Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:30 PM GMT

PDB ID	:	4P0S
Title	:	human Mus81-Eme1-3'flap DNA complex
Authors	:	Gwon, G.H.; Baek, K.; Cho, Y.
Deposited on	:	2014-02-22
Resolution	:	6.00 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

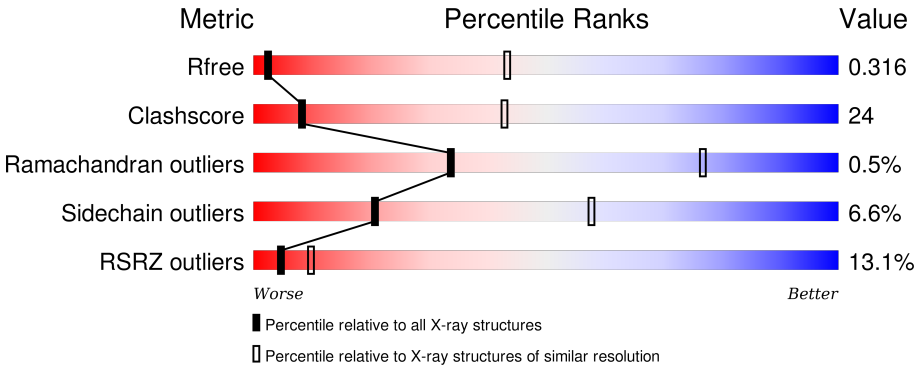
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 6.00 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}	91344	1002 (8.30-3.66)
Clashscore	102246	1050 (8.30-3.70)
Ramachandran outliers	100387	1023 (8.30-3.66)
Sidechain outliers	100360	1012 (8.30-3.64)
RSRZ outliers	91569	1001 (8.30-3.66)

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. 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	306	8% 52% 34% • 10%
1	C	306	4% 53% 32% • 10%
1	E	306	14% 53% 35% • 10%
1	G	306	7% 49% 36% 5% 10%
2	B	393	6% 41% 27% 5% 28%

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Mol	Chain	Length	Quality of chain
2	D	393	9% 43% 25% 28%
2	F	393	19% 42% 25% 5% 28%
2	H	393	8% 42% 24% 5% 28%
3	I	12	25% 25% 42% 33%
3	M	12	25% 17% 33% 50%
3	Q	12	67% 25% 58% 17%
3	U	12	42% 42% 17%
4	J	24	8% 25% 50% 21%
4	N	24	13% 8% 17% 54% 21%
4	R	24	58% 42% 33% 21%
4	V	24	33% 8% 29% 42% 21%
5	L	13	8% 15% 54% 31%
5	P	13	15% 15% 38% 31%
5	T	13	54% 15% 15% 38% 31%
5	X	13	31% 38% 31%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 20884 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 Crossover junction endonuclease MUS81.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	0	0
			2173	1364	403	398	8			
1	C	275	Total	C	N	O	S	0	0	0
			2173	1364	403	398	8			
1	E	275	Total	C	N	O	S	0	0	0
			2173	1364	403	398	8			
1	G	275	Total	C	N	O	S	0	0	0
			2173	1364	403	398	8			

- Molecule 2 is a protein called Crossover junction endonuclease EME1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	284	Total	C	N	O	S	0	0	0
			2227	1401	397	415	14			
2	D	284	Total	C	N	O	S	0	0	0
			2227	1401	397	415	14			
2	F	284	Total	C	N	O	S	0	0	0
			2227	1401	397	415	14			
2	H	284	Total	C	N	O	S	0	0	0
			2227	1401	397	415	14			

- Molecule 3 is a DNA chain called DNA GAATGTGTGTCT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	12	Total	C	N	O	P	0	0	0
			249	119	43	75	12			
3	M	12	Total	C	N	O	P	0	0	0
			249	119	43	75	12			
3	Q	12	Total	C	N	O	P	0	0	0
			249	119	43	75	12			
3	U	12	Total	C	N	O	P	0	0	0
			249	119	43	75	12			

- Molecule 4 is a DNA chain called DNA TAGACACACATTCGGGACATGCAG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	J	19	Total	C	N	O	P	0	0	0
			389	185	76	109	19			
4	N	19	Total	C	N	O	P	0	0	0
			389	185	76	109	19			
4	R	19	Total	C	N	O	P	0	0	0
			389	185	76	109	19			
4	V	19	Total	C	N	O	P	0	0	0
			389	185	76	109	19			

- Molecule 5 is a DNA chain called DNA TCTGCATGTCATT.

