Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2024 – 09:41 AM EDT

PDB ID	:	1T3N
Title	:	Structure of the catalytic core of DNA polymerase Iota in complex with DNA and dTTP
Authors	:	Nair, D.T.; Johnson, R.E.; Prakash, S.; Prakash, L.; Aggarwal, A.K.
Deposited on	:	2004-04-27
Resolution	:	2.30 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 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:

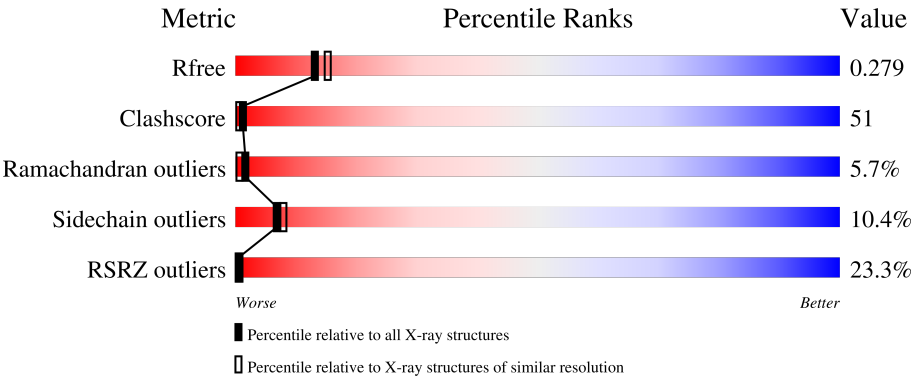
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 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	1-T	14	14% 43% 57%
1	2-T	14	14% 43% 57%
2	1-P	13	31% 69%
2	2-P	13	31% 69%
3	1-A	388	23% 49% 41% 8% .

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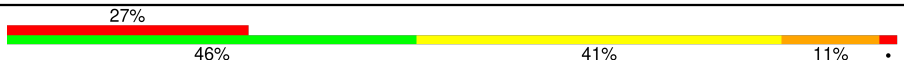
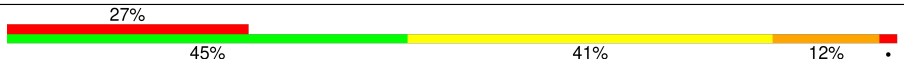
Mol	Chain	Length	Quality of chain
3	1-B	388	
3	2-A	388	
3	2-B	388	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 13538 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 Template DNA strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1-T	14	Total	C	N	O	P	0	0	0
			277	133	47	84	13			
1	2-T	14	Total	C	N	O	P	0	0	0
			277	133	47	84	13			

- Molecule 2 is a DNA chain called Primer DNA strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1-P	13	Total	C	N	O	P	0	0	0
			270	127	59	72	12			
2	2-P	13	Total	C	N	O	P	0	0	0
			270	127	59	72	12			

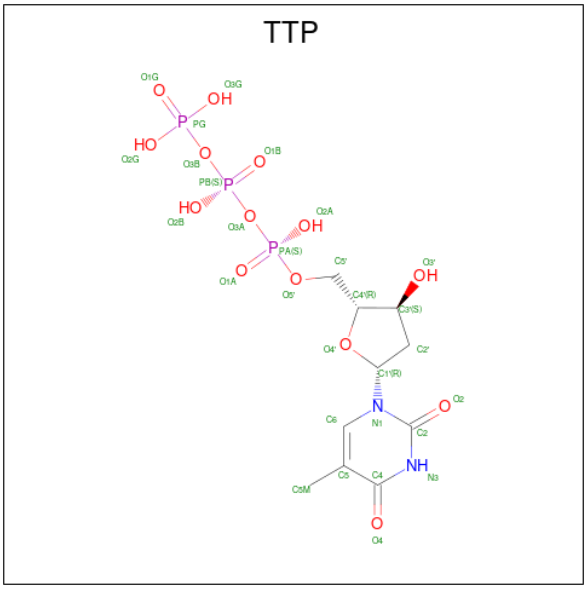
- Molecule 3 is a protein called polymerase (DNA directed) iota.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	1-A	388	Total	C	N	O	S	0	0	0
			2868	1801	502	547	18			
3	2-A	388	Total	C	N	O	S	0	0	0
			2868	1801	502	547	18			
3	1-B	388	Total	C	N	O	S	0	0	0
			2886	1812	509	547	18			
3	2-B	388	Total	C	N	O	S	0	0	0
			2886	1812	509	547	18			

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	1-B	1	Total	Mg	0	0
			1	1		
4	2-B	1	Total	Mg	0	0
			1	1		

- Molecule 5 is THYMIDINE-5'-TRIPHOSPHATE (three-letter code: TTP) (formula: $C_{10}H_{17}N_2O_{14}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	1-B	1	Total	C	N	O	P	0	0
			29	10	2	14	3		
5	2-B	1	Total	C	N	O	P	0	0
			29	10	2	14	3		

- Molecule 6 is water.

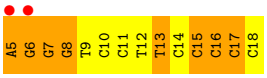
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	1-T	11	Total	O	0	0
			11	11		
6	2-T	209	Total	O	0	0
			209	209		
6	1-P	12	Total	O	0	0
			12	12		
6	2-P	208	Total	O	0	0
			208	208		
6	1-A	207	Total	O	0	0
			207	207		
6	2-A	11	Total	O	0	0
			11	11		
6	1-B	208	Total	O	0	0
			208	208		
6	2-B	10	Total	O	0	0
			10	10		

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.

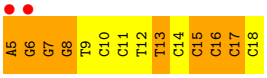
• Molecule 1: Template DNA strand

Chain 1-T:



• Molecule 1: Template DNA strand

Chain 2-T:



• Molecule 2: Primer DNA strand

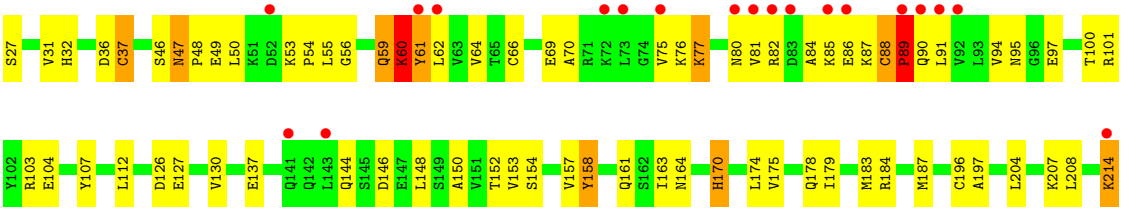
Chain 1-P:

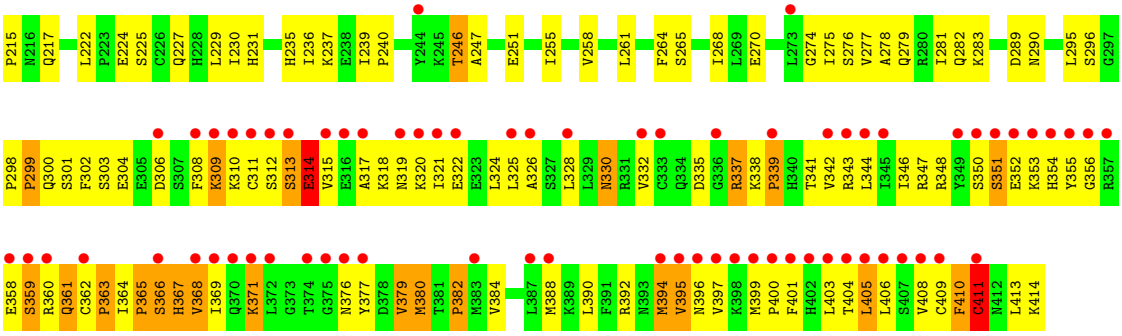
• Molecule 2: Primer DNA strand

Chain 2-P:

• Molecule 3: polymerase (DNA directed) iota

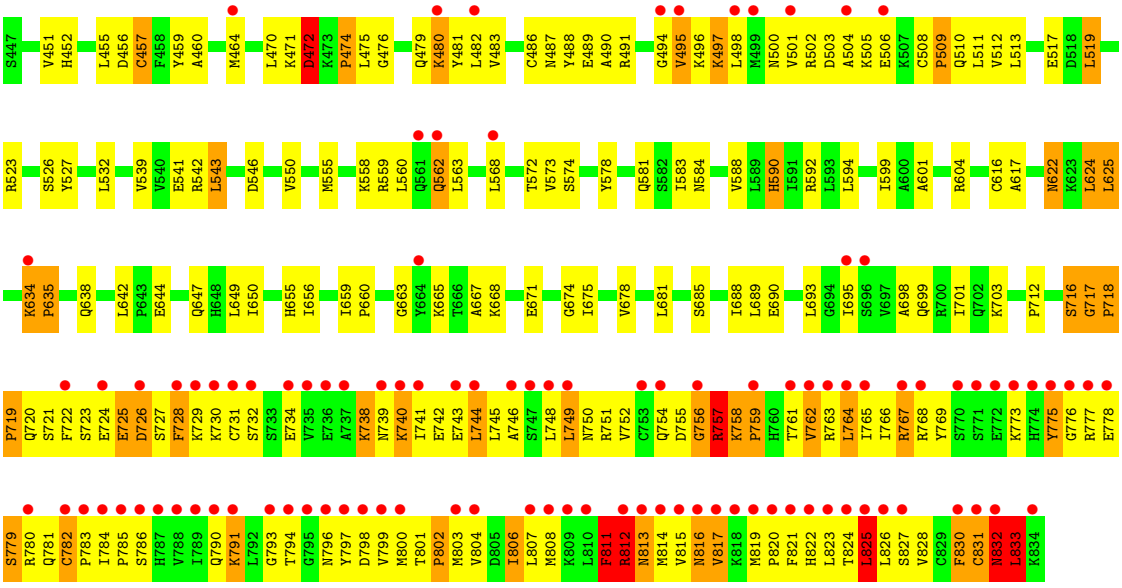
Chain 1-A:





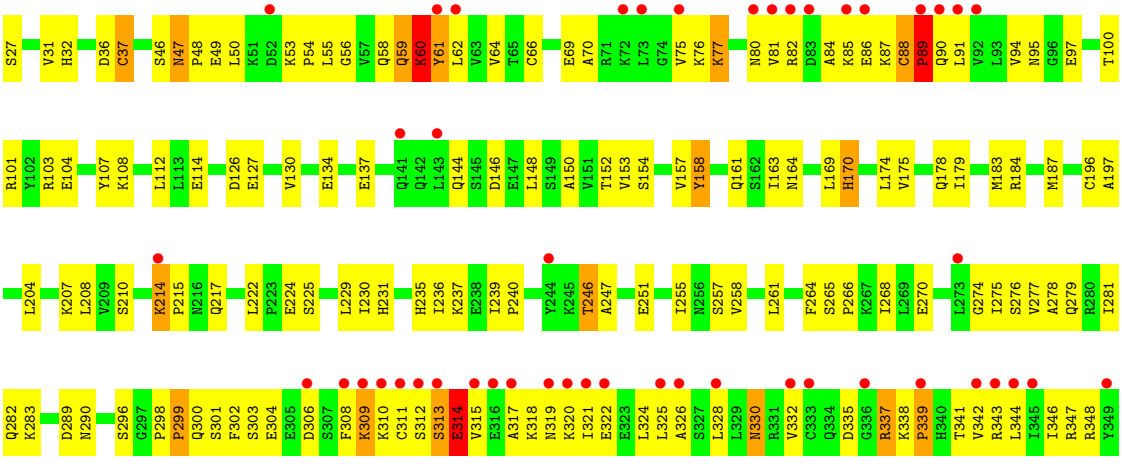
• Molecule 3: polymerase (DNA directed) iota

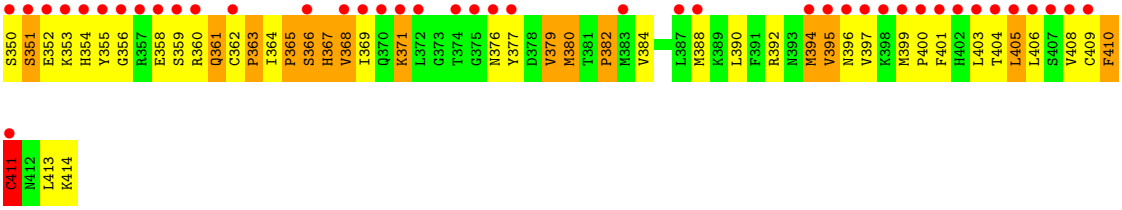
Chain 1-B:



• Molecule 3: polymerase (DNA directed) iota

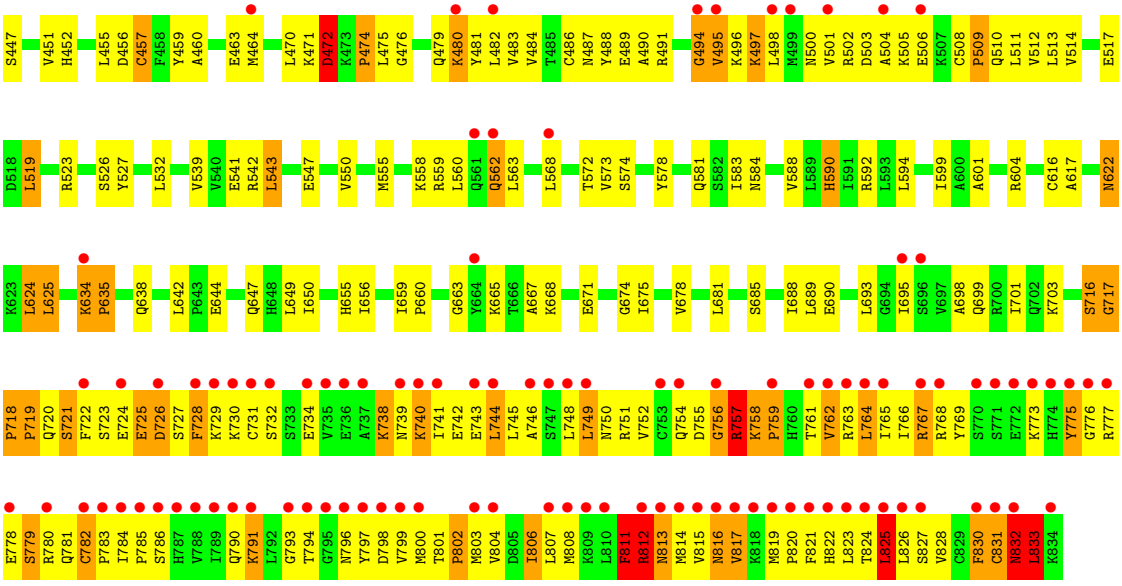
Chain 2-A:





• Molecule 3: polymerase (DNA directed) iota

Chain 2-B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	98.83Å 98.83Å 202.75Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.30 39.43 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.00-2.30) 96.9 (39.43-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.41 (at 2.29Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.265 , 0.286 0.258 , 0.279	Depositor DCC
R_{free} test set	4842 reflections (9.75%)	wwPDB-VP
Wilson B-factor (Å^2)	42.1	Xtriage
Anisotropy	0.408	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 67.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.478 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	13538	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: TTP, 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	1-T	0.77	0/308	1.22	3/472 (0.6%)
1	2-T	0.76	0/308	1.22	3/472 (0.6%)
2	1-P	1.20	2/285 (0.7%)	1.55	7/440 (1.6%)
2	2-P	1.20	2/285 (0.7%)	1.54	7/440 (1.6%)
3	1-A	0.51	1/2908 (0.0%)	0.85	8/3946 (0.2%)
3	1-B	0.63	2/2928 (0.1%)	0.99	20/3975 (0.5%)
3	2-A	0.50	1/2908 (0.0%)	0.85	8/3946 (0.2%)
3	2-B	0.63	3/2928 (0.1%)	0.99	21/3975 (0.5%)
All	All	0.62	11/12858 (0.1%)	0.98	77/17666 (0.4%)

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	1-T	1	6
1	2-T	1	6
2	1-P	0	3
2	2-P	0	3
3	1-B	0	1
3	2-B	0	1
All	All	2	20

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1-P	12	DC	C3'-O3'	-12.37	1.27	1.44
2	2-P	12	DC	C3'-O3'	-12.34	1.27	1.44
3	1-B	832	ASN	N-CA	7.35	1.61	1.46
3	2-B	832	ASN	N-CA	7.33	1.61	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2-A	60	LYS	CB-CG	-6.49	1.35	1.52
3	1-A	60	LYS	CB-CG	-6.46	1.35	1.52
3	2-B	816	ASN	C-O	-6.18	1.11	1.23
3	1-B	816	ASN	C-O	-6.18	1.11	1.23
3	2-B	721	SER	N-CA	5.81	1.57	1.46
2	1-P	11	DC	O3'-P	-5.58	1.54	1.61
2	2-P	11	DC	O3'-P	-5.41	1.54	1.61

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	1-A	60	LYS	CB-CG-CD	-12.63	78.75	111.60
3	2-A	60	LYS	CB-CG-CD	-12.63	78.77	111.60
3	2-B	757	ARG	CB-CG-CD	10.15	138.00	111.60
3	1-B	757	ARG	CB-CG-CD	10.15	138.00	111.60
3	1-B	831	CYS	N-CA-C	9.52	136.71	111.00
3	2-B	831	CYS	N-CA-C	9.51	136.67	111.00
3	1-B	831	CYS	C-N-CA	8.07	141.88	121.70
3	2-B	831	CYS	C-N-CA	8.07	141.88	121.70
3	1-B	819	MET	C-N-CD	-8.05	102.88	120.60
3	2-B	819	MET	C-N-CD	-8.04	102.91	120.60
3	1-B	811	PHE	C-N-CA	7.78	141.16	121.70
3	1-B	757	ARG	CA-CB-CG	7.77	130.49	113.40
3	2-B	811	PHE	C-N-CA	7.75	141.06	121.70
3	2-B	757	ARG	CA-CB-CG	7.74	130.43	113.40
3	1-B	756	GLY	CA-C-N	-7.67	100.33	117.20
3	2-B	756	GLY	CA-C-N	-7.65	100.37	117.20
3	1-A	394	MET	C-N-CA	7.35	140.08	121.70
3	2-A	394	MET	C-N-CA	7.35	140.08	121.70
3	2-B	811	PHE	CB-CG-CD2	7.01	125.71	120.80
2	1-P	11	DC	O3'-P-O5'	-6.99	90.72	104.00
3	1-B	816	ASN	C-N-CA	-6.96	104.29	121.70
3	1-B	811	PHE	CB-CG-CD2	6.95	125.66	120.80
3	2-B	816	ASN	C-N-CA	-6.95	104.34	121.70
3	1-A	394	MET	CA-C-N	-6.90	102.02	117.20
3	2-B	811	PHE	CA-C-N	-6.89	102.04	117.20
3	2-A	394	MET	CA-C-N	-6.89	102.04	117.20
3	2-A	411	CYS	C-N-CA	6.87	138.88	121.70
3	1-A	411	CYS	C-N-CA	6.87	138.88	121.70
3	1-B	817	VAL	N-CA-C	6.86	129.53	111.00
3	1-B	811	PHE	CA-C-N	-6.86	102.10	117.20
3	2-B	817	VAL	N-CA-C	6.84	129.47	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	2-B	756	GLY	C-N-CA	6.77	138.63	121.70
3	2-A	60	LYS	CA-CB-CG	6.76	128.28	113.40
3	1-A	60	LYS	CA-CB-CG	6.76	128.26	113.40
3	1-B	756	GLY	C-N-CA	6.75	138.57	121.70
3	1-A	59	GLN	CA-C-N	-6.61	102.66	117.20
2	2-P	3	DG	C5'-C4'-C3'	-6.61	102.20	114.10
3	2-A	59	GLN	CA-C-N	-6.61	102.67	117.20
2	1-P	3	DG	C5'-C4'-C3'	-6.60	102.22	114.10
3	2-B	764	LEU	N-CA-C	-6.43	93.64	111.00
3	1-B	764	LEU	N-CA-C	-6.40	93.73	111.00
1	1-T	15	DC	C2'-C3'-O3'	6.39	133.69	112.60
1	2-T	15	DC	C2'-C3'-O3'	6.37	133.62	112.60
2	2-P	11	DC	C4'-C3'-O3'	6.27	125.37	109.70
2	1-P	11	DC	C4'-C3'-O3'	6.25	125.33	109.70
3	1-A	394	MET	O-C-N	6.03	132.35	122.70
2	2-P	11	DC	O3'-P-O5'	-6.03	92.55	104.00
3	2-A	394	MET	O-C-N	6.01	132.32	122.70
2	2-P	12	DC	O4'-C4'-C3'	-5.98	102.11	104.50
2	1-P	12	DC	O4'-C4'-C3'	-5.87	102.15	104.50
3	1-B	833	LEU	CA-CB-CG	5.83	128.70	115.30
3	2-B	833	LEU	CA-CB-CG	5.83	128.70	115.30
2	1-P	12	DC	N1-C1'-C2'	5.80	123.62	112.60
3	2-B	832	ASN	C-N-CA	5.79	136.17	121.70
2	2-P	12	DC	N1-C1'-C2'	5.78	123.58	112.60
3	1-B	832	ASN	C-N-CA	5.72	136.01	121.70
1	1-T	13	DT	C4'-C3'-O3'	5.56	123.60	109.70
1	2-T	13	DT	C4'-C3'-O3'	5.53	123.52	109.70
3	1-B	758	LYS	N-CA-C	5.51	125.89	111.00
3	2-B	758	LYS	N-CA-C	5.51	125.87	111.00
3	1-B	832	ASN	CA-C-N	-5.45	105.20	117.20
3	2-B	831	CYS	O-C-N	5.43	131.39	122.70
3	2-B	832	ASN	CA-C-N	-5.43	105.26	117.20
3	1-B	831	CYS	O-C-N	5.41	131.36	122.70
3	2-B	634	LYS	N-CA-C	5.38	125.53	111.00
3	1-B	634	LYS	N-CA-C	5.37	125.50	111.00
1	2-T	13	DT	C4'-C3'-C2'	5.31	107.88	103.10
2	2-P	4	DG	C5'-C4'-C3'	-5.27	104.61	114.10
2	1-P	4	DG	C5'-C4'-C3'	-5.25	104.65	114.10
1	1-T	13	DT	C4'-C3'-C2'	5.23	107.81	103.10
3	1-B	756	GLY	O-C-N	5.21	131.04	122.70
3	2-B	756	GLY	O-C-N	5.21	131.03	122.70
3	1-A	214	LYS	N-CA-C	5.18	124.99	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	2-A	214	LYS	N-CA-C	5.15	124.91	111.00
2	2-P	7	DA	C4'-C3'-O3'	5.12	122.53	112.30
2	1-P	7	DA	C4'-C3'-O3'	5.06	122.42	112.30
3	2-B	757	ARG	N-CA-CB	5.05	119.68	110.60

