Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 06:06 pm BST

PDB ID	:	4L62
Title	:	Crystal Structure of Pseudomonas aeruginosa transcriptional regulator PA2196 bound to its operator DNA
Authors	:	Choe, J.W.; Kim, Y.W.
Deposited on	:	2013-06-11
Resolution	:	2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

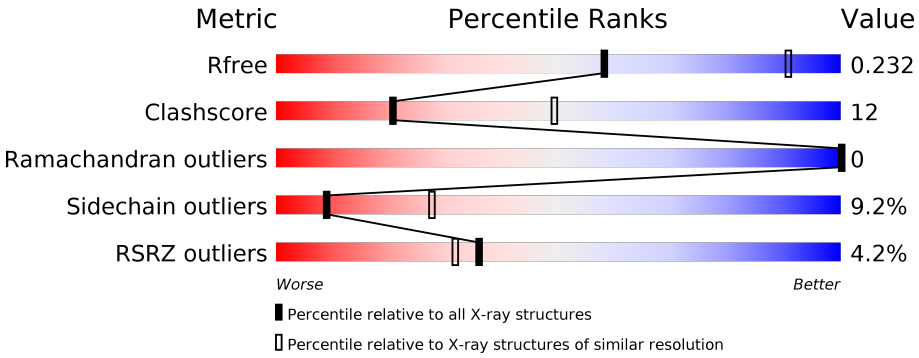
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 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.



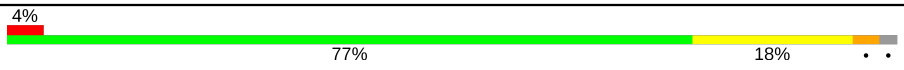
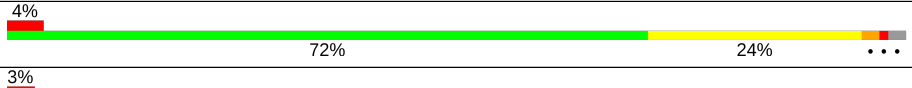
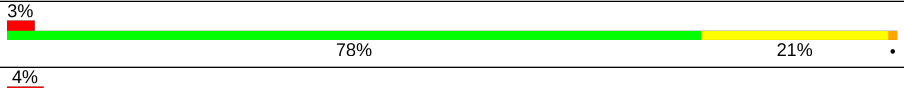
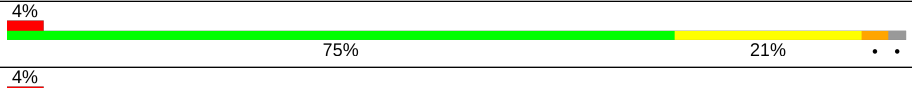
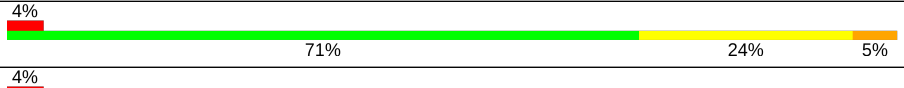
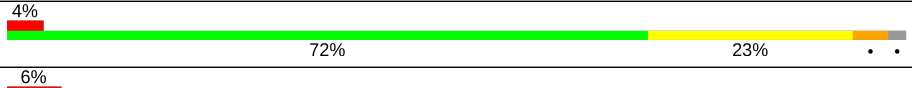
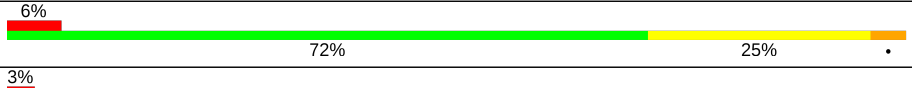
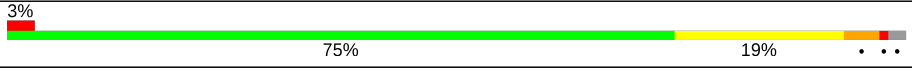
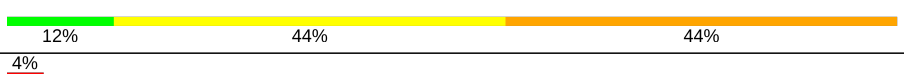
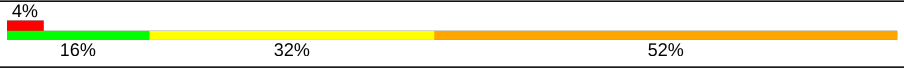
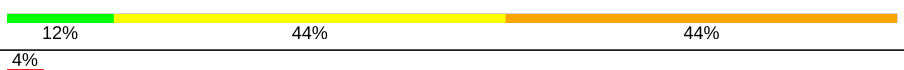
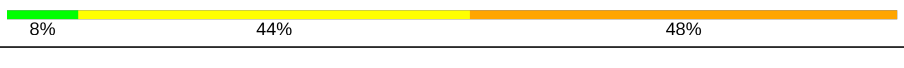
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	190	3% 73% 24% •
1	B	190	4% 78% 16% • •
1	C	190	5% 76% 21% •
1	D	190	3% 75% 21% • • •
1	E	190	4% 71% 24% 5%
1	F	190	7% 68% 24% 6% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	190	
1	H	190	
1	I	190	
1	J	190	
1	K	190	
1	L	190	
1	M	190	
1	N	190	
1	O	190	
1	P	190	
2	Q	25	
2	S	25	
2	U	25	
2	W	25	
3	R	25	
3	T	25	
3	V	25	
3	X	25	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 27921 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Transcriptional regulator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	190	Total	C	N	O	S	0	0	0
			1491	935	263	282	11			
1	B	187	Total	C	N	O	S	0	0	0
			1465	919	260	275	11			
1	C	190	Total	C	N	O	S	0	0	0
			1491	935	263	282	11			
1	D	187	Total	C	N	O	S	0	0	0
			1465	919	260	275	11			
1	E	190	Total	C	N	O	S	0	0	0
			1491	935	263	282	11			
1	F	187	Total	C	N	O	S	0	0	0
			1465	919	260	275	11			
1	G	187	Total	C	N	O	S	0	0	0
			1465	919	260	275	11			
1	H	190	Total	C	N	O	S	0	0	0
			1491	935	263	282	11			
1	I	190	Total	C	N	O	S	0	0	0
			1491	935	263	282	11			
1	J	187	Total	C	N	O	S	0	0	0
			1465	919	260	275	11			
1	K	190	Total	C	N	O	S	0	0	0
			1491	935	263	282	11			
1	L	187	Total	C	N	O	S	0	0	0
			1465	919	260	275	11			
1	M	190	Total	C	N	O	S	0	0	0
			1491	935	263	282	11			
1	N	187	Total	C	N	O	S	0	0	0
			1465	919	260	275	11			
1	O	190	Total	C	N	O	S	0	0	0
			1491	935	263	282	11			
1	P	187	Total	C	N	O	S	0	0	0
			1465	919	260	275	11			

- Molecule 2 is a DNA chain called DNA (25-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Q	25	Total	C	N	O	P	0	0	0
			505	239	88	153	25			
2	S	25	Total	C	N	O	P	0	0	0
			505	239	88	153	25			
2	U	25	Total	C	N	O	P	0	0	0
			505	239	88	153	25			
2	W	25	Total	C	N	O	P	0	0	0
			505	239	88	153	25			

- Molecule 3 is a DNA chain called DNA (25-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	R	25	Total	C	N	O	P	0	0	0
			511	242	97	147	25			
3	T	25	Total	C	N	O	P	0	0	0
			511	242	97	147	25			
3	V	25	Total	C	N	O	P	0	0	0
			511	242	97	147	25			
3	X	25	Total	C	N	O	P	0	0	0
			511	242	97	147	25			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	19	Total	O	0	0
			19	19		
4	B	31	Total	O	0	0
			31	31		
4	C	5	Total	O	0	0
			5	5		
4	D	3	Total	O	0	0
			3	3		
4	E	12	Total	O	0	0
			12	12		
4	F	5	Total	O	0	0
			5	5		
4	G	24	Total	O	0	0
			24	24		
4	H	13	Total	O	0	0
			13	13		
4	I	4	Total	O	0	0
			4	4		

Continued on next page...

Continued from previous page...

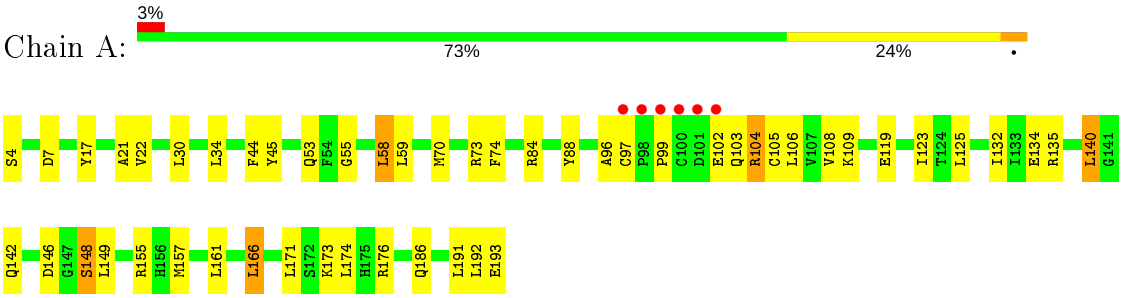
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	J	1	Total O 1 1	0	0
4	K	15	Total O 15 15	0	0
4	L	19	Total O 19 19	0	0
4	M	8	Total O 8 8	0	0
4	N	4	Total O 4 4	0	0
4	Q	3	Total O 3 3	0	0
4	R	2	Total O 2 2	0	0
4	S	13	Total O 13 13	0	0
4	T	7	Total O 7 7	0	0
4	U	12	Total O 12 12	0	0
4	V	9	Total O 9 9	0	0

3 Residue-property plots (i)

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

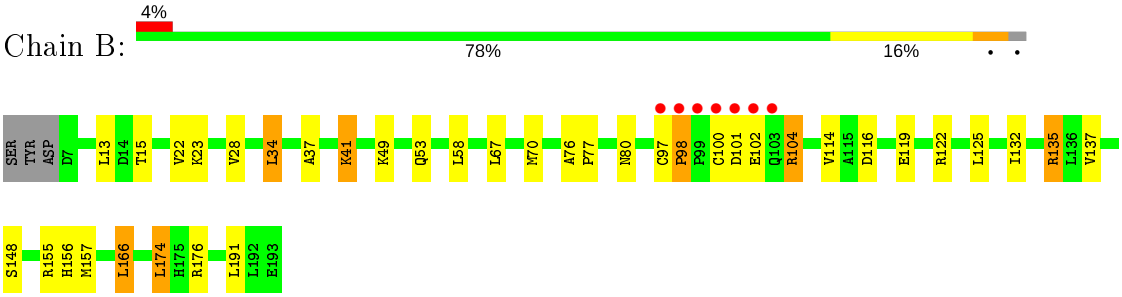
- Molecule 1: Transcriptional regulator

Chain A:



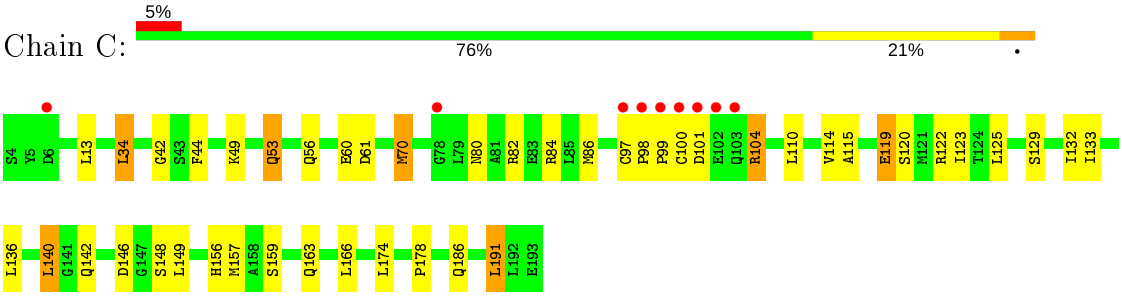
- Molecule 1: Transcriptional regulator

Chain B:



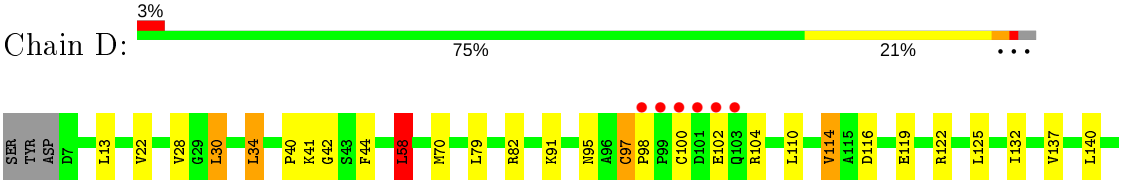
- Molecule 1: Transcriptional regulator

Chain C:

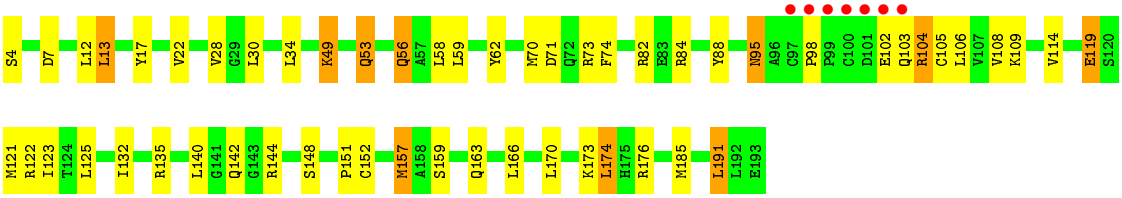


- Molecule 1: Transcriptional regulator

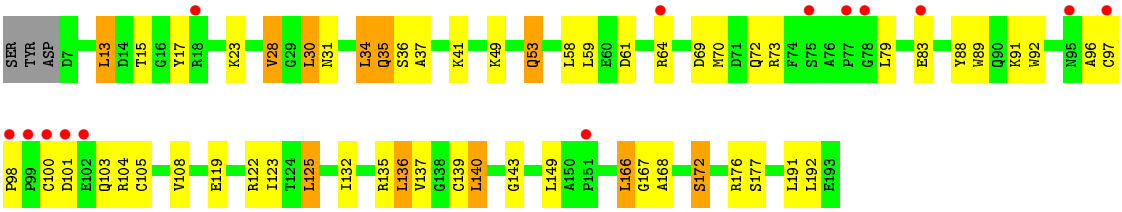
Chain D:



