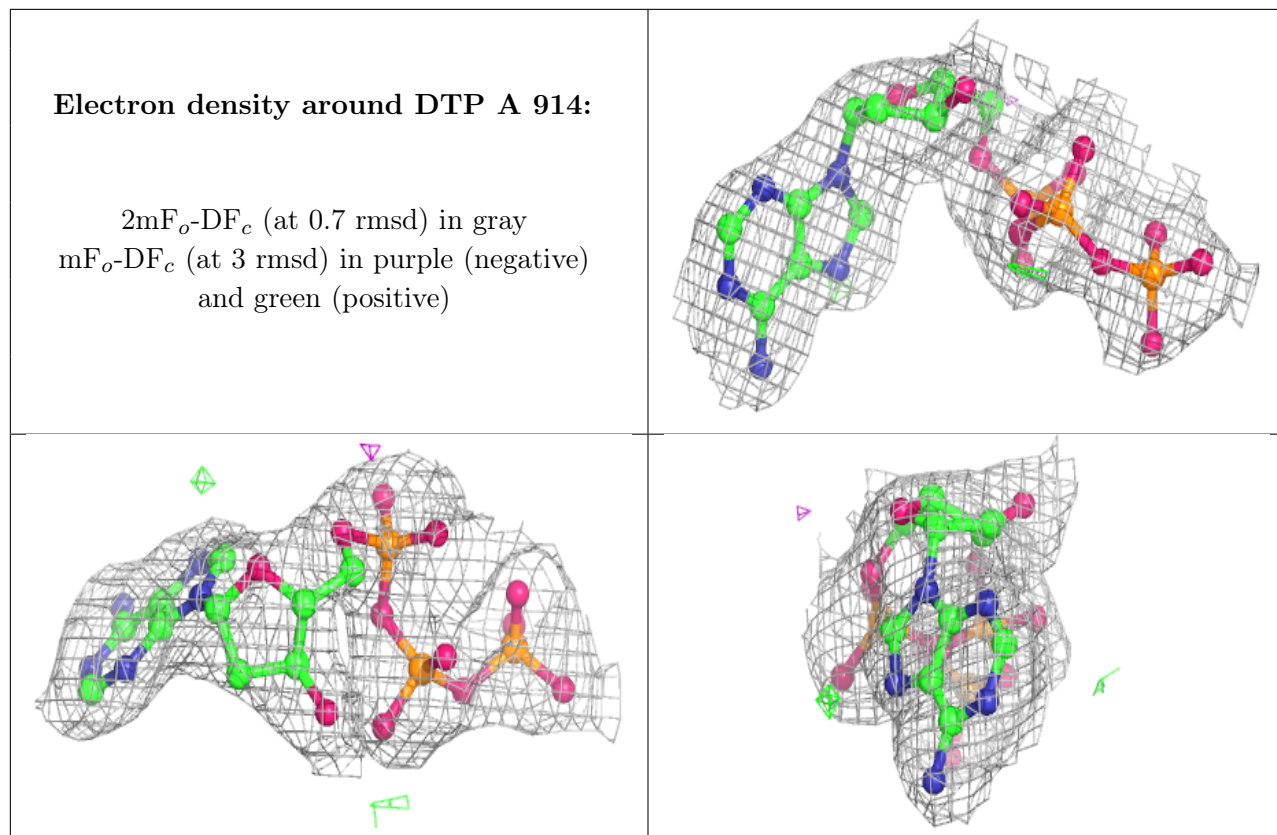| Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	3DR	T	804	11/12	0.95	0.17	21,29,37,37	0
3	DOC	P	913	18/19	0.96	0.13	5,16,19,19	0

6.3 Carbohydrates ⓘ

There are no monosaccharides 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	MG	A	1002	1/1	0.86	0.20	17,17,17,17	0
5	MG	A	1001	1/1	0.95	0.10	23,23,23,23	0
4	DTP	A	914	30/30	0.97	0.13	9,16,19,20	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 914:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.