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	1-T	13	DT	C3'
1	2-T	13	DT	C3'

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	1-B	816	ASN	Mainchain
2	1-P	1	DG	Sidechain
2	1-P	2	DG	Sidechain
2	1-P	8	DG	Sidechain
1	1-T	16	DC	Sidechain
1	1-T	17	DC	Sidechain
1	1-T	5	DA	Sidechain
1	1-T	6	DG	Sidechain
1	1-T	7	DG	Sidechain
1	1-T	8	DG	Sidechain
3	2-B	816	ASN	Mainchain
2	2-P	1	DG	Sidechain
2	2-P	2	DG	Sidechain
2	2-P	8	DG	Sidechain
1	2-T	16	DC	Sidechain
1	2-T	17	DC	Sidechain
1	2-T	5	DA	Sidechain
1	2-T	6	DG	Sidechain
1	2-T	7	DG	Sidechain
1	2-T	8	DG	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	1-T	277	0	159	59	0
1	2-T	277	0	159	55	0
2	1-P	270	0	145	46	0
2	2-P	270	0	145	39	0
3	1-A	2868	0	2764	247	0
3	1-B	2886	0	2789	306	0
3	2-A	2868	0	2764	252	0
3	2-B	2886	0	2789	306	0
4	1-B	1	0	0	0	0
4	2-B	1	0	0	0	0
5	1-B	29	0	10	2	0
5	2-B	29	0	10	4	0
6	1-A	207	0	0	18	0
6	1-B	208	0	0	20	0
6	1-P	12	0	0	0	0
6	1-T	11	0	0	1	0
6	2-A	11	0	0	0	0
6	2-B	10	0	0	1	0
6	2-P	208	0	0	18	0
6	2-T	209	0	0	29	0
All	All	13538	0	11734	1236	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 51.