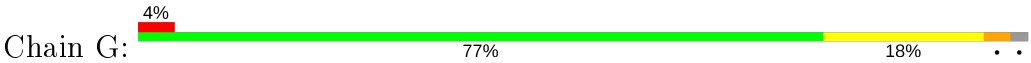
• Molecule 1: Transcriptional regulator

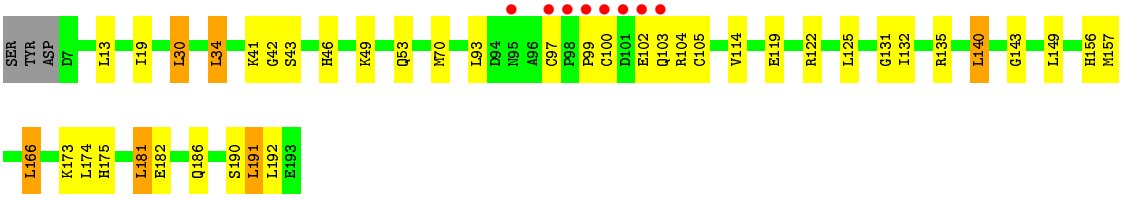


• Molecule 1: Transcriptional regulator

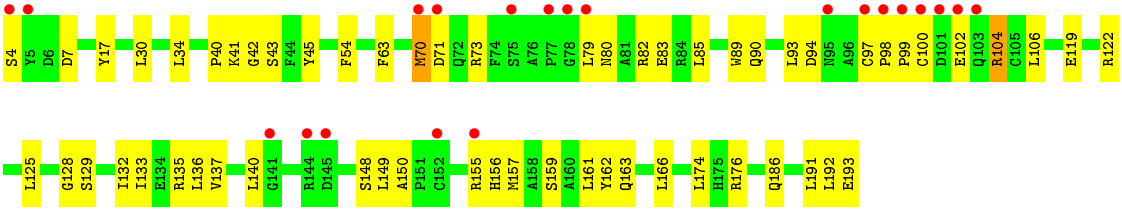


• Molecule 1: Transcriptional regulator

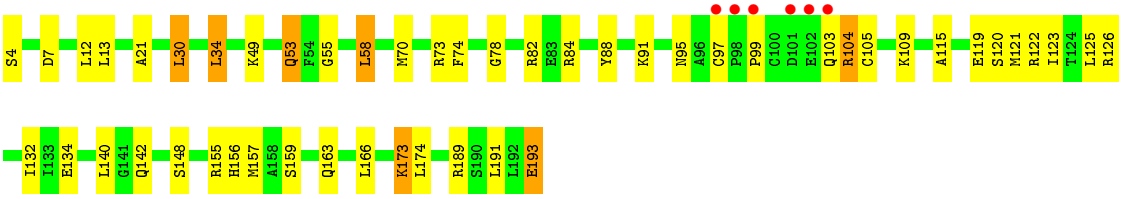




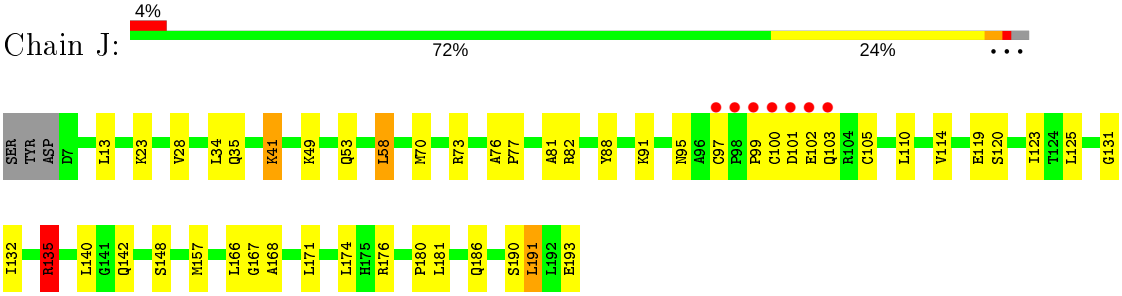
• Molecule 1: Transcriptional regulator



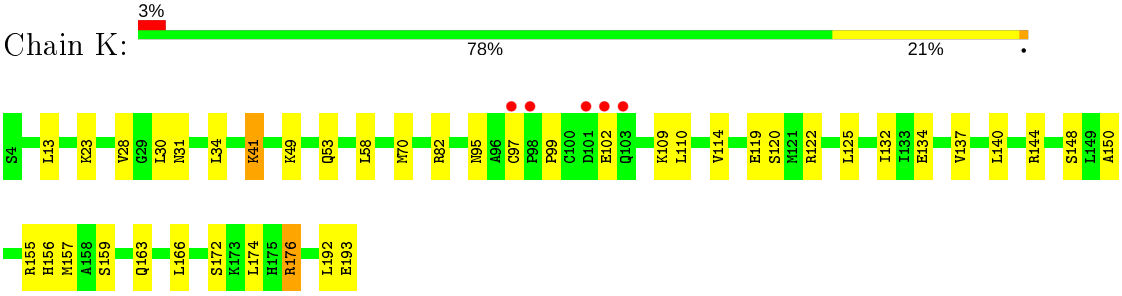
• Molecule 1: Transcriptional regulator



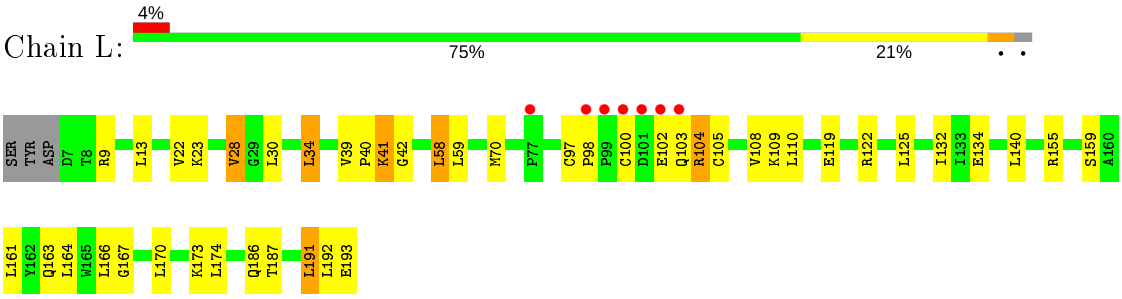
• Molecule 1: Transcriptional regulator



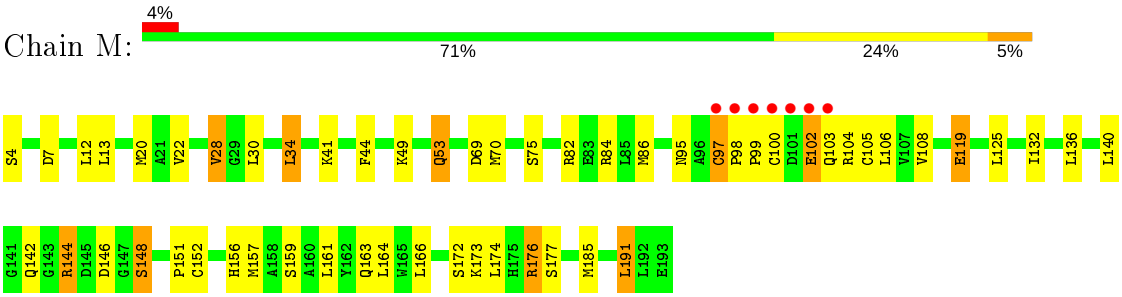
• Molecule 1: Transcriptional regulator



• Molecule 1: Transcriptional regulator

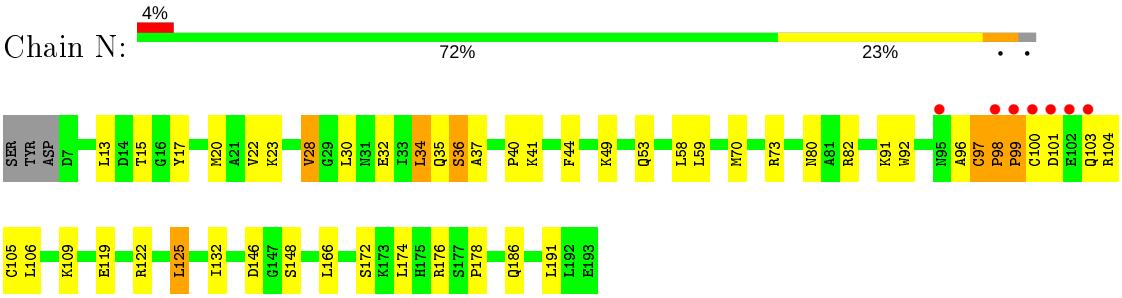


• Molecule 1: Transcriptional regulator



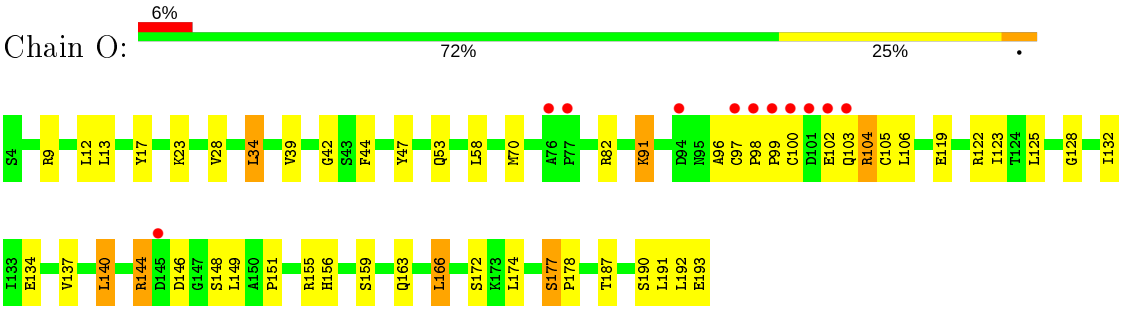
• Molecule 1: Transcriptional regulator

Chain N:



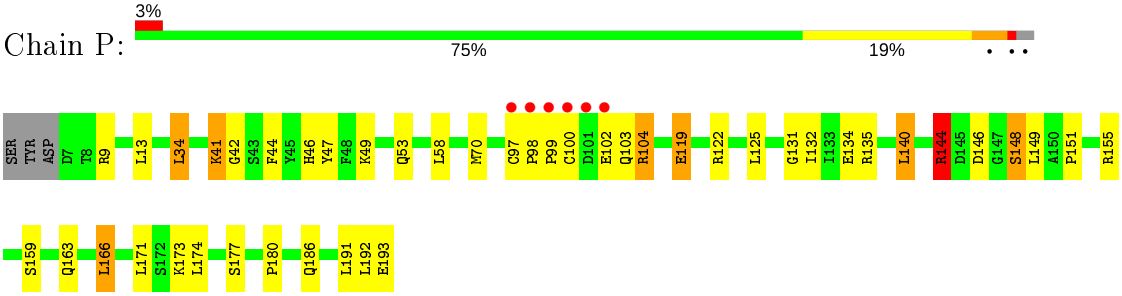
• Molecule 1: Transcriptional regulator

Chain O:



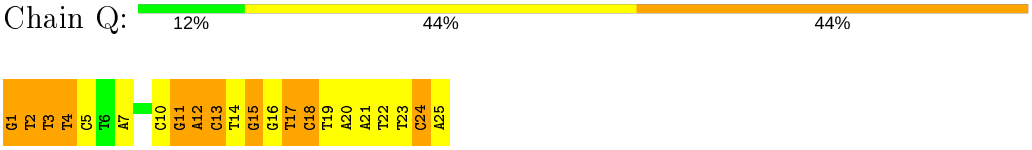
• Molecule 1: Transcriptional regulator

Chain P:



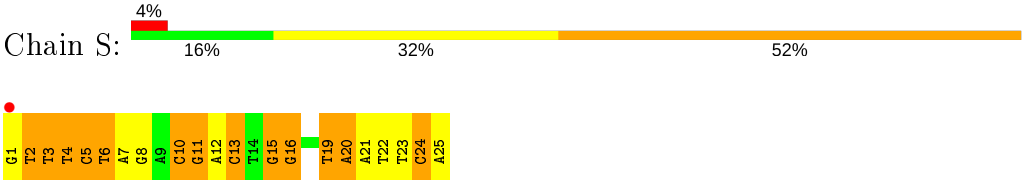
• Molecule 2: DNA (25-MER)

Chain Q:



• Molecule 2: DNA (25-MER)

Chain S:

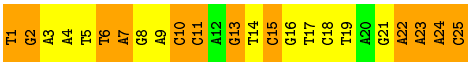


• Molecule 2: DNA (25-MER)

Chain U:

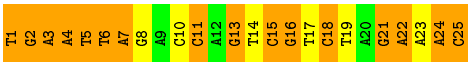
• Molecule 2: DNA (25-MER)

• Molecule 3: DNA (25-MER)



• Molecule 3: DNA (25-MER)

• Molecule 3: DNA (25-MER)



• Molecule 3: DNA (25-MER)

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	211.99Å 211.99Å 282.77Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.95 – 2.90 19.95 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.95-2.90) 93.8 (19.95-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.50 (at 2.88Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.198 , 0.238 0.194 , 0.232	Depositor DCC
R_{free} test set	8138 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	51.5	Xtriage
Anisotropy	0.401	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 38.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.036 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	27921	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.72% 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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.67	0/1521	0.81	1/2052 (0.0%)
1	B	0.73	0/1494	0.85	3/2015 (0.1%)
1	C	0.60	0/1521	0.81	0/2052
1	D	0.59	0/1494	0.80	2/2015 (0.1%)
1	E	0.63	0/1521	0.86	1/2052 (0.0%)
1	F	0.55	0/1494	0.84	1/2015 (0.0%)
1	G	0.63	0/1494	0.79	0/2015
1	H	0.54	0/1521	0.77	1/2052 (0.0%)
1	I	0.68	0/1521	0.87	5/2052 (0.2%)
1	J	0.71	0/1494	0.86	3/2015 (0.1%)
1	K	0.61	0/1521	0.79	2/2052 (0.1%)
1	L	0.60	0/1494	0.78	2/2015 (0.1%)
1	M	0.62	1/1521 (0.1%)	0.81	2/2052 (0.1%)
1	N	0.58	0/1494	0.81	2/2015 (0.1%)
1	O	0.55	0/1521	0.77	0/2052
1	P	0.66	0/1494	0.82	2/2015 (0.1%)
2	Q	1.72	15/565 (2.7%)	3.14	86/867 (9.9%)
2	S	1.60	6/565 (1.1%)	2.89	76/867 (8.8%)
2	U	1.86	20/565 (3.5%)	3.53	97/867 (11.2%)
2	W	1.60	6/565 (1.1%)	3.13	78/867 (9.0%)
3	R	1.61	11/574 (1.9%)	3.11	75/882 (8.5%)
3	T	1.59	11/574 (1.9%)	2.74	69/882 (7.8%)
3	V	1.76	15/574 (2.6%)	3.19	88/882 (10.0%)
3	X	1.60	8/574 (1.4%)	2.94	78/882 (8.8%)
All	All	0.88	93/28676 (0.3%)	1.50	674/39532 (1.7%)

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	C	0	1

All (93) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	V	4	DA	N9-C4	-10.39	1.31	1.37
2	W	13	DC	N1-C2	10.30	1.50	1.40
3	X	1	DT	N1-C2	10.24	1.46	1.38
2	U	2	DT	N1-C2	9.62	1.45	1.38
2	S	13	DC	N1-C2	8.55	1.48	1.40
3	R	1	DT	N1-C2	8.49	1.44	1.38
3	V	1	DT	N1-C2	8.13	1.44	1.38
2	U	11	DG	C5-C6	-7.95	1.34	1.42
2	Q	11	DG	C2-N3	7.87	1.39	1.32
2	Q	1	DG	P-O5'	7.67	1.67	1.59
2	U	11	DG	C2-N3	7.65	1.38	1.32
2	W	15	DG	C5-C6	-7.48	1.34	1.42
2	U	15	DG	C5-C6	-7.46	1.34	1.42
3	V	13	DG	N1-C2	7.39	1.43	1.37
3	R	15	DC	N1-C2	7.27	1.47	1.40
3	V	15	DC	N1-C2	7.22	1.47	1.40
3	X	13	DG	C3'-O3'	-7.16	1.34	1.44
3	R	4	DA	N9-C4	-7.15	1.33	1.37
3	X	13	DG	C5-C6	-7.12	1.35	1.42
2	Q	22	DT	N1-C2	7.08	1.43	1.38
2	W	13	DC	C1'-N1	6.99	1.58	1.49
3	T	24	DA	C6-N1	6.89	1.40	1.35
3	T	3	DA	N9-C4	-6.86	1.33	1.37
2	U	15	DG	C2-N3	6.82	1.38	1.32
2	Q	2	DT	N1-C2	6.81	1.43	1.38
3	T	1	DT	N1-C2	6.71	1.43	1.38
3	R	15	DC	C4-C5	6.63	1.48	1.43
2	U	22	DT	N1-C2	6.62	1.43	1.38
2	S	3	DT	N1-C2	6.55	1.43	1.38
2	Q	4	DT	C1'-N1	6.46	1.57	1.49
3	R	13	DG	C5-C6	-6.42	1.35	1.42
2	Q	23	DT	C1'-N1	6.36	1.57	1.49
2	U	23	DT	N1-C2	6.36	1.43	1.38
2	U	13	DC	N1-C2	6.33	1.46	1.40
2	U	4	DT	C1'-N1	6.31	1.57	1.49
2	Q	11	DG	C2-N2	6.23	1.40	1.34
2	Q	15	DG	C5-C6	-6.21	1.36	1.42
2	U	15	DG	C3'-O3'	-6.21	1.35	1.44
2	U	3	DT	N1-C2	6.19	1.43	1.38
3	X	3	DA	N9-C4	-6.18	1.34	1.37
3	R	22	DA	N9-C4	-6.17	1.34	1.37
2	U	25	DA	N7-C5	-6.12	1.35	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	V	13	DG	C2-N3	6.04	1.37	1.32
3	T	16	DG	C3'-O3'	-5.99	1.36	1.44
3	V	13	DG	C5-C6	-5.99	1.36	1.42
3	V	11	DC	C4-C5	5.97	1.47	1.43
2	U	22	DT	C1'-N1	5.97	1.57	1.49
2	Q	11	DG	C5-C6	-5.94	1.36	1.42
3	X	15	DC	C1'-N1	5.89	1.56	1.49
2	U	4	DT	N1-C2	5.89	1.42	1.38
3	V	24	DA	C6-N1	5.84	1.39	1.35
2	U	15	DG	N7-C5	-5.77	1.35	1.39
3	V	13	DG	C3'-O3'	-5.77	1.36	1.44
3	T	13	DG	C5-C6	-5.74	1.36	1.42
2	S	22	DT	N1-C2	5.70	1.42	1.38
2	U	11	DG	C2-N2	5.67	1.40	1.34
2	U	11	DG	N1-C2	5.66	1.42	1.37
2	Q	11	DG	N1-C2	5.62	1.42	1.37
3	T	13	DG	N1-C2	5.62	1.42	1.37
2	Q	15	DG	C2-N3	5.61	1.37	1.32
3	X	13	DG	N1-C2	5.61	1.42	1.37
3	R	13	DG	C3'-O3'	-5.61	1.36	1.44
3	T	11	DC	C1'-N1	5.58	1.56	1.49
2	Q	12	DA	C3'-O3'	-5.58	1.36	1.44
2	Q	3	DT	N1-C2	5.57	1.42	1.38
2	Q	13	DC	N1-C2	5.56	1.45	1.40
3	V	11	DC	N1-C2	5.56	1.45	1.40
3	V	23	DA	C3'-O3'	-5.54	1.36	1.44
3	V	13	DG	C1'-N9	-5.54	1.39	1.47
2	Q	23	DT	N1-C2	5.50	1.42	1.38
2	S	3	DT	C1'-N1	5.47	1.56	1.49
2	S	23	DT	N1-C2	5.42	1.42	1.38
3	T	18	DC	C3'-O3'	-5.41	1.36	1.44
2	U	11	DG	N7-C5	-5.40	1.36	1.39
3	T	13	DG	C6-N1	5.39	1.43	1.39
3	R	7	DA	C3'-O3'	-5.39	1.36	1.44
3	R	24	DA	C6-N1	5.34	1.39	1.35
3	X	4	DA	N9-C4	-5.27	1.34	1.37
3	R	11	DC	N1-C2	5.26	1.45	1.40
2	W	3	DT	N1-C2	5.26	1.42	1.38
3	V	23	DA	N9-C4	-5.23	1.34	1.37
3	T	4	DA	N9-C4	-5.21	1.34	1.37
2	W	8	DG	C3'-O3'	-5.20	1.37	1.44
2	U	15	DG	N1-C2	5.20	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	X	18	DC	C3'-O3'	-5.20	1.37	1.44
1	M	102	GLU	CG-CD	5.19	1.59	1.51
3	V	15	DC	C4-C5	5.15	1.47	1.43
3	T	9	DA	C3'-O3'	-5.14	1.37	1.44
3	R	13	DG	N1-C2	5.14	1.41	1.37
2	U	13	DC	C1'-N1	5.11	1.55	1.49
2	W	23	DT	N1-C2	5.09	1.42	1.38
2	S	24	DC	N1-C2	5.03	1.45	1.40
3	V	13	DG	N9-C4	-5.03	1.33	1.38