All (1236) 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:729:LYS:O	3:B:730:LYS:HG2	1.26	1.34
3:B:729:LYS:O	3:B:730:LYS:HG2	1.26	1.33
3:B:763:ARG:O	3:B:828:VAL:HG13	1.33	1.28
3:B:763:ARG:O	3:B:828:VAL:HG13	1.33	1.27
3:A:60:LYS:O	3:A:61:TYR:HD1	1.22	1.21
3:B:807:LEU:O	3:B:811:PHE:CD1	1.95	1.20
2:P:8:DG:H3'	3:B:776:GLY:O	1.42	1.19
2:P:8:DG:H3'	3:B:776:GLY:O	1.41	1.19
3:A:409:CYS:SG	3:A:411:CYS:HB2	1.82	1.18
3:A:60:LYS:O	3:A:61:TYR:HD1	1.22	1.18
3:B:807:LEU:O	3:B:811:PHE:CD1	1.95	1.18
3:A:409:CYS:SG	3:A:411:CYS:HB2	1.82	1.18
3:B:780:ARG:NH2	3:B:812:ARG:O	1.77	1.17
3:B:807:LEU:O	3:B:811:PHE:HD1	1.26	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:60:LYS:O	3:A:61:TYR:CD1	1.98	1.17
3:B:780:ARG:NH2	3:B:812:ARG:O	1.77	1.17
3:A:60:LYS:O	3:A:61:TYR:CD1	1.98	1.17
1:T:6:DG:H2"	1:T:7:DG:H5'	1.19	1.15
3:A:366:SER:O	3:A:367:HIS:CG	2.00	1.15
2:P:8:DG:C3'	3:B:776:GLY:O	1.94	1.14
2:P:8:DG:C3'	3:B:776:GLY:O	1.96	1.13
3:A:366:SER:O	3:A:367:HIS:CG	2.00	1.13
1:T:6:DG:H2"	1:T:7:DG:H5'	1.19	1.09
1:T:11:DC:H2"	1:T:12:DT:H5"	1.25	1.09
3:B:778:GLU:O	3:B:779:SER:HB3	1.51	1.08
3:B:825:LEU:HD23	3:B:825:LEU:H	1.18	1.08
3:A:342:VAL:HG13	3:A:364:ILE:HD11	1.14	1.08
3:B:825:LEU:HD23	3:B:825:LEU:H	1.18	1.08
3:A:342:VAL:HG13	3:A:364:ILE:HD11	1.14	1.08
1:T:11:DC:H2"	1:T:12:DT:H5"	1.25	1.07
3:A:380:MET:O	3:A:384:VAL:HG23	1.55	1.07
3:B:807:LEU:O	3:B:811:PHE:HD1	1.26	1.06
1:T:11:DC:C2'	1:T:12:DT:H5"	1.87	1.05
3:A:380:MET:O	3:A:384:VAL:HG23	1.55	1.05
1:T:11:DC:C2'	1:T:12:DT:H5"	1.87	1.05
6:T:185:HOH:O	3:A:158:TYR:O	1.72	1.05
3:B:501:VAL:HG12	3:B:502:ARG:H	1.19	1.04
1:T:17:DC:OP1	3:A:246:THR:OG1	1.75	1.04
3:B:791:LYS:HB3	3:B:794:THR:CG2	1.87	1.04
3:B:791:LYS:HB3	3:B:794:THR:CG2	1.87	1.04
3:A:392:ARG:O	3:A:395:VAL:CB	2.06	1.04
3:B:791:LYS:HB3	3:B:794:THR:HG21	1.39	1.03
3:B:763:ARG:O	3:B:828:VAL:CG1	2.06	1.03
3:B:763:ARG:O	3:B:828:VAL:CG1	2.06	1.03
3:A:342:VAL:HG13	3:A:364:ILE:CD1	1.89	1.03
3:A:342:VAL:HG13	3:A:364:ILE:CD1	1.89	1.02
3:B:501:VAL:HG12	3:B:502:ARG:H	1.19	1.02
3:B:778:GLU:O	3:B:779:SER:HB3	1.51	1.02
3:A:392:ARG:O	3:A:395:VAL:CB	2.06	1.02
3:B:729:LYS:O	3:B:730:LYS:CG	2.08	1.02
3:A:365:PRO:HB2	3:A:369:ILE:HD13	1.42	1.01
1:T:17:DC:OP1	3:A:246:THR:OG1	1.75	1.01
3:B:729:LYS:O	3:B:730:LYS:CG	2.08	1.01
6:T:182:HOH:O	3:A:103:ARG:HD2	1.59	1.01
3:B:791:LYS:HB3	3:B:794:THR:HG21	1.39	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:P:198:HOH:O	3:B:486:CYS:SG	2.18	1.01
3:B:723:SER:HB2	3:B:828:VAL:O	1.61	1.01
2:P:1:DG:H2"	2:P:2:DG:H5"	1.42	1.00
3:A:365:PRO:HB2	3:A:369:ILE:HD13	1.42	1.00
3:A:328:LEU:O	3:A:332:VAL:HG23	1.60	1.00
3:B:723:SER:HB2	3:B:828:VAL:O	1.61	0.99
3:A:328:LEU:O	3:A:332:VAL:HG23	1.61	0.99
3:A:366:SER:O	3:A:367:HIS:ND1	1.95	0.99
3:B:752:VAL:O	3:B:755:ASP:O	1.81	0.99
1:T:14:DC:H2"	1:T:15:DC:H5'	1.42	0.99
3:B:752:VAL:O	3:B:755:ASP:O	1.81	0.99
3:A:107:TYR:OH	3:A:299:PRO:HG3	1.63	0.99
3:A:107:TYR:OH	3:A:299:PRO:HG3	1.64	0.98
3:A:366:SER:O	3:A:367:HIS:ND1	1.95	0.98
2:P:1:DG:H2"	2:P:2:DG:H5"	1.42	0.97
1:T:14:DC:H2"	1:T:15:DC:H5'	1.42	0.97
2:P:8:DG:OP2	3:B:779:SER:OG	1.82	0.96
2:P:8:DG:OP2	3:B:779:SER:OG	1.83	0.96
3:A:404:THR:HG22	3:A:405:LEU:H	1.29	0.96
2:P:8:DG:O5'	3:B:777:ARG:HA	1.66	0.95
3:A:308:PHE:CB	3:A:405:LEU:HD22	1.97	0.95
3:A:404:THR:HG22	3:A:405:LEU:H	1.29	0.94
3:A:308:PHE:CB	3:A:405:LEU:HD22	1.97	0.94
6:T:211:HOH:O	3:A:290:ASN:HB2	1.66	0.94
2:P:8:DG:O5'	3:B:777:ARG:HA	1.64	0.93
3:B:826:LEU:HD12	3:B:826:LEU:O	1.69	0.93
3:B:734:GLU:OE2	3:B:821:PHE:HA	1.68	0.93
1:T:12:DT:OP1	3:A:363:PRO:CD	2.15	0.93
3:B:826:LEU:HD12	3:B:826:LEU:O	1.68	0.93
3:A:103:ARG:HD2	6:A:581:HOH:O	1.68	0.92
3:A:366:SER:O	3:A:367:HIS:CE1	2.22	0.92
3:B:759:PRO:HD3	3:B:833:LEU:CD1	1.99	0.92
3:B:734:GLU:OE2	3:B:821:PHE:HA	1.68	0.92
3:B:759:PRO:HD3	3:B:833:LEU:CD1	1.99	0.92
6:T:123:HOH:O	3:A:289:ASP:OD1	1.87	0.92
3:A:366:SER:O	3:A:367:HIS:CE1	2.22	0.92
6:T:231:HOH:O	3:A:27:SER:N	2.02	0.91
3:B:542:ARG:HG3	3:B:716:SER:OG	1.70	0.91
3:A:317:ALA:HA	3:A:320:LYS:HG3	1.52	0.91
3:B:542:ARG:HG3	3:B:716:SER:OG	1.70	0.91
3:B:791:LYS:O	3:B:794:THR:HG22	1.72	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:6:DG:H2"	1:T:7:DG:C5'	2.01	0.90
1:T:12:DT:OP1	3:A:363:PRO:HD2	1.71	0.90
1:T:6:DG:H2"	1:T:7:DG:C5'	2.00	0.90
3:B:762:VAL:HG21	3:B:803:MET:CE	2.01	0.90
3:A:317:ALA:HA	3:A:320:LYS:HG3	1.51	0.90
3:B:724:GLU:O	3:B:744:LEU:HD12	1.72	0.90
3:B:791:LYS:O	3:B:794:THR:HG22	1.72	0.89
3:B:822:HIS:O	3:B:823:LEU:HG	1.72	0.89
3:A:346:ILE:O	3:A:358:GLU:CB	2.21	0.89
3:B:762:VAL:HG21	3:B:803:MET:CE	2.01	0.89
3:A:392:ARG:O	3:A:395:VAL:CA	2.21	0.89
3:B:822:HIS:O	3:B:823:LEU:HG	1.72	0.89
2:P:6:DA:H2'	2:P:7:DA:C8	2.08	0.89
3:A:346:ILE:O	3:A:358:GLU:CB	2.21	0.89
6:P:226:HOH:O	3:B:717:GLY:HA3	1.71	0.89
3:B:724:GLU:O	3:B:744:LEU:HD12	1.72	0.89
3:A:366:SER:O	3:A:367:HIS:CD2	2.26	0.88
3:A:348:ARG:HA	3:A:403:LEU:CB	2.04	0.88
3:A:348:ARG:HA	3:A:403:LEU:CB	2.04	0.88
3:A:392:ARG:O	3:A:395:VAL:CA	2.21	0.88
6:T:122:HOH:O	3:A:231:HIS:ND1	2.05	0.88
3:A:366:SER:O	3:A:367:HIS:CD2	2.26	0.88
3:B:486:CYS:SG	6:B:1098:HOH:O	2.29	0.88
2:P:6:DA:H2'	2:P:7:DA:C8	2.08	0.88
3:A:371:LYS:H	3:A:371:LYS:HD3	1.39	0.87
3:A:290:ASN:HB2	6:A:610:HOH:O	1.73	0.86
3:B:763:ARG:C	3:B:764:LEU:HD12	1.95	0.86
3:B:763:ARG:C	3:B:764:LEU:HD12	1.95	0.86
3:A:360:ARG:HB3	3:A:390:LEU:HD22	1.58	0.86
6:T:270:HOH:O	3:A:94:VAL:HG13	1.74	0.86
3:A:347:ARG:CB	3:A:356:GLY:O	2.23	0.86
3:A:347:ARG:CB	3:A:356:GLY:O	2.23	0.86
3:A:164:ASN:H	3:A:170:HIS:HD2	1.20	0.85
3:A:164:ASN:H	3:A:170:HIS:HD2	1.20	0.85
3:A:343:ARG:O	3:A:344:LEU:HD12	1.77	0.85
3:A:371:LYS:H	3:A:371:LYS:HD3	1.39	0.85
1:T:6:DG:C2'	1:T:7:DG:H5'	2.05	0.85
3:A:343:ARG:O	3:A:344:LEU:HD12	1.76	0.85
3:B:471:LYS:HD3	3:B:472:ASP:H	1.43	0.84
3:B:756:GLY:O	3:B:757:ARG:HD3	1.77	0.84
3:B:756:GLY:O	3:B:757:ARG:HD3	1.78	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:759:PRO:HD3	3:B:833:LEU:HD11	1.57	0.84
3:B:471:LYS:HD3	3:B:472:ASP:H	1.43	0.84
3:B:762:VAL:HG21	3:B:803:MET:HE1	1.58	0.84
3:B:724:GLU:HG2	3:B:748:LEU:HD23	1.60	0.84
3:B:762:VAL:HG21	3:B:803:MET:HE1	1.59	0.84
3:B:475:LEU:O	3:B:486:CYS:HB2	1.78	0.84
3:A:313:SER:O	3:A:315:VAL:N	2.11	0.83
3:A:313:SER:O	3:A:315:VAL:HG12	1.78	0.83
3:B:759:PRO:HD3	3:B:833:LEU:HD11	1.57	0.83
3:A:313:SER:O	3:A:315:VAL:HG12	1.78	0.83
3:B:763:ARG:O	3:B:764:LEU:HD12	1.78	0.83
3:A:313:SER:O	3:A:315:VAL:N	2.11	0.83
3:A:360:ARG:HB3	3:A:390:LEU:HD22	1.58	0.83
3:B:763:ARG:O	3:B:764:LEU:HD12	1.78	0.83
1:T:6:DG:C2'	1:T:7:DG:H5'	2.05	0.83
3:B:475:LEU:O	3:B:486:CYS:HB2	1.78	0.83
3:B:584:ASN:H	3:B:590:HIS:HD2	1.23	0.82
1:T:12:DT:OP1	3:A:363:PRO:CD	2.26	0.82
1:T:12:DT:H2"	1:T:13:DT:C6	2.13	0.82
3:A:365:PRO:O	3:A:369:ILE:HB	1.79	0.82
3:A:365:PRO:O	3:A:369:ILE:HB	1.80	0.82
6:P:220:HOH:O	3:B:674:GLY:C	2.17	0.82
3:B:584:ASN:H	3:B:590:HIS:HD2	1.24	0.82
3:B:724:GLU:HG2	3:B:748:LEU:HD23	1.60	0.82
1:T:12:DT:H2"	1:T:13:DT:C6	2.13	0.82
3:B:755:ASP:OD2	3:B:756:GLY:O	1.97	0.82
3:B:755:ASP:OD2	3:B:756:GLY:O	1.97	0.81
6:P:206:HOH:O	3:B:523:ARG:HD3	1.80	0.81
3:A:314:GLU:CD	3:A:401:PHE:CB	2.50	0.81
3:A:367:HIS:CD2	3:A:368:VAL:HG22	2.16	0.81
3:B:721:SER:HB3	3:B:831:CYS:HB2	1.62	0.81
3:A:367:HIS:CD2	3:A:368:VAL:HG22	2.16	0.80
3:A:314:GLU:CD	3:A:401:PHE:CB	2.50	0.80
1:T:15:DC:H2"	1:T:16:DC:H5"	1.62	0.80
3:B:721:SER:HB3	3:B:831:CYS:HB2	1.63	0.80
3:B:690:GLU:HG3	3:B:695:ILE:HA	1.64	0.80
3:B:690:GLU:HG3	3:B:695:ILE:HA	1.64	0.80
3:A:409:CYS:SG	3:A:411:CYS:CB	2.69	0.80
3:A:306:ASP:O	3:A:405:LEU:HB3	1.81	0.80
3:B:763:ARG:HB3	3:B:781:GLN:HG2	1.63	0.80
3:A:158:TYR:O	6:A:584:HOH:O	2.00	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:812:ARG:HG3	3:B:812:ARG:HH11	1.48	0.79
3:B:802:PRO:O	3:B:806:ILE:HG23	1.82	0.79
3:A:409:CYS:SG	3:A:411:CYS:CB	2.69	0.79
3:B:685:SER:HB3	3:B:688:ILE:HG22	1.63	0.79
1:T:15:DC:H2"	1:T:16:DC:H5"	1.62	0.79
3:B:685:SER:HB3	3:B:688:ILE:HG22	1.63	0.79
3:B:802:PRO:O	3:B:806:ILE:HG23	1.82	0.79
3:B:822:HIS:O	3:B:823:LEU:CG	2.30	0.79
3:B:812:ARG:HG3	3:B:812:ARG:HH11	1.48	0.79
3:A:306:ASP:O	3:A:405:LEU:HB3	1.81	0.79
3:A:371:LYS:HD3	3:A:371:LYS:N	1.98	0.79
3:A:94:VAL:HG13	6:A:668:HOH:O	1.84	0.78
3:A:404:THR:HG22	3:A:405:LEU:N	1.99	0.78
3:B:763:ARG:HB3	3:B:781:GLN:HG2	1.63	0.78
3:B:734:GLU:OE2	3:B:821:PHE:CA	2.32	0.78
3:B:800:MET:O	3:B:804:VAL:HG23	1.84	0.78
3:B:734:GLU:OE2	3:B:821:PHE:CB	2.31	0.78
3:B:822:HIS:O	3:B:823:LEU:CG	2.30	0.78
1:T:7:DG:H5"	3:B:519:LEU:HG	1.65	0.78
1:T:12:DT:H2'	1:T:13:DT:H72	1.65	0.78
3:B:721:SER:HB2	3:B:831:CYS:HB3	1.66	0.78
3:A:404:THR:HG22	3:A:405:LEU:N	1.99	0.78
3:B:825:LEU:H	3:B:825:LEU:CD2	1.89	0.77
3:A:371:LYS:HD3	3:A:371:LYS:N	1.98	0.77
3:B:734:GLU:OE2	3:B:821:PHE:CB	2.31	0.77
1:T:12:DT:OP1	3:A:363:PRO:HD2	1.84	0.77
3:B:807:LEU:O	3:B:811:PHE:CE1	2.37	0.77
3:B:800:MET:O	3:B:804:VAL:HG23	1.84	0.77
3:B:734:GLU:OE2	3:B:821:PHE:CA	2.32	0.77
1:T:12:DT:OP1	3:A:363:PRO:HD3	1.85	0.77
3:A:324:LEU:O	3:A:328:LEU:HG	1.85	0.76
3:B:717:GLY:HA3	6:B:1126:HOH:O	1.84	0.76
3:B:825:LEU:H	3:B:825:LEU:CD2	1.89	0.76
3:B:727:SER:HB2	3:B:825:LEU:HB3	1.66	0.76
3:B:740:LYS:O	3:B:744:LEU:HD23	1.85	0.76
1:T:11:DC:H2"	1:T:12:DT:C5'	2.13	0.76
1:T:12:DT:H2'	1:T:13:DT:H72	1.65	0.76
3:B:791:LYS:HB3	3:B:794:THR:HG22	1.68	0.76
3:B:807:LEU:O	3:B:811:PHE:CE1	2.37	0.76
3:B:501:VAL:HG12	3:B:502:ARG:N	1.98	0.76
3:A:377:TYR:HD1	3:A:377:TYR:O	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:721:SER:HB2	3:B:831:CYS:HB3	1.66	0.76
3:A:377:TYR:HD1	3:A:377:TYR:O	1.68	0.76
3:A:85:LYS:HA	3:A:91:LEU:HD23	1.67	0.75
1:T:7:DG:H5"	3:B:519:LEU:HG	1.67	0.75
3:A:85:LYS:HA	3:A:91:LEU:HD23	1.67	0.75
3:B:790:GLN:O	3:B:791:LYS:NZ	2.16	0.75
3:A:324:LEU:O	3:A:328:LEU:HG	1.85	0.75
3:B:740:LYS:O	3:B:744:LEU:HD23	1.85	0.75
3:B:725:GLU:HB2	3:B:827:SER:HA	1.69	0.75
3:B:791:LYS:HE3	3:B:791:LYS:HA	1.69	0.75
3:A:59:GLN:O	3:A:62:LEU:N	2.19	0.75
3:A:59:GLN:O	3:A:62:LEU:N	2.19	0.75
3:A:289:ASP:OD1	6:A:523:HOH:O	2.03	0.75
3:B:825:LEU:HD23	3:B:825:LEU:N	2.01	0.75
3:B:791:LYS:HE3	3:B:791:LYS:HA	1.69	0.75
2:P:8:DG:O5'	3:B:777:ARG:CA	2.35	0.74
3:A:314:GLU:OE2	3:A:401:PHE:CB	2.35	0.74
3:B:727:SER:HB2	3:B:825:LEU:HB3	1.66	0.74
3:B:724:GLU:HG2	3:B:748:LEU:CD2	2.18	0.74
3:B:791:LYS:HB3	3:B:794:THR:HG22	1.68	0.74
3:B:825:LEU:HD23	3:B:825:LEU:N	2.01	0.74
1:T:13:DT:H2'	1:T:14:DC:C6	2.23	0.74
3:B:725:GLU:HB2	3:B:827:SER:HA	1.68	0.74
3:A:365:PRO:HB2	3:A:369:ILE:CD1	2.17	0.74
3:A:395:VAL:O	3:A:397:VAL:N	2.21	0.74
3:B:725:GLU:OE1	3:B:827:SER:HB3	1.88	0.74
1:T:11:DC:H2"	1:T:12:DT:C5'	2.13	0.74
3:A:395:VAL:O	3:A:397:VAL:N	2.21	0.74
3:B:743:GLU:O	3:B:746:ALA:HB3	1.88	0.74
3:B:778:GLU:O	3:B:779:SER:CB	2.32	0.73
1:T:13:DT:H2'	1:T:14:DC:C6	2.23	0.73
3:A:377:TYR:O	3:A:377:TYR:CD1	2.41	0.73
3:B:501:VAL:HG12	3:B:502:ARG:N	1.98	0.73
3:B:592:ARG:HG2	3:B:592:ARG:HH11	1.51	0.73
3:B:724:GLU:HG2	3:B:748:LEU:CD2	2.17	0.73
3:B:743:GLU:O	3:B:746:ALA:HB3	1.88	0.73
3:A:314:GLU:OE1	3:A:401:PHE:CB	2.36	0.73
3:B:725:GLU:OE1	3:B:827:SER:HB3	1.88	0.73
3:B:592:ARG:HG2	3:B:592:ARG:HH11	1.51	0.73
3:B:762:VAL:HG11	3:B:806:ILE:HD11	1.71	0.73
3:A:339:PRO:HG3	3:A:413:LEU:CD2	2.19	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:342:VAL:CG1	3:A:364:ILE:HD11	2.08	0.73
3:A:314:GLU:OE2	3:A:401:PHE:CB	2.35	0.73
3:B:767:ARG:HB2	3:B:775:TYR:O	1.88	0.73
3:A:365:PRO:HB2	3:A:369:ILE:CD1	2.17	0.73
3:A:377:TYR:O	3:A:377:TYR:CD1	2.41	0.73
2:P:2:DG:H2"	2:P:3:DG:O5'	1.89	0.72
2:P:8:DG:C4'	3:B:776:GLY:O	2.36	0.72
3:A:342:VAL:CG1	3:A:364:ILE:HD11	2.08	0.72
3:B:767:ARG:HB2	3:B:775:TYR:O	1.88	0.72
2:P:2:DG:H2"	2:P:3:DG:O5'	1.89	0.72
3:B:762:VAL:HB	3:B:784:ILE:HD11	1.71	0.72
3:A:314:GLU:OE1	3:A:401:PHE:CB	2.36	0.72
3:B:727:SER:CB	3:B:825:LEU:HB3	2.20	0.72
2:P:8:DG:O5'	3:B:777:ARG:CA	2.38	0.72
3:A:337:ARG:HG2	3:A:414:LYS:O	1.89	0.72
3:B:762:VAL:HG11	3:B:806:ILE:HD11	1.71	0.72
3:A:379:VAL:O	3:A:382:PRO:CD	2.38	0.72
3:A:379:VAL:O	3:A:382:PRO:CD	2.38	0.72
3:A:339:PRO:HG3	3:A:413:LEU:CD2	2.19	0.72
3:A:337:ARG:HG2	3:A:414:LYS:O	1.89	0.72
3:B:727:SER:CB	3:B:825:LEU:HB3	2.20	0.72
3:B:721:SER:HB3	3:B:831:CYS:CB	2.19	0.71
3:A:270:GLU:HG3	3:A:275:ILE:HA	1.70	0.71
6:T:172:HOH:O	3:A:239:ILE:O	2.09	0.71
3:A:88:CYS:O	3:A:90:GLN:N	2.24	0.71
3:A:303:SER:HB2	3:A:409:CYS:HA	1.73	0.71
3:B:724:GLU:N	3:B:748:LEU:HD21	2.05	0.71
3:B:762:VAL:HB	3:B:784:ILE:HD11	1.71	0.71
3:B:801:THR:CB	3:B:802:PRO:CD	2.69	0.71
6:T:256:HOH:O	3:A:58:GLN:OE1	2.08	0.71
3:B:801:THR:CB	3:B:802:PRO:CD	2.69	0.71
1:T:14:DC:H2'	1:T:15:DC:C5	2.26	0.71
3:B:721:SER:HB3	3:B:831:CYS:CB	2.20	0.71
3:A:88:CYS:O	3:A:90:GLN:N	2.24	0.71
3:A:270:GLU:HG3	3:A:275:ILE:HA	1.70	0.71
3:B:724:GLU:N	3:B:748:LEU:HD21	2.05	0.70
3:B:790:GLN:O	3:B:791:LYS:NZ	2.16	0.70
3:B:573:VAL:HB	3:B:594:LEU:HD22	1.72	0.70
3:B:622:ASN:ND2	3:B:625:LEU:H	1.89	0.70
3:B:674:GLY:C	6:B:1120:HOH:O	2.29	0.70
3:B:778:GLU:O	3:B:779:SER:CB	2.32	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:622:ASN:ND2	3:B:625:LEU:H	1.89	0.70
3:B:721:SER:CB	3:B:831:CYS:HB3	2.21	0.70
1:T:14:DC:H2'	1:T:15:DC:C5	2.26	0.70
3:A:84:ALA:HA	3:A:87:LYS:HG2	1.74	0.70
3:B:573:VAL:HB	3:B:594:LEU:HD22	1.71	0.70
3:B:721:SER:CB	3:B:831:CYS:HB3	2.21	0.70
3:A:303:SER:HB2	3:A:409:CYS:HA	1.72	0.70
3:A:47:ASN:ND2	3:A:49:GLU:HG2	2.07	0.70
2:P:8:DG:C4'	3:B:776:GLY:O	2.38	0.70
3:A:84:ALA:HA	3:A:87:LYS:HG2	1.74	0.70
3:B:762:VAL:HG21	3:B:803:MET:HE3	1.73	0.70
1:T:12:DT:OP1	3:A:363:PRO:HD3	1.91	0.70
1:T:11:DC:C3'	1:T:12:DT:H5"	2.22	0.70
1:T:12:DT:O2	6:B:1005:HOH:O	2.07	0.70
3:B:584:ASN:H	3:B:590:HIS:CD2	2.09	0.70
1:T:14:DC:H2'	1:T:15:DC:C6	2.27	0.70
3:B:734:GLU:HG3	3:B:821:PHE:CB	2.22	0.69
3:A:366:SER:C	3:A:367:HIS:CG	2.63	0.69
3:B:721:SER:HA	3:B:833:LEU:HD23	1.73	0.69
1:T:14:DC:H2'	1:T:15:DC:C6	2.27	0.69
3:A:409:CYS:HG	3:A:411:CYS:HB2	1.57	0.69
3:B:526:SER:OG	3:B:542:ARG:NH2	2.26	0.69
3:B:734:GLU:HG3	3:B:821:PHE:CB	2.22	0.69
3:B:812:ARG:HH11	3:B:812:ARG:CG	2.06	0.69
3:A:47:ASN:ND2	3:A:49:GLU:HG2	2.07	0.69
3:A:366:SER:C	3:A:367:HIS:CG	2.63	0.69
3:B:584:ASN:H	3:B:590:HIS:CD2	2.09	0.69
3:B:768:ARG:HH21	3:B:812:ARG:NH2	1.91	0.69
1:T:18:DC:OP1	6:T:172:HOH:O	2.11	0.69
1:T:11:DC:C3'	1:T:12:DT:H5"	2.22	0.69
2:P:11:DC:H2"	2:P:12:DC:O4'	1.92	0.69
3:A:371:LYS:HE2	3:A:376:ASN:HB2	1.75	0.69
3:B:768:ARG:HH21	3:B:812:ARG:NH2	1.91	0.69
1:T:5:DA:H4'	3:B:480:LYS:HB2	1.75	0.68
3:B:812:ARG:HH11	3:B:812:ARG:CG	2.06	0.68
3:A:164:ASN:H	3:A:170:HIS:CD2	2.09	0.68
3:A:371:LYS:HE2	3:A:376:ASN:HB2	1.75	0.68
3:B:721:SER:HA	3:B:833:LEU:HD23	1.74	0.68
3:B:526:SER:OG	3:B:542:ARG:NH2	2.25	0.68
3:A:27:SER:N	6:A:630:HOH:O	2.27	0.68
3:B:523:ARG:HD3	6:B:1106:HOH:O	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:729:LYS:HA	3:B:825:LEU:CD2	2.23	0.68
3:B:763:ARG:HA	3:B:780:ARG:O	1.94	0.68
3:B:729:LYS:HA	3:B:825:LEU:CD2	2.23	0.67
3:A:107:TYR:OH	3:A:299:PRO:CG	2.40	0.67
3:A:320:LYS:HB2	3:A:406:LEU:CD1	2.25	0.67
3:A:164:ASN:H	3:A:170:HIS:CD2	2.08	0.67
3:B:457:CYS:HA	5:B:902:TTP:O1B	1.94	0.67
3:A:343:ARG:C	3:A:344:LEU:HD12	2.15	0.67
3:A:306:ASP:OD1	3:A:405:LEU:HD23	1.95	0.67
3:B:762:VAL:HG21	3:B:803:MET:HE3	1.74	0.67
1:T:5:DA:H2"	1:T:6:DG:O5'	1.95	0.67
3:A:95:ASN:HD21	3:A:97:GLU:HB2	1.59	0.67
3:B:745:LEU:HD21	3:B:828:VAL:HG11	1.76	0.67
3:A:343:ARG:C	3:A:344:LEU:HD12	2.15	0.67
3:A:320:LYS:HB2	3:A:406:LEU:CD1	2.25	0.67
3:A:306:ASP:OD1	3:A:405:LEU:HD23	1.95	0.66
6:T:230:HOH:O	3:A:296:SER:O	2.12	0.66
6:P:253:HOH:O	3:B:504:ALA:HB2	1.95	0.66
3:B:763:ARG:HA	3:B:780:ARG:O	1.94	0.66
3:A:341:THR:HG23	3:A:362:CYS:O	1.95	0.66
3:B:745:LEU:HD21	3:B:828:VAL:HG11	1.76	0.66
1:T:5:DA:H2"	1:T:6:DG:O5'	1.95	0.66
6:P:220:HOH:O	3:B:675:ILE:N	2.29	0.66
3:A:341:THR:HG23	3:A:362:CYS:O	1.95	0.66
1:T:7:DG:H4'	3:B:519:LEU:HD12	1.78	0.66
3:A:95:ASN:HD21	3:A:97:GLU:HB2	1.59	0.66
3:A:112:LEU:C	3:A:112:LEU:HD23	2.15	0.66
3:B:451:VAL:CG1	3:B:550:VAL:HB	2.26	0.66
3:B:685:SER:HB3	3:B:688:ILE:CG2	2.25	0.66
6:T:117:HOH:O	3:A:210:SER:OG	2.13	0.66
3:A:112:LEU:C	3:A:112:LEU:HD23	2.15	0.66
1:T:10:DC:H2"	1:T:11:DC:O5'	1.96	0.66
6:T:159:HOH:O	3:A:137:GLU:HG3	1.94	0.66
3:B:568:LEU:O	3:B:568:LEU:HD23	1.96	0.66
3:B:685:SER:HB3	3:B:688:ILE:CG2	2.24	0.66
3:A:59:GLN:O	3:A:61:TYR:N	2.23	0.65
3:B:568:LEU:O	3:B:568:LEU:HD23	1.97	0.65
1:T:10:DC:H2"	1:T:11:DC:O5'	1.96	0.65
3:B:451:VAL:CG1	3:B:550:VAL:HB	2.27	0.65
3:B:762:VAL:CG2	3:B:803:MET:HE1	2.27	0.65
2:P:11:DC:H2"	2:P:12:DC:O4'	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:392:ARG:O	3:A:395:VAL:HA	1.95	0.65
3:B:622:ASN:HD21	3:B:625:LEU:H	1.44	0.65
3:A:107:TYR:OH	3:A:299:PRO:CG	2.41	0.65
3:A:392:ARG:O	3:A:395:VAL:HA	1.95	0.65
3:B:808:MET:HA	3:B:811:PHE:HB2	1.79	0.65
3:A:299:PRO:HD3	6:A:502:HOH:O	1.97	0.65
3:A:409:CYS:HG	3:A:411:CYS:HB2	1.61	0.65
2:P:4:DG:H2"	2:P:5:DG:H8	1.62	0.65
2:P:4:DG:H2"	2:P:5:DG:H8	1.62	0.64
1:T:5:DA:H4'	3:B:480:LYS:HB2	1.77	0.64
3:B:740:LYS:HZ2	3:B:741:ILE:HG13	1.62	0.64
3:B:622:ASN:HD21	3:B:625:LEU:H	1.45	0.64
3:A:88:CYS:SG	3:A:91:LEU:HB2	2.37	0.64
6:T:102:HOH:O	3:A:299:PRO:HD3	1.96	0.64
3:B:721:SER:CB	3:B:831:CYS:CB	2.76	0.64
3:B:762:VAL:CG2	3:B:803:MET:HE1	2.28	0.64
3:A:88:CYS:SG	3:A:91:LEU:HB2	2.38	0.64
3:B:808:MET:HA	3:B:811:PHE:HB2	1.79	0.64
3:A:59:GLN:O	3:A:61:TYR:N	2.23	0.63
3:A:59:GLN:CD	3:A:64:VAL:HG11	2.18	0.63
3:B:721:SER:CB	3:B:831:CYS:CB	2.76	0.63
1:T:14:DC:C2'	1:T:15:DC:C6	2.81	0.63
3:A:319:ASN:HA	3:A:322:GLU:OE1	1.99	0.63
3:B:622:ASN:C	3:B:622:ASN:HD22	2.02	0.63
3:B:767:ARG:CB	3:B:775:TYR:O	2.45	0.63
1:T:7:DG:H4'	3:B:519:LEU:HD12	1.81	0.63
3:B:765:ILE:N	3:B:827:SER:O	2.22	0.63
3:A:347:ARG:HA	3:A:356:GLY:O	1.99	0.63
1:T:14:DC:C2'	1:T:15:DC:C6	2.81	0.63
3:A:309:LYS:O	3:A:310:LYS:HE3	1.99	0.63
3:B:767:ARG:CB	3:B:775:TYR:O	2.45	0.63
3:A:371:LYS:HE2	3:A:376:ASN:O	1.99	0.62
3:B:527:TYR:OH	3:B:719:PRO:HG3	1.99	0.62
3:A:371:LYS:HE2	3:A:376:ASN:O	1.99	0.62
3:A:59:GLN:CD	3:A:64:VAL:HG11	2.18	0.62
3:A:319:ASN:HA	3:A:322:GLU:OE1	1.99	0.62
3:B:729:LYS:O	3:B:730:LYS:CB	2.48	0.62
3:A:309:LYS:O	3:A:310:LYS:HE3	1.99	0.62
3:A:347:ARG:HA	3:A:356:GLY:O	1.99	0.62
3:B:717:GLY:O	3:B:718:PRO:O	2.18	0.62
3:B:622:ASN:C	3:B:622:ASN:HD22	2.02	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:318:LYS:O	3:A:322:GLU:HG3	2.00	0.62
3:A:379:VAL:O	3:A:382:PRO:N	2.32	0.62
3:A:163:ILE:HG21	3:A:174:LEU:HD11	1.82	0.62
3:A:318:LYS:O	3:A:322:GLU:HG3	2.00	0.62
3:B:717:GLY:O	3:B:718:PRO:O	2.18	0.62
3:B:723:SER:C	3:B:748:LEU:HD21	2.20	0.62
3:A:55:LEU:HD12	3:A:56:GLY:H	1.64	0.62
3:B:729:LYS:O	3:B:730:LYS:CB	2.48	0.62
3:A:163:ILE:HG21	3:A:174:LEU:HD11	1.82	0.61
3:A:343:ARG:O	3:A:344:LEU:CD1	2.48	0.61
3:B:765:ILE:N	3:B:827:SER:O	2.22	0.61
3:A:55:LEU:HD12	3:A:56:GLY:H	1.64	0.61
3:A:379:VAL:O	3:A:382:PRO:HD2	2.00	0.61
3:A:371:LYS:NZ	3:A:376:ASN:HB2	2.15	0.61
2:P:4:DG:H2"	2:P:5:DG:C8	2.35	0.61
3:B:495:VAL:HG12	3:B:497:LYS:HE2	1.82	0.61
3:B:527:TYR:OH	3:B:719:PRO:HG3	1.99	0.61
3:B:740:LYS:NZ	3:B:741:ILE:HG13	2.15	0.61
3:A:347:ARG:CA	3:A:356:GLY:O	2.48	0.61
3:B:464:MET:HE2	3:B:471:LYS:HA	1.82	0.61
3:A:347:ARG:CA	3:A:356:GLY:O	2.48	0.61
3:A:379:VAL:O	3:A:382:PRO:N	2.33	0.61
3:B:504:ALA:HB2	6:B:1152:HOH:O	2.01	0.61
3:B:555:MET:CE	3:B:599:ILE:HD12	2.31	0.61
3:B:740:LYS:NZ	3:B:741:ILE:HG13	2.15	0.61
3:A:379:VAL:O	3:A:382:PRO:HD2	2.00	0.61
3:A:371:LYS:NZ	3:A:376:ASN:HB2	2.15	0.61
3:B:718:PRO:HG3	6:B:1123:HOH:O	2.00	0.61
3:A:107:TYR:HH	3:A:299:PRO:HG3	1.63	0.61
3:A:371:LYS:CE	3:A:376:ASN:HB2	2.29	0.61
3:A:384:VAL:O	3:A:388:MET:HG2	2.01	0.61
3:B:532:LEU:C	3:B:532:LEU:HD23	2.22	0.60
3:B:532:LEU:C	3:B:532:LEU:HD23	2.22	0.60
3:A:322:GLU:O	3:A:326:ALA:HB2	2.02	0.60
3:A:59:GLN:C	3:A:61:TYR:H	2.04	0.60
3:A:371:LYS:CE	3:A:376:ASN:HB2	2.30	0.60
2:P:4:DG:H2"	2:P:5:DG:C8	2.35	0.60
3:A:343:ARG:O	3:A:344:LEU:CD1	2.48	0.60
3:B:457:CYS:HA	5:B:902:TTP:O1B	2.01	0.60
3:B:740:LYS:HZ2	3:B:741:ILE:HG13	1.66	0.60
6:T:128:HOH:O	3:A:158:TYR:OH	2.15	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:723:SER:C	3:B:748:LEU:HD21	2.20	0.60
3:B:764:LEU:O	3:B:779:SER:HA	2.02	0.60
3:B:475:LEU:HD12	3:B:476:GLY:H	1.67	0.60
3:A:384:VAL:O	3:A:388:MET:HG2	2.01	0.60
3:B:555:MET:CE	3:B:599:ILE:HD12	2.31	0.60
1:T:15:DC:H2"	1:T:16:DC:C5'	2.32	0.60
3:A:161:GLN:NE2	3:A:225:SER:OG	2.35	0.60
3:B:495:VAL:HG12	3:B:497:LYS:HE2	1.82	0.60
3:B:690:GLU:HA	3:B:698:ALA:CB	2.32	0.60
3:B:689:LEU:HD11	3:B:701:ILE:HD11	1.83	0.60
3:B:764:LEU:O	3:B:779:SER:HA	2.02	0.60
3:B:689:LEU:HD11	3:B:701:ILE:HD11	1.84	0.59
3:A:59:GLN:C	3:A:61:TYR:H	2.04	0.59
3:A:322:GLU:O	3:A:326:ALA:HB2	2.02	0.59
3:B:475:LEU:HD12	3:B:476:GLY:H	1.67	0.59
2:P:12:DC:H5"	2:P:13:DOC:OP2	2.02	0.59
3:B:479:GLN:O	3:B:482:LEU:N	2.33	0.59
1:T:8:DG:H2'	1:T:9:DT:H72	1.84	0.59
1:T:15:DC:H2"	1:T:16:DC:C5'	2.32	0.59
3:B:690:GLU:HA	3:B:698:ALA:CB	2.31	0.59
3:B:722:PHE:O	3:B:830:PHE:HB2	2.03	0.59
1:T:12:DT:H2'	1:T:13:DT:C7	2.32	0.59
3:A:309:LYS:O	3:A:310:LYS:HB2	2.03	0.59
3:A:314:GLU:OE1	3:A:314:GLU:CA	2.51	0.59
3:B:479:GLN:O	3:B:482:LEU:N	2.33	0.59
2:P:6:DA:H5'	3:B:781:GLN:HB2	1.85	0.59
3:B:659:ILE:HD11	3:B:678:VAL:HG22	1.85	0.59
1:T:13:DT:C2'	1:T:14:DC:C6	2.85	0.59
3:A:161:GLN:NE2	3:A:225:SER:OG	2.36	0.59
3:A:215:PRO:O	3:A:217:GLN:HG3	2.03	0.58
3:A:311:CYS:O	3:A:312:SER:HB3	2.03	0.58
3:B:767:ARG:CG	3:B:775:TYR:O	2.51	0.58
1:T:12:DT:H2'	1:T:13:DT:C7	2.32	0.58
3:B:659:ILE:HD11	3:B:678:VAL:HG22	1.86	0.58
3:B:497:LYS:H	3:B:497:LYS:HD2	1.68	0.58
3:A:50:LEU:HD23	3:A:53:LYS:HD3	1.85	0.58
3:A:314:GLU:OE1	3:A:314:GLU:CA	2.51	0.58
1:T:13:DT:C2'	1:T:14:DC:C6	2.85	0.58
3:A:215:PRO:O	3:A:217:GLN:HG3	2.04	0.58
3:A:50:LEU:HD23	3:A:53:LYS:HD3	1.85	0.58
3:A:50:LEU:HA	3:A:53:LYS:HD3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:317:ALA:HA	3:A:320:LYS:CG	2.31	0.58
3:B:767:ARG:CG	3:B:775:TYR:O	2.51	0.58
3:A:59:GLN:NE2	3:A:64:VAL:HG11	2.19	0.58
1:T:8:DG:H2'	1:T:9:DT:H72	1.84	0.58
3:B:464:MET:HE2	3:B:471:LYS:HA	1.86	0.58
3:A:54:PRO:O	3:A:91:LEU:HD12	2.04	0.58
3:A:311:CYS:O	3:A:312:SER:HB3	2.03	0.58
3:A:54:PRO:O	3:A:91:LEU:HD12	2.04	0.58
3:B:801:THR:CB	3:B:802:PRO:HD3	2.33	0.58
3:B:675:ILE:N	6:B:1120:HOH:O	2.37	0.58
1:T:5:DA:C2'	1:T:6:DG:O5'	2.51	0.57
2:P:7:DA:H5"	6:B:1149:HOH:O	2.04	0.57
2:P:6:DA:H5'	3:B:781:GLN:HB2	1.86	0.57
3:A:50:LEU:HA	3:A:53:LYS:HD3	1.84	0.57
3:B:739:ASN:O	3:B:742:GLU:HG3	2.05	0.57
3:B:801:THR:CB	3:B:802:PRO:HD3	2.33	0.57
3:A:59:GLN:NE2	3:A:64:VAL:HG11	2.19	0.57
3:A:309:LYS:O	3:A:310:LYS:HB2	2.03	0.57
3:B:739:ASN:O	3:B:742:GLU:HG3	2.05	0.57
3:B:560:LEU:HD12	3:B:592:ARG:NH1	2.19	0.57
3:A:314:GLU:OE1	3:A:314:GLU:N	2.37	0.57
1:T:5:DA:C2'	1:T:6:DG:O5'	2.51	0.57
3:B:497:LYS:H	3:B:497:LYS:HD2	1.68	0.57
3:B:722:PHE:O	3:B:830:PHE:HB2	2.03	0.57
1:T:14:DC:H2"	1:T:15:DC:C5'	2.28	0.57
3:A:314:GLU:OE1	3:A:314:GLU:N	2.37	0.57
3:A:306:ASP:HB2	3:A:324:LEU:HD21	1.86	0.57
3:A:367:HIS:HD2	3:A:368:VAL:HG22	1.70	0.57
3:B:560:LEU:HD12	3:B:592:ARG:NH1	2.19	0.57
3:B:592:ARG:HG2	3:B:592:ARG:NH1	2.20	0.57
3:A:36:ASP:O	3:A:37:CYS:C	2.43	0.57
3:A:317:ALA:O	3:A:321:ILE:HD13	2.05	0.56
3:B:456:ASP:O	3:B:457:CYS:C	2.43	0.56
3:B:742:GLU:O	3:B:746:ALA:HB2	2.05	0.56
3:A:366:SER:O	3:A:367:HIS:NE2	2.38	0.56
3:B:456:ASP:O	3:B:457:CYS:C	2.43	0.56
3:A:36:ASP:O	3:A:37:CYS:C	2.43	0.56
3:A:279:GLN:O	3:A:283:LYS:HG3	2.06	0.56
3:B:497:LYS:NZ	3:B:497:LYS:HB3	2.20	0.56
3:A:306:ASP:HB2	3:A:324:LEU:HD21	1.86	0.56
3:A:317:ALA:O	3:A:321:ILE:HD13	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:380:MET:O	3:A:384:VAL:CG2	2.44	0.56
3:B:464:MET:CE	3:B:487:ASN:HD22	2.19	0.56
3:B:740:LYS:HD3	3:B:741:ILE:N	2.19	0.56
2:P:11:DC:OP1	3:B:665:LYS:CB	2.54	0.56
3:B:497:LYS:NZ	3:B:497:LYS:HB3	2.20	0.56
1:T:7:DG:H2"	1:T:8:DG:OP2	2.05	0.56
3:A:366:SER:O	3:A:367:HIS:NE2	2.38	0.56
3:B:592:ARG:HG2	3:B:592:ARG:NH1	2.20	0.56
2:P:6:DA:H2"	2:P:7:DA:O4'	2.05	0.56
3:B:742:GLU:O	3:B:746:ALA:HB2	2.05	0.56
3:B:782:CYS:SG	3:B:806:ILE:HD12	2.46	0.56
3:A:204:LEU:CD1	3:A:240:PRO:HD2	2.35	0.56
1:T:7:DG:H5"	3:B:519:LEU:CG	2.36	0.56
2:P:8:DG:C5'	3:B:777:ARG:HA	2.36	0.56
3:A:279:GLN:O	3:A:283:LYS:HG3	2.05	0.56
3:B:740:LYS:HD3	3:B:741:ILE:N	2.20	0.56
3:B:782:CYS:SG	3:B:806:ILE:HD12	2.46	0.56
3:A:204:LEU:CD1	3:A:240:PRO:HD2	2.36	0.55
3:A:261:LEU:HD23	3:A:261:LEU:O	2.07	0.55
3:B:699:GLN:O	3:B:703:LYS:HG2	2.07	0.55
3:A:47:ASN:HD21	3:A:49:GLU:HG2	1.72	0.55
6:T:269:HOH:O	3:A:94:VAL:HA	2.06	0.55
2:P:11:DC:OP1	3:B:665:LYS:CB	2.55	0.55
1:T:14:DC:H2"	1:T:15:DC:C5'	2.28	0.55
3:A:157:VAL:HG11	3:A:161:GLN:O	2.07	0.55
3:A:54:PRO:CA	3:A:70:ALA:HB2	2.37	0.55
3:A:339:PRO:HD3	3:A:413:LEU:HD22	1.89	0.55
6:T:269:HOH:O	3:A:95:ASN:N	2.23	0.55
3:A:137:GLU:HG3	6:A:559:HOH:O	2.07	0.55
3:A:157:VAL:HG11	3:A:161:GLN:O	2.07	0.55
3:A:339:PRO:HD3	3:A:413:LEU:HD22	1.89	0.55
3:B:464:MET:CE	3:B:487:ASN:HD22	2.19	0.55
1:T:7:DG:H2"	1:T:8:DG:OP2	2.05	0.55
3:A:261:LEU:HD23	3:A:261:LEU:O	2.07	0.55
3:B:583:ILE:HG21	3:B:594:LEU:HD11	1.89	0.55
3:B:699:GLN:O	3:B:703:LYS:HG2	2.07	0.55
3:B:716:SER:OG	3:B:716:SER:O	2.23	0.55
3:A:231:HIS:ND1	6:A:522:HOH:O	2.33	0.55
3:B:762:VAL:CG1	3:B:806:ILE:HD11	2.36	0.55
3:B:738:LYS:CB	3:B:808:MET:SD	2.95	0.55
3:B:491:ARG:HA	3:B:496:LYS:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:738:LYS:CB	3:B:808:MET:SD	2.95	0.55
3:B:729:LYS:HA	3:B:825:LEU:HD22	1.89	0.54
6:T:210:HOH:O	3:A:277:VAL:HG21	2.07	0.54
2:P:6:DA:H2"	2:P:7:DA:O4'	2.05	0.54
3:B:728:PHE:CZ	3:B:740:LYS:HG3	2.42	0.54
3:A:308:PHE:O	3:A:310:LYS:N	2.37	0.54
3:B:779:SER:H	3:B:811:PHE:HE2	1.55	0.54
3:B:721:SER:HA	3:B:833:LEU:CD2	2.38	0.54
3:B:491:ARG:HA	3:B:496:LYS:O	2.07	0.54
3:B:583:ILE:HG21	3:B:594:LEU:HD11	1.89	0.54
1:T:7:DG:OP2	3:B:725:GLU:N	2.33	0.54
3:B:741:ILE:HA	3:B:744:LEU:HD21	1.89	0.54
3:B:741:ILE:HA	3:B:744:LEU:HD21	1.89	0.54
3:B:762:VAL:CG1	3:B:806:ILE:HD11	2.36	0.54
3:A:341:THR:O	3:A:411:CYS:O	2.25	0.54
2:P:4:DG:OP2	3:A:300:GLN:NE2	2.40	0.54
3:B:745:LEU:O	3:B:749:LEU:HD22	2.08	0.54
3:A:47:ASN:HD21	3:A:49:GLU:HG2	1.72	0.54
3:A:367:HIS:HD2	3:A:368:VAL:HG22	1.69	0.54
3:B:728:PHE:HZ	3:B:740:LYS:HG3	1.73	0.54
3:B:506:GLU:O	3:B:509:PRO:HD3	2.08	0.54
2:P:8:DG:C5'	3:B:777:ARG:HA	2.38	0.54
3:A:163:ILE:HD13	3:A:174:LEU:HD11	1.90	0.54
3:A:247:ALA:O	3:A:251:GLU:HG3	2.08	0.54
3:A:341:THR:O	3:A:411:CYS:O	2.25	0.54
3:A:343:ARG:HG3	3:A:361:GLN:HB2	1.90	0.54
3:B:509:PRO:C	3:B:511:LEU:H	2.11	0.54
3:A:388:MET:N	3:A:388:MET:HE2	2.23	0.54
3:B:474:PRO:HG3	3:B:489:GLU:O	2.07	0.54
3:B:506:GLU:O	3:B:509:PRO:HD3	2.08	0.54
3:B:509:PRO:C	3:B:511:LEU:H	2.11	0.54
3:B:726:ASP:HB3	3:B:744:LEU:HB3	1.90	0.54
3:A:163:ILE:HD13	3:A:174:LEU:HD11	1.90	0.54
3:B:647:GLN:O	3:B:650:ILE:HG22	2.08	0.54
3:A:54:PRO:CA	3:A:70:ALA:HB2	2.37	0.54
3:A:126:ASP:OD1	3:A:127:GLU:HG3	2.09	0.53
1:T:7:DG:H5"	3:B:519:LEU:CG	2.38	0.53
3:A:126:ASP:OD1	3:A:127:GLU:HG3	2.08	0.53
3:B:723:SER:O	3:B:751:ARG:NH2	2.41	0.53
3:A:343:ARG:HG3	3:A:361:GLN:HB2	1.90	0.53
3:A:84:ALA:HA	3:A:87:LYS:NZ	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:88:CYS:N	3:A:89:PRO:CD	2.71	0.53
3:B:558:LYS:NZ	6:B:1131:HOH:O	2.41	0.53
6:P:231:HOH:O	3:B:558:LYS:NZ	2.41	0.53
3:A:337:ARG:CG	3:A:414:LYS:O	2.56	0.53
3:B:464:MET:HE1	3:B:487:ASN:HD22	1.74	0.53
3:B:491:ARG:CZ	3:B:498:LEU:HD11	2.39	0.53
3:B:604:ARG:HE	3:B:638:GLN:HE21	1.55	0.53
3:B:729:LYS:HA	3:B:825:LEU:HD22	1.89	0.53
2:P:7:DA:C5'	6:B:1149:HOH:O	2.57	0.53
3:B:474:PRO:HG3	3:B:489:GLU:O	2.07	0.53
3:B:728:PHE:HZ	3:B:740:LYS:HG3	1.72	0.53
1:T:14:DC:C2'	1:T:15:DC:H5'	2.28	0.53
3:A:350:SER:O	3:A:351:SER:O	2.26	0.53
3:A:247:ALA:O	3:A:251:GLU:HG3	2.08	0.53
3:B:745:LEU:O	3:B:749:LEU:HD22	2.08	0.53
6:T:227:HOH:O	3:A:290:ASN:ND2	2.29	0.53
3:A:84:ALA:HA	3:A:87:LYS:NZ	2.23	0.53
3:B:728:PHE:CZ	3:B:740:LYS:HG3	2.43	0.53
3:B:604:ARG:HE	3:B:638:GLN:HE21	1.54	0.53
3:B:723:SER:O	3:B:751:ARG:NH2	2.41	0.53
3:B:495:VAL:HG12	3:B:495:VAL:O	2.09	0.53
3:A:161:GLN:OE1	3:A:224:GLU:HB2	2.09	0.53
3:A:337:ARG:CG	3:A:414:LYS:O	2.56	0.53
3:A:350:SER:O	3:A:351:SER:O	2.26	0.53
3:A:314:GLU:OE1	3:A:314:GLU:HA	2.09	0.53
3:A:317:ALA:HA	3:A:320:LYS:CG	2.30	0.53
3:A:360:ARG:NH1	3:A:394:MET:SD	2.82	0.53
3:B:471:LYS:CD	3:B:472:ASP:H	2.19	0.53
3:B:647:GLN:O	3:B:650:ILE:HG22	2.09	0.53
3:B:766:ILE:CB	3:B:778:GLU:CB	2.86	0.53
3:B:539:VAL:CG2	6:B:1077:HOH:O	2.57	0.53
3:A:31:VAL:HG12	3:A:130:VAL:HB	1.91	0.53
3:B:495:VAL:HG12	3:B:495:VAL:O	2.09	0.53
6:P:182:HOH:O	3:B:720:GLN:NE2	2.42	0.53
3:B:766:ILE:CB	3:B:778:GLU:CB	2.86	0.53
3:B:716:SER:OG	3:B:716:SER:O	2.23	0.53
3:A:360:ARG:NH1	3:A:394:MET:SD	2.82	0.52
3:B:616:CYS:SG	3:B:634:LYS:O	2.67	0.52
3:A:161:GLN:OE1	3:A:224:GLU:HB2	2.09	0.52
2:P:2:DG:H2'	6:A:597:HOH:O	2.10	0.52
3:A:328:LEU:O	3:A:332:VAL:CG2	2.47	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:726:ASP:HB3	3:B:744:LEU:HB3	1.90	0.52
3:B:797:TYR:CD1	3:B:797:TYR:O	2.62	0.52
3:A:88:CYS:N	3:A:89:PRO:CD	2.71	0.52
3:A:314:GLU:OE1	3:A:314:GLU:HA	2.09	0.52
3:A:31:VAL:HG12	3:A:130:VAL:HB	1.90	0.52
3:A:371:LYS:HZ1	3:A:376:ASN:HB2	1.74	0.52
1:T:14:DC:C2'	1:T:15:DC:H5'	2.28	0.52
3:A:321:ILE:O	3:A:325:LEU:HB2	2.09	0.52
3:B:471:LYS:CD	3:B:472:ASP:H	2.19	0.52
6:T:126:HOH:O	3:A:134:GLU:HG3	2.08	0.52
3:B:616:CYS:SG	3:B:634:LYS:O	2.67	0.52
3:B:488:TYR:C	3:B:490:ALA:H	2.12	0.52
3:B:491:ARG:CZ	3:B:498:LEU:HD11	2.39	0.52
3:B:562:GLN:HE21	3:B:562:GLN:N	2.07	0.52
3:A:196:CYS:SG	3:A:214:LYS:O	2.67	0.52
3:A:320:LYS:HB2	3:A:406:LEU:HD12	1.92	0.52
3:B:471:LYS:HD3	3:B:472:ASP:N	2.20	0.52
3:B:681:LEU:HD12	3:B:681:LEU:O	2.10	0.52
1:T:5:DA:N3	1:T:5:DA:O5'	2.39	0.52
2:P:8:DG:O3'	3:B:776:GLY:O	2.27	0.52
3:B:779:SER:H	3:B:811:PHE:HE2	1.55	0.52
3:A:88:CYS:O	3:A:91:LEU:N	2.41	0.52
3:A:320:LYS:HB2	3:A:406:LEU:HD12	1.92	0.52
3:B:488:TYR:C	3:B:490:ALA:H	2.12	0.52
3:B:491:ARG:NH2	3:B:498:LEU:HD11	2.25	0.52
3:B:555:MET:HE1	3:B:599:ILE:HD12	1.92	0.52
2:P:4:DG:OP2	3:A:300:GLN:NE2	2.43	0.52
3:A:196:CYS:SG	3:A:214:LYS:O	2.67	0.52
3:A:313:SER:O	3:A:315:VAL:CG1	2.56	0.52
3:B:721:SER:HA	3:B:833:LEU:CD2	2.38	0.52
2:P:8:DG:OP1	3:B:777:ARG:C	2.49	0.51
3:A:332:VAL:HG21	3:A:410:PHE:CE1	2.45	0.51
3:B:741:ILE:HD12	3:B:808:MET:SD	2.50	0.51
3:B:797:TYR:CD1	3:B:797:TYR:O	2.62	0.51
3:B:741:ILE:HD12	3:B:808:MET:SD	2.50	0.51
3:A:332:VAL:HG21	3:A:410:PHE:CE1	2.45	0.51
3:B:681:LEU:HD12	3:B:681:LEU:O	2.10	0.51
3:A:94:VAL:HA	6:A:667:HOH:O	2.10	0.51
3:A:103:ARG:HD3	6:A:603:HOH:O	2.10	0.51
3:A:330:ASN:O	3:A:330:ASN:ND2	2.44	0.51
3:B:741:ILE:HA	3:B:744:LEU:CD2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:248:HOH:O	3:A:169:LEU:HD12	2.10	0.51
3:A:31:VAL:CG1	3:A:130:VAL:HB	2.39	0.51
3:A:330:ASN:ND2	3:A:330:ASN:O	2.44	0.51
3:B:738:LYS:CB	3:B:808:MET:CE	2.88	0.51
3:B:624:LEU:HD21	3:B:660:PRO:HD2	1.93	0.51
3:B:451:VAL:HG12	3:B:550:VAL:HB	1.92	0.51
2:P:5:DG:C2'	2:P:6:DA:O5'	2.59	0.51
3:A:321:ILE:O	3:A:325:LEU:HB2	2.09	0.51
3:B:624:LEU:HD21	3:B:660:PRO:HD2	1.93	0.51
3:B:741:ILE:HA	3:B:744:LEU:CD2	2.40	0.51
3:B:451:VAL:HG12	3:B:550:VAL:HB	1.92	0.51
3:B:532:LEU:HD23	3:B:532:LEU:O	2.10	0.51
3:B:501:VAL:C	3:B:503:ASP:N	2.63	0.51
3:B:511:LEU:HD23	3:B:512:VAL:O	2.11	0.51
3:A:31:VAL:CG1	3:A:130:VAL:HB	2.40	0.51
3:B:573:VAL:HG12	6:B:1037:HOH:O	2.11	0.51
3:B:745:LEU:HD21	3:B:828:VAL:CG1	2.41	0.51
3:A:270:GLU:HA	3:A:278:ALA:CB	2.41	0.51
3:B:532:LEU:HD23	3:B:532:LEU:O	2.10	0.51
3:B:562:GLN:HE21	3:B:562:GLN:N	2.08	0.51
3:B:738:LYS:CB	3:B:808:MET:CE	2.88	0.51
3:B:740:LYS:HD3	3:B:741:ILE:HG13	1.92	0.51
3:B:497:LYS:O	3:B:500:ASN:ND2	2.44	0.51
3:B:539:VAL:HG23	6:B:1077:HOH:O	2.11	0.51
3:A:236:ILE:HD12	3:A:237:LYS:N	2.26	0.51
3:B:797:TYR:O	3:B:797:TYR:HD1	1.93	0.51
6:T:101:HOH:O	3:A:161:GLN:NE2	2.43	0.50
3:A:127:GLU:OE1	3:A:207:LYS:NZ	2.41	0.50
3:A:308:PHE:O	3:A:310:LYS:N	2.37	0.50
3:A:388:MET:N	3:A:388:MET:HE2	2.26	0.50
3:A:88:CYS:O	3:A:91:LEU:N	2.41	0.50
1:T:14:DC:H5"	1:T:14:DC:H6	1.77	0.50
2:P:5:DG:C2'	2:P:6:DA:O5'	2.59	0.50
3:B:491:ARG:NH2	3:B:498:LEU:HD11	2.25	0.50
3:B:740:LYS:HD3	3:B:741:ILE:HG13	1.92	0.50
3:B:797:TYR:O	3:B:797:TYR:HD1	1.93	0.50
2:P:8:DG:OP1	3:B:777:ARG:C	2.50	0.50
3:B:497:LYS:O	3:B:500:ASN:ND2	2.43	0.50
3:A:328:LEU:O	3:A:332:VAL:CG2	2.47	0.50
3:B:498:LEU:N	3:B:498:LEU:HD12	2.26	0.50
3:B:764:LEU:HD13	3:B:807:LEU:HA	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:511:LEU:HD23	3:B:512:VAL:O	2.11	0.50
3:B:812:ARG:CG	3:B:812:ARG:NH1	2.74	0.50
3:A:317:ALA:CA	3:A:320:LYS:HG3	2.33	0.50
3:A:332:VAL:HG21	3:A:410:PHE:CD1	2.46	0.50
1:T:14:DC:H2"	1:T:15:DC:C6	2.47	0.50
3:A:270:GLU:HA	3:A:278:ALA:CB	2.41	0.50
3:B:498:LEU:N	3:B:498:LEU:HD12	2.26	0.50
3:A:320:LYS:HB2	3:A:406:LEU:HD11	1.93	0.50
3:B:471:LYS:HD3	3:B:472:ASP:N	2.20	0.50
3:A:82:ARG:HA	3:A:85:LYS:HB2	1.94	0.50
3:A:235:HIS:ND1	3:A:237:LYS:HG2	2.27	0.50
1:T:14:DC:H5"	1:T:14:DC:H6	1.77	0.49
1:T:8:DG:H2"	1:T:9:DT:C6	2.47	0.49
3:B:761:THR:HG22	3:B:762:VAL:N	2.27	0.49
3:B:826:LEU:HD12	3:B:826:LEU:C	2.31	0.49
1:T:5:DA:N3	1:T:5:DA:O5'	2.39	0.49
3:A:239:ILE:HD11	3:A:258:VAL:HG22	1.94	0.49
3:A:236:ILE:HD12	3:A:237:LYS:N	2.27	0.49
3:A:239:ILE:HD11	3:A:258:VAL:HG22	1.95	0.49
3:B:501:VAL:CG1	3:B:502:ARG:H	2.04	0.49
3:B:501:VAL:C	3:B:503:ASP:N	2.64	0.49
3:B:767:ARG:NH1	3:B:824:THR:HB	2.27	0.49
2:P:8:DG:H2"	2:P:9:DG:H8	1.77	0.49
3:A:82:ARG:HA	3:A:85:LYS:HB2	1.94	0.49
3:A:235:HIS:ND1	3:A:237:LYS:HG2	2.28	0.49
3:A:332:VAL:HG21	3:A:410:PHE:CD1	2.46	0.49
3:A:371:LYS:HZ1	3:A:376:ASN:HB2	1.76	0.49
2:P:5:DG:H2'	2:P:6:DA:H8	1.78	0.49
2:P:5:DG:H2'	2:P:6:DA:H8	1.77	0.49
3:A:88:CYS:O	3:A:88:CYS:SG	2.71	0.49
3:A:50:LEU:O	3:A:53:LYS:HG2	2.13	0.49
3:A:88:CYS:O	3:A:88:CYS:SG	2.71	0.49
3:B:764:LEU:HD13	3:B:807:LEU:HA	1.94	0.49
3:B:767:ARG:NH1	3:B:824:THR:HB	2.27	0.49
1:T:8:DG:H2"	1:T:9:DT:C6	2.47	0.49
3:B:491:ARG:HH22	5:B:902:TTP:PG	2.36	0.49
3:B:601:ALA:HA	3:B:638:GLN:HE22	1.77	0.49
2:P:12:DC:H2"	3:B:543:LEU:HD21	1.94	0.49
3:A:404:THR:CG2	3:A:405:LEU:N	2.73	0.49
3:B:501:VAL:CG1	3:B:502:ARG:H	2.04	0.49
1:T:14:DC:H2"	1:T:15:DC:C6	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:601:ALA:HA	3:B:638:GLN:HE22	1.77	0.49
3:B:808:MET:O	3:B:811:PHE:HB2	2.13	0.49
3:B:808:MET:O	3:B:811:PHE:HB2	2.13	0.49
1:T:5:DA:O3'	3:B:480:LYS:HG2	2.13	0.48
3:A:100:THR:O	3:A:104:GLU:HG3	2.13	0.48
2:P:11:DC:C2'	2:P:12:DC:O5'	2.61	0.48
3:A:84:ALA:HA	3:A:87:LYS:HZ3	1.78	0.48
3:A:410:PHE:HD2	3:A:410:PHE:HA	1.60	0.48
3:A:50:LEU:O	3:A:53:LYS:HG2	2.13	0.48
3:B:761:THR:HG22	3:B:762:VAL:N	2.27	0.48
2:P:8:DG:H2"	2:P:9:DG:H8	1.77	0.48
3:B:826:LEU:HD12	3:B:826:LEU:C	2.31	0.48
3:A:55:LEU:HD12	3:A:56:GLY:N	2.27	0.48
3:A:320:LYS:HB2	3:A:406:LEU:HD11	1.93	0.48
3:A:343:ARG:HB3	3:A:409:CYS:HB3	1.96	0.48
3:A:343:ARG:HB3	3:A:409:CYS:HB3	1.96	0.48
1:T:5:DA:H8	3:B:479:GLN:OE1	1.97	0.48
3:A:380:MET:O	3:A:384:VAL:CG2	2.44	0.48
2:P:7:DA:H5'	3:B:779:SER:O	2.14	0.48
3:A:303:SER:OG	3:A:408:VAL:O	2.24	0.48
3:B:799:VAL:O	3:B:803:MET:HG2	2.14	0.48
3:A:161:GLN:NE2	6:A:501:HOH:O	2.46	0.48
3:A:369:ILE:HG13	3:A:379:VAL:HG21	1.96	0.48
3:B:734:GLU:CG	3:B:821:PHE:CB	2.91	0.48
6:P:177:HOH:O	3:B:539:VAL:HG23	2.14	0.48
3:A:46:SER:O	3:A:48:PRO:HD3	2.13	0.48
3:A:150:ALA:O	3:A:152:THR:HG23	2.14	0.48
3:A:318:LYS:HE2	3:A:322:GLU:OE2	2.14	0.48
3:B:763:ARG:O	3:B:764:LEU:CD1	2.57	0.48
3:B:779:SER:N	3:B:811:PHE:CE2	2.82	0.48
3:A:46:SER:O	3:A:48:PRO:HD3	2.13	0.48
3:A:318:LYS:HE2	3:A:322:GLU:OE2	2.14	0.48
3:B:763:ARG:O	3:B:764:LEU:CD1	2.57	0.48