All (674) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	W	13	DC	N1-C2-O2	21.02	131.51	118.90
2	W	13	DC	N3-C2-O2	-19.31	108.39	121.90
2	U	15	DG	O4'-C1'-N9	-19.23	94.54	108.00
2	U	11	DG	O4'-C1'-N9	-17.58	95.69	108.00
3	R	13	DG	N1-C6-O6	17.07	130.14	119.90
3	V	13	DG	N1-C6-O6	17.01	130.11	119.90
2	U	13	DC	N3-C2-O2	-16.85	110.10	121.90
2	U	11	DG	N1-C6-O6	16.65	129.89	119.90
3	R	23	DA	O4'-C1'-N9	-16.55	96.41	108.00
3	V	11	DC	N3-C2-O2	-16.43	110.40	121.90
2	U	15	DG	N1-C6-O6	16.32	129.69	119.90
3	R	15	DC	N3-C2-O2	-16.29	110.50	121.90
2	Q	15	DG	N1-C6-O6	15.81	129.39	119.90
2	U	13	DC	N1-C2-O2	15.68	128.31	118.90
2	U	11	DG	C4-C5-N7	15.65	117.06	110.80
3	X	13	DG	N1-C6-O6	15.57	129.24	119.90
2	U	11	DG	C6-C5-N7	-15.46	121.12	130.40
3	X	1	DT	N3-C2-O2	-15.31	113.11	122.30
2	Q	13	DC	N3-C2-O2	-15.31	111.18	121.90
3	R	1	DT	N3-C2-O2	-15.17	113.19	122.30
2	S	13	DC	N3-C2-O2	-15.16	111.28	121.90
2	W	23	DT	N3-C2-O2	-15.04	113.28	122.30
2	Q	22	DT	N3-C2-O2	-14.86	113.39	122.30
2	W	15	DG	N1-C6-O6	14.79	128.78	119.90
2	U	11	DG	C5-C6-O6	-14.35	119.99	128.60
2	U	15	DG	C6-C5-N7	-13.75	122.15	130.40
2	Q	15	DG	C6-C5-N7	-13.65	122.21	130.40
3	R	13	DG	C5-C6-O6	-13.62	120.43	128.60
2	U	2	DT	N3-C2-O2	-13.55	114.17	122.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Q	23	DT	N3-C2-O2	-13.55	114.17	122.30
2	W	15	DG	C4-C5-N7	13.53	116.21	110.80
2	W	15	DG	C6-C5-N7	-13.52	122.29	130.40
3	R	3	DA	N1-C6-N6	13.43	126.66	118.60
2	W	21	DA	O4'-C1'-N9	13.39	117.38	108.00
2	Q	11	DG	N1-C6-O6	13.34	127.91	119.90
3	R	13	DG	O4'-C1'-N9	-13.23	98.74	108.00
3	V	13	DG	C5-C6-O6	-13.22	120.67	128.60
3	V	7	DA	O4'-C1'-N9	-13.19	98.77	108.00
2	U	22	DT	N3-C2-O2	-13.16	114.40	122.30
3	V	4	DA	C2-N3-C4	-13.10	104.05	110.60
2	U	15	DG	C5-C6-O6	-13.09	120.75	128.60
2	Q	11	DG	C4-C5-N7	13.07	116.03	110.80
3	V	13	DG	O4'-C1'-N9	-13.04	98.88	108.00
2	S	25	DA	O4'-C1'-N9	-12.94	98.94	108.00
3	T	13	DG	N1-C6-O6	12.91	127.64	119.90
3	R	7	DA	O4'-C1'-N9	-12.85	99.00	108.00
2	W	15	DG	C5-C6-O6	-12.85	120.89	128.60
3	R	11	DC	N3-C2-O2	-12.84	112.91	121.90
3	X	1	DT	N1-C2-O2	12.84	133.37	123.10
2	S	13	DC	N1-C2-O2	12.78	126.57	118.90
2	Q	13	DC	N1-C2-O2	12.78	126.57	118.90
2	U	11	DG	N9-C4-C5	-12.77	100.29	105.40
2	Q	11	DG	N9-C4-C5	-12.65	100.34	105.40
2	Q	11	DG	C5-C6-O6	-12.60	121.04	128.60
2	U	2	DT	O4'-C1'-C2'	-12.56	95.85	105.90
3	V	13	DG	C6-C5-N7	-12.54	122.87	130.40
2	U	23	DT	N3-C2-O2	-12.54	114.78	122.30
3	X	11	DC	N3-C2-O2	-12.45	113.18	121.90
2	U	21	DA	O4'-C1'-N9	12.42	116.69	108.00
2	Q	3	DT	N3-C2-O2	-12.36	114.89	122.30
3	R	13	DG	C4-C5-N7	12.34	115.73	110.80
2	S	15	DG	O4'-C1'-N9	-12.30	99.39	108.00
2	S	3	DT	N3-C2-O2	-12.13	115.02	122.30
2	Q	15	DG	C5-C6-O6	-11.99	121.41	128.60
2	U	3	DT	N3-C2-O2	-11.95	115.13	122.30
3	T	13	DG	C5-C6-O6	-11.91	121.45	128.60
2	Q	11	DG	O4'-C1'-N9	-11.91	99.66	108.00
2	Q	2	DT	N3-C2-O2	-11.90	115.16	122.30
2	Q	11	DG	C6-C5-N7	-11.89	123.27	130.40
2	U	15	DG	C4-C5-N7	11.89	115.56	110.80
3	V	2	DG	O4'-C1'-N9	-11.86	99.70	108.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	W	25	DA	O4'-C1'-N9	-11.83	99.72	108.00
2	Q	15	DG	C4-C5-N7	11.71	115.48	110.80
3	V	3	DA	N1-C6-N6	11.71	125.63	118.60
3	X	23	DA	O4'-C1'-N9	-11.69	99.82	108.00
3	V	15	DC	N3-C2-O2	-11.63	113.76	121.90
3	T	11	DC	N3-C2-O2	-11.60	113.78	121.90
2	U	4	DT	C4-C5-C6	11.57	124.94	118.00
3	X	13	DG	C6-C5-N7	-11.49	123.51	130.40
3	R	15	DC	N1-C2-O2	11.46	125.78	118.90
3	V	4	DA	N1-C6-N6	11.45	125.47	118.60
3	X	15	DC	N3-C2-O2	-11.44	113.89	121.90
3	V	13	DG	C4-C5-N7	11.42	115.37	110.80
2	U	2	DT	N1-C2-O2	11.38	132.21	123.10
3	X	8	DG	O4'-C1'-N9	11.35	115.94	108.00
3	V	5	DT	O4'-C1'-N1	-11.21	100.15	108.00
3	X	13	DG	O4'-C1'-N9	-11.20	100.16	108.00
3	R	13	DG	C6-C5-N7	-11.19	123.69	130.40
2	U	4	DT	N3-C2-O2	-11.09	115.64	122.30
2	S	15	DG	C4-C5-N7	11.08	115.23	110.80
3	T	7	DA	O4'-C1'-N9	-11.06	100.25	108.00
3	T	1	DT	N3-C2-O2	-11.04	115.68	122.30
2	S	22	DT	N3-C2-O2	-10.96	115.72	122.30
3	R	22	DA	O4'-C1'-N9	-10.96	100.33	108.00
3	V	5	DT	O4'-C4'-C3'	-10.94	99.44	106.00
2	U	4	DT	N1-C2-N3	10.92	121.15	114.60
2	S	24	DC	N3-C2-O2	-10.92	114.26	121.90
2	W	19	DT	N3-C4-O4	10.85	126.41	119.90
3	V	11	DC	C4-C5-C6	10.82	122.81	117.40
3	R	11	DC	N1-C2-O2	10.77	125.36	118.90
3	T	15	DC	N3-C2-O2	-10.76	114.37	121.90
3	X	13	DG	C5-C6-O6	-10.71	122.18	128.60
2	W	11	DG	N1-C6-O6	10.70	126.32	119.90
3	R	1	DT	N1-C2-O2	10.69	131.65	123.10
3	V	25	DC	O4'-C4'-C3'	-10.63	99.62	106.00
3	V	13	DG	N9-C4-C5	-10.61	101.16	105.40
3	R	13	DG	N9-C4-C5	-10.60	101.16	105.40
3	V	4	DA	N3-C4-C5	10.60	134.22	126.80
2	Q	25	DA	O4'-C1'-N9	-10.59	100.58	108.00
3	X	3	DA	N1-C6-N6	10.56	124.94	118.60
2	S	13	DC	O4'-C1'-N1	10.54	115.38	108.00
3	X	11	DC	N1-C2-O2	10.51	125.20	118.90
3	V	11	DC	N1-C2-O2	10.50	125.20	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Q	21	DA	O4'-C1'-N9	10.50	115.35	108.00
3	V	22	DA	N1-C6-N6	10.47	124.88	118.60
3	V	15	DC	O4'-C1'-N1	10.45	115.32	108.00
3	T	22	DA	N1-C6-N6	10.41	124.85	118.60
2	W	11	DG	C5-C6-O6	-10.35	122.39	128.60
2	W	13	DC	O4'-C1'-N1	10.31	115.22	108.00
3	X	3	DA	C2-N3-C4	-10.20	105.50	110.60
2	U	4	DT	C2-N3-C4	-10.17	121.10	127.20
3	V	11	DC	O4'-C1'-C2'	-10.16	97.77	105.90
2	W	22	DT	C2-N3-C4	-10.16	121.11	127.20
2	U	8	DG	O4'-C1'-N9	10.14	115.10	108.00
2	W	11	DG	C4-C5-N7	10.09	114.84	110.80
2	S	23	DT	N3-C2-O2	-10.09	116.25	122.30
3	V	4	DA	C5-N7-C8	-10.03	98.88	103.90
3	V	23	DA	O4'-C1'-N9	-10.03	100.98	108.00
3	R	4	DA	O4'-C1'-N9	-10.00	101.00	108.00
2	S	15	DG	N1-C6-O6	9.91	125.85	119.90
2	S	13	DC	C4-C5-C6	9.88	122.34	117.40
2	U	3	DT	C2-N3-C4	-9.81	121.32	127.20
2	Q	4	DT	N3-C2-O2	-9.80	116.42	122.30
2	W	4	DT	C2-N3-C4	-9.80	121.32	127.20
2	W	24	DC	N3-C2-O2	-9.74	115.08	121.90
2	U	22	DT	N1-C2-N3	9.72	120.43	114.60
3	X	2	DG	N1-C6-O6	9.71	125.73	119.90
3	V	1	DT	N3-C2-O2	-9.70	116.48	122.30
3	X	11	DC	O4'-C1'-N1	9.68	114.78	108.00
3	R	23	DA	N1-C6-N6	9.62	124.38	118.60
3	R	4	DA	C2-N3-C4	-9.59	105.81	110.60
3	T	1	DT	N1-C2-O2	9.54	130.73	123.10
2	W	15	DG	O4'-C1'-N9	-9.53	101.33	108.00
3	R	25	DC	N3-C2-O2	-9.52	115.24	121.90
2	U	25	DA	N1-C6-N6	9.52	124.31	118.60
2	S	15	DG	C5-C6-O6	-9.49	122.91	128.60
2	Q	4	DT	C4-C5-C6	9.49	123.69	118.00
3	R	4	DA	N1-C6-N6	9.45	124.27	118.60
3	T	2	DG	C2-N3-C4	-9.43	107.18	111.90
2	Q	4	DT	N1-C2-N3	9.42	120.25	114.60
3	V	4	DA	O4'-C1'-N9	-9.37	101.44	108.00
2	W	19	DT	C5-C4-O4	-9.36	118.35	124.90
2	W	1	DG	O4'-C1'-N9	-9.35	101.46	108.00
3	T	23	DA	O4'-C1'-N9	-9.34	101.46	108.00
2	U	4	DT	C5-C6-N1	-9.33	118.10	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	W	15	DG	N9-C4-C5	-9.33	101.67	105.40
3	R	15	DC	O4'-C1'-N1	9.29	114.51	108.00
2	W	11	DG	C6-C5-N7	-9.26	124.84	130.40
2	Q	13	DC	C4-C5-C6	9.25	122.03	117.40
3	X	2	DG	C6-C5-N7	-9.25	124.85	130.40
3	X	3	DA	O4'-C1'-N9	-9.24	101.53	108.00
3	V	25	DC	N3-C2-O2	-9.19	115.47	121.90
3	X	5	DT	O4'-C1'-N1	-9.17	101.58	108.00
3	R	15	DC	C5-C6-N1	-9.14	116.43	121.00
3	T	3	DA	O4'-C1'-N9	-9.14	101.60	108.00
3	R	15	DC	C4-C5-C6	9.11	121.95	117.40
3	V	4	DA	N3-C4-N9	-9.10	120.12	127.40
2	U	19	DT	N3-C4-O4	9.08	125.35	119.90
2	U	23	DT	C2-N3-C4	-9.07	121.76	127.20
2	Q	13	DC	C5-C6-N1	-9.06	116.47	121.00
2	S	21	DA	N1-C2-N3	-9.06	124.77	129.30
3	R	22	DA	C2-N3-C4	-9.02	106.09	110.60
3	T	4	DA	N1-C6-N6	8.99	124.00	118.60
3	T	15	DC	N1-C2-O2	8.95	124.27	118.90
3	V	1	DT	N1-C2-O2	8.94	130.25	123.10
2	U	1	DG	N1-C6-O6	8.93	125.26	119.90
2	U	22	DT	C2-N3-C4	-8.86	121.88	127.20
3	X	22	DA	N1-C6-N6	8.84	123.90	118.60
2	U	3	DT	C5-C6-N1	-8.83	118.40	123.70
2	U	15	DG	C5-N7-C8	-8.83	99.89	104.30
2	W	22	DT	N1-C2-N3	8.80	119.88	114.60
3	X	4	DA	N1-C6-N6	8.79	123.87	118.60
2	U	3	DT	N1-C2-N3	8.77	119.86	114.60
2	S	11	DG	O4'-C1'-N9	-8.76	101.87	108.00
2	U	13	DC	O4'-C1'-C2'	-8.76	98.89	105.90
2	W	3	DT	N1-C1'-C2'	8.76	129.24	112.60
3	R	15	DC	N3-C4-N4	-8.71	111.90	118.00
2	S	4	DT	O4'-C1'-C2'	-8.70	98.94	105.90
2	Q	2	DT	O4'-C1'-N1	8.70	114.09	108.00
3	V	15	DC	C2-N3-C4	-8.70	115.55	119.90
2	W	3	DT	N3-C2-O2	-8.69	117.08	122.30
3	X	2	DG	C2-N3-C4	-8.65	107.57	111.90
3	V	5	DT	O4'-C1'-C2'	-8.65	98.98	105.90
2	Q	15	DG	O4'-C1'-N9	-8.60	101.98	108.00
3	X	2	DG	O4'-C1'-N9	-8.59	101.99	108.00
3	R	5	DT	O4'-C1'-N1	-8.59	101.99	108.00
2	W	22	DT	N3-C2-O2	-8.56	117.16	122.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	T	5	DT	O4'-C1'-N1	-8.47	102.07	108.00
3	V	3	DA	C2-N3-C4	-8.46	106.37	110.60
2	W	4	DT	N1-C2-N3	8.46	119.67	114.60
2	W	13	DC	O4'-C1'-C2'	-8.46	99.13	105.90
2	W	15	DG	C5-N7-C8	-8.45	100.08	104.30
3	R	3	DA	O4'-C1'-N9	-8.43	102.10	108.00
2	S	2	DT	O4'-C1'-N1	8.43	113.90	108.00
3	V	11	DC	C5-C6-N1	-8.42	116.79	121.00
3	R	13	DG	N3-C4-C5	8.42	132.81	128.60
2	W	3	DT	C1'-O4'-C4'	-8.35	101.75	110.10
3	T	3	DA	C5-N7-C8	-8.27	99.76	103.90
2	S	8	DG	O4'-C1'-N9	8.26	113.78	108.00
3	V	23	DA	N1-C6-N6	8.24	123.54	118.60
2	S	3	DT	N1-C1'-C2'	8.17	128.12	112.60
2	W	23	DT	C5-C6-N1	-8.15	118.81	123.70
2	U	14	DT	N3-C4-O4	8.09	124.76	119.90
3	T	25	DC	N1-C1'-C2'	8.08	127.95	112.60
2	W	4	DT	N3-C2-O2	-8.07	117.46	122.30
3	X	4	DA	O4'-C1'-N9	-8.07	102.35	108.00
2	S	25	DA	N1-C6-N6	8.06	123.44	118.60
3	T	4	DA	O4'-C1'-N9	-8.05	102.36	108.00
2	S	15	DG	N9-C4-C5	-8.05	102.18	105.40
3	R	15	DC	C5-C4-N4	8.03	125.82	120.20
3	T	2	DG	C6-C5-N7	-8.02	125.59	130.40
2	U	5	DC	N3-C4-C5	8.02	125.11	121.90
2	S	15	DG	C6-C5-N7	-8.00	125.60	130.40
2	U	15	DG	C2-N3-C4	-7.99	107.91	111.90
2	U	11	DG	C5-N7-C8	-7.99	100.31	104.30
3	T	2	DG	N1-C6-O6	7.97	124.69	119.90
3	V	3	DA	C5-C6-N1	-7.95	113.72	117.70
2	S	21	DA	N1-C6-N6	7.95	123.37	118.60
2	S	13	DC	C5-C6-N1	-7.93	117.03	121.00
2	Q	4	DT	C5-C6-N1	-7.90	118.96	123.70
2	S	13	DC	C2-N3-C4	-7.89	115.95	119.90
2	Q	3	DT	O4'-C1'-C2'	-7.89	99.59	105.90
3	R	3	DA	C5-C6-N6	-7.88	117.40	123.70
2	U	23	DT	N1-C2-N3	7.87	119.32	114.60
2	Q	13	DC	N3-C4-N4	-7.87	112.49	118.00
2	S	21	DA	N9-C4-C5	-7.86	102.66	105.80
2	U	13	DC	C5-C4-N4	7.85	125.69	120.20
2	W	23	DT	N1-C2-N3	7.83	119.30	114.60
2	Q	2	DT	N1-C2-O2	7.83	129.36	123.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Q	4	DT	C2-N3-C4	-7.83	122.50	127.20
3	R	2	DG	O4'-C1'-N9	-7.82	102.53	108.00
2	W	11	DG	O4'-C1'-N9	-7.82	102.53	108.00
2	U	22	DT	C4-C5-C6	7.81	122.69	118.00
3	X	13	DG	C4-C5-N7	7.80	113.92	110.80
2	W	22	DT	C5-C6-N1	-7.80	119.02	123.70
2	Q	15	DG	C5-N7-C8	-7.80	100.40	104.30
3	R	25	DC	O4'-C4'-C3'	-7.79	101.33	106.00
2	Q	15	DG	N9-C4-C5	-7.79	102.29	105.40
3	X	13	DG	C2-N3-C4	-7.78	108.01	111.90
2	S	24	DC	N3-C4-N4	-7.77	112.56	118.00
2	W	13	DC	N3-C4-N4	-7.76	112.57	118.00
2	U	1	DG	C6-C5-N7	-7.76	125.75	130.40
2	Q	1	DG	O4'-C4'-C3'	-7.75	101.35	106.00
3	V	15	DC	N3-C4-N4	-7.72	112.60	118.00
3	R	4	DA	N3-C4-C5	7.71	132.20	126.80
2	Q	22	DT	N1-C2-O2	7.71	129.27	123.10
3	T	11	DC	N1-C2-O2	7.69	123.51	118.90
3	X	3	DA	C5-N7-C8	-7.68	100.06	103.90
3	T	3	DA	N3-C4-C5	7.65	132.16	126.80
2	U	5	DC	C4-C5-C6	-7.64	113.58	117.40
2	S	23	DT	C2-N3-C4	-7.61	122.64	127.20
3	T	13	DG	C4-C5-N7	7.61	113.84	110.80
3	V	13	DG	C8-N9-C4	7.60	109.44	106.40
3	X	13	DG	N9-C4-C5	-7.58	102.37	105.40
2	W	24	DC	N1-C2-O2	7.57	123.44	118.90
3	X	3	DA	N3-C4-C5	7.57	132.10	126.80
3	V	13	DG	N3-C4-C5	7.55	132.38	128.60
2	S	22	DT	C2-N3-C4	-7.55	122.67	127.20
2	Q	13	DC	C5-C4-N4	7.55	125.48	120.20
3	V	4	DA	C5-C6-N1	-7.54	113.93	117.70
2	U	13	DC	N3-C4-N4	-7.53	112.73	118.00
3	X	1	DT	C5-C6-N1	-7.53	119.18	123.70
2	Q	2	DT	O4'-C1'-C2'	-7.51	99.89	105.90
2	W	13	DC	C4-C5-C6	7.51	121.15	117.40
3	R	15	DC	C2-N3-C4	-7.50	116.15	119.90
2	S	16	DG	O4'-C1'-N9	7.48	113.23	108.00
3	T	2	DG	O4'-C1'-N9	-7.45	102.79	108.00
3	V	22	DA	O4'-C1'-N9	-7.44	102.80	108.00
3	V	11	DC	N1-C2-N3	7.43	124.40	119.20
1	F	100	CYS	N-CA-C	-7.42	90.96	111.00
3	V	13	DG	C2-N3-C4	-7.41	108.20	111.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	W	2	DT	O4'-C1'-N1	7.39	113.17	108.00
3	X	15	DC	C4-C5-C6	7.38	121.09	117.40
2	W	11	DG	C5-N7-C8	-7.37	100.61	104.30
3	T	2	DG	C5-C6-N1	-7.36	107.82	111.50
3	V	15	DC	N1-C2-O2	7.35	123.31	118.90
2	W	23	DT	C2-N3-C4	-7.34	122.80	127.20
3	R	13	DG	C8-N9-C4	7.33	109.33	106.40
2	Q	1	DG	C4'-C3'-C2'	7.33	109.69	103.10
3	V	1	DT	O4'-C1'-N1	7.32	113.12	108.00
3	V	11	DC	C2-N3-C4	-7.29	116.25	119.90
3	V	4	DA	C4-C5-N7	7.28	114.34	110.70
3	R	25	DC	N1-C2-O2	7.27	123.26	118.90
2	S	5	DC	O4'-C1'-N1	7.25	113.08	108.00
3	T	11	DC	O4'-C1'-N1	7.25	113.08	108.00
3	T	13	DG	C6-C5-N7	-7.24	126.06	130.40
3	X	23	DA	C2-N3-C4	-7.24	106.98	110.60
3	R	22	DA	N1-C6-N6	7.22	122.94	118.60
3	R	13	DG	C5-N7-C8	-7.21	100.70	104.30
3	X	1	DT	C6-N1-C1'	-7.21	109.59	120.40
2	U	23	DT	C4-C5-C6	7.19	122.31	118.00
2	U	13	DC	C4-C5-C6	7.17	120.99	117.40
3	V	23	DA	C5-N7-C8	-7.17	100.31	103.90
3	R	11	DC	C4-C5-C6	7.17	120.98	117.40
2	Q	11	DG	N3-C2-N2	7.16	124.91	119.90
2	Q	15	DG	C2-N3-C4	-7.15	108.33	111.90
2	S	15	DG	C5-N7-C8	-7.13	100.73	104.30
3	R	23	DA	C2-N3-C4	-7.11	107.04	110.60
3	X	22	DA	C2-N3-C4	-7.11	107.05	110.60
2	W	17	DT	C5-C4-O4	-7.11	119.92	124.90
3	R	1	DT	O4'-C1'-C2'	-7.09	100.23	105.90
2	Q	18	DC	O4'-C1'-N1	7.05	112.93	108.00
2	S	21	DA	O4'-C1'-N9	7.03	112.92	108.00
2	S	24	DC	N1-C2-O2	7.01	123.11	118.90
2	Q	1	DG	N1-C6-O6	7.00	124.10	119.90
3	X	5	DT	C1'-O4'-C4'	-6.99	103.11	110.10
2	Q	3	DT	N1-C2-N3	6.98	118.79	114.60
3	X	2	DG	C5-N7-C8	-6.97	100.81	104.30
3	X	4	DA	C5-N7-C8	-6.97	100.42	103.90
3	X	22	DA	C5-N7-C8	-6.95	100.43	103.90
3	V	15	DC	C4-C5-C6	6.94	120.87	117.40
3	X	4	DA	C2-N3-C4	-6.91	107.14	110.60
2	W	16	DG	O4'-C1'-N9	6.90	112.83	108.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	X	1	DT	O4'-C4'-C3'	-6.90	101.74	104.50
3	X	14	DT	O4'-C4'-C3'	-6.90	101.74	104.50
2	S	22	DT	C5-C6-N1	-6.88	119.57	123.70
2	Q	23	DT	N1-C1'-C2'	6.86	125.64	112.60
2	U	1	DG	C2-N3-C4	-6.86	108.47	111.90
3	V	24	DA	N1-C6-N6	6.85	122.71	118.60
3	R	11	DC	C5-C4-N4	6.83	124.98	120.20
2	U	13	DC	O4'-C1'-N1	6.82	112.78	108.00
2	W	23	DT	N1-C1'-C2'	6.82	125.56	112.60
3	X	3	DA	C5-C6-N1	-6.82	114.29	117.70
2	W	21	DA	N1-C6-N6	6.82	122.69	118.60
2	Q	11	DG	C5-N7-C8	-6.82	100.89	104.30
2	Q	3	DT	C2-N3-C4	-6.81	123.11	127.20
2	W	15	DG	C2-N3-C4	-6.81	108.50	111.90
1	D	58	LEU	CA-CB-CG	6.79	130.93	115.30
3	T	25	DC	O4'-C1'-N1	-6.79	103.24	108.00
2	U	15	DG	O4'-C4'-C3'	-6.79	101.78	104.50
2	U	24	DC	N3-C2-O2	-6.78	117.15	121.90
2	W	22	DT	C4-C5-C6	6.78	122.07	118.00
1	M	98	PRO	C-N-CD	6.77	142.62	128.40
2	U	11	DG	N3-C2-N2	6.77	124.64	119.90
2	Q	21	DA	O4'-C1'-C2'	-6.77	100.49	105.90
2	W	13	DC	C5-C6-N1	-6.76	117.62	121.00
3	X	13	DG	N3-C4-C5	6.75	131.97	128.60
3	R	13	DG	C2-N3-C4	-6.74	108.53	111.90