6:P:137:HOH:O	3:B:573:VAL:HG12	2.14	0.48
3:B:634:LYS:O	3:B:635:PRO:O	2.32	0.48
3:B:689:LEU:HD11	3:B:693:LEU:HD12	1.95	0.47
2:P:8:DG:O3'	3:B:776:GLY:O	2.30	0.47
2:P:13:DOC:H5'	3:B:547:GLU:OE2	2.14	0.47
3:A:100:THR:O	3:A:104:GLU:HG3	2.14	0.47
3:B:779:SER:N	3:B:811:PHE:CE2	2.82	0.47
3:A:365:PRO:CB	3:A:369:ILE:HD13	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:55:LEU:HD12	3:A:56:GLY:N	2.27	0.47
3:B:799:VAL:O	3:B:803:MET:HG2	2.14	0.47
1:T:6:DG:OP1	3:B:517:GLU:HG2	2.14	0.47
3:A:150:ALA:O	3:A:152:THR:HG23	2.14	0.47
3:B:801:THR:CB	3:B:802:PRO:HD2	2.45	0.47
3:A:161:GLN:NE2	3:A:222:LEU:HB2	2.30	0.47
3:B:456:ASP:OD1	3:B:635:PRO:O	2.32	0.47
3:B:734:GLU:CG	3:B:821:PHE:CB	2.91	0.47
3:A:304:GLU:HB2	3:A:328:LEU:HD21	1.97	0.47
3:B:495:VAL:O	3:B:497:LYS:HD2	2.15	0.47
3:B:634:LYS:O	3:B:635:PRO:O	2.32	0.47
3:B:734:GLU:CD	3:B:821:PHE:CB	2.82	0.47
6:T:198:HOH:O	2:P:2:DG:H2'	2.13	0.47
6:T:200:HOH:O	3:A:343:ARG:NH2	2.43	0.47
2:P:12:DC:H5"	2:P:13:DOC:OP2	2.15	0.47
3:A:161:GLN:NE2	3:A:222:LEU:HB2	2.30	0.47
1:T:5:DA:O3'	3:B:480:LYS:HG2	2.15	0.47
2:P:5:DG:H2"	2:P:6:DA:O4'	2.15	0.47
3:B:759:PRO:HG2	3:B:830:PHE:CD1	2.50	0.47
3:B:767:ARG:HH11	3:B:824:THR:HB	1.79	0.47
2:P:11:DC:C2'	2:P:12:DC:O5'	2.61	0.47
3:A:81:VAL:O	3:A:85:LYS:HB2	2.15	0.47
3:A:184:ARG:HA	3:A:187:MET:CE	2.45	0.47
3:B:456:ASP:OD1	3:B:635:PRO:O	2.32	0.47
3:B:502:ARG:HD3	3:B:505:LYS:CB	2.45	0.47
3:B:539:VAL:N	6:B:1067:HOH:O	2.30	0.47
3:B:624:LEU:CD2	3:B:660:PRO:HD2	2.45	0.47
3:B:813:ASN:O	3:B:814:MET:C	2.52	0.47
3:A:184:ARG:HA	3:A:187:MET:CE	2.45	0.47
3:A:369:ILE:HG13	3:A:379:VAL:HG21	1.96	0.47
3:B:502:ARG:HD3	3:B:505:LYS:CB	2.44	0.47
3:B:734:GLU:CD	3:B:821:PHE:CB	2.82	0.47
3:B:745:LEU:HD21	3:B:828:VAL:CG1	2.41	0.47
3:B:779:SER:N	3:B:811:PHE:CZ	2.82	0.47
3:B:798:ASP:O	3:B:802:PRO:HD2	2.15	0.47
3:B:767:ARG:HH11	3:B:824:THR:HB	1.79	0.47
3:B:779:SER:N	3:B:811:PHE:CZ	2.82	0.47
3:B:791:LYS:CB	3:B:794:THR:HG21	2.26	0.47
3:B:798:ASP:O	3:B:802:PRO:HD2	2.15	0.47
3:A:81:VAL:O	3:A:85:LYS:HB2	2.15	0.47
1:T:8:DG:H2'	1:T:9:DT:C7	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:759:PRO:HG2	3:B:830:PHE:CD1	2.50	0.47
1:T:6:DG:H4'	1:T:6:DG:OP1	2.15	0.47
6:T:129:HOH:O	3:A:114:GLU:OE1	2.20	0.47
3:B:624:LEU:CD2	3:B:660:PRO:HD2	2.45	0.47
3:B:794:THR:HG23	3:B:796:ASN:ND2	2.30	0.47
3:B:497:LYS:HB3	3:B:497:LYS:HZ2	1.79	0.47
1:T:8:DG:H2'	1:T:9:DT:C7	2.45	0.47
6:P:297:HOH:O	3:B:572:THR:HG21	2.15	0.47
1:T:6:DG:OP1	1:T:6:DG:H4'	2.15	0.46
2:P:5:DG:H2"	2:P:6:DA:O4'	2.15	0.46
3:A:54:PRO:HB3	3:A:70:ALA:HB2	1.97	0.46
3:A:379:VAL:N	6:A:593:HOH:O	2.48	0.46
3:B:588:VAL:O	3:B:592:ARG:HG3	2.15	0.46
3:A:388:MET:CE	3:A:388:MET:HA	2.45	0.46
3:B:689:LEU:HD11	3:B:693:LEU:HD12	1.96	0.46
1:T:12:DT:C2'	1:T:13:DT:C6	2.93	0.46
3:A:54:PRO:HB3	3:A:70:ALA:HB2	1.97	0.46
3:A:61:TYR:O	3:A:62:LEU:HD23	2.14	0.46
3:B:495:VAL:O	3:B:497:LYS:HD2	2.15	0.46
3:B:665:LYS:O	3:B:668:LYS:HB2	2.16	0.46
3:B:740:LYS:NZ	3:B:741:ILE:CG1	2.78	0.46
3:B:782:CYS:SG	3:B:782:CYS:O	2.73	0.46
3:A:296:SER:O	6:A:629:HOH:O	2.20	0.46
3:A:317:ALA:CA	3:A:320:LYS:HG3	2.33	0.46
3:B:464:MET:HE1	3:B:487:ASN:HD22	1.80	0.46
3:B:665:LYS:O	3:B:668:LYS:HB2	2.16	0.46
6:T:248:HOH:O	3:A:169:LEU:CD1	2.64	0.46
3:A:304:GLU:HB2	3:A:328:LEU:HD21	1.97	0.46
3:B:588:VAL:O	3:B:592:ARG:HG3	2.15	0.46
1:T:12:DT:C2'	1:T:13:DT:C6	2.93	0.46
3:A:410:PHE:O	3:A:411:CYS:O	2.33	0.46
3:B:762:VAL:O	3:B:781:GLN:HG2	2.15	0.46
3:A:302:PHE:O	3:A:328:LEU:HD22	2.16	0.46
1:T:5:DA:H8	3:B:479:GLN:OE1	1.99	0.46
6:T:101:HOH:O	3:A:222:LEU:HB2	2.14	0.46
3:A:50:LEU:HA	3:A:53:LYS:CD	2.46	0.46
2:P:9:DG:P	3:B:776:GLY:H	2.38	0.46
3:A:302:PHE:O	3:A:328:LEU:HD22	2.16	0.46
3:B:555:MET:HE2	3:B:599:ILE:HD12	1.98	0.46
3:B:791:LYS:CB	3:B:794:THR:HG21	2.27	0.46
3:A:127:GLU:OE1	3:A:207:LYS:NZ	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:301:SER:O	3:A:302:PHE:HD2	1.98	0.46
3:B:460:ALA:O	3:B:464:MET:HG3	2.16	0.46
3:B:782:CYS:SG	3:B:782:CYS:O	2.73	0.46
1:T:12:DT:H2"	1:T:13:DT:H6	1.76	0.46
6:P:257:HOH:O	3:B:447:SER:HB2	2.16	0.46
3:A:313:SER:O	3:A:315:VAL:CG1	2.56	0.46
3:B:459:TYR:CZ	5:B:902:TTP:H1'	2.51	0.46
3:A:339:PRO:HG2	3:A:410:PHE:CD1	2.51	0.46
3:A:54:PRO:HG3	3:A:69:GLU:HG3	1.98	0.46
3:A:301:SER:O	3:A:302:PHE:HD2	1.98	0.46
3:A:339:PRO:HG2	3:A:410:PHE:CD1	2.51	0.46
3:B:501:VAL:C	3:B:503:ASP:H	2.19	0.46
3:A:61:TYR:O	3:A:62:LEU:HD23	2.14	0.46
3:A:146:ASP:C	3:A:148:LEU:H	2.20	0.46
3:A:153:VAL:HG22	3:A:154:SER:N	2.31	0.46
3:A:410:PHE:O	3:A:411:CYS:O	2.33	0.46
3:B:740:LYS:NZ	3:B:741:ILE:CG1	2.78	0.46
3:B:794:THR:HG23	3:B:796:ASN:ND2	2.30	0.45
3:B:762:VAL:O	3:B:781:GLN:HG2	2.15	0.45
3:B:813:ASN:O	3:B:814:MET:C	2.52	0.45
2:P:12:DC:H2"	3:B:543:LEU:HD21	1.98	0.45
3:A:86:GLU:O	3:A:89:PRO:HD3	2.16	0.45
3:A:354:HIS:O	3:A:355:TYR:C	2.55	0.45
3:B:592:ARG:NH1	3:B:592:ARG:CG	2.80	0.45
3:B:725:GLU:HB2	3:B:827:SER:CA	2.43	0.45
3:B:501:VAL:C	3:B:503:ASP:H	2.19	0.45
6:P:177:HOH:O	3:B:539:VAL:CG2	2.64	0.45
3:A:54:PRO:HG3	3:A:69:GLU:HG3	1.97	0.45
3:A:392:ARG:O	3:A:395:VAL:N	2.50	0.45
3:A:50:LEU:HA	3:A:53:LYS:CG	2.47	0.45
3:A:365:PRO:CB	3:A:369:ILE:HD13	2.30	0.45
3:B:460:ALA:O	3:B:464:MET:HG3	2.16	0.45
3:B:592:ARG:NH1	3:B:592:ARG:CG	2.80	0.45
3:B:728:PHE:HB2	3:B:731:CYS:HB2	1.99	0.45
3:A:388:MET:CE	3:A:388:MET:HA	2.45	0.45
3:B:822:HIS:O	3:B:823:LEU:CB	2.64	0.45
1:T:6:DG:OP1	3:B:517:GLU:HG2	2.17	0.45
3:A:86:GLU:O	3:A:89:PRO:HD3	2.16	0.45
3:A:265:SER:OG	3:A:268:ILE:HB	2.17	0.45
3:A:60:LYS:O	3:A:61:TYR:CG	2.63	0.45
3:A:388:MET:N	3:A:388:MET:CE	2.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:667:ALA:O	3:B:671:GLU:HG3	2.17	0.45
3:B:720:GLN:NE2	6:B:1082:HOH:O	2.46	0.45
2:P:1:DG:H2"	2:P:2:DG:C5'	2.31	0.45
3:A:341:THR:CG2	3:A:362:CYS:O	2.64	0.45
3:A:354:HIS:O	3:A:355:TYR:C	2.55	0.45
3:A:388:MET:N	3:A:388:MET:CE	2.80	0.45
3:B:667:ALA:O	3:B:671:GLU:HG3	2.17	0.45
1:T:10:DC:C2'	1:T:11:DC:O5'	2.62	0.45
1:T:8:DG:C8	1:T:9:DT:H72	2.52	0.45
6:P:230:HOH:O	3:B:539:VAL:HG11	2.17	0.45
3:A:184:ARG:HA	3:A:187:MET:HE3	1.99	0.45
3:A:410:PHE:O	3:A:411:CYS:C	2.55	0.45
3:B:822:HIS:O	3:B:823:LEU:CB	2.64	0.45
1:T:8:DG:C8	1:T:9:DT:H72	2.52	0.45
2:P:5:DG:H2"	2:P:6:DA:O5'	2.17	0.45
3:A:265:SER:OG	3:A:268:ILE:HB	2.17	0.45
3:A:175:VAL:O	3:A:178:GLN:HB2	2.17	0.45
3:B:479:GLN:O	3:B:480:LYS:C	2.56	0.44
3:B:512:VAL:HG12	3:B:513:LEU:N	2.32	0.44
1:T:10:DC:C2'	1:T:11:DC:O5'	2.62	0.44
2:P:5:DG:H2"	2:P:6:DA:O5'	2.17	0.44
6:P:249:HOH:O	3:B:781:GLN:HG3	2.16	0.44
3:A:208:LEU:HD21	3:A:240:PRO:HD3	2.00	0.44
3:B:728:PHE:HB2	3:B:731:CYS:HB2	1.98	0.44
3:B:512:VAL:HG12	3:B:513:LEU:N	2.32	0.44
1:T:5:DA:C8	3:B:479:GLN:OE1	2.71	0.44
3:A:55:LEU:O	3:A:66:CYS:HB2	2.17	0.44
3:A:175:VAL:O	3:A:178:GLN:HB2	2.17	0.44
3:B:479:GLN:O	3:B:480:LYS:C	2.56	0.44
3:A:75:VAL:HG12	3:A:75:VAL:O	2.17	0.44
3:A:153:VAL:HG22	3:A:154:SER:N	2.32	0.44
3:A:335:ASP:OD1	3:A:337:ARG:HB2	2.18	0.44
3:B:725:GLU:HB2	3:B:827:SER:CA	2.43	0.44
3:A:75:VAL:HG12	3:A:75:VAL:O	2.17	0.44
3:A:335:ASP:OD1	3:A:337:ARG:HB2	2.18	0.44
3:A:347:ARG:CB	3:A:356:GLY:HA3	2.48	0.44
3:A:410:PHE:O	3:A:411:CYS:C	2.55	0.44
3:B:559:ARG:CZ	3:B:599:ILE:CD1	2.96	0.44
3:B:750:ASN:O	3:B:754:GLN:HB2	2.18	0.44
3:A:60:LYS:O	3:A:61:TYR:CG	2.63	0.44
3:A:392:ARG:O	3:A:395:VAL:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:750:ASN:O	3:B:754:GLN:HB2	2.18	0.44
3:B:801:THR:CB	3:B:802:PRO:HD2	2.45	0.44
3:A:346:ILE:N	3:A:358:GLU:O	2.51	0.44
3:B:802:PRO:O	3:B:806:ILE:CG2	2.60	0.44
6:T:148:HOH:O	3:A:257:SER:HB2	2.18	0.44
3:A:301:SER:O	3:A:302:PHE:CD2	2.71	0.44
3:A:405:LEU:HA	3:A:405:LEU:HD12	1.67	0.44
3:B:685:SER:CB	3:B:688:ILE:HG22	2.42	0.44
3:A:50:LEU:HA	3:A:53:LYS:CG	2.47	0.44
1:T:17:DC:H2"	1:T:18:DC:OP2	2.18	0.44
3:A:55:LEU:O	3:A:66:CYS:HB2	2.17	0.44
3:A:146:ASP:C	3:A:148:LEU:H	2.20	0.44
1:T:13:DT:H2"	1:T:14:DC:O4'	2.18	0.43
3:A:54:PRO:HB3	3:A:70:ALA:CB	2.48	0.43
3:B:459:TYR:CZ	5:B:902:TTP:H1'	2.53	0.43
3:B:471:LYS:O	3:B:472:ASP:OD1	2.35	0.43
3:B:539:VAL:HG11	6:B:1130:HOH:O	2.18	0.43
3:B:743:GLU:O	3:B:746:ALA:CB	2.63	0.43
3:B:744:LEU:HD11	3:B:828:VAL:HG23	2.00	0.43
1:T:17:DC:H2"	1:T:18:DC:OP2	2.18	0.43
3:A:101:ARG:HG3	3:A:101:ARG:HH11	1.83	0.43
3:B:560:LEU:HD23	3:B:563:LEU:HD12	2.00	0.43
3:A:270:GLU:HA	3:A:278:ALA:HB2	2.00	0.43
2:P:1:DG:H2"	2:P:2:DG:C5'	2.31	0.43
3:A:301:SER:O	3:A:302:PHE:CD2	2.71	0.43
3:B:573:VAL:HG22	3:B:574:SER:N	2.33	0.43
2:P:8:DG:C5'	3:B:776:GLY:O	2.66	0.43
3:A:208:LEU:HD21	3:A:240:PRO:HD3	1.99	0.43
3:B:560:LEU:HD23	3:B:563:LEU:HD12	2.00	0.43
3:B:764:LEU:HA	3:B:828:VAL:HA	2.01	0.43
3:A:88:CYS:N	3:A:89:PRO:HD3	2.33	0.43
3:B:622:ASN:ND2	3:B:622:ASN:C	2.72	0.43
3:B:822:HIS:O	3:B:823:LEU:CD2	2.66	0.43
1:T:13:DT:H2"	1:T:14:DC:O4'	2.18	0.43
3:B:559:ARG:CZ	3:B:599:ILE:CD1	2.96	0.43
3:B:716:SER:O	3:B:717:GLY:O	2.36	0.43
3:A:346:ILE:N	3:A:358:GLU:O	2.51	0.43
3:A:347:ARG:CB	3:A:356:GLY:HA3	2.48	0.43
3:B:508:CYS:C	3:B:510:GLN:H	2.21	0.43
3:B:759:PRO:CD	3:B:833:LEU:HD11	2.40	0.43
3:A:50:LEU:HA	3:A:53:LYS:CD	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:50:LEU:HA	3:A:53:LYS:HG2	2.01	0.43
3:A:318:LYS:HD3	3:A:318:LYS:C	2.39	0.43
3:A:371:LYS:HE2	3:A:376:ASN:CB	2.47	0.43
3:A:101:ARG:HG3	3:A:101:ARG:HH11	1.83	0.43
3:A:335:ASP:OD1	3:A:335:ASP:C	2.57	0.43
2:P:8:DG:O5'	3:B:777:ARG:C	2.56	0.43
3:A:335:ASP:OD1	3:A:335:ASP:C	2.56	0.43
3:B:508:CYS:C	3:B:510:GLN:H	2.21	0.43
3:B:572:THR:HG21	6:B:1197:HOH:O	2.18	0.43
1:T:5:DA:C8	3:B:479:GLN:OE1	2.72	0.43
3:A:388:MET:CE	3:A:388:MET:CA	2.97	0.43
3:B:716:SER:O	3:B:717:GLY:O	2.36	0.43
3:A:255:ILE:HD11	3:A:264:PHE:CD1	2.53	0.43
3:A:46:SER:C	3:A:48:PRO:HD3	2.39	0.43
3:A:54:PRO:HB3	3:A:70:ALA:CB	2.48	0.43
3:A:318:LYS:HD3	3:A:318:LYS:C	2.39	0.43
3:B:471:LYS:O	3:B:472:ASP:OD1	2.35	0.43
3:B:802:PRO:O	3:B:806:ILE:CG2	2.60	0.43
1:T:14:DC:OP1	3:A:360:ARG:NH2	2.52	0.43
3:A:46:SER:C	3:A:48:PRO:HD3	2.39	0.43
3:A:388:MET:CE	3:A:388:MET:CA	2.97	0.43
3:B:581:GLN:OE1	3:B:642:LEU:HB2	2.19	0.43
2:P:7:DA:H5'	3:B:779:SER:O	2.19	0.43
3:A:179:ILE:O	3:A:183:MET:HG3	2.19	0.43
3:A:255:ILE:HD11	3:A:264:PHE:CD1	2.53	0.43
3:B:508:CYS:O	3:B:510:GLN:N	2.52	0.43
3:B:573:VAL:HG22	3:B:574:SER:N	2.33	0.43
1:T:12:DT:H2"	1:T:13:DT:H6	1.75	0.42
3:A:405:LEU:HA	3:A:405:LEU:HD12	1.67	0.42
3:B:744:LEU:HD11	3:B:828:VAL:HG23	2.00	0.42
3:B:484:VAL:HG21	5:B:902:TTP:O2	2.18	0.42
3:B:764:LEU:HG	3:B:828:VAL:HG22	2.00	0.42
3:A:295:LEU:HD22	6:A:698:HOH:O	2.18	0.42
3:B:483:VAL:HG23	3:B:501:VAL:HA	2.01	0.42
3:A:320:LYS:CB	3:A:406:LEU:HD12	2.50	0.42
1:T:7:DG:C4'	3:B:519:LEU:HD12	2.47	0.42
3:A:112:LEU:HD23	3:A:112:LEU:O	2.19	0.42
3:B:712:PRO:HB3	6:B:1127:HOH:O	2.20	0.42
3:A:88:CYS:N	3:A:89:PRO:HD3	2.33	0.42
3:A:95:ASN:N	6:A:667:HOH:O	2.37	0.42
3:A:179:ILE:O	3:A:183:MET:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:270:GLU:HA	3:A:278:ALA:HB2	2.00	0.42
3:A:320:LYS:CB	3:A:406:LEU:HD12	2.50	0.42
3:A:341:THR:CG2	3:A:362:CYS:O	2.64	0.42
3:A:408:VAL:CG1	3:A:409:CYS:N	2.82	0.42
3:B:761:THR:CG2	3:B:762:VAL:N	2.82	0.42
1:T:18:DC:OP1	6:T:103:HOH:O	2.22	0.42
3:A:54:PRO:CB	3:A:70:ALA:HB2	2.49	0.42
3:B:483:VAL:HG23	3:B:501:VAL:HA	2.01	0.42
3:B:560:LEU:HD12	3:B:592:ARG:HH12	1.83	0.42
3:A:75:VAL:O	3:A:77:LYS:N	2.52	0.42
2:P:9:DG:P	3:B:776:GLY:H	2.43	0.42
3:B:767:ARG:HD3	3:B:769:TYR:CB	2.50	0.42
3:B:824:THR:HG22	3:B:825:LEU:HG	2.02	0.42
3:B:508:CYS:O	3:B:510:GLN:N	2.52	0.42
3:B:560:LEU:HD12	3:B:592:ARG:HH12	1.83	0.42
3:B:685:SER:CB	3:B:688:ILE:HG22	2.43	0.42
3:B:761:THR:CG2	3:B:762:VAL:N	2.82	0.42
6:P:223:HOH:O	3:B:718:PRO:HG3	2.20	0.42
3:B:584:ASN:N	3:B:590:HIS:HD2	2.04	0.42
1:T:12:DT:P	3:A:363:PRO:HD3	2.58	0.42
3:B:511:LEU:HD23	3:B:511:LEU:C	2.40	0.42
3:B:743:GLU:O	3:B:746:ALA:CB	2.63	0.42
3:B:764:LEU:HG	3:B:828:VAL:HG22	2.00	0.42
3:A:75:VAL:O	3:A:77:LYS:N	2.52	0.42
3:B:581:GLN:NE2	3:B:644:GLU:HB2	2.35	0.42
6:T:235:HOH:O	3:A:108:LYS:NZ	2.45	0.42
2:P:8:DG:H2"	2:P:9:DG:C8	2.54	0.42
2:P:11:DC:H2"	2:P:12:DC:O5'	2.19	0.42
3:A:32:HIS:O	3:A:197:ALA:HA	2.20	0.42
3:A:214:LYS:HB2	3:A:215:PRO:HD3	2.02	0.42
3:A:281:ILE:HG22	3:A:282:GLN:N	2.35	0.42
3:A:369:ILE:HG13	3:A:379:VAL:CG2	2.50	0.42
3:A:408:VAL:CG1	3:A:409:CYS:N	2.82	0.42
3:B:481:TYR:C	3:B:501:VAL:HG13	2.40	0.42
3:B:562:GLN:HE21	3:B:562:GLN:H	1.68	0.42
3:B:722:PHE:N	3:B:722:PHE:CD1	2.88	0.42
3:B:755:ASP:CG	3:B:756:GLY:O	2.58	0.42
3:B:780:ARG:NH2	3:B:812:ARG:C	2.66	0.42
3:B:822:HIS:O	3:B:823:LEU:CD2	2.66	0.42
2:P:8:DG:C5'	3:B:776:GLY:O	2.67	0.41
3:A:54:PRO:CB	3:A:70:ALA:HB2	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:321:ILE:O	3:A:325:LEU:HD13	2.20	0.41
3:A:369:ILE:HG13	3:A:379:VAL:CG2	2.50	0.41
3:B:722:PHE:HE1	3:B:833:LEU:HG	1.85	0.41
3:B:824:THR:HG22	3:B:825:LEU:HG	2.02	0.41
3:A:50:LEU:HA	3:A:53:LYS:HG2	2.00	0.41
3:A:342:VAL:HG12	3:A:410:PHE:CD2	2.55	0.41
3:B:581:GLN:OE1	3:B:642:LEU:HB2	2.19	0.41
3:B:685:SER:O	3:B:688:ILE:HG22	2.20	0.41
3:B:555:MET:HE1	3:B:599:ILE:HD12	2.02	0.41
3:B:562:GLN:HE21	3:B:562:GLN:H	1.68	0.41
3:B:581:GLN:NE2	3:B:644:GLU:HB2	2.35	0.41
3:B:655:HIS:CE1	3:B:656:ILE:HG12	2.56	0.41
3:B:767:ARG:HD3	3:B:769:TYR:CB	2.50	0.41
3:A:395:VAL:C	3:A:397:VAL:H	2.24	0.41
3:B:541:GLU:HA	3:B:716:SER:HB3	2.03	0.41
3:B:764:LEU:HA	3:B:828:VAL:HA	2.01	0.41
3:A:321:ILE:O	3:A:325:LEU:HD13	2.20	0.41
3:B:616:CYS:SG	3:B:635:PRO:O	2.79	0.41
3:B:722:PHE:HE1	3:B:833:LEU:HG	1.85	0.41
2:P:5:DG:H2'	2:P:6:DA:C8	2.56	0.41
2:P:6:DA:C2'	2:P:7:DA:C8	2.93	0.41
3:A:60:LYS:O	3:A:61:TYR:CB	2.68	0.41
3:B:452:HIS:O	3:B:617:ALA:HA	2.21	0.41
3:B:685:SER:O	3:B:688:ILE:HG22	2.20	0.41
1:T:10:DC:H2"	1:T:11:DC:H6	1.85	0.41
3:A:112:LEU:HD23	3:A:112:LEU:O	2.19	0.41
3:B:479:GLN:O	3:B:481:TYR:N	2.54	0.41
3:B:655:HIS:CE1	3:B:656:ILE:HG12	2.55	0.41
3:B:716:SER:C	3:B:717:GLY:O	2.59	0.41
1:T:8:DG:H2"	1:T:9:DT:H6	1.85	0.41
3:A:338:LYS:HA	3:A:339:PRO:HD2	1.94	0.41
3:B:470:LEU:HD13	3:B:475:LEU:CD2	2.50	0.41
3:B:616:CYS:SG	3:B:635:PRO:O	2.78	0.41
3:B:758:LYS:HA	3:B:759:PRO:HD2	1.89	0.41
1:T:7:DG:C4'	3:B:519:LEU:HD12	2.49	0.41
3:A:265:SER:HA	3:A:266:PRO:HD3	1.94	0.41
3:B:470:LEU:HD13	3:B:475:LEU:CD2	2.50	0.41
3:B:532:LEU:C	3:B:532:LEU:CD2	2.89	0.41
3:B:541:GLU:HA	3:B:716:SER:HB3	2.03	0.41
1:T:5:DA:H1'	3:B:479:GLN:HB3	2.03	0.41
3:B:559:ARG:CZ	3:B:599:ILE:HD13	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:8:DG:H4'	3:B:777:ARG:HA	2.03	0.41
3:B:475:LEU:HD12	3:B:476:GLY:N	2.34	0.41
3:B:483:VAL:HB	3:B:500:ASN:O	2.21	0.41
3:B:759:PRO:CD	3:B:833:LEU:CD1	2.84	0.41
1:T:14:DC:OP1	3:A:359:SER:O	2.38	0.41
2:P:8:DG:H2"	2:P:9:DG:C8	2.54	0.41
3:B:479:GLN:O	3:B:481:TYR:N	2.54	0.41
1:T:8:DG:H2"	1:T:9:DT:H6	1.85	0.41
2:P:8:DG:O5'	3:B:777:ARG:C	2.59	0.41
2:P:10:DA:H2"	2:P:11:DC:H5"	2.03	0.41
3:A:214:LYS:HB2	3:A:215:PRO:HD3	2.02	0.41
3:B:744:LEU:HG	3:B:745:LEU:N	2.36	0.41
1:T:10:DC:H2"	1:T:11:DC:H6	1.85	0.41
2:P:10:DA:H2"	2:P:11:DC:H5"	2.03	0.41
3:A:84:ALA:CA	3:A:87:LYS:HG2	2.47	0.41
3:A:274:GLY:O	3:A:278:ALA:HB2	2.21	0.41
3:A:302:PHE:HZ	3:A:335:ASP:OD2	2.04	0.41
3:B:509:PRO:C	3:B:511:LEU:N	2.74	0.41
3:B:559:ARG:CZ	3:B:599:ILE:HD13	2.51	0.41
3:B:604:ARG:HH21	3:B:638:GLN:HE21	1.69	0.41
3:B:716:SER:C	3:B:717:GLY:O	2.59	0.41
3:B:722:PHE:N	3:B:722:PHE:CD1	2.88	0.41
3:B:744:LEU:HG	3:B:745:LEU:N	2.36	0.41
6:P:253:HOH:O	3:B:504:ALA:CB	2.60	0.41
3:A:60:LYS:O	3:A:61:TYR:CB	2.68	0.41
3:A:60:LYS:C	3:A:61:TYR:CD1	2.85	0.41
3:A:230:ILE:HD12	3:A:230:ILE:HA	1.97	0.41
3:A:274:GLY:O	3:A:278:ALA:HB2	2.21	0.41
3:A:371:LYS:HE2	3:A:376:ASN:CB	2.48	0.41
3:A:395:VAL:C	3:A:397:VAL:H	2.24	0.41
3:B:511:LEU:HD23	3:B:511:LEU:C	2.40	0.41
3:B:573:VAL:CB	3:B:594:LEU:HD22	2.47	0.41
3:B:758:LYS:HA	3:B:759:PRO:HD2	1.89	0.41
2:P:1:DG:O5'	3:A:304:GLU:HA	2.21	0.41
2:P:9:DG:OP2	3:B:776:GLY:N	2.54	0.41
3:A:32:HIS:O	3:A:197:ALA:HA	2.20	0.41
3:B:584:ASN:N	3:B:590:HIS:HD2	2.04	0.41
3:B:781:GLN:HG3	6:B:1149:HOH:O	2.20	0.41
3:B:799:VAL:O	3:B:799:VAL:HG12	2.21	0.41
1:T:5:DA:N3	1:T:5:DA:C5'	2.84	0.41
3:A:84:ALA:CA	3:A:87:LYS:HG2	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:351:SER:O	3:A:353:LYS:N	2.54	0.41
3:B:562:GLN:N	3:B:562:GLN:NE2	2.69	0.41
1:T:5:DA:N3	1:T:5:DA:C5'	2.84	0.40
3:A:227:GLN:O	3:A:230:ILE:HG22	2.21	0.40
3:A:342:VAL:HG12	3:A:410:PHE:CD2	2.55	0.40
3:B:546:ASP:HA	6:B:1046:HOH:O	2.19	0.40
3:B:604:ARG:HH21	3:B:638:GLN:HE21	1.69	0.40
3:B:481:TYR:C	3:B:501:VAL:HG13	2.41	0.40
3:B:604:ARG:HE	3:B:638:GLN:NE2	2.19	0.40
3:B:812:ARG:HD3	3:B:812:ARG:HA	1.94	0.40
3:B:452:HIS:O	3:B:617:ALA:HA	2.21	0.40
3:B:494:GLY:C	3:B:496:LYS:N	2.73	0.40
3:B:497:LYS:HB3	3:B:497:LYS:HZ2	1.84	0.40
2:P:9:DG:P	3:B:775:TYR:CB	3.09	0.40
2:P:12:DC:OP2	3:B:663:GLY:HA2	2.21	0.40
3:A:53:LYS:HA	3:A:54:PRO:HD3	1.97	0.40
3:A:230:ILE:HD12	3:A:230:ILE:HA	1.98	0.40
3:A:351:SER:O	3:A:353:LYS:N	2.54	0.40
3:B:501:VAL:O	3:B:503:ASP:N	2.54	0.40
3:A:281:ILE:HG22	3:A:282:GLN:N	2.35	0.40
3:A:338:LYS:HA	3:A:339:PRO:HD2	1.94	0.40
3:B:748:LEU:O	3:B:751:ARG:N	2.53	0.40
2:P:8:DG:OP1	3:B:778:GLU:CA	2.69	0.40
2:P:8:DG:OP1	3:B:777:ARG:O	2.38	0.40
3:A:303:SER:CB	3:A:409:CYS:HA	2.49	0.40
3:A:303:SER:CB	3:A:409:CYS:HA	2.48	0.40
3:B:463:GLU:HG3	3:B:514:VAL:HG21	2.04	0.40
3:B:501:VAL:O	3:B:503:ASP:N	2.55	0.40
3:A:277:VAL:HG21	6:A:609:HOH:O	2.22	0.40
3:B:475:LEU:HD12	3:B:476:GLY:N	2.34	0.40
2:P:7:DA:H5"	6:P:249:HOH:O	2.22	0.40
2:P:12:DC:OP2	3:B:663:GLY:HA2	2.21	0.40
3:B:764:LEU:O	3:B:779:SER:CB	2.69	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	1-A	386/388 (100%)	338 (88%)	27 (7%)	21 (5%)	2	1
3	1-B	386/388 (100%)	319 (83%)	44 (11%)	23 (6%)	1	0
3	2-A	386/388 (100%)	337 (87%)	28 (7%)	21 (5%)	2	1
3	2-B	386/388 (100%)	319 (83%)	44 (11%)	23 (6%)	1	0
All	All	1544/1552 (100%)	1313 (85%)	143 (9%)	88 (6%)	1	1

All (88) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	1-A	60	LYS
3	1-A	61	TYR
3	1-A	76	LYS
3	1-A	80	ASN
3	1-A	89	PRO
3	1-A	309	LYS
3	1-A	314	GLU
3	1-A	351	SER
3	1-A	352	GLU
3	1-A	395	VAL
3	1-A	396	ASN
3	1-A	399	MET
3	1-A	400	PRO
3	1-A	411	CYS
3	1-B	480	LYS
3	1-B	635	PRO
3	1-B	773	LYS
3	1-B	779	SER
3	1-B	812	ARG
3	1-B	815	VAL
3	1-B	825	LEU
3	1-B	832	ASN

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Mol	Chain	Res	Type
3	1-B	833	LEU
3	2-A	60	LYS
3	2-A	61	TYR
3	2-A	76	LYS
3	2-A	80	ASN
3	2-A	89	PRO
3	2-A	309	LYS
3	2-A	314	GLU
3	2-A	351	SER
3	2-A	352	GLU
3	2-A	395	VAL
3	2-A	396	ASN
3	2-A	399	MET
3	2-A	400	PRO
3	2-A	411	CYS
3	2-B	480	LYS
3	2-B	635	PRO
3	2-B	773	LYS
3	2-B	779	SER
3	2-B	812	ARG
3	2-B	815	VAL
3	2-B	825	LEU
3	2-B	832	ASN
3	2-B	833	LEU
3	1-A	77	LYS
3	1-A	380	MET
3	1-B	717	GLY
3	1-B	718	PRO
3	1-B	738	LYS
3	2-A	77	LYS
3	2-A	380	MET
3	2-B	717	GLY
3	2-B	718	PRO
3	2-B	738	LYS
3	1-A	37	CYS
3	1-A	158	TYR
3	1-B	457	CYS
3	1-B	472	ASP
3	1-B	474	PRO
3	1-B	817	VAL
3	2-A	37	CYS
3	2-B	457	CYS