2	S	3	DT	C1'-O4'-C4'	-6.73	103.37	110.10
3	V	3	DA	O4'-C1'-N9	-6.73	103.29	108.00
2	S	11	DG	N1-C6-O6	6.72	123.93	119.90
2	W	17	DT	N3-C4-O4	6.71	123.92	119.90
2	U	23	DT	C5-C6-N1	-6.70	119.68	123.70
3	R	3	DA	N9-C4-C5	-6.68	103.13	105.80
2	U	15	DG	N9-C4-C5	-6.66	102.74	105.40
3	T	15	DC	C4-C5-C6	6.65	120.72	117.40
3	T	4	DA	C5-N7-C8	-6.64	100.58	103.90
3	X	23	DA	N1-C6-N6	6.61	122.57	118.60
3	X	2	DG	C4-C5-N7	6.60	113.44	110.80
2	S	4	DT	N3-C2-O2	-6.59	118.34	122.30
3	R	17	DT	C5-C4-O4	-6.59	120.29	124.90
2	W	11	DG	N9-C4-C5	-6.55	102.78	105.40
2	W	15	DG	O4'-C1'-C2'	6.52	111.12	105.90
3	T	3	DA	C2-N3-C4	-6.52	107.34	110.60
3	T	3	DA	N1-C6-N6	6.52	122.51	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	R	11	DC	O4'-C1'-C2'	-6.51	100.69	105.90
2	U	2	DT	C6-N1-C1'	-6.51	110.64	120.40
3	V	13	DG	C5-N7-C8	-6.51	101.05	104.30
3	V	25	DC	N1-C2-O2	6.49	122.79	118.90
3	V	22	DA	C5-N7-C8	-6.49	100.66	103.90
2	S	22	DT	N1-C2-N3	6.48	118.49	114.60
3	R	25	DC	N3-C4-N4	-6.48	113.47	118.00
3	R	15	DC	N1-C2-N3	6.46	123.73	119.20
3	R	25	DC	C5-C4-N4	6.45	124.71	120.20
2	S	2	DT	N3-C2-O2	-6.42	118.45	122.30
2	S	23	DT	C5-C6-N1	-6.42	119.85	123.70
1	J	135	ARG	NE-CZ-NH1	6.38	123.49	120.30
2	U	3	DT	N1-C1'-C2'	6.38	124.72	112.60
3	T	1	DT	O4'-C1'-C2'	-6.36	100.81	105.90
2	U	21	DA	N1-C6-N6	6.36	122.42	118.60
2	S	3	DT	O4'-C1'-C2'	-6.36	100.81	105.90
3	X	15	DC	N1-C2-O2	6.35	122.71	118.90
2	U	7	DA	C1'-O4'-C4'	-6.35	103.75	110.10
3	X	17	DT	N3-C4-O4	6.33	123.70	119.90
3	V	2	DG	C6-C5-N7	-6.32	126.61	130.40
3	R	3	DA	C4-C5-N7	6.30	113.85	110.70
2	S	21	DA	C5-C6-N6	-6.29	118.67	123.70
3	X	11	DC	O4'-C1'-C2'	-6.28	100.87	105.90
3	R	11	DC	N3-C4-N4	-6.28	113.60	118.00
2	W	13	DC	C2-N1-C1'	6.28	125.71	118.80
3	X	4	DA	N3-C4-C5	6.27	131.19	126.80
3	X	13	DG	C4-C5-C6	6.26	122.56	118.80
2	W	4	DT	C4-C5-C6	6.26	121.76	118.00
3	V	21	DG	N1-C2-N3	6.26	127.66	123.90
2	W	21	DA	N9-C4-C5	-6.26	103.30	105.80
3	T	4	DA	C2-N3-C4	-6.25	107.47	110.60
2	W	3	DT	C4-C5-C6	6.25	121.75	118.00
3	V	1	DT	O4'-C1'-C2'	-6.25	100.90	105.90
2	S	21	DA	C1'-O4'-C4'	-6.24	103.86	110.10
2	U	14	DT	C5-C4-O4	-6.23	120.54	124.90
1	I	58	LEU	CA-CB-CG	6.23	129.63	115.30
3	R	16	DG	O5'-P-OP2	-6.23	100.09	105.70
3	T	25	DC	O4'-C1'-C2'	-6.23	100.92	105.90
3	V	2	DG	C2-N3-C4	-6.23	108.79	111.90
2	Q	11	DG	N1-C2-N3	-6.22	120.17	123.90
2	S	23	DT	N1-C2-N3	6.20	118.32	114.60
2	S	24	DC	C5-C4-N4	6.20	124.54	120.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	U	13	DC	C5-C6-N1	-6.20	117.90	121.00
2	U	1	DG	C4-C5-N7	6.19	113.28	110.80
2	Q	23	DT	N1-C2-N3	6.18	118.31	114.60
3	T	2	DG	N3-C4-C5	6.18	131.69	128.60
3	V	16	DG	O4'-C1'-N9	6.15	112.31	108.00
2	Q	18	DC	C1'-O4'-C4'	-6.14	103.96	110.10
3	X	3	DA	C4-C5-N7	6.13	113.77	110.70
3	T	2	DG	C5-N7-C8	-6.13	101.24	104.30
2	Q	7	DA	C1'-O4'-C4'	-6.11	103.99	110.10
2	W	21	DA	N1-C2-N3	-6.11	126.24	129.30
3	V	6	DT	O4'-C1'-C2'	-6.11	101.01	105.90
2	S	11	DG	N3-C4-C5	6.09	131.65	128.60
2	U	21	DA	N1-C2-N3	-6.09	126.25	129.30
3	T	22	DA	C5-N7-C8	-6.09	100.86	103.90
2	U	14	DT	O4'-C1'-N1	-6.09	103.74	108.00
2	U	25	DA	C5-C6-N6	-6.09	118.83	123.70
3	T	22	DA	C2-N3-C4	-6.09	107.56	110.60
1	L	58	LEU	CA-CB-CG	6.08	129.29	115.30
2	W	23	DT	C4-C5-C6	6.08	121.65	118.00
2	U	1	DG	C5-C6-O6	-6.08	124.95	128.60
2	U	11	DG	C8-N9-C4	6.08	108.83	106.40
3	R	14	DT	O4'-C4'-C3'	-6.07	102.07	104.50
2	Q	11	DG	C8-N9-C4	6.07	108.83	106.40
3	T	22	DA	C4-C5-N7	6.07	113.73	110.70
3	R	2	DG	C2-N3-C4	-6.07	108.87	111.90
2	Q	24	DC	N3-C4-N4	-6.04	113.77	118.00
3	V	22	DA	C2-N3-C4	-6.03	107.59	110.60
3	R	1	DT	O4'-C4'-C3'	6.01	109.61	106.00
3	T	3	DA	C4-C5-N7	6.00	113.70	110.70
3	X	15	DC	N1-C2-N3	6.00	123.40	119.20
2	S	21	DA	C8-N9-C4	5.99	108.19	105.80
3	X	24	DA	O4'-C1'-N9	5.98	112.19	108.00
2	Q	4	DT	N1-C1'-C2'	5.97	123.95	112.60
3	T	15	DC	C5-C6-N1	-5.97	118.02	121.00
2	U	2	DT	C2-N1-C1'	5.95	127.72	118.20
2	U	11	DG	N3-C4-C5	5.94	131.57	128.60
2	U	23	DT	N1-C1'-C2'	5.92	123.85	112.60
2	S	7	DA	P-O5'-C5'	-5.91	111.44	120.90
2	U	16	DG	O4'-C1'-N9	5.91	112.14	108.00
2	U	25	DA	C6-C5-N7	-5.89	128.18	132.30
3	T	4	DA	N3-C4-C5	5.89	130.92	126.80
2	S	11	DG	C2-N3-C4	-5.88	108.96	111.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	U	1	DG	C5-N7-C8	-5.87	101.36	104.30
2	U	5	DC	C5-C6-N1	5.87	123.94	121.00
3	R	23	DA	C5-N7-C8	-5.87	100.97	103.90
3	X	1	DT	C6-N1-C2	5.86	124.23	121.30
3	V	1	DT	C6-N1-C1'	-5.86	111.61	120.40
2	Q	12	DA	O4'-C1'-N9	5.86	112.10	108.00
2	S	25	DA	C2-N3-C4	-5.84	107.68	110.60
2	S	22	DT	P-O5'-C5'	-5.84	111.55	120.90
3	V	25	DC	O4'-C1'-N1	5.84	112.09	108.00
2	W	3	DT	N1-C2-N3	5.84	118.11	114.60
3	X	2	DG	C5-C6-N1	-5.84	108.58	111.50
3	X	13	DG	C5-C6-N1	-5.84	108.58	111.50
2	S	10	DC	C6-N1-C2	5.83	122.63	120.30
2	U	25	DA	C5-N7-C8	-5.83	100.98	103.90
2	S	6	DT	O4'-C1'-N1	-5.83	103.92	108.00
3	V	15	DC	C5-C6-N1	-5.83	118.09	121.00
2	Q	15	DG	C4-C5-C6	5.82	122.29	118.80
3	V	1	DT	C5-C4-O4	-5.82	120.83	124.90
3	R	3	DA	C6-C5-N7	-5.81	128.23	132.30
3	V	11	DC	O4'-C1'-N1	5.81	112.07	108.00
2	W	3	DT	O4'-C1'-C2'	-5.81	101.25	105.90
2	U	11	DG	C2-N3-C4	-5.81	109.00	111.90
3	T	13	DG	N1-C2-N3	-5.80	120.42	123.90
3	X	11	DC	C4-C5-C6	5.80	120.30	117.40
3	T	24	DA	N1-C2-N3	-5.80	126.40	129.30
2	U	15	DG	C4-C5-C6	5.80	122.28	118.80
2	Q	1	DG	C5-C6-O6	-5.79	125.12	128.60
3	V	25	DC	N3-C4-N4	-5.78	113.95	118.00
2	W	5	DC	C5-C6-N1	5.78	123.89	121.00
2	W	13	DC	C6-N1-C1'	-5.78	113.87	120.80
2	U	3	DT	C4-C5-C6	5.78	121.47	118.00
2	W	4	DT	C5-C6-N1	-5.76	120.25	123.70
2	W	5	DC	C4-C5-C6	-5.75	114.53	117.40
3	X	14	DT	N3-C4-O4	5.73	123.34	119.90
2	S	19	DT	C6-C5-C7	-5.73	119.46	122.90
3	T	18	DC	O4'-C1'-N1	-5.72	104.00	108.00
2	U	19	DT	C5-C4-O4	-5.72	120.89	124.90
2	Q	22	DT	C2-N3-C4	-5.72	123.77	127.20
1	K	102	GLU	N-CA-C	-5.71	95.58	111.00
3	V	17	DT	N3-C4-O4	5.70	123.32	119.90
2	W	10	DC	C1'-O4'-C4'	-5.69	104.41	110.10
3	R	11	DC	O4'-C1'-N1	5.68	111.98	108.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Q	13	DC	C2-N3-C4	-5.68	117.06	119.90
3	V	21	DG	N9-C4-C5	5.68	107.67	105.40
2	Q	13	DC	C1'-O4'-C4'	-5.68	104.42	110.10
2	W	13	DC	C5-C4-N4	5.68	124.18	120.20
2	W	3	DT	O4'-C4'-C3'	-5.68	102.23	104.50
3	T	2	DG	C4-C5-N7	5.68	113.07	110.80
2	Q	3	DT	C5-C6-N1	-5.67	120.30	123.70
3	T	19	DT	N3-C4-O4	5.65	123.29	119.90
2	S	19	DT	C4-C5-C7	5.65	122.39	119.00
3	T	24	DA	C4'-C3'-C2'	-5.65	98.01	103.10
1	M	97	CYS	N-CA-C	-5.64	95.77	111.00
2	Q	1	DG	C6-C5-N7	-5.64	127.02	130.40
2	S	24	DC	N1-C1'-C2'	5.64	123.31	112.60
3	T	4	DA	C4-C5-N7	5.63	113.52	110.70
2	U	22	DT	N1-C1'-C2'	5.63	123.29	112.60
3	X	15	DC	C2-N3-C4	-5.62	117.09	119.90
2	Q	17	DT	C6-C5-C7	-5.61	119.53	122.90
3	V	8	DG	C1'-O4'-C4'	-5.61	104.49	110.10
2	U	10	DC	C1'-O4'-C4'	-5.60	104.50	110.10
3	X	13	DG	O4'-C1'-C2'	5.60	110.38	105.90
3	R	14	DT	N3-C4-O4	5.60	123.26	119.90
2	U	21	DA	O4'-C1'-C2'	-5.60	101.42	105.90
1	I	34	LEU	CA-CB-CG	5.60	128.18	115.30
3	R	17	DT	N3-C4-O4	5.60	123.26	119.90
2	W	12	DA	O4'-C1'-N9	5.59	111.91	108.00
2	Q	3	DT	N1-C1'-C2'	5.57	123.19	112.60
2	U	21	DA	C1'-O4'-C4'	-5.57	104.53	110.10
3	T	22	DA	C5-C6-N6	-5.56	119.25	123.70
2	S	23	DT	N1-C1'-C2'	5.56	123.17	112.60
3	X	5	DT	C5-C6-N1	-5.56	120.37	123.70
2	Q	13	DC	O4'-C1'-C2'	-5.55	101.46	105.90
2	W	21	DA	C1'-O4'-C4'	-5.55	104.55	110.10
2	Q	3	DT	C4'-C3'-C2'	-5.55	98.11	103.10
3	X	10	DC	C1'-O4'-C4'	-5.53	104.57	110.10
1	I	173	LYS	CD-CE-NZ	-5.53	98.98	111.70
2	Q	3	DT	C4-C5-C6	5.53	121.32	118.00
1	P	58	LEU	CA-CB-CG	5.53	128.01	115.30
2	Q	1	DG	O4'-C1'-N9	-5.53	104.13	108.00
3	V	15	DC	C5-C4-N4	5.52	124.06	120.20
2	Q	23	DT	N1-C2-O2	5.51	127.51	123.10
2	W	14	DT	C6-C5-C7	-5.51	119.59	122.90
2	U	24	DC	C4-C5-C6	5.50	120.15	117.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	101	ASP	CB-CG-OD2	-5.50	113.35	118.30
2	S	3	DT	C4-C5-C6	5.50	121.30	118.00
3	R	4	DA	C8-N9-C4	5.49	108.00	105.80
2	U	2	DT	O4'-C1'-N1	5.49	111.85	108.00
1	B	135	ARG	NE-CZ-NH2	-5.48	117.56	120.30
3	X	7	DA	O4'-C1'-N9	-5.48	104.17	108.00
3	V	3	DA	C6-C5-N7	-5.48	128.47	132.30
1	D	97	CYS	CA-CB-SG	5.47	123.86	114.00
2	S	5	DC	C4'-C3'-C2'	5.47	108.03	103.10
3	X	18	DC	O4'-C1'-N1	-5.47	104.17	108.00
3	X	21	DG	O4'-C1'-N9	-5.47	104.17	108.00
2	Q	5	DC	C4-C5-C6	-5.46	114.67	117.40
2	W	2	DT	N3-C2-O2	-5.46	119.02	122.30
3	X	13	DG	C8-N9-C4	5.46	108.59	106.40
2	W	3	DT	C5-C6-N1	-5.46	120.42	123.70
1	I	121	MET	CG-SD-CE	-5.46	91.47	100.20
2	S	23	DT	C4-C5-C6	5.45	121.27	118.00
2	S	7	DA	O5'-P-OP1	-5.45	100.80	105.70
3	R	21	DG	P-O5'-C5'	-5.45	112.19	120.90
2	S	21	DA	C4-C5-N7	5.45	113.42	110.70
2	Q	23	DT	O4'-C1'-C2'	-5.44	101.55	105.90
3	X	15	DC	C6-N1-C2	-5.44	118.12	120.30
3	X	24	DA	C4'-C3'-C2'	-5.44	98.21	103.10
3	R	11	DC	C5-C6-N1	-5.43	118.28	121.00
3	V	25	DC	C5-C4-N4	5.43	124.00	120.20
2	U	22	DT	O4'-C1'-C2'	-5.42	101.56	105.90
3	T	13	DG	N3-C4-C5	5.42	131.31	128.60
2	S	24	DC	C2-N3-C4	-5.42	117.19	119.90
3	R	22	DA	C5-N7-C8	-5.40	101.20	103.90
3	X	4	DA	C4-C5-N7	5.40	113.40	110.70
3	T	19	DT	C5-C4-O4	-5.40	121.12	124.90
2	S	3	DT	N1-C2-N3	5.40	117.84	114.60
3	T	11	DC	C4-C5-C6	5.40	120.10	117.40
2	W	23	DT	N1-C2-O2	5.40	127.42	123.10
2	W	25	DA	N1-C6-N6	5.40	121.84	118.60
3	X	2	DG	N7-C8-N9	5.39	115.80	113.10
3	V	1	DT	C2-N1-C1'	5.39	126.82	118.20
3	X	11	DC	C5-C6-N1	-5.39	118.31	121.00
2	S	5	DC	C6-N1-C2	-5.39	118.14	120.30
3	V	3	DA	C5-N7-C8	-5.38	101.21	103.90
2	Q	1	DG	O5'-P-OP1	5.37	117.14	110.70
2	S	15	DG	N3-C4-C5	5.37	131.28	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	T	3	DA	C6-N1-C2	5.36	121.82	118.60
2	Q	11	DG	N3-C4-N9	5.35	129.21	126.00
3	X	14	DT	C5-C4-O4	-5.35	121.15	124.90
1	N	99	PRO	N-CA-C	5.35	126.01	112.10
2	Q	16	DG	O4'-C1'-N9	5.35	111.75	108.00
1	P	144	ARG	NE-CZ-NH1	5.35	122.97	120.30
2	U	11	DG	O4'-C1'-C2'	5.34	110.18	105.90
3	T	11	DC	C6-N1-C2	-5.34	118.16	120.30
2	W	24	DC	N3-C4-N4	-5.34	114.27	118.00
2	S	21	DA	C3'-C2'-C1'	-5.33	96.11	102.50
1	B	98	PRO	N-CA-C	5.33	125.95	112.10
3	V	15	DC	N1-C2-N3	5.33	122.93	119.20
2	Q	11	DG	O4'-C1'-C2'	5.32	110.16	105.90
3	V	3	DA	N3-C4-C5	5.31	130.52	126.80
3	T	13	DG	O4'-C1'-N9	-5.31	104.28	108.00
3	T	24	DA	C5-C6-N6	-5.31	119.45	123.70
3	T	25	DC	C5-C6-N1	-5.30	118.35	121.00
3	X	1	DT	C1'-O4'-C4'	-5.30	104.80	110.10
3	V	3	DA	C6-N1-C2	5.30	121.78	118.60
3	T	1	DT	C6-N1-C1'	-5.29	112.47	120.40
1	I	126	ARG	NE-CZ-NH1	-5.29	117.66	120.30
3	T	23	DA	N1-C6-N6	5.29	121.77	118.60
3	X	21	DG	N1-C2-N2	-5.27	111.45	116.20
2	Q	25	DA	N1-C6-N6	5.27	121.76	118.60
3	T	12	DA	O4'-C1'-N9	5.27	111.69	108.00
3	R	3	DA	C5-N7-C8	-5.27	101.27	103.90
3	T	17	DT	C5-C4-O4	-5.26	121.22	124.90
3	V	22	DA	C4-C5-N7	5.26	113.33	110.70
2	W	3	DT	C2-N3-C4	-5.26	124.04	127.20
3	V	11	DC	N1-C1'-C2'	5.26	122.59	112.60
3	V	10	DC	N1-C1'-C2'	5.26	122.59	112.60
1	A	58	LEU	CA-CB-CG	5.25	127.36	115.30
3	T	3	DA	N3-C4-N9	-5.23	123.22	127.40
3	R	22	DA	N3-C4-C5	5.22	130.46	126.80
3	X	17	DT	C5-C4-O4	-5.22	121.25	124.90
3	R	10	DC	O4'-C1'-N1	-5.22	104.35	108.00
2	U	15	DG	N3-C4-C5	5.21	131.21	128.60
2	S	22	DT	C4-C5-C6	5.21	121.12	118.00
3	T	13	DG	N9-C4-C5	-5.20	103.32	105.40
2	Q	21	DA	C1'-O4'-C4'	-5.20	104.91	110.10
2	S	5	DC	C5'-C4'-C3'	-5.20	104.75	114.10
2	Q	5	DC	N3-C4-C5	5.19	123.98	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	U	17	DT	C5-C4-O4	-5.19	121.27	124.90
3	T	24	DA	N1-C6-N6	5.18	121.71	118.60
3	X	5	DT	O4'-C4'-C3'	-5.18	102.43	104.50
3	V	23	DA	C5-C6-N6	-5.18	119.56	123.70
3	V	11	DC	C5-C4-N4	5.17	123.82	120.20
2	W	14	DT	N3-C4-O4	5.17	123.00	119.90
3	V	3	DA	C4-C5-N7	5.16	113.28	110.70
3	V	17	DT	C5-C4-O4	-5.16	121.28	124.90
2	Q	5	DC	C2-N1-C1'	-5.16	113.12	118.80
3	R	4	DA	C4-C5-N7	5.16	113.28	110.70
2	Q	21	DA	N1-C2-N3	-5.15	126.72	129.30
2	U	22	DT	C6-N1-C2	-5.15	118.72	121.30
2	S	8	DG	N1-C6-O6	-5.15	116.81	119.90
1	H	98	PRO	C-N-CD	5.14	139.20	128.40
2	S	20	DA	O4'-C1'-N9	-5.14	104.40	108.00
1	J	191	LEU	CA-CB-CG	5.14	127.12	115.30
3	T	8	DG	C1'-O4'-C4'	-5.14	104.96	110.10
2	Q	14	DT	C5-C4-O4	-5.13	121.31	124.90
3	X	11	DC	C5-C4-N4	5.13	123.79	120.20
3	R	4	DA	O4'-C1'-C2'	5.13	110.00	105.90
3	R	6	DT	O4'-C1'-C2'	-5.13	101.80	105.90
2	U	22	DT	C5-C6-N1	-5.12	120.62	123.70
3	V	18	DC	O4'-C1'-N1	-5.12	104.41	108.00
3	R	1	DT	C4'-C3'-C2'	-5.12	98.49	103.10
2	U	22	DT	N3-C4-O4	5.11	122.97	119.90
3	V	13	DG	N9-C1'-C2'	-5.11	102.88	112.60
2	U	24	DC	C5-C6-N1	-5.11	118.45	121.00
2	Q	15	DG	N3-C4-C5	5.10	131.15	128.60
1	L	28	VAL	CB-CA-C	-5.09	101.73	111.40
3	T	13	DG	O4'-C1'-C2'	5.08	109.96	105.90
2	S	13	DC	C1'-O4'-C4'	-5.08	105.02	110.10
2	W	21	DA	C5-C6-N6	-5.08	119.64	123.70
2	S	21	DA	C6-N1-C2	5.07	121.64	118.60
3	X	14	DT	OP1-P-OP2	5.07	127.20	119.60
3	R	21	DG	N1-C2-N3	5.06	126.94	123.90
1	E	98	PRO	C-N-CD	5.06	139.02	128.40
2	Q	1	DG	P-O5'-C5'	5.06	128.99	120.90
1	J	58	LEU	CA-CB-CG	5.06	126.93	115.30
3	X	15	DC	O4'-C1'-N1	5.06	111.54	108.00
2	Q	22	DT	N1-C1'-C2'	5.05	122.20	112.60
3	T	2	DG	N7-C8-N9	5.05	115.63	113.10
2	Q	5	DC	N3-C4-N4	-5.05	114.47	118.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	V	7	DA	O4'-C1'-C2'	-5.05	101.86	105.90
2	W	10	DC	C6-N1-C2	5.05	122.32	120.30
2	S	3	DT	N1-C2-O2	5.04	127.13	123.10
1	K	95	ASN	CB-CA-C	5.04	120.47	110.40
2	Q	17	DT	C4-C5-C7	5.03	122.02	119.00
3	R	24	DA	C3'-C2'-C1'	-5.03	96.46	102.50
2	U	11	DG	C4-C5-C6	5.03	121.82	118.80
2	S	22	DT	C5'-C4'-C3'	-5.02	105.06	114.10
3	V	23	DA	C4-C5-N7	5.02	113.21	110.70
2	U	7	DA	O4'-C1'-N9	-5.02	104.49	108.00
2	Q	1	DG	C2-N3-C4	-5.02	109.39	111.90
2	U	4	DT	N3-C4-O4	5.01	122.91	119.90
1	N	98	PRO	N-CA-C	5.01	125.12	112.10
3	R	15	DC	OP2-P-O3'	5.00	116.21	105.20
3	T	11	DC	N1-C2-N3	5.00	122.70	119.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	97	CYS	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1491	0	1461	39	0
1	B	1465	0	1443	26	0
1	C	1491	0	1461	29	0
1	D	1465	0	1443	30	0
1	E	1491	0	1461	39	0
1	F	1465	0	1443	39	0
1	G	1465	0	1443	32	0
1	H	1491	0	1461	38	0
1	I	1491	0	1461	30	0
1	J	1465	0	1443	25	2
1	K	1491	0	1461	20	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	1465	0	1443	36	0
1	M	1491	0	1461	33	0
1	N	1465	0	1443	35	0
1	O	1491	0	1461	36	0
1	P	1465	0	1443	34	0
2	Q	505	0	267	29	0
2	S	505	0	267	30	0
2	U	505	0	267	32	0
2	W	505	0	267	27	0
3	R	511	0	273	30	0
3	T	511	0	273	31	0
3	V	511	0	273	36	0
3	X	511	0	273	34	0
4	A	19	0	0	2	2
4	B	31	0	0	4	0
4	C	5	0	0	0	0
4	D	3	0	0	1	0
4	E	12	0	0	4	0
4	F	5	0	0	2	0
4	G	24	0	0	0	0
4	H	13	0	0	8	0
4	I	4	0	0	0	0
4	J	1	0	0	0	0
4	K	15	0	0	3	0
4	L	19	0	0	5	0
4	M	8	0	0	1	0
4	N	4	0	0	0	0
4	Q	3	0	0	0	0
4	R	2	0	0	0	0
4	S	13	0	0	0	0
4	T	7	0	0	0	0
4	U	12	0	0	0	0
4	V	9	0	0	0	0
All	All	27921	0	25392	625	2