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Mol	Chain	Res	Type
3	2-B	472	ASP
3	2-B	474	PRO
3	2-B	817	VAL
3	1-A	88	CYS
3	1-A	367	HIS
3	1-A	405	LEU
3	1-B	578	TYR
3	1-B	775	TYR
3	1-B	793	GLY
3	2-A	88	CYS
3	2-A	158	TYR
3	2-A	367	HIS
3	2-A	405	LEU
3	2-B	578	TYR
3	2-B	775	TYR
3	2-B	793	GLY
3	2-B	757	ARG
3	1-B	757	ARG
3	1-B	494	GLY
3	1-B	509	PRO
3	2-B	494	GLY
3	2-B	509	PRO
3	1-B	495	VAL
3	2-B	495	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
3	1-A	299/353 (85%)	274 (92%)	25 (8%)	11 13
3	1-B	304/353 (86%)	266 (88%)	38 (12%)	4 5
3	2-A	299/353 (85%)	274 (92%)	25 (8%)	11 13
3	2-B	304/353 (86%)	266 (88%)	38 (12%)	4 5
All	All	1206/1412 (85%)	1080 (90%)	126 (10%)	7 8

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1-A	47	ASN
3	1-A	60	LYS
3	1-A	89	PRO
3	1-A	144	GLN
3	1-A	170	HIS
3	1-A	229	LEU
3	1-A	246	THR
3	1-A	276	SER
3	1-A	298	PRO
3	1-A	299	PRO
3	1-A	313	SER
3	1-A	314	GLU
3	1-A	330	ASN
3	1-A	337	ARG
3	1-A	339	PRO
3	1-A	359	SER
3	1-A	361	GLN
3	1-A	363	PRO
3	1-A	365	PRO
3	1-A	366	SER
3	1-A	368	VAL
3	1-A	371	LYS
3	1-A	379	VAL
3	1-A	382	PRO
3	1-A	410	PHE
3	1-B	455	LEU
3	1-B	472	ASP
3	1-B	497	LYS
3	1-B	519	LEU
3	1-B	543	LEU
3	1-B	562	GLN
3	1-B	590	HIS
3	1-B	622	ASN
3	1-B	624	LEU
3	1-B	625	LEU
3	1-B	649	LEU
3	1-B	716	SER
3	1-B	719	PRO
3	1-B	725	GLU
3	1-B	726	ASP
3	1-B	728	PHE
3	1-B	732	SER

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Mol	Chain	Res	Type
3	1-B	740	LYS
3	1-B	744	LEU
3	1-B	749	LEU
3	1-B	757	ARG
3	1-B	759	PRO
3	1-B	762	VAL
3	1-B	767	ARG
3	1-B	782	CYS
3	1-B	783	PRO
3	1-B	785	PRO
3	1-B	786	SER
3	1-B	791	LYS
3	1-B	802	PRO
3	1-B	806	ILE
3	1-B	811	PHE
3	1-B	812	ARG
3	1-B	813	ASN
3	1-B	820	PRO
3	1-B	825	LEU
3	1-B	830	PHE
3	1-B	832	ASN
3	2-A	47	ASN
3	2-A	60	LYS
3	2-A	89	PRO
3	2-A	144	GLN
3	2-A	170	HIS
3	2-A	229	LEU
3	2-A	246	THR
3	2-A	276	SER
3	2-A	298	PRO
3	2-A	299	PRO
3	2-A	313	SER
3	2-A	314	GLU
3	2-A	330	ASN
3	2-A	337	ARG
3	2-A	339	PRO
3	2-A	359	SER
3	2-A	361	GLN
3	2-A	363	PRO
3	2-A	365	PRO
3	2-A	366	SER
3	2-A	368	VAL

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Mol	Chain	Res	Type
3	2-A	371	LYS
3	2-A	379	VAL
3	2-A	382	PRO
3	2-A	410	PHE
3	2-B	455	LEU
3	2-B	472	ASP
3	2-B	497	LYS
3	2-B	519	LEU
3	2-B	543	LEU
3	2-B	562	GLN
3	2-B	590	HIS
3	2-B	622	ASN
3	2-B	624	LEU
3	2-B	625	LEU
3	2-B	649	LEU
3	2-B	716	SER
3	2-B	719	PRO
3	2-B	725	GLU
3	2-B	726	ASP
3	2-B	728	PHE
3	2-B	732	SER
3	2-B	740	LYS
3	2-B	744	LEU
3	2-B	749	LEU
3	2-B	757	ARG
3	2-B	759	PRO
3	2-B	762	VAL
3	2-B	767	ARG
3	2-B	782	CYS
3	2-B	783	PRO
3	2-B	785	PRO
3	2-B	786	SER
3	2-B	791	LYS
3	2-B	802	PRO
3	2-B	806	ILE
3	2-B	811	PHE
3	2-B	812	ARG
3	2-B	813	ASN
3	2-B	820	PRO
3	2-B	825	LEU
3	2-B	830	PHE
3	2-B	832	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
3	1-A	47	ASN
3	1-A	59	GLN
3	1-A	95	ASN
3	1-A	161	GLN
3	1-A	170	HIS
3	1-A	227	GLN
3	1-A	256	ASN
3	1-A	262	GLN
3	1-A	367	HIS
3	1-B	478	GLN
3	1-B	487	ASN
3	1-B	562	GLN
3	1-B	590	HIS
3	1-B	622	ASN
3	1-B	638	GLN
3	1-B	682	GLN
3	1-B	699	GLN
3	1-B	760	HIS
3	1-B	813	ASN
3	2-A	47	ASN
3	2-A	59	GLN
3	2-A	95	ASN
3	2-A	161	GLN
3	2-A	170	HIS
3	2-A	227	GLN
3	2-A	256	ASN
3	2-A	262	GLN
3	2-A	330	ASN
3	2-A	367	HIS
3	2-B	478	GLN
3	2-B	487	ASN
3	2-B	562	GLN
3	2-B	590	HIS
3	2-B	622	ASN
3	2-B	638	GLN
3	2-B	682	GLN
3	2-B	699	GLN
3	2-B	760	HIS
3	2-B	813	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)

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	$\#\|Z\| > 2$
2	DOC	1-P	13	1,2	16,19,20	0.78	0	20,26,29	0.78	1 (5%)
2	DOC	2-P	13	1,2	16,19,20	0.78	0	20,26,29	0.78	1 (5%)

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
2	DOC	1-P	13	1,2	-	0/7/18/19	0/2/2/2
2	DOC	2-P	13	1,2	-	0/7/18/19	0/2/2/2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	1-P	13	DOC	O4'-C1'-N1	2.29	111.92	107.86
2	2-P	13	DOC	O4'-C1'-N1	2.28	111.91	107.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	1-P	13	DOC	1	0
2	2-P	13	DOC	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 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	$\#\|Z\| > 2$
5	TTP	2-B	902	4	29,30,30	5.40	13 (44%)	43,47,47	2.50	15 (34%)
5	TTP	1-B	902	4	29,30,30	5.38	12 (41%)	43,47,47	2.52	15 (34%)

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
5	TTP	2-B	902	4	-	3/22/34/34	0/2/2/2
5	TTP	1-B	902	4	-	3/22/34/34	0/2/2/2

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	2-B	902	TTP	C5M-C5	-21.55	0.98	1.50
5	1-B	902	TTP	C5M-C5	-21.49	0.98	1.50
5	2-B	902	TTP	PA-O3A	9.73	1.70	1.59
5	1-B	902	TTP	PA-O3A	9.64	1.69	1.59
5	2-B	902	TTP	PB-O3A	8.26	1.68	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	1-B	902	TTP	PB-O3B	7.91	1.68	1.59
5	1-B	902	TTP	PB-O3A	7.83	1.67	1.59
5	2-B	902	TTP	PB-O3B	7.67	1.67	1.59
5	1-B	902	TTP	O4-C4	5.26	1.33	1.23
5	2-B	902	TTP	O4-C4	5.17	1.33	1.23
5	1-B	902	TTP	PA-O5'	-4.93	1.40	1.59
5	1-B	902	TTP	PA-O1A	-4.90	1.33	1.50
5	2-B	902	TTP	C1'-N1	4.84	1.60	1.48
5	2-B	902	TTP	PA-O5'	-4.81	1.40	1.59
5	2-B	902	TTP	PA-O1A	-4.79	1.34	1.50
5	1-B	902	TTP	C1'-N1	4.78	1.60	1.48
5	1-B	902	TTP	O5'-C5'	4.63	1.62	1.44
5	2-B	902	TTP	O5'-C5'	4.53	1.61	1.44
5	2-B	902	TTP	C6-C5	4.46	1.41	1.34
5	1-B	902	TTP	C6-C5	4.40	1.41	1.34
5	1-B	902	TTP	C2-N1	2.83	1.42	1.38
5	2-B	902	TTP	C2-N1	2.80	1.42	1.38
5	1-B	902	TTP	PG-O1G	2.40	1.57	1.50
5	2-B	902	TTP	PG-O1G	2.33	1.57	1.50
5	2-B	902	TTP	PB-O1B	2.04	1.57	1.50

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	2-B	902	TTP	C5-C4-N3	6.15	120.67	115.32
5	2-B	902	TTP	N3-C2-N1	6.01	122.72	114.89
5	1-B	902	TTP	N3-C2-N1	5.98	122.68	114.89
5	1-B	902	TTP	C5-C4-N3	5.74	120.31	115.32
5	1-B	902	TTP	C6-N1-C2	-5.55	115.78	121.30
5	1-B	902	TTP	C4-N3-C2	-5.35	120.32	127.34
5	2-B	902	TTP	C6-N1-C2	-5.24	116.08	121.30
5	2-B	902	TTP	C4-N3-C2	-5.15	120.59	127.34
5	2-B	902	TTP	C1'-N1-C6	4.68	128.61	120.74
5	1-B	902	TTP	C1'-N1-C6	4.63	128.52	120.74
5	1-B	902	TTP	C2'-C1'-N1	-4.37	102.89	113.81
5	2-B	902	TTP	C2'-C1'-N1	-4.06	103.66	113.81
5	1-B	902	TTP	O2-C2-N3	-3.89	114.31	121.49
5	2-B	902	TTP	O2-C2-N3	-3.77	114.54	121.49
5	1-B	902	TTP	O2A-PA-O5'	3.42	123.06	107.57
5	2-B	902	TTP	O2A-PA-O5'	3.42	123.06	107.57
5	1-B	902	TTP	C6-C5-C4	-3.35	115.26	118.02
5	2-B	902	TTP	C5M-C5-C4	3.31	122.32	118.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	2-B	902	TTP	C6-C5-C4	-2.91	115.62	118.02
5	1-B	902	TTP	C5M-C5-C4	2.81	121.78	118.78
5	2-B	902	TTP	O5'-C5'-C4'	2.66	118.05	108.99
5	1-B	902	TTP	O5'-C5'-C4'	2.65	118.01	108.99
5	1-B	902	TTP	O4-C4-N3	-2.47	115.48	120.11
5	1-B	902	TTP	O2A-PA-O1A	-2.36	101.47	112.44
5	2-B	902	TTP	O2A-PA-O1A	-2.34	101.54	112.44
5	2-B	902	TTP	O4-C4-N3	-2.34	115.72	120.11
5	2-B	902	TTP	O3A-PB-O1B	-2.21	104.06	110.70
5	1-B	902	TTP	O3G-PG-O3B	2.18	111.94	104.64
5	2-B	902	TTP	O3G-PG-O3B	2.18	111.93	104.64
5	1-B	902	TTP	O3A-PB-O1B	-2.14	104.27	110.70

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	1-B	902	TTP	PG-O3B-PB-O2B
5	2-B	902	TTP	PG-O3B-PB-O2B
5	1-B	902	TTP	PB-O3A-PA-O1A
5	2-B	902	TTP	PB-O3A-PA-O1A
5	1-B	902	TTP	PB-O3A-PA-O2A
5	2-B	902	TTP	PB-O3A-PA-O2A

There are no ring outliers.