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 12.

All (625) 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)
2:U:24:DC:N3	3:V:2:DG:N2	2.03	1.07
2:Q:1:DG:N2	3:R:25:DC:N3	2.03	1.06
1:P:100:CYS:SG	1:P:104:ARG:NH2	2.31	1.03
2:U:1:DG:N2	3:V:25:DC:N3	2.06	1.01
1:C:98:PRO:HB3	1:C:178:PRO:HD3	1.40	0.99
2:U:15:DG:H1	3:V:11:DC:H42	1.09	0.99
2:U:1:DG:H1	3:V:25:DC:H42	1.03	0.98
1:F:103:GLN:HG3	1:F:105:CYS:H	1.29	0.97
2:Q:11:DG:H1	3:R:15:DC:H42	1.11	0.97
2:U:24:DC:H42	3:V:2:DG:H1	1.05	0.94
2:Q:24:DC:N3	3:R:2:DG:N2	2.14	0.94
2:S:11:DG:H1	3:T:15:DC:H42	1.14	0.94
2:Q:15:DG:H1	3:R:11:DC:H42	1.14	0.93
2:S:24:DC:H42	3:T:2:DG:H1	0.94	0.93
1:I:103:GLN:HE21	1:I:105:CYS:H	1.09	0.93
2:U:2:DT:N3	3:V:24:DA:N1	2.17	0.92
1:A:105:CYS:SG	4:A:218:HOH:O	2.28	0.92
2:S:24:DC:N3	3:T:2:DG:N2	2.18	0.91
2:Q:24:DC:H42	3:R:2:DG:H1	1.03	0.91
2:U:15:DG:N2	3:V:11:DC:N3	2.18	0.91
2:S:1:DG:H1	3:T:25:DC:H42	1.15	0.90
2:W:24:DC:H42	3:X:2:DG:H1	1.11	0.90
1:P:42:GLY:HA3	3:X:11:DC:H41	1.36	0.90
1:N:22:VAL:HG13	1:N:101:ASP:HB3	1.54	0.90
2:U:11:DG:H1	3:V:15:DC:H42	1.19	0.89
1:I:103:GLN:OE1	1:I:173:LYS:NZ	2.07	0.88
1:O:100:CYS:SG	1:O:104:ARG:NH2	2.47	0.88
2:W:13:DC:H42	3:X:13:DG:H1	1.17	0.88
1:H:70:MET:HE1	1:H:132:ILE:HA	1.56	0.87
1:G:42:GLY:HA3	3:T:11:DC:H41	1.38	0.87
1:L:70:MET:HE1	1:L:132:ILE:HA	1.54	0.87
1:D:70:MET:HE1	1:D:132:ILE:HA	1.58	0.85
2:W:13:DC:N3	3:X:13:DG:N2	2.25	0.85
1:I:70:MET:HE1	1:I:132:ILE:HA	1.58	0.84
1:C:100:CYS:SG	1:C:104:ARG:NH2	2.51	0.84
1:D:41:LYS:HE2	2:Q:13:DC:H5	1.42	0.84
1:H:119:GLU:OE2	1:H:122:ARG:NH1	2.10	0.83
2:U:13:DC:O2	3:V:13:DG:N2	2.11	0.83
1:D:42:GLY:HA3	3:R:11:DC:H41	1.45	0.81
1:G:119:GLU:OE2	1:G:122:ARG:NH1	2.12	0.81
1:F:61:ASP:OD1	1:F:64:ARG:NH2	2.13	0.81
1:F:15:THR:HG21	1:F:37:ALA:HB2	1.61	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:13:DC:O2	3:T:13:DG:N2	2.14	0.80
1:E:59:LEU:HD12	4:E:209:HOH:O	1.82	0.80
1:J:70:MET:HE1	1:J:132:ILE:HA	1.62	0.80
2:U:15:DG:H1	3:V:11:DC:N4	1.78	0.80
2:Q:15:DG:N2	3:R:11:DC:N3	2.30	0.79
1:D:100:CYS:SG	1:D:104:ARG:NH2	2.57	0.78
3:X:1:DT:H2'	3:X:2:DG:C8	2.19	0.78
1:A:103:GLN:OE1	1:A:173:LYS:HD2	1.85	0.77
1:E:103:GLN:HG2	1:E:109:LYS:HB2	1.67	0.77
1:L:41:LYS:HD3	2:U:13:DC:H41	1.50	0.77
2:U:15:DG:N2	3:V:11:DC:O2	2.17	0.77
1:G:103:GLN:HE21	1:G:105:CYS:H	1.33	0.77
1:M:4:SER:HA	1:M:7:ASP:HB2	1.66	0.77
1:E:103:GLN:HE22	1:E:173:LYS:HD2	1.51	0.76
2:Q:13:DC:H42	3:R:13:DG:H1	1.35	0.75
2:S:15:DG:H1	3:T:11:DC:H42	1.33	0.75
1:J:103:GLN:HE21	1:J:105:CYS:H	1.35	0.74
2:Q:11:DG:N2	3:R:15:DC:N3	2.35	0.74
1:F:143:GLY:HA3	1:F:149:LEU:HD12	1.70	0.73
1:O:34:LEU:HD21	1:O:44:PHE:HB2	1.70	0.72
1:P:146:ASP:OD1	1:P:148:SER:HB2	1.88	0.72
1:L:105:CYS:SG	4:L:214:HOH:O	2.47	0.72
1:B:100:CYS:HB3	1:B:104:ARG:HH22	1.54	0.72
1:P:41:LYS:HE2	2:W:13:DC:H5	1.53	0.72
2:W:24:DC:N3	3:X:2:DG:N2	2.30	0.72
1:M:22:VAL:HG22	1:M:102:GLU:HA	1.70	0.72
1:E:103:GLN:NE2	1:E:173:LYS:HD2	2.05	0.71
1:B:97:CYS:HB2	4:B:224:HOH:O	1.90	0.71
2:W:11:DG:H1	3:X:15:DC:H42	1.37	0.71
2:S:13:DC:H42	3:T:13:DG:H1	1.38	0.70
1:I:84:ARG:NH1	1:I:142:GLN:OE1	2.24	0.70
2:S:5:DC:H2"	2:S:6:DT:H5'	1.73	0.70
1:K:150:ALA:O	4:K:206:HOH:O	2.09	0.69
2:Q:15:DG:H1	3:R:11:DC:N4	1.87	0.69
2:U:11:DG:N2	3:V:15:DC:N3	2.39	0.69
2:S:11:DG:H1	3:T:15:DC:N4	1.88	0.69
1:M:146:ASP:OD1	1:M:148:SER:OG	2.09	0.69
1:I:103:GLN:HE21	1:I:105:CYS:N	1.88	0.69
2:Q:11:DG:H1	3:R:15:DC:N4	1.88	0.69
1:K:134:GLU:OE1	1:K:155:ARG:NH2	2.26	0.69
1:L:42:GLY:HA3	3:V:11:DC:H41	1.56	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:2:DT:O4	3:R:24:DA:N6	2.17	0.69
2:Q:4:DT:H3	3:R:22:DA:H2	1.39	0.68
1:N:146:ASP:OD1	1:N:148:SER:OG	2.11	0.68
3:R:1:DT:H2"	3:R:2:DG:C8	2.28	0.68
2:S:13:DC:N3	3:T:13:DG:N2	2.40	0.68
1:G:149:LEU:HD22	1:G:192:LEU:HD22	1.76	0.68
1:F:105:CYS:SG	1:F:108:VAL:HG23	2.33	0.68
1:H:193:GLU:OE2	4:H:211:HOH:O	2.12	0.68
1:M:176:ARG:NH2	1:N:119:GLU:OE2	2.27	0.68
1:G:103:GLN:OE1	1:G:173:LYS:NZ	2.23	0.68
2:S:1:DG:H1	3:T:25:DC:N4	1.91	0.68
2:S:1:DG:N2	3:T:25:DC:N3	2.32	0.67
1:G:41:LYS:HZ2	2:S:13:DC:H5	1.41	0.67
2:S:3:DT:H2"	2:S:4:DT:H5'	1.76	0.67
2:S:11:DG:N2	3:T:15:DC:N3	2.38	0.67
1:K:97:CYS:SG	1:K:99:PRO:HD2	2.35	0.67
1:M:97:CYS:O	1:M:99:PRO:HD2	1.94	0.66
1:O:103:GLN:HG3	1:O:105:CYS:H	1.61	0.66
1:A:103:GLN:HE21	1:A:105:CYS:H	1.42	0.66
1:E:144:ARG:NH1	1:E:152:CYS:O	2.28	0.66
1:E:119:GLU:O	1:E:123:ILE:HG12	1.97	0.65
1:F:23:LYS:HB2	1:F:28:VAL:HG13	1.77	0.65
1:I:159:SER:O	1:I:163:GLN:HG3	1.96	0.65
1:P:70:MET:HE2	1:P:132:ILE:HG12	1.79	0.65
1:K:119:GLU:OE2	1:K:122:ARG:NH1	2.29	0.65
3:V:1:DT:H2"	3:V:2:DG:C8	2.31	0.65
1:C:146:ASP:OD1	1:C:148:SER:OG	2.11	0.65
1:L:103:GLN:HG2	1:L:173:LYS:NZ	2.12	0.65
1:F:69:ASP:OD2	1:F:73:ARG:NH1	2.27	0.64
1:O:134:GLU:OE1	1:O:155:ARG:NH2	2.31	0.64
1:I:4:SER:HA	1:I:7:ASP:HB2	1.80	0.64
1:D:192:LEU:O	1:D:193:GLU:HG2	1.98	0.64
1:K:70:MET:HE1	1:K:132:ILE:HA	1.78	0.64
1:E:4:SER:HA	1:E:7:ASP:HB2	1.79	0.64
1:H:150:ALA:O	4:H:213:HOH:O	2.14	0.64
1:A:146:ASP:OD1	1:A:148:SER:OG	2.15	0.64
1:F:103:GLN:HG3	1:F:105:CYS:N	2.08	0.63
1:P:70:MET:HE1	1:P:132:ILE:HA	1.79	0.63
1:L:42:GLY:H	3:V:11:DC:H5	1.46	0.63
1:C:42:GLY:HA3	2:Q:4:DT:C5	2.33	0.63
1:M:70:MET:HE1	1:M:132:ILE:HG12	1.79	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:70:MET:HE1	1:E:132:ILE:HG12	1.79	0.63
1:E:163:GLN:OE1	1:F:168:ALA:HB2	1.99	0.62
1:G:70:MET:HE1	1:G:132:ILE:HG12	1.79	0.62
1:L:41:LYS:HD3	2:U:13:DC:N4	2.13	0.62
1:J:100:CYS:SG	1:J:102:GLU:HG2	2.39	0.62
1:E:70:MET:HE3	1:E:132:ILE:HA	1.81	0.62
2:Q:18:DC:H2"	2:Q:19:DT:H72	1.82	0.62
1:F:136:LEU:O	1:F:140:LEU:HD12	2.00	0.62
1:A:70:MET:HE1	1:A:132:ILE:HG12	1.80	0.62
2:W:11:DG:H1	3:X:15:DC:N4	1.97	0.62
1:A:70:MET:CE	1:A:132:ILE:HA	2.30	0.61
1:F:72:GLN:NE2	4:F:201:HOH:O	2.32	0.61
2:W:13:DC:N4	3:X:13:DG:H1	1.95	0.61
2:U:11:DG:H1	3:V:15:DC:N4	1.93	0.61
1:A:84:ARG:NH1	1:A:142:GLN:OE1	2.33	0.61
1:M:119:GLU:OE1	1:N:176:ARG:NH2	2.29	0.61
1:G:97:CYS:C	1:G:99:PRO:HD2	2.22	0.60
1:N:103:GLN:HG3	1:N:105:CYS:H	1.65	0.60
2:W:11:DG:N2	3:X:15:DC:N3	2.48	0.60
1:F:59:LEU:HD13	1:F:125:LEU:HD13	1.82	0.60
1:B:70:MET:HE2	1:B:132:ILE:HG12	1.83	0.60
2:Q:24:DC:N4	3:R:2:DG:H1	1.87	0.60
1:D:91:LYS:HE3	1:D:95:ASN:HD22	1.66	0.60
1:M:84:ARG:HH12	1:M:142:GLN:HE22	1.50	0.60
1:H:45:TYR:HB2	4:H:203:HOH:O	2.02	0.59
1:N:80:ASN:HD22	1:N:148:SER:HB3	1.67	0.59
1:G:42:GLY:H	3:T:11:DC:H5	1.51	0.59
2:S:15:DG:N2	3:T:11:DC:N3	2.51	0.59
1:E:22:VAL:HG22	1:E:102:GLU:HA	1.84	0.59
2:S:13:DC:N4	3:T:13:DG:H1	2.00	0.59
2:Q:15:DG:N2	3:R:11:DC:C2	2.71	0.59
1:D:42:GLY:H	3:R:11:DC:H5	1.49	0.59
1:B:70:MET:HE1	1:B:132:ILE:HA	1.83	0.59
1:O:156:HIS:NE2	1:P:186:GLN:HG2	2.17	0.59
1:D:41:LYS:HE2	2:Q:13:DC:C5	2.31	0.59
1:E:62:TYR:CG	1:E:106:LEU:HD12	2.37	0.59
1:H:140:LEU:HD12	1:H:149:LEU:HD13	1.83	0.59
1:J:97:CYS:C	1:J:99:PRO:HD2	2.23	0.59
2:W:15:DG:H1	3:X:11:DC:H42	1.51	0.59
1:E:73:ARG:HD3	1:E:88:TYR:HB2	1.86	0.58
1:J:91:LYS:HE3	1:J:95:ASN:HD22	1.69	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:103:GLN:HE21	1:P:173:LYS:NZ	2.01	0.58
2:U:23:DT:H3	3:V:3:DA:H2	1.49	0.58
1:A:103:GLN:N	4:B:210:HOH:O	2.35	0.58
1:B:70:MET:CE	1:B:132:ILE:HA	2.33	0.58
1:C:98:PRO:CB	1:C:178:PRO:HD3	2.26	0.58
3:V:13:DG:H2"	3:V:14:DT:H5'	1.86	0.58
1:A:70:MET:HE3	1:A:132:ILE:HA	1.86	0.58
1:H:100:CYS:SG	1:H:104:ARG:NH2	2.76	0.58
2:W:15:DG:N2	3:X:11:DC:N3	2.52	0.58
1:F:70:MET:HE1	1:F:132:ILE:HA	1.85	0.57
1:E:82:ARG:HB2	1:E:148:SER:HB3	1.85	0.57
1:N:98:PRO:N	1:N:99:PRO:HD2	2.19	0.57
1:O:42:GLY:HA3	2:W:4:DT:C5	2.39	0.57
1:L:9:ARG:HD2	4:L:202:HOH:O	2.03	0.57
1:M:70:MET:HE3	1:M:132:ILE:HA	1.86	0.57
1:P:42:GLY:CA	3:X:11:DC:H41	2.14	0.57
1:H:79:LEU:HD22	1:H:83:GLU:HB3	1.87	0.57
1:D:119:GLU:OE2	1:D:122:ARG:NH1	2.38	0.57
1:G:41:LYS:NZ	2:S:13:DC:H5	2.02	0.57
2:U:15:DG:N2	3:V:11:DC:C2	2.64	0.57
1:G:49:LYS:HG2	1:G:53:GLN:OE1	2.04	0.57
1:C:80:ASN:HD22	1:C:148:SER:HB3	1.70	0.57
1:E:95:ASN:ND2	1:E:104:ARG:HD2	2.20	0.56
1:F:89:TRP:CZ2	1:F:136:LEU:HD11	2.40	0.56
1:O:17:TYR:HB2	1:O:58:LEU:HD21	1.87	0.56
1:N:70:MET:HE2	1:N:132:ILE:HG12	1.87	0.56
1:N:99:PRO:HB3	1:N:176:ARG:O	2.05	0.56
2:U:13:DC:H42	3:V:13:DG:H1	1.52	0.56
1:N:70:MET:HE1	1:N:132:ILE:HA	1.87	0.56
1:A:22:VAL:HG22	1:A:102:GLU:HA	1.87	0.56
1:H:97:CYS:HB3	1:H:99:PRO:HD2	1.88	0.56
1:O:96:ALA:HB2	1:O:103:GLN:HE22	1.71	0.56
1:A:119:GLU:O	1:A:123:ILE:HG12	2.05	0.56
1:J:41:LYS:HE2	3:V:16:DG:N7	2.20	0.56
1:F:49:LYS:HG2	1:F:53:GLN:NE2	2.20	0.56
1:H:162:TYR:HA	4:H:207:HOH:O	2.05	0.56
1:H:45:TYR:OH	3:T:19:DT:H2"	2.05	0.56
1:J:82:ARG:HB2	1:J:148:SER:HB3	1.88	0.56
1:K:82:ARG:HB2	1:K:148:SER:HB3	1.88	0.56
1:F:17:TYR:OH	1:F:104:ARG:HD3	2.05	0.56
1:B:67:LEU:HD23	1:B:70:MET:HE3	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:22:VAL:HG22	1:D:102:GLU:HA	1.88	0.56
2:S:15:DG:H1	3:T:11:DC:N4	2.03	0.56
3:T:23:DA:H1'	3:T:24:DA:H5'	1.86	0.56
1:B:100:CYS:HB3	1:B:104:ARG:NH2	2.20	0.55
1:D:137:VAL:HG22	1:D:155:ARG:HA	1.88	0.55
1:I:82:ARG:HB2	1:I:148:SER:HB3	1.87	0.55
1:N:73:ARG:NH2	1:N:91:LYS:HD3	2.22	0.55
1:H:128:GLY:O	1:H:132:ILE:HG12	2.07	0.55
1:P:49:LYS:HG2	1:P:53:GLN:OE1	2.05	0.55
2:Q:19:DT:H2"	2:Q:20:DA:C8	2.42	0.55
1:L:41:LYS:HE2	2:U:13:DC:H5	1.72	0.55
1:O:70:MET:HE1	1:O:132:ILE:HA	1.88	0.55
1:G:175:HIS:HE1	4:H:209:HOH:O	1.90	0.55
1:H:40:PRO:HG2	1:H:43:SER:OG	2.06	0.55
1:D:70:MET:CE	1:D:132:ILE:HA	2.35	0.54
1:L:105:CYS:SG	1:L:108:VAL:HG23	2.47	0.54
3:T:18:DC:H2'	3:T:19:DT:C6	2.42	0.54
3:X:1:DT:H2'	3:X:2:DG:N7	2.22	0.54
3:T:15:DC:H2"	3:T:16:DG:O5'	2.06	0.54
1:C:99:PRO:HG3	1:K:176:ARG:HD2	1.89	0.54
1:H:63:PHE:CE2	1:H:128:GLY:HA3	2.42	0.54
2:Q:1:DG:N2	3:R:25:DC:C2	2.75	0.54
2:U:4:DT:H3	3:V:22:DA:H2	1.55	0.54
1:H:42:GLY:HA3	2:S:4:DT:C5	2.43	0.54
1:M:34:LEU:HD21	1:M:44:PHE:HB2	1.88	0.54
1:I:119:GLU:O	1:I:123:ILE:HG12	2.08	0.54
1:N:99:PRO:O	1:N:176:ARG:HD3	2.08	0.54
1:G:42:GLY:CA	3:T:11:DC:H41	2.15	0.54
1:P:134:GLU:OE1	1:P:155:ARG:NH2	2.40	0.54
2:W:1:DG:H1	3:X:25:DC:N4	2.06	0.54
1:M:144:ARG:HD2	1:M:151:PRO:HA	1.89	0.53
1:O:192:LEU:O	1:O:193:GLU:HG2	2.08	0.53
3:V:2:DG:H1'	3:V:3:DA:H5'	1.89	0.53
1:E:159:SER:O	1:E:163:GLN:HG3	2.08	0.53
2:S:19:DT:H2"	2:S:20:DA:C8	2.43	0.53
2:W:1:DG:H1	3:X:25:DC:H42	1.55	0.53
1:N:70:MET:CE	1:N:132:ILE:HA	2.39	0.53
2:S:15:DG:H2'	2:S:16:DG:C8	2.43	0.53
1:A:119:GLU:OE2	1:B:176:ARG:NH1	2.41	0.53
1:F:79:LEU:HA	1:F:83:GLU:OE1	2.08	0.53
1:G:100:CYS:HB2	1:G:102:GLU:HG2	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:84:ARG:NH1	1:M:142:GLN:HE22	2.06	0.53
2:Q:1:DG:H1	3:R:25:DC:H42	1.56	0.53
1:D:40:PRO:HB3	3:R:10:DC:H2'	1.90	0.53
2:U:19:DT:H2"	2:U:20:DA:C8	2.43	0.53
1:F:101:ASP:OD2	1:F:176:ARG:NH1	2.35	0.53
1:J:97:CYS:O	1:J:99:PRO:HD2	2.09	0.53
1:M:49:LYS:HB2	1:M:53:GLN:HG2	1.90	0.53
1:A:96:ALA:HB2	4:A:211:HOH:O	2.08	0.53
1:G:93:LEU:HD11	1:G:182:GLU:HG3	1.91	0.53
1:N:98:PRO:HG2	1:N:178:PRO:HA	1.90	0.53
1:F:119:GLU:OE2	1:F:122:ARG:NH1	2.41	0.52
1:O:128:GLY:O	1:O:132:ILE:HG12	2.09	0.52
1:J:135:ARG:HH11	1:J:135:ARG:CG	2.22	0.52
1:G:93:LEU:HA	1:G:181:LEU:HD12	1.92	0.52
1:L:103:GLN:HG2	1:L:173:LYS:HZ1	1.72	0.52
1:O:119:GLU:OE2	1:O:122:ARG:NH1	2.42	0.52
1:P:42:GLY:H	3:X:11:DC:H5	1.56	0.52
2:S:11:DG:H2'	2:S:12:DA:C8	2.43	0.52
2:S:24:DC:N4	3:T:2:DG:H1	1.80	0.52
1:L:134:GLU:OE1	1:L:155:ARG:NH2	2.42	0.52
1:E:121:MET:HG2	4:E:209:HOH:O	2.10	0.52
1:B:22:VAL:HG22	1:B:102:GLU:HA	1.92	0.52
1:C:156:HIS:NE2	1:D:186:GLN:HG2	2.25	0.52
1:J:70:MET:CE	1:J:132:ILE:HA	2.35	0.52
1:H:97:CYS:CB	1:H:99:PRO:HD2	2.40	0.52
1:K:23:LYS:HB2	1:K:28:VAL:HG22	1.92	0.52
2:Q:13:DC:N3	3:R:13:DG:N2	2.52	0.52
1:I:134:GLU:OE1	1:I:155:ARG:NH2	2.43	0.52
1:I:91:LYS:HE3	1:I:95:ASN:HD22	1.75	0.52
3:R:1:DT:H2"	3:R:2:DG:N7	2.25	0.52
1:A:59:LEU:HD23	1:A:106:LEU:HD13	1.91	0.51
2:Q:3:DT:H3	3:R:23:DA:H2	1.58	0.51
1:A:186:GLN:HG2	1:B:156:HIS:CE1	2.46	0.51
1:C:70:MET:HE1	1:C:132:ILE:HA	1.93	0.51
1:E:70:MET:CE	1:E:132:ILE:HA	2.40	0.51
1:I:73:ARG:HG2	1:I:74:PHE:CD1	2.44	0.51
1:N:59:LEU:HD13	1:N:125:LEU:HD13	1.93	0.51
1:H:4:SER:HA	1:H:7:ASP:HB2	1.93	0.51
1:H:79:LEU:HD12	4:H:204:HOH:O	2.11	0.51
1:I:49:LYS:H	1:I:53:GLN:HG2	1.75	0.51
1:A:104:ARG:HB2	1:A:104:ARG:HH11	1.76	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:92:TRP:O	1:F:96:ALA:HB3	2.09	0.51
1:H:90:GLN:HG3	1:H:94:ASP:OD2	2.11	0.51
1:G:46:HIS:CD2	3:T:8:DG:H2'	2.46	0.51
1:N:100:CYS:SG	1:N:101:ASP:N	2.81	0.51
1:I:78:GLY:O	3:X:1:DT:H1'	2.11	0.51
1:H:80:ASN:ND2	1:H:148:SER:OG	2.44	0.51
1:M:156:HIS:CE1	1:N:186:GLN:HG2	2.46	0.51
1:A:102:GLU:O	1:A:102:GLU:HG2	2.10	0.50
2:W:1:DG:H2'	2:W:2:DT:C6	2.46	0.50
1:F:41:LYS:HE2	3:T:16:DG:N7	2.26	0.50
1:D:34:LEU:HD11	1:D:44:PHE:HB2	1.93	0.50
1:N:103:GLN:HG3	1:N:105:CYS:N	2.26	0.50
3:X:1:DT:H3'	3:X:1:DT:OP2	2.12	0.50
1:G:70:MET:HE3	1:G:132:ILE:HA	1.92	0.50
1:P:119:GLU:OE2	1:P:122:ARG:NH1	2.44	0.50
2:Q:13:DC:N4	3:R:13:DG:H1	2.06	0.50
2:W:15:DG:N2	3:X:11:DC:C2	2.79	0.50
1:G:186:GLN:HG2	1:H:156:HIS:NE2	2.26	0.50
3:V:6:DT:H2"	3:V:7:DA:N7	2.26	0.50
1:N:40:PRO:HB3	2:W:7:DA:H2'	1.94	0.50
1:P:41:LYS:CE	2:W:13:DC:H5	2.25	0.50
1:C:56:GLN:HG2	1:C:60:GLU:OE2	2.11	0.50
1:N:20:MET:HG2	1:N:28:VAL:HG21	1.93	0.50
1:P:34:LEU:HD11	1:P:44:PHE:HB2	1.94	0.50
1:A:97:CYS:C	1:A:99:PRO:HD2	2.32	0.50
1:E:71:ASP:OD1	1:E:135:ARG:NE	2.41	0.50
3:T:1:DT:H2"	3:T:2:DG:C8	2.46	0.50
2:U:1:DG:N2	3:V:25:DC:C2	2.77	0.50
1:H:137:VAL:HG22	1:H:155:ARG:HA	1.94	0.49
3:V:13:DG:H2"	3:V:14:DT:C5'	2.42	0.49
1:N:22:VAL:HG13	1:N:101:ASP:CB	2.35	0.49
1:A:34:LEU:HD11	1:A:44:PHE:CD2	2.47	0.49
1:H:97:CYS:C	1:H:99:PRO:HD2	2.32	0.49
1:P:34:LEU:HD23	1:P:41:LYS:HD2	1.95	0.49
3:X:13:DG:H2"	3:X:14:DT:H5'	1.93	0.49
2:S:1:DG:H2'	2:S:2:DT:C6	2.48	0.49
3:T:21:DG:H2"	3:T:22:DA:C8	2.47	0.49
1:E:144:ARG:HD2	1:E:151:PRO:HA	1.94	0.49
1:O:70:MET:CE	1:O:132:ILE:HA	2.42	0.49
1:A:140:LEU:HD12	1:A:149:LEU:HD13	1.94	0.49
1:A:4:SER:HA	1:A:7:ASP:HB2	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:73:ARG:HG2	1:E:74:PHE:CD1	2.46	0.49
1:L:59:LEU:HD21	1:L:110:LEU:HD12	1.95	0.49
2:Q:11:DG:H2'	2:Q:12:DA:C8	2.48	0.49
1:A:105:CYS:SG	1:A:108:VAL:HG23	2.52	0.49
1:E:84:ARG:NH1	1:E:142:GLN:NE2	2.60	0.49
1:E:176:ARG:HD2	4:F:204:HOH:O	2.12	0.49
1:D:42:GLY:CA	3:R:11:DC:H41	2.21	0.49
1:B:116:ASP:OD1	4:B:210:HOH:O	2.20	0.49
1:I:103:GLN:HG2	1:I:109:LYS:HB2	1.94	0.48
1:O:12:LEU:HD21	1:O:39:VAL:HG21	1.94	0.48
3:R:22:DA:H2"	3:R:23:DA:C8	2.47	0.48
3:V:18:DC:H2'	3:V:19:DT:C6	2.48	0.48
1:D:91:LYS:HE3	1:D:95:ASN:ND2	2.28	0.48
1:H:157:MET:HG3	4:H:206:HOH:O	2.13	0.48
1:K:70:MET:CE	1:K:132:ILE:HA	2.43	0.48
1:L:70:MET:CE	1:L:132:ILE:HA	2.35	0.48
1:M:103:GLN:HE21	1:M:173:LYS:HD2	1.78	0.48
1:A:73:ARG:HG2	1:A:74:PHE:CD1	2.48	0.48
1:J:135:ARG:HG2	1:J:135:ARG:HH11	1.78	0.48
1:N:92:TRP:O	1:N:96:ALA:HB3	2.14	0.48
1:L:105:CYS:O	4:L:219:HOH:O	2.20	0.48
1:P:9:ARG:HG3	1:P:47:TYR:HB3	1.96	0.48
3:X:1:DT:H3'	3:X:1:DT:P	2.54	0.48
1:K:159:SER:O	1:K:163:GLN:HG3	2.14	0.48
1:L:100:CYS:SG	1:L:104:ARG:NH1	2.87	0.48
1:P:34:LEU:HD21	1:P:41:LYS:HA	1.96	0.48
1:A:70:MET:HE1	1:A:132:ILE:HA	1.96	0.48
1:H:17:TYR:HD1	1:H:106:LEU:HD11	1.78	0.48
1:A:21:ALA:HB1	1:A:103:GLN:O	2.14	0.47
1:G:70:MET:CE	1:G:132:ILE:HA	2.44	0.47
1:O:119:GLU:O	1:O:123:ILE:HG12	2.14	0.47
1:C:119:GLU:HG2	1:O:178:PRO:HG3	1.96	0.47
1:N:99:PRO:HA	1:N:176:ARG:HA	1.96	0.47
1:A:134:GLU:OE1	1:A:155:ARG:NH2	2.45	0.47
1:A:73:ARG:HD3	1:A:88:TYR:HB2	1.95	0.47
1:I:30:LEU:HD12	1:I:30:LEU:HA	1.75	0.47
1:F:88:TYR:HH	1:F:92:TRP:HZ3	1.60	0.47
1:L:100:CYS:SG	1:L:104:ARG:NH2	2.88	0.47
1:M:144:ARG:NH1	1:M:152:CYS:H	2.12	0.47
1:M:97:CYS:C	1:M:99:PRO:HD2	2.35	0.47
1:P:98:PRO:HG2	1:P:177:SER:N	2.30	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:56:GLN:HA	4:E:209:HOH:O	2.13	0.47
1:L:97:CYS:HB3	1:L:98:PRO:CD	2.45	0.47
1:O:140:LEU:HD12	1:O:140:LEU:HA	1.76	0.47
1:O:163:GLN:HE21	1:P:180:PRO:HB3	1.80	0.47
1:O:96:ALA:CB	1:O:103:GLN:HE22	2.28	0.47
1:G:131:GLY:O	1:G:135:ARG:HG2	2.15	0.47
1:L:103:GLN:HG2	1:L:173:LYS:HZ2	1.80	0.47
1:M:49:LYS:H	1:M:53:GLN:HG2	1.80	0.47
1:G:191:LEU:HA	1:G:191:LEU:HD12	1.58	0.46
1:H:79:LEU:HA	1:H:83:GLU:OE1	2.15	0.46
1:C:159:SER:O	1:C:163:GLN:HG3	2.15	0.46
1:J:168:ALA:HB1	1:J:181:LEU:HD23	1.97	0.46
1:M:70:MET:CE	1:M:132:ILE:HA	2.45	0.46
1:P:119:GLU:OE1	1:P:119:GLU:HA	2.15	0.46
1:J:110:LEU:O	1:J:114:VAL:HB	2.15	0.46
1:L:97:CYS:HB3	1:L:98:PRO:HD2	1.96	0.46
1:N:82:ARG:HB2	1:N:148:SER:HB2	1.98	0.46
1:O:97:CYS:C	1:O:99:PRO:HD2	2.36	0.46
2:U:11:DG:H2"	2:U:12:DA:H5'	1.97	0.46
3:X:18:DC:H2'	3:X:19:DT:C6	2.51	0.46
1:L:39:VAL:HA	1:L:40:PRO:HD3	1.76	0.46
1:E:105:CYS:SG	1:E:108:VAL:HG23	2.55	0.46
1:J:171:LEU:HA	1:J:171:LEU:HD23	1.78	0.46
1:P:131:GLY:O	1:P:135:ARG:HG2	2.15	0.46
2:W:3:DT:H3	3:X:23:DA:H2	1.64	0.46
1:A:103:GLN:HG2	1:A:109:LYS:HB2	1.98	0.46
1:K:176:ARG:NH2	1:L:119:GLU:OE1	2.49	0.46
1:O:98:PRO:HG2	1:O:177:SER:C	2.36	0.46
1:G:41:LYS:HZ2	2:S:13:DC:H41	1.63	0.46
1:O:98:PRO:HG2	1:O:177:SER:CA	2.46	0.46
3:R:18:DC:H2'	3:R:19:DT:C6	2.50	0.46
1:A:55:GLY:O	1:A:58:LEU:HB3	2.15	0.45
1:H:63:PHE:CD2	1:H:128:GLY:HA3	2.50	0.45
1:N:104:ARG:HA	1:N:104:ARG:HD3	1.85	0.45
1:O:144:ARG:HD2	1:O:151:PRO:HA	1.98	0.45
2:U:24:DC:N4	3:V:2:DG:H1	1.90	0.45
1:B:174:LEU:HA	1:B:174:LEU:HD12	1.80	0.45
1:E:140:LEU:HD21	1:E:157:MET:HB3	1.99	0.45
1:F:31:ASN:O	1:F:35:GLN:HB2	2.16	0.45
1:I:163:GLN:O	1:J:167:GLY:HA3	2.16	0.45
1:J:49:LYS:HG2	1:J:53:GLN:OE1	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:97:CYS:HA	1:N:98:PRO:HD3	1.60	0.45
1:O:9:ARG:HG3	1:O:47:TYR:HB3	1.97	0.45
1:N:98:PRO:HB3	1:N:172:SER:OG	2.16	0.45
2:W:1:DG:N2	3:X:25:DC:N3	2.60	0.45
1:E:84:ARG:NH1	1:E:142:GLN:HE22	2.14	0.45
1:P:159:SER:O	1:P:163:GLN:HG3	2.16	0.45
2:U:23:DT:O4	3:V:3:DA:N1	2.50	0.45
2:W:15:DG:H2'	2:W:16:DG:C8	2.51	0.45
1:E:82:ARG:CB	1:E:148:SER:HB3	2.47	0.45
1:L:41:LYS:CE	2:U:13:DC:H5	2.29	0.45
1:C:129:SER:HA	1:C:132:ILE:HG13	1.98	0.45
1:O:159:SER:O	1:O:163:GLN:HG3	2.17	0.45
3:X:5:DT:H2"	3:X:6:DT:O5'	2.16	0.45
1:D:137:VAL:CG2	1:D:155:ARG:HA	2.47	0.45
1:J:119:GLU:O	1:J:123:ILE:HG12	2.16	0.45
1:C:99:PRO:HG3	1:K:176:ARG:CD	2.46	0.45
1:F:70:MET:CE	1:F:132:ILE:HA	2.46	0.45
1:I:163:GLN:NE2	1:J:180:PRO:HB3	2.31	0.45
1:K:31:ASN:OD1	1:K:41:LYS:HD2	2.17	0.45
1:N:103:GLN:HE21	1:N:105:CYS:H	1.63	0.45
1:N:34:LEU:HD11	1:N:44:PHE:HB2	1.98	0.45
1:O:17:TYR:HD1	1:O:106:LEU:HD11	1.82	0.45
1:M:105:CYS:SG	1:M:108:VAL:HG23	2.56	0.44
1:M:34:LEU:HD23	1:M:41:LYS:HA	1.99	0.44
3:T:1:DT:P	3:T:1:DT:H3'	2.57	0.44
1:A:140:LEU:HA	1:A:140:LEU:HD12	1.63	0.44
1:B:97:CYS:O	1:B:100:CYS:SG	2.76	0.44
1:F:135:ARG:HG3	1:F:135:ARG:HH11	1.82	0.44
1:L:109:LYS:HE3	4:L:207:HOH:O	2.18	0.44
2:U:15:DG:C2	3:V:11:DC:N3	2.83	0.44
3:X:14:DT:H2'	3:X:15:DC:C6	2.52	0.44
1:L:42:GLY:CA	3:V:11:DC:H41	2.28	0.44
1:M:12:LEU:HD21	1:M:34:LEU:HD12	1.99	0.44
2:S:13:DC:N3	3:T:13:DG:N1	2.65	0.44
1:E:49:LYS:H	1:E:53:GLN:HG2	1.83	0.44
1:M:172:SER:HB2	1:M:177:SER:O	2.16	0.44
3:T:14:DT:H2'	3:T:15:DC:C6	2.53	0.44
1:B:15:THR:HG21	1:B:37:ALA:HB2	2.00	0.44
1:O:163:GLN:HG2	1:P:171:LEU:HD12	1.99	0.44
1:D:30:LEU:HA	1:D:30:LEU:HD12	1.75	0.44
1:E:122:ARG:NH1	1:F:176:ARG:HE	2.16	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:12:LEU:HD23	1:E:12:LEU:HA	1.80	0.44
1:I:104:ARG:HB2	1:I:104:ARG:HE	1.34	0.44
1:J:81:ALA:HB2	1:J:142:GLN:HG2	2.00	0.44
1:M:161:LEU:O	1:M:164:LEU:HB3	2.18	0.44
3:R:6:DT:H2"	3:R:7:DA:N7	2.33	0.44
1:C:110:LEU:O	1:C:114:VAL:HB	2.18	0.44
1:C:133:ILE:O	1:C:136:LEU:HB2	2.17	0.44
2:U:22:DT:H3	3:V:4:DA:H2	1.65	0.44
2:W:23:DT:H3	3:X:3:DA:H2	1.58	0.44
1:F:92:TRP:HD1	1:F:92:TRP:O	2.00	0.44
1:H:79:LEU:HB3	1:H:83:GLU:HB2	2.00	0.44
1:L:163:GLN:NE2	4:L:206:HOH:O	2.41	0.44
1:B:98:PRO:HD2	4:B:224:HOH:O	2.18	0.43
1:C:115:ALA:HA	1:C:122:ARG:HG3	2.00	0.43
1:D:82:ARG:HB2	1:D:148:SER:HB3	1.99	0.43
1:G:97:CYS:O	1:G:99:PRO:HD2	2.17	0.43
1:O:53:GLN:HG2	1:O:53:GLN:O	2.18	0.43
1:P:192:LEU:O	1:P:193:GLU:HG2	2.17	0.43
1:B:119:GLU:OE2	1:B:122:ARG:NH1	2.51	0.43
1:B:49:LYS:HG2	1:B:53:GLN:NE2	2.33	0.43
1:E:17:TYR:HB2	1:E:58:LEU:HD11	2.00	0.43
1:M:159:SER:O	1:M:163:GLN:HG3	2.17	0.43
1:O:187:THR:O	1:O:191:LEU:HB2	2.17	0.43
1:F:15:THR:CG2	1:F:37:ALA:HB2	2.40	0.43
1:H:159:SER:O	1:H:163:GLN:HG3	2.18	0.43
1:L:161:LEU:O	1:L:164:LEU:HB3	2.18	0.43
1:N:49:LYS:HD3	1:N:49:LYS:HA	1.69	0.43
2:W:15:DG:H1	3:X:11:DC:N4	2.15	0.43
1:N:17:TYR:HD1	1:N:106:LEU:HD11	1.82	0.43
1:C:140:LEU:HD12	1:C:149:LEU:HD13	1.98	0.43
1:D:110:LEU:O	1:D:114:VAL:HB	2.17	0.43
1:K:137:VAL:HG22	1:K:155:ARG:HA	2.01	0.43
1:P:140:LEU:HD12	1:P:149:LEU:HD13	2.01	0.43
1:P:46:HIS:CD2	3:X:8:DG:H2'	2.53	0.43
1:C:119:GLU:O	1:C:123:ILE:HG12	2.19	0.43
1:E:140:LEU:HD21	1:E:157:MET:HG2	2.01	0.43
1:F:166:LEU:HD12	1:F:166:LEU:HA	1.75	0.43
2:Q:18:DC:H2"	2:Q:19:DT:C7	2.49	0.43
1:C:101:ASP:HB2	1:D:116:ASP:OD1	2.19	0.43
1:H:102:GLU:HG3	1:H:102:GLU:O	2.17	0.43
1:M:103:GLN:NE2	4:M:208:HOH:O	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:LEU:C	1:A:193:GLU:HG3	2.39	0.43
1:B:137:VAL:HG22	1:B:155:ARG:HA	2.01	0.43
1:F:30:LEU:HA	1:F:30:LEU:HD12	1.83	0.43
1:F:34:LEU:HD21	1:F:41:LYS:HA	1.99	0.43
1:K:109:LYS:HE3	4:K:203:HOH:O	2.17	0.43
1:P:102:GLU:O	1:P:102:GLU:HG3	2.18	0.43
1:A:17:TYR:N	1:A:58:LEU:HD21	2.34	0.43
1:B:23:LYS:HB2	1:B:28:VAL:HG22	2.00	0.43
1:C:34:LEU:HD21	1:C:44:PHE:HB2	2.01	0.43
1:F:97:CYS:HA	1:F:98:PRO:HD3	1.61	0.43
1:I:189:ARG:O	1:I:193:GLU:HG2	2.19	0.43
1:P:144:ARG:HG2	1:P:151:PRO:HA	2.01	0.43
1:B:80:ASN:ND2	1:B:148:SER:OG	2.52	0.42
1:O:23:LYS:HB2	1:O:28:VAL:HG22	2.01	0.42
1:E:121:MET:HE3	4:E:209:HOH:O	2.19	0.42
1:E:163:GLN:O	1:F:167:GLY:HA3	2.19	0.42
1:F:30:LEU:O	1:F:34:LEU:HB2	2.19	0.42
1:D:97:CYS:HA	1:D:98:PRO:HD3	1.79	0.42
1:G:30:LEU:HA	1:G:30:LEU:HD12	1.69	0.42
1:I:97:CYS:SG	1:I:99:PRO:HD2	2.59	0.42
1:P:166:LEU:HD12	1:P:166:LEU:HA	1.78	0.42
1:C:84:ARG:NH1	1:C:142:GLN:OE1	2.47	0.42
1:E:191:LEU:HD11	1:F:191:LEU:CD1	2.49	0.42
1:G:30:LEU:O	1:G:34:LEU:HD22	2.20	0.42
1:K:163:GLN:O	1:L:167:GLY:HA3	2.19	0.42
1:M:106:LEU:HD23	1:M:106:LEU:HA	1.76	0.42
1:P:98:PRO:HG2	1:P:177:SER:C	2.39	0.42
1:B:34:LEU:CD2	1:B:41:LYS:HD3	2.49	0.42
1:G:143:GLY:HA3	1:G:149:LEU:HD12	2.01	0.42
1:H:71:ASP:OD1	1:H:135:ARG:NE	2.52	0.42
1:K:192:LEU:O	1:K:193:GLU:HG2	2.19	0.42
1:M:144:ARG:HH11	1:M:152:CYS:H	1.65	0.42
2:Q:10:DC:H2"	2:Q:11:DG:H8	1.85	0.42
1:A:45:TYR:HE1	2:Q:17:DT:H72	1.85	0.42
1:F:172:SER:O	1:F:176:ARG:N	2.52	0.42
2:W:22:DT:H3	3:X:4:DA:H2	1.66	0.42
1:C:140:LEU:HA	1:C:140:LEU:HD12	1.87	0.42
1:E:174:LEU:HD11	1:F:125:LEU:HD23	2.02	0.42
1:I:115:ALA:HA	1:I:122:ARG:HG3	2.02	0.42
1:L:34:LEU:HA	1:L:34:LEU:HD12	1.80	0.42
1:M:82:ARG:O	1:M:86:MET:HG2	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:191:LEU:HA	1:C:191:LEU:HD12	1.63	0.42
1:C:49:LYS:HB2	1:C:53:GLN:HG2	2.00	0.42
1:F:13:LEU:HD12	1:F:58:LEU:HA	2.02	0.42
1:K:144:ARG:HG2	4:K:206:HOH:O	2.18	0.42
1:K:156:HIS:CE1	1:L:186:GLN:HG2	2.54	0.42
1:L:23:LYS:HB2	1:L:28:VAL:HG22	2.02	0.42
1:O:137:VAL:HG22	1:O:155:ARG:HA	2.01	0.42
1:D:41:LYS:CE	2:Q:13:DC:H5	2.23	0.42
3:V:5:DT:H2"	3:V:6:DT:O5'	2.20	0.42
2:W:5:DC:H2"	2:W:6:DT:O5'	2.19	0.42
1:G:140:LEU:HD12	1:G:149:LEU:HD13	2.01	0.42
1:P:97:CYS:C	1:P:99:PRO:HD2	2.40	0.42
1:A:135:ARG:HG3	1:A:135:ARG:HH11	1.85	0.42
1:A:161:LEU:HD23	1:A:161:LEU:HA	1.87	0.42
1:D:122:ARG:NH2	4:D:201:HOH:O	2.42	0.42
1:G:166:LEU:HA	1:G:166:LEU:HD12	1.84	0.42
1:H:82:ARG:H	1:H:148:SER:HB3	1.84	0.42
1:L:159:SER:O	1:L:163:GLN:HG3	2.19	0.42
1:M:103:GLN:NE2	1:M:173:LYS:HD2	2.34	0.42
1:O:82:ARG:HB2	1:O:148:SER:HB3	2.01	0.42
1:G:102:GLU:O	1:G:102:GLU:HG3	2.19	0.41
1:A:21:ALA:O	1:A:103:GLN:HB3	2.19	0.41
1:E:49:LYS:HB2	1:E:49:LYS:NZ	2.34	0.41
1:H:34:LEU:HD23	1:H:41:LYS:HA	2.02	0.41
1:N:15:THR:HG21	1:N:37:ALA:HB2	2.01	0.41
1:B:135:ARG:HG3	1:B:135:ARG:HH11	1.86	0.41
1:C:163:GLN:HG2	1:D:171:LEU:HD12	2.01	0.41
1:I:55:GLY:O	1:I:58:LEU:HB3	2.20	0.41
1:L:192:LEU:O	1:L:193:GLU:HG2	2.19	0.41
3:R:8:DG:H2"	3:R:9:DA:H8	1.84	0.41
1:N:119:GLU:OE1	1:N:119:GLU:HA	2.21	0.41
2:S:15:DG:N2	3:T:11:DC:C2	2.89	0.41
1:D:159:SER:O	1:D:163:GLN:HG3	2.19	0.41
1:I:156:HIS:CE1	1:J:186:GLN:HG2	2.55	0.41
1:J:97:CYS:SG	1:J:99:PRO:HD2	2.60	0.41
2:U:10:DC:H2"	2:U:11:DG:H8	1.86	0.41
2:W:19:DT:H2"	2:W:20:DA:C8	2.55	0.41
1:I:73:ARG:HD3	1:I:88:TYR:HB2	2.02	0.41
1:L:22:VAL:HG22	1:L:102:GLU:HA	2.01	0.41
1:L:119:GLU:OE2	1:L:122:ARG:NH1	2.54	0.41
1:C:119:GLU:OE2	1:C:122:ARG:NH1	2.44	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:164:LEU:HD21	1:D:187:THR:HB	2.03	0.41
1:G:156:HIS:CE1	1:H:186:GLN:HG2	2.55	0.41
1:H:73:ARG:HD2	4:H:208:HOH:O	2.20	0.41
1:M:136:LEU:HA	1:M:136:LEU:HD23	1.76	0.41
1:N:32:GLU:O	1:N:36:SER:HB3	2.21	0.41
1:O:91:LYS:HE2	1:O:91:LYS:HB2	1.84	0.41
1:G:181:LEU:HD22	1:G:181:LEU:HA	1.95	0.41
1:O:102:GLU:HG2	1:O:102:GLU:O	2.21	0.41
1:B:67:LEU:HD23	1:B:70:MET:CE	2.50	0.41
1:B:76:ALA:HA	1:B:77:PRO:HD3	1.92	0.41
1:H:89:TRP:CZ2	1:H:161:LEU:HD13	2.55	0.41
1:L:187:THR:O	1:L:191:LEU:HB2	2.20	0.41
2:S:3:DT:C2'	2:S:4:DT:H5'	2.48	0.41
1:A:176:ARG:NH2	1:B:119:GLU:OE1	2.54	0.41
1:H:192:LEU:O	1:H:193:GLU:HG2	2.21	0.41
1:J:131:GLY:O	1:J:135:ARG:HG3	2.21	0.41
1:P:70:MET:CE	1:P:132:ILE:HA	2.49	0.41
2:U:4:DT:O4	3:V:22:DA:N1	2.53	0.41
3:V:21:DG:H2"	3:V:22:DA:C8	2.55	0.41
3:X:2:DG:O5'	3:X:2:DG:H8	2.03	0.41
1:A:166:LEU:HD12	1:A:166:LEU:HA	1.96	0.40
1:C:82:ARG:HB2	1:C:148:SER:HB2	2.03	0.40
1:E:13:LEU:HD12	1:E:13:LEU:HA	1.87	0.40
1:H:133:ILE:O	1:H:136:LEU:HB2	2.21	0.40
1:I:21:ALA:O	1:I:103:GLN:HB3	2.21	0.40
1:J:76:ALA:HA	1:J:77:PRO:HD3	1.78	0.40
2:U:13:DC:N4	3:V:13:DG:H1	2.18	0.40
1:C:163:GLN:NE2	1:D:180:PRO:HB3	2.36	0.40
1:J:73:ARG:HD3	1:J:88:TYR:HA	2.04	0.40
1:K:110:LEU:O	1:K:114:VAL:HB	2.21	0.40
1:M:191:LEU:HA	1:M:191:LEU:HD13	1.95	0.40
1:N:106:LEU:HD23	1:N:106:LEU:HA	1.81	0.40
1:P:34:LEU:CD2	1:P:41:LYS:HD2	2.50	0.40
2:S:10:DC:H2"	2:S:11:DG:O5'	2.21	0.40
1:B:166:LEU:HD12	1:B:166:LEU:HA	1.88	0.40
1:D:58:LEU:C	1:D:58:LEU:HD12	2.41	0.40
1:I:12:LEU:HD23	1:I:12:LEU:HA	1.81	0.40
1:I:70:MET:CE	1:I:132:ILE:HG12	2.52	0.40
1:I:21:ALA:HB1	1:I:103:GLN:HB3	2.04	0.40
1:J:23:LYS:HB2	1:J:28:VAL:HG22	2.02	0.40
1:M:20:MET:HG2	1:M:28:VAL:HG21	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:22:DA:H2"	3:R:23:DA:O5'	2.21	0.40
2:U:11:DG:H2'	2:U:12:DA:C8	2.56	0.40
3:X:14:DT:C4	3:X:15:DC:N4	2.90	0.40
1:A:171:LEU:HA	1:A:171:LEU:HD23	1.93	0.40
1:F:119:GLU:O	1:F:123:ILE:HG12	2.21	0.40
1:I:70:MET:HE2	1:I:132:ILE:HG12	2.04	0.40
1:O:104:ARG:H	1:O:104:ARG:HG2	1.64	0.40
1:O:166:LEU:HA	1:O:166:LEU:HD12	1.93	0.40
2:W:25:DA:C2	3:X:2:DG:N2	2.89	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:176:ARG:NH1	4:A:201:HOH:O[2_874]	2.05	0.15
1:J:101:ASP:OD2	4:A:205:HOH:O[2_874]	2.18	0.02