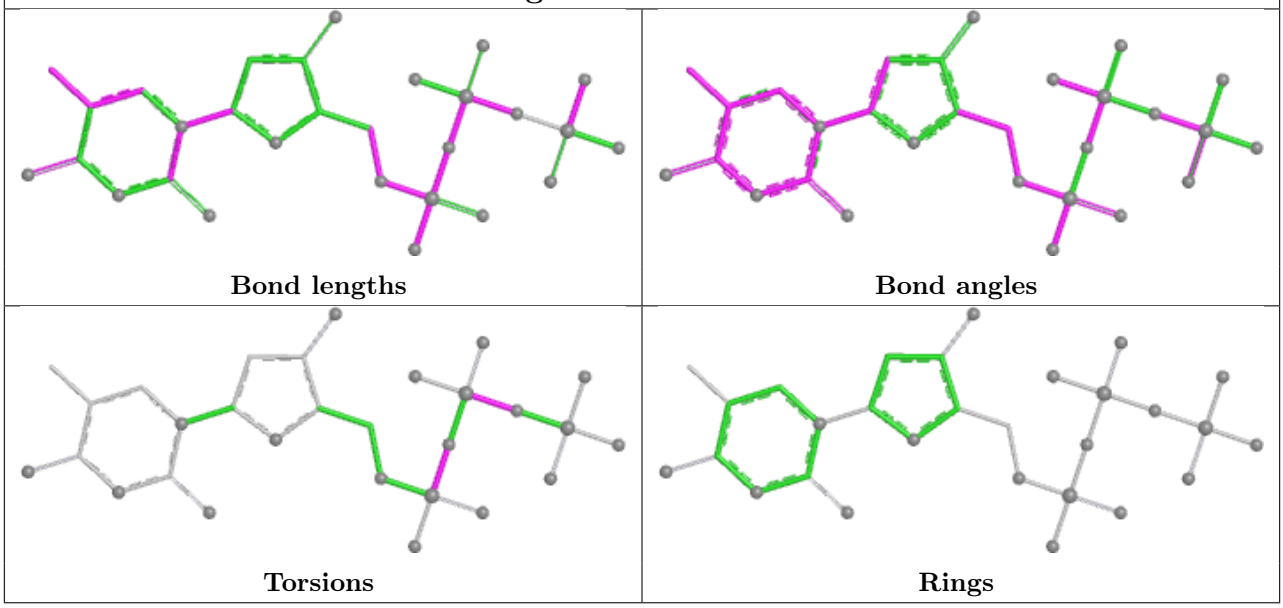
2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	2-B	902	TTP	4	0
5	1-B	902	TTP	2	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 TTP B 902



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, 95^{th} 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	1-T	14/14 (100%)	0.33	2 (14%) 2 3	42, 50, 59, 66	14 (100%)
1	2-T	14/14 (100%)	0.33	2 (14%) 2 3	42, 50, 59, 66	14 (100%)
2	1-P	12/13 (92%)	0.38	0 100 100	47, 59, 70, 73	12 (100%)
2	2-P	12/13 (92%)	0.38	0 100 100	47, 59, 70, 73	12 (100%)
3	1-A	388/388 (100%)	1.36	89 (22%) 0 1	20, 51, 100, 100	388 (100%)
3	1-B	388/388 (100%)	1.23	103 (26%) 0 0	23, 51, 100, 100	388 (100%)
3	2-A	388/388 (100%)	1.36	89 (22%) 0 1	20, 51, 100, 100	388 (100%)
3	2-B	388/388 (100%)	1.23	103 (26%) 0 0	23, 51, 100, 100	388 (100%)
All	All	1604/1606 (99%)	1.26	388 (24%) 0 0	20, 51, 100, 100	1604 (100%)

All (388) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	1-A	354	HIS	23.0
3	2-A	354	HIS	23.0
3	1-A	399	MET	20.2
3	2-A	399	MET	20.2
3	1-A	397	VAL	18.8
3	2-A	397	VAL	18.8
3	1-A	401	PHE	18.0
3	2-A	401	PHE	18.0
3	1-B	815	VAL	17.6
3	2-B	815	VAL	17.6
3	1-A	400	PRO	16.8
3	2-A	400	PRO	16.8
3	1-A	353	LYS	16.4
3	2-A	353	LYS	16.4
3	1-B	774	HIS	16.0
3	2-B	774	HIS	16.0

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Mol	Chain	Res	Type	RSRZ
3	1-A	355	TYR	15.1
3	2-A	355	TYR	15.1
3	1-B	816	ASN	13.6
3	2-B	816	ASN	13.6
3	1-A	352	GLU	13.4
3	2-A	352	GLU	13.4
3	1-A	398	LYS	12.1
3	2-A	398	LYS	12.1
3	1-A	356	GLY	11.9
3	2-A	356	GLY	11.9
3	1-A	82	ARG	11.3
3	2-A	82	ARG	11.3
3	1-B	797	TYR	11.2
3	2-B	797	TYR	11.2
3	1-B	821	PHE	11.0
3	2-B	821	PHE	11.0
3	1-B	764	LEU	10.9
3	2-B	764	LEU	10.9
3	1-B	729	LYS	10.3
3	2-B	729	LYS	10.3
3	1-A	407	SER	9.8
3	2-A	407	SER	9.8
3	1-A	406	LEU	9.7
3	2-A	406	LEU	9.7
3	1-A	405	LEU	9.0
3	2-A	405	LEU	9.0
3	1-B	731	CYS	9.0
3	2-B	731	CYS	9.0
3	1-B	765	ILE	8.7
3	2-B	765	ILE	8.7
3	1-B	818	LYS	8.6
3	2-B	818	LYS	8.6
3	1-B	817	VAL	8.4
3	2-B	817	VAL	8.4
3	1-A	90	GLN	8.3
3	2-A	90	GLN	8.3
3	1-A	369	ILE	8.0
3	2-A	369	ILE	8.0
3	1-B	813	ASN	7.9
3	2-B	813	ASN	7.9
3	1-A	89	PRO	7.8
3	2-A	89	PRO	7.8

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Mol	Chain	Res	Type	RSRZ
3	1-B	790	GLN	7.7
3	2-B	790	GLN	7.7
3	1-A	316	GLU	7.6
3	2-A	316	GLU	7.6
3	1-A	351	SER	7.5
3	2-A	351	SER	7.5
3	1-B	732	SER	7.3
3	2-B	732	SER	7.3
3	1-A	244	TYR	7.1
3	2-A	244	TYR	7.1
3	1-A	81	VAL	6.8
3	2-A	81	VAL	6.8
3	1-B	784	ILE	6.8
3	2-B	784	ILE	6.8
3	1-B	740	LYS	6.8
3	2-B	740	LYS	6.8
3	1-B	825	LEU	6.6
3	2-B	825	LEU	6.6
3	1-A	310	LYS	6.5
3	2-A	310	LYS	6.5
3	1-A	371	LYS	6.5
3	2-A	371	LYS	6.5
3	1-A	311	CYS	6.4
3	2-A	311	CYS	6.4
3	1-A	214	LYS	6.3
3	2-A	214	LYS	6.3
3	1-A	395	VAL	6.2
3	2-A	395	VAL	6.2
3	1-B	775	TYR	6.0
3	2-B	775	TYR	6.0
3	1-B	814	MET	6.0
3	2-B	814	MET	6.0
3	1-B	771	SER	5.9
3	2-B	771	SER	5.9
3	1-B	824	THR	5.8
3	2-B	824	THR	5.8
3	1-A	306	ASP	5.7
3	2-A	306	ASP	5.7
3	1-A	372	LEU	5.6
3	2-A	372	LEU	5.6
3	1-B	786	SER	5.5
3	2-B	786	SER	5.5

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Mol	Chain	Res	Type	RSRZ
3	1-A	377	TYR	5.4
3	2-A	377	TYR	5.4
3	1-B	772	GLU	5.4
3	2-B	772	GLU	5.4
3	1-B	730	LYS	5.3
3	2-B	730	LYS	5.3
3	1-B	803	MET	5.3
3	2-B	803	MET	5.3
3	1-B	494	GLY	5.3
3	2-B	494	GLY	5.3
3	1-B	773	LYS	5.3
3	2-B	773	LYS	5.3
3	1-A	358	GLU	5.2
3	2-A	358	GLU	5.2
3	1-A	343	ARG	5.1
3	2-A	343	ARG	5.1
3	1-A	404	THR	5.1
3	2-A	404	THR	5.1
3	1-A	315	VAL	5.0
3	2-A	315	VAL	5.0
3	1-B	495	VAL	5.0
3	2-B	495	VAL	5.0
3	1-A	333	CYS	5.0
3	2-A	333	CYS	5.0
3	1-A	366	SER	5.0
3	2-A	366	SER	5.0
3	1-A	368	VAL	5.0
3	2-A	368	VAL	5.0
3	1-B	504	ALA	5.0
3	2-B	504	ALA	5.0
3	1-B	763	ARG	4.7
3	2-B	763	ARG	4.7
3	1-B	739	ASN	4.7
3	2-B	739	ASN	4.7
3	1-B	820	PRO	4.7
3	2-B	820	PRO	4.7
3	1-B	822	HIS	4.7
3	2-B	822	HIS	4.7
3	1-B	498	LEU	4.6
3	2-B	498	LEU	4.6
3	1-B	482	LEU	4.6
3	2-B	482	LEU	4.6

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Mol	Chain	Res	Type	RSRZ
3	1-B	795	GLY	4.6
3	2-B	795	GLY	4.6
3	1-A	313	SER	4.5
3	2-A	313	SER	4.5
3	1-B	787	HIS	4.5
3	2-B	787	HIS	4.5
3	1-A	273	LEU	4.5
3	2-A	273	LEU	4.5
3	1-B	734	GLU	4.5
3	2-B	734	GLU	4.5
3	1-A	350	SER	4.4
3	2-A	350	SER	4.4
3	1-B	776	GLY	4.4
3	2-B	776	GLY	4.4
3	1-B	823	LEU	4.4
3	2-B	823	LEU	4.4
3	1-B	728	PHE	4.4
3	2-B	728	PHE	4.4
3	1-A	345	ILE	4.4
3	2-A	345	ILE	4.4
3	1-B	695	ILE	4.3
3	2-B	695	ILE	4.3
3	1-B	726	ASP	4.3
3	2-B	726	ASP	4.3
3	1-A	402	HIS	4.2
3	2-A	402	HIS	4.2
3	1-B	634	LYS	4.2
3	2-B	634	LYS	4.2
3	1-A	344	LEU	4.1
3	2-A	344	LEU	4.1
3	1-B	826	LEU	4.1
3	2-B	826	LEU	4.1
3	1-A	357	ARG	4.1
3	2-A	357	ARG	4.1
3	1-A	394	MET	4.0
3	2-A	394	MET	4.0
3	1-A	73	LEU	3.9
3	1-B	791	LYS	3.9
3	2-A	73	LEU	3.9
3	2-B	791	LYS	3.9
3	1-A	62	LEU	3.9
3	2-A	62	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
3	1-A	408	VAL	3.8
3	2-A	408	VAL	3.8
3	1-A	362	CYS	3.8
3	2-A	362	CYS	3.8
3	1-B	785	PRO	3.8
3	2-B	785	PRO	3.8
3	1-A	396	ASN	3.7
3	2-A	396	ASN	3.7
3	1-B	770	SER	3.7
3	2-B	770	SER	3.7
3	1-B	741	ILE	3.7
3	2-B	741	ILE	3.7
3	1-B	819	MET	3.6
3	2-B	819	MET	3.6
3	1-A	411	CYS	3.5
3	1-B	831	CYS	3.5
3	2-A	411	CYS	3.5
3	2-B	831	CYS	3.5
3	1-A	375	GLY	3.5
3	2-A	375	GLY	3.5
3	1-A	317	ALA	3.5
3	2-A	317	ALA	3.5
3	1-A	141	GLN	3.4
3	2-A	141	GLN	3.4
3	1-B	827	SER	3.4
3	2-B	827	SER	3.4
3	1-A	342	VAL	3.4
3	2-A	342	VAL	3.4
3	1-B	768	ARG	3.4
3	2-B	768	ARG	3.4
3	1-B	809	LYS	3.4
3	2-B	809	LYS	3.4
3	1-A	312	SER	3.4
3	2-A	312	SER	3.4
3	1-B	782	CYS	3.3
3	2-B	782	CYS	3.3
3	1-B	788	VAL	3.3
3	2-B	788	VAL	3.3
3	1-B	506	GLU	3.3
3	2-B	506	GLU	3.3
3	1-A	409	CYS	3.2
3	2-A	409	CYS	3.2

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Mol	Chain	Res	Type	RSRZ
3	1-B	747	SER	3.2
3	2-B	747	SER	3.2
3	1-A	92	VAL	3.2
3	2-A	92	VAL	3.2
3	1-B	807	LEU	3.2
3	2-B	807	LEU	3.2
3	1-A	336	GLY	3.2
3	2-A	336	GLY	3.2
3	1-B	796	ASN	3.2
3	2-B	796	ASN	3.2
3	1-A	325	LEU	3.2
3	2-A	325	LEU	3.2
3	1-A	321	ILE	3.1
3	2-A	321	ILE	3.1
3	1-B	746	ALA	3.1
3	2-B	746	ALA	3.1
3	1-A	85	LYS	3.1
3	2-A	85	LYS	3.1
3	1-A	376	ASN	3.1
3	2-A	376	ASN	3.1
3	1-B	832	ASN	3.1
3	2-B	832	ASN	3.1
3	1-A	383	MET	3.1
3	2-A	383	MET	3.1
3	1-A	326	ALA	3.1
3	2-A	326	ALA	3.1
3	1-A	308	PHE	3.0
3	2-A	308	PHE	3.0
3	1-A	359	SER	3.0
3	2-A	359	SER	3.0
3	1-A	387	LEU	3.0
3	2-A	387	LEU	3.0
3	1-A	86	GLU	3.0
3	2-A	86	GLU	3.0
3	1-B	789	ILE	3.0
3	2-B	789	ILE	3.0
3	1-A	349	TYR	2.9
3	2-A	349	TYR	2.9
3	1-B	744	LEU	2.9
3	2-B	744	LEU	2.9
3	1-B	767	ARG	2.8
3	2-B	767	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
3	1-A	80	ASN	2.8
3	2-A	80	ASN	2.8
3	1-B	499	MET	2.8
3	2-B	499	MET	2.8
3	1-A	75	VAL	2.8
3	2-A	75	VAL	2.8
3	1-A	320	LYS	2.8
3	1-B	808	MET	2.8
3	2-A	320	LYS	2.8
3	2-B	808	MET	2.8
3	1-A	52	ASP	2.7
3	2-A	52	ASP	2.7
3	1-B	793	GLY	2.7
3	2-B	793	GLY	2.7
3	1-B	780	ARG	2.7
3	2-B	780	ARG	2.7
3	1-A	83	ASP	2.7
3	2-A	83	ASP	2.7
3	1-B	754	GLN	2.7
3	2-B	754	GLN	2.7
3	1-A	339	PRO	2.7
3	2-A	339	PRO	2.7
3	1-A	91	LEU	2.6
3	1-A	143	LEU	2.6
3	2-A	91	LEU	2.6
3	2-A	143	LEU	2.6
3	1-A	319	ASN	2.6
3	1-B	561	GLN	2.6
3	2-A	319	ASN	2.6
3	2-B	561	GLN	2.6
3	1-B	568	LEU	2.6
3	1-B	664	TYR	2.6
3	2-B	568	LEU	2.6
3	2-B	664	TYR	2.6
1	1-T	6	DG	2.6
1	2-T	6	DG	2.6
3	1-B	830	PHE	2.6
3	2-B	830	PHE	2.6
3	1-A	61	TYR	2.6
3	2-A	61	TYR	2.6
3	1-A	403	LEU	2.5
3	2-A	403	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	1-T	5	DA	2.5
1	2-T	5	DA	2.5
3	1-B	737	ALA	2.5
3	2-B	737	ALA	2.5
3	1-B	778	GLU	2.5
3	2-B	778	GLU	2.5
3	1-B	810	LEU	2.5
3	2-B	810	LEU	2.5
3	1-B	812	ARG	2.5
3	2-B	812	ARG	2.5
3	1-B	799	VAL	2.5
3	2-B	799	VAL	2.5
3	1-A	72	LYS	2.5
3	2-A	72	LYS	2.5
3	1-B	724	GLU	2.5
3	2-B	724	GLU	2.5
3	1-B	783	PRO	2.4
3	2-B	783	PRO	2.4
3	1-A	388	MET	2.4
3	2-A	388	MET	2.4
3	1-B	735	VAL	2.4
3	2-B	735	VAL	2.4
3	1-B	756	GLY	2.4
3	2-B	756	GLY	2.4
3	1-A	328	LEU	2.4
3	2-A	328	LEU	2.4
3	1-B	804	VAL	2.4
3	2-B	804	VAL	2.4
3	1-A	360	ARG	2.4
3	2-A	360	ARG	2.4
3	1-A	322	GLU	2.4
3	2-A	322	GLU	2.4
3	1-B	753	CYS	2.4
3	2-B	753	CYS	2.4
3	1-A	309	LYS	2.3
3	2-A	309	LYS	2.3
3	1-B	777	ARG	2.3
3	2-B	777	ARG	2.3
3	1-B	798	ASP	2.2
3	2-B	798	ASP	2.2
3	1-B	722	PHE	2.2
3	2-B	722	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
3	1-B	761	THR	2.2
3	2-B	761	THR	2.2
3	1-B	743	GLU	2.2
3	2-B	743	GLU	2.2
3	1-B	800	MET	2.2
3	2-B	800	MET	2.2
3	1-B	762	VAL	2.2
3	2-B	762	VAL	2.2
3	1-A	370	GLN	2.1
3	2-A	370	GLN	2.1
3	1-B	759	PRO	2.1
3	2-B	759	PRO	2.1
3	1-B	501	VAL	2.1
3	2-B	501	VAL	2.1
3	1-B	736	GLU	2.1
3	2-B	736	GLU	2.1
3	1-B	696	SER	2.1
3	2-B	696	SER	2.1
3	1-B	749	LEU	2.1
3	2-B	749	LEU	2.1
3	1-B	480	LYS	2.1
3	1-B	794	THR	2.1
3	2-B	480	LYS	2.1
3	2-B	794	THR	2.1
3	1-B	834	LYS	2.0
3	2-B	834	LYS	2.0
3	1-B	748	LEU	2.0
3	2-B	748	LEU	2.0
3	1-B	464	MET	2.0
3	2-B	464	MET	2.0
3	1-A	332	VAL	2.0
3	2-A	332	VAL	2.0
3	1-B	562	GLN	2.0
3	2-B	562	GLN	2.0
3	1-A	374	THR	2.0
3	2-A	374	THR	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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	DOC	1-P	13	18/19	0.93	0.21	25,30,37,37	18
2	DOC	2-P	13	18/19	0.93	0.21	25,31,34,36	18

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

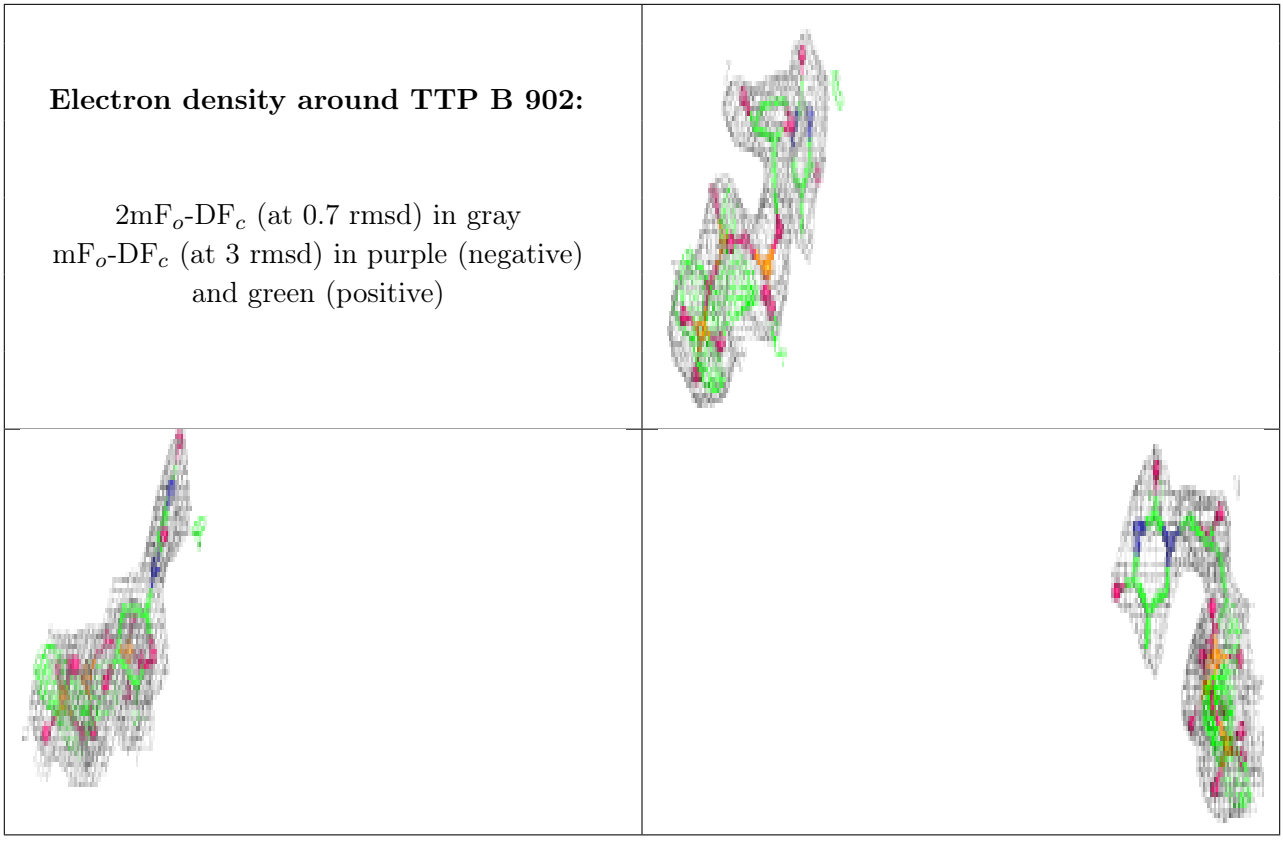
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	TTP	1-B	902	29/29	0.87	0.22	28,31,37,38	29
5	TTP	2-B	902	29/29	0.87	0.22	27,33,36,38	29
4	MG	1-B	901	1/1	0.91	0.17	35,35,35,35	1
4	MG	2-B	901	1/1	0.91	0.17	35,35,35,35	1

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 TTP B 902:

$2mF_o$-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.