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	188/190 (99%)	186 (99%)	2 (1%)	0	100	100
1	B	185/190 (97%)	181 (98%)	4 (2%)	0	100	100
1	C	188/190 (99%)	184 (98%)	4 (2%)	0	100	100
1	D	185/190 (97%)	182 (98%)	3 (2%)	0	100	100
1	E	188/190 (99%)	187 (100%)	1 (0%)	0	100	100
1	F	185/190 (97%)	184 (100%)	1 (0%)	0	100	100
1	G	185/190 (97%)	183 (99%)	2 (1%)	0	100	100
1	H	188/190 (99%)	185 (98%)	3 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	188/190 (99%)	186 (99%)	2 (1%)	0	100	100
1	J	185/190 (97%)	181 (98%)	4 (2%)	0	100	100
1	K	188/190 (99%)	185 (98%)	3 (2%)	0	100	100
1	L	185/190 (97%)	182 (98%)	3 (2%)	0	100	100
1	M	188/190 (99%)	185 (98%)	3 (2%)	0	100	100
1	N	185/190 (97%)	180 (97%)	5 (3%)	0	100	100
1	O	188/190 (99%)	184 (98%)	4 (2%)	0	100	100
1	P	185/190 (97%)	182 (98%)	3 (2%)	0	100	100
All	All	2984/3040 (98%)	2937 (98%)	47 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	159/159 (100%)	149 (94%)	10 (6%)	18	46
1	B	156/159 (98%)	145 (93%)	11 (7%)	14	40
1	C	159/159 (100%)	143 (90%)	16 (10%)	7	23
1	D	156/159 (98%)	143 (92%)	13 (8%)	11	32
1	E	159/159 (100%)	141 (89%)	18 (11%)	6	18
1	F	156/159 (98%)	139 (89%)	17 (11%)	6	19
1	G	156/159 (98%)	141 (90%)	15 (10%)	8	25
1	H	159/159 (100%)	147 (92%)	12 (8%)	13	37
1	I	159/159 (100%)	146 (92%)	13 (8%)	11	32
1	J	156/159 (98%)	141 (90%)	15 (10%)	8	25
1	K	159/159 (100%)	144 (91%)	15 (9%)	8	26
1	L	156/159 (98%)	144 (92%)	12 (8%)	13	35
1	M	159/159 (100%)	138 (87%)	21 (13%)	4	12

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	N	156/159 (98%)	139 (89%)	17 (11%)	6 19
1	O	159/159 (100%)	145 (91%)	14 (9%)	10 30
1	P	156/159 (98%)	144 (92%)	12 (8%)	13 35
All	All	2520/2544 (99%)	2289 (91%)	231 (9%)	9 27

All (231) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	LEU
1	A	53	GLN
1	A	104	ARG
1	A	125	LEU
1	A	140	LEU
1	A	148	SER
1	A	157	MET
1	A	166	LEU
1	A	174	LEU
1	A	191	LEU
1	B	13	LEU
1	B	34	LEU
1	B	41	LYS
1	B	58	LEU
1	B	104	ARG
1	B	114	VAL
1	B	125	LEU
1	B	157	MET
1	B	166	LEU
1	B	174	LEU
1	B	191	LEU
1	C	13	LEU
1	C	34	LEU
1	C	53	GLN
1	C	61	ASP
1	C	70	MET
1	C	86	MET
1	C	104	ARG
1	C	119	GLU
1	C	120	SER
1	C	125	LEU
1	C	140	LEU
1	C	157	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	166	LEU
1	C	174	LEU
1	C	186	GLN
1	C	191	LEU
1	D	13	LEU
1	D	28	VAL
1	D	30	LEU
1	D	34	LEU
1	D	58	LEU
1	D	79	LEU
1	D	114	VAL
1	D	125	LEU
1	D	140	LEU
1	D	166	LEU
1	D	170	LEU
1	D	174	LEU
1	D	191	LEU
1	E	13	LEU
1	E	28	VAL
1	E	30	LEU
1	E	34	LEU
1	E	49	LYS
1	E	53	GLN
1	E	56	GLN
1	E	95	ASN
1	E	104	ARG
1	E	114	VAL
1	E	119	GLU
1	E	125	LEU
1	E	157	MET
1	E	166	LEU
1	E	170	LEU
1	E	174	LEU
1	E	185	MET
1	E	191	LEU
1	F	13	LEU
1	F	28	VAL
1	F	30	LEU
1	F	34	LEU
1	F	35	GLN
1	F	36	SER
1	F	53	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	91	LYS
1	F	125	LEU
1	F	136	LEU
1	F	137	VAL
1	F	139	CYS
1	F	140	LEU
1	F	166	LEU
1	F	172	SER
1	F	177	SER
1	F	192	LEU
1	G	13	LEU
1	G	19	ILE
1	G	30	LEU
1	G	34	LEU
1	G	43	SER
1	G	104	ARG
1	G	114	VAL
1	G	125	LEU
1	G	140	LEU
1	G	157	MET
1	G	166	LEU
1	G	174	LEU
1	G	181	LEU
1	G	190	SER
1	G	191	LEU
1	H	30	LEU
1	H	54	PHE
1	H	70	MET
1	H	85	LEU
1	H	93	LEU
1	H	104	ARG
1	H	125	LEU
1	H	129	SER
1	H	166	LEU
1	H	174	LEU
1	H	176	ARG
1	H	191	LEU
1	I	13	LEU
1	I	30	LEU
1	I	34	LEU
1	I	53	GLN
1	I	104	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	120	SER
1	I	125	LEU
1	I	140	LEU
1	I	157	MET
1	I	166	LEU
1	I	174	LEU
1	I	191	LEU
1	I	193	GLU
1	J	13	LEU
1	J	34	LEU
1	J	35	GLN
1	J	41	LYS
1	J	58	LEU
1	J	120	SER
1	J	125	LEU
1	J	135	ARG
1	J	140	LEU
1	J	157	MET
1	J	166	LEU
1	J	174	LEU
1	J	190	SER
1	J	191	LEU
1	J	193	GLU
1	K	13	LEU
1	K	30	LEU
1	K	34	LEU
1	K	41	LYS
1	K	49	LYS
1	K	53	GLN
1	K	58	LEU
1	K	120	SER
1	K	125	LEU
1	K	140	LEU
1	K	157	MET
1	K	166	LEU
1	K	172	SER
1	K	174	LEU
1	K	176	ARG
1	L	13	LEU
1	L	30	LEU
1	L	34	LEU
1	L	41	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	58	LEU
1	L	104	ARG
1	L	125	LEU
1	L	140	LEU
1	L	166	LEU
1	L	170	LEU
1	L	174	LEU
1	L	191	LEU
1	M	13	LEU
1	M	28	VAL
1	M	30	LEU
1	M	34	LEU
1	M	53	GLN
1	M	69	ASP
1	M	75	SER
1	M	95	ASN
1	M	100	CYS
1	M	104	ARG
1	M	119	GLU
1	M	125	LEU
1	M	140	LEU
1	M	144	ARG
1	M	148	SER
1	M	157	MET
1	M	166	LEU
1	M	174	LEU
1	M	176	ARG
1	M	185	MET
1	M	191	LEU
1	N	13	LEU
1	N	23	LYS
1	N	28	VAL
1	N	30	LEU
1	N	34	LEU
1	N	35	GLN
1	N	36	SER
1	N	41	LYS
1	N	53	GLN
1	N	58	LEU
1	N	97	CYS
1	N	109	LYS
1	N	122	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	N	125	LEU
1	N	166	LEU
1	N	174	LEU
1	N	191	LEU
1	O	13	LEU
1	O	34	LEU
1	O	91	LYS
1	O	104	ARG
1	O	125	LEU
1	O	140	LEU
1	O	144	ARG
1	O	146	ASP
1	O	149	LEU
1	O	166	LEU
1	O	172	SER
1	O	174	LEU
1	O	177	SER
1	O	190	SER
1	P	13	LEU
1	P	34	LEU
1	P	41	LYS
1	P	104	ARG
1	P	119	GLU
1	P	125	LEU
1	P	140	LEU
1	P	144	ARG
1	P	148	SER
1	P	166	LEU
1	P	174	LEU
1	P	191	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	163	GLN
1	I	163	GLN
1	J	103	GLN
1	M	142	GLN
1	N	103	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	A	190/190 (100%)	-0.41	6 (3%) 47 43	20, 29, 53, 127	0
1	B	187/190 (98%)	-0.29	7 (3%) 41 37	17, 31, 55, 128	0
1	C	190/190 (100%)	-0.13	9 (4%) 31 28	21, 43, 75, 135	0
1	D	187/190 (98%)	-0.29	6 (3%) 47 43	23, 38, 67, 145	0
1	E	190/190 (100%)	-0.24	7 (3%) 41 37	22, 42, 73, 122	0
1	F	187/190 (98%)	0.09	14 (7%) 14 11	31, 53, 92, 160	0
1	G	187/190 (98%)	-0.22	8 (4%) 35 31	22, 37, 73, 161	0
1	H	190/190 (100%)	0.37	21 (11%) 5 4	28, 68, 99, 146	0
1	I	190/190 (100%)	-0.39	6 (3%) 47 43	17, 27, 52, 132	0
1	J	187/190 (98%)	-0.32	7 (3%) 41 37	14, 28, 54, 138	0
1	K	190/190 (100%)	-0.33	5 (2%) 56 52	21, 36, 64, 130	0
1	L	187/190 (98%)	-0.37	7 (3%) 41 37	18, 33, 63, 141	0
1	M	190/190 (100%)	-0.26	7 (3%) 41 37	20, 37, 61, 132	0
1	N	187/190 (98%)	-0.14	7 (3%) 41 37	27, 46, 78, 136	0
1	O	190/190 (100%)	-0.05	11 (5%) 23 19	23, 49, 88, 136	0
1	P	187/190 (98%)	-0.38	6 (3%) 47 43	21, 32, 67, 138	0
2	Q	25/25 (100%)	-0.71	0 100 100	19, 31, 47, 50	0
2	S	25/25 (100%)	-0.39	1 (4%) 38 33	25, 39, 55, 70	0
2	U	25/25 (100%)	-0.71	0 100 100	18, 26, 40, 55	0
2	W	25/25 (100%)	-0.37	1 (4%) 38 33	22, 36, 45, 66	0
3	R	25/25 (100%)	-0.58	0 100 100	23, 30, 51, 71	0
3	T	25/25 (100%)	-0.38	0 100 100	27, 35, 54, 58	0
3	V	25/25 (100%)	-0.73	0 100 100	17, 24, 42, 67	0
3	X	25/25 (100%)	-0.40	0 100 100	25, 32, 48, 56	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
All	All	3216/3240 (99%)	-0.23	136 (4%) 36 32	14, 38, 84, 161	0

All (136) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	101	ASP	15.9
1	G	99	PRO	12.4
1	F	101	ASP	12.2
1	B	98	PRO	11.7
1	F	100	CYS	10.5
1	D	101	ASP	10.1
1	B	99	PRO	9.9
1	M	102	GLU	9.6
1	F	99	PRO	9.4
1	K	101	ASP	8.9
1	N	100	CYS	8.8
1	I	98	PRO	8.8
1	A	98	PRO	8.3
1	J	101	ASP	8.2
1	N	98	PRO	7.9
1	J	100	CYS	7.9
1	L	101	ASP	7.9
1	G	100	CYS	7.8
1	F	98	PRO	7.6
1	H	101	ASP	7.6
1	E	101	ASP	7.2
1	H	102	GLU	7.1
1	D	98	PRO	7.0
1	H	98	PRO	6.9
1	M	98	PRO	6.7
1	C	98	PRO	6.6
1	C	99	PRO	6.5
1	C	101	ASP	6.5
1	P	101	ASP	6.5
1	K	103	GLN	6.3
1	C	100	CYS	6.2
1	M	101	ASP	6.2
1	K	102	GLU	6.1
1	I	99	PRO	6.1
1	O	101	ASP	6.1
1	E	102	GLU	6.0
1	N	99	PRO	6.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	O	99	PRO	6.0
1	J	98	PRO	6.0
1	M	97	CYS	5.9
1	O	98	PRO	5.8
1	P	99	PRO	5.8
1	M	100	CYS	5.7
1	J	102	GLU	5.7
1	L	102	GLU	5.5
1	N	102	GLU	5.4
1	O	102	GLU	5.3
1	G	98	PRO	5.2
1	I	101	ASP	5.2
1	D	102	GLU	5.2
1	F	102	GLU	5.1
1	I	102	GLU	5.0
1	A	101	ASP	4.9
1	C	103	GLN	4.9
1	E	98	PRO	4.8
1	B	102	GLU	4.7
1	L	100	CYS	4.7
1	P	98	PRO	4.7
1	E	100	CYS	4.6
1	M	99	PRO	4.6
1	G	102	GLU	4.6
1	O	77	PRO	4.6
1	B	101	ASP	4.6
1	H	99	PRO	4.4
1	G	101	ASP	4.3
1	A	99	PRO	4.2
1	H	75	SER	4.0
1	K	98	PRO	4.0
1	H	145	ASP	4.0
1	O	103	GLN	4.0
1	M	103	GLN	3.9
1	O	100	CYS	3.9
1	I	103	GLN	3.8
1	A	100	CYS	3.7
1	P	97	CYS	3.7
1	P	102	GLU	3.7
1	A	102	GLU	3.6
1	L	99	PRO	3.6
1	C	102	GLU	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	103	GLN	3.5
1	G	97	CYS	3.5
1	D	99	PRO	3.4
1	D	103	GLN	3.4
2	S	1	DG	3.4
1	H	103	GLN	3.4
1	J	99	PRO	3.4
1	O	97	CYS	3.4
1	F	95	ASN	3.3
1	E	103	GLN	3.3
1	H	97	CYS	3.3
1	I	97	CYS	3.3
2	W	1	DG	3.2
1	E	97	CYS	3.2
1	J	103	GLN	3.2
1	F	97	CYS	3.1
1	L	98	PRO	3.0
1	H	78	GLY	3.0
1	H	100	CYS	2.8
1	F	77	PRO	2.8
1	L	103	GLN	2.8
1	C	97	CYS	2.7
1	H	70	MET	2.7
1	N	103	GLN	2.7
1	D	100	CYS	2.7
1	B	97	CYS	2.7
1	H	77	PRO	2.7
1	F	78	GLY	2.6
1	H	95	ASN	2.6
1	H	144	ARG	2.6
1	A	97	CYS	2.6
1	C	78	GLY	2.6
1	L	77	PRO	2.6
1	H	71	ASP	2.6
1	H	155	ARG	2.6
1	H	4	SER	2.4
1	H	79	LEU	2.4
1	B	100	CYS	2.4
1	H	5	TYR	2.3
1	P	100	CYS	2.3
1	F	64	ARG	2.3
1	O	145	ASP	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	N	95	ASN	2.3
1	H	141	GLY	2.2
1	G	103	GLN	2.2
1	F	18	ARG	2.2
1	G	95	ASN	2.2
1	F	151	PRO	2.2
1	E	99	PRO	2.2
1	C	6	ASP	2.1
1	J	97	CYS	2.1
1	H	152	CYS	2.1
1	F	75	SER	2.1
1	K	97	CYS	2.1
1	F	83	GLU	2.0
1	O	94	ASP	2.0
1	O	76	ALA	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.