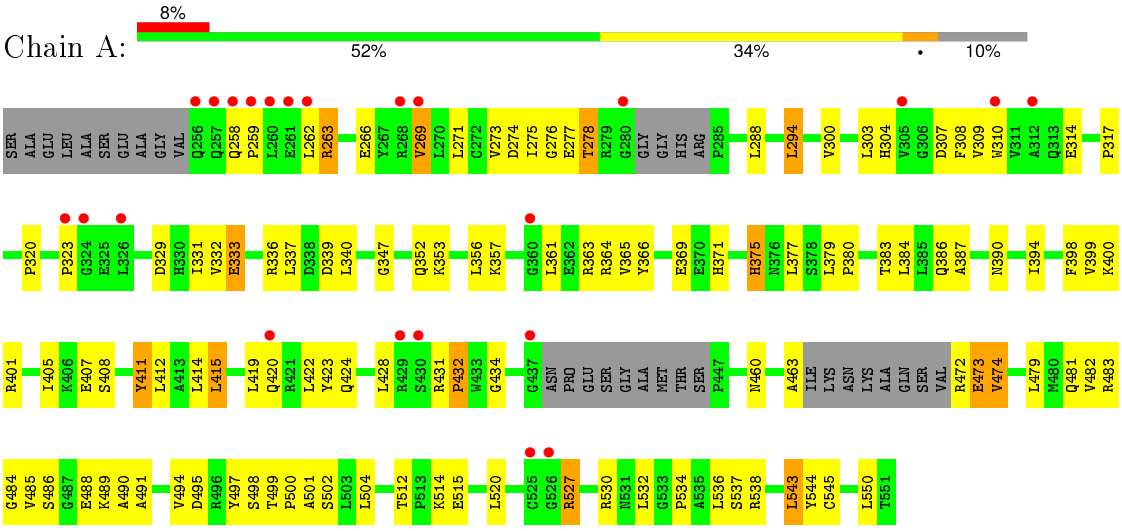
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	L	9	Total	C	N	O	P	0	0	0
			183	88	29	57	9			
5	P	9	Total	C	N	O	P	0	0	0
			183	88	29	57	9			
5	T	9	Total	C	N	O	P	0	0	0
			183	88	29	57	9			
5	X	9	Total	C	N	O	P	0	0	0
			183	88	29	57	9			

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 errors 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.

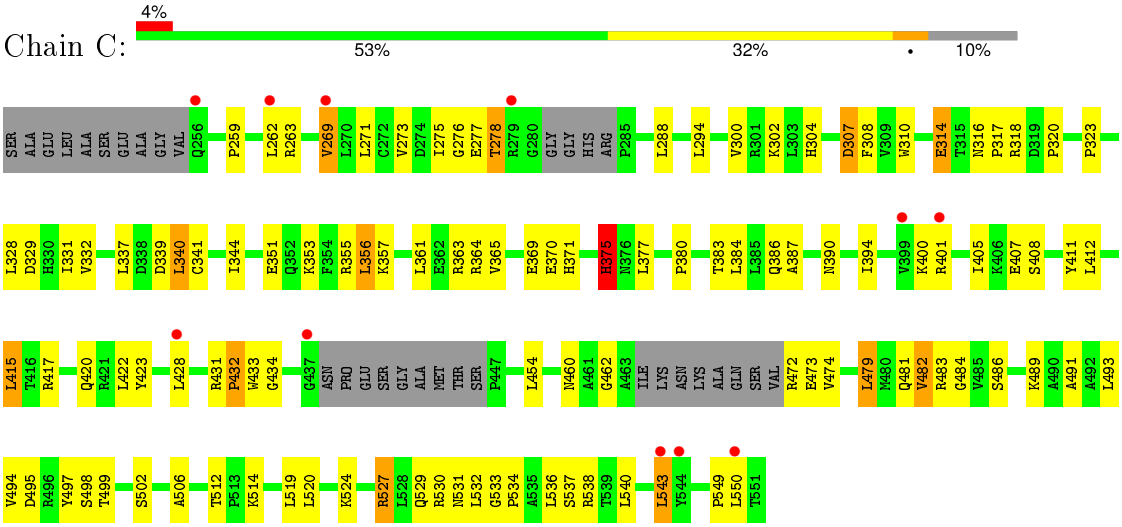
- Molecule 1: Crossover junction endonuclease MUS81

Chain A:



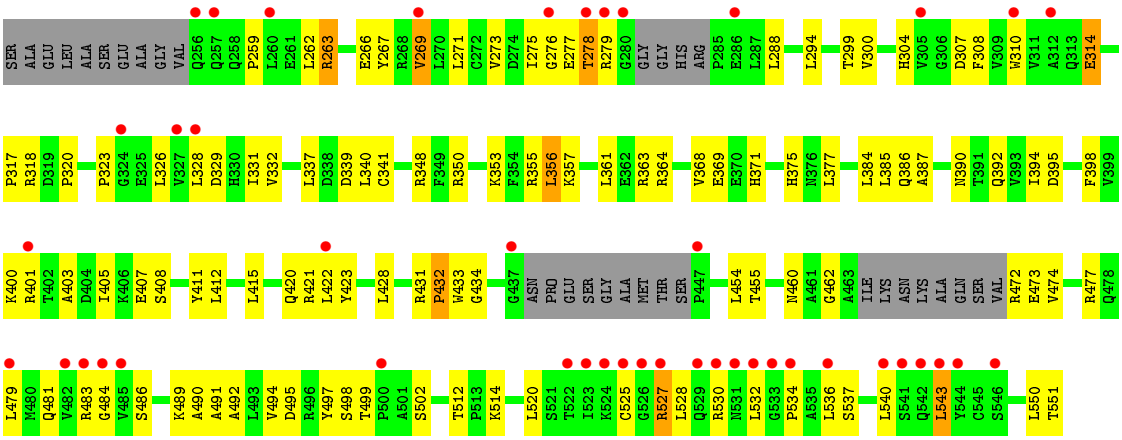
- Molecule 1: Crossover junction endonuclease MUS81

Chain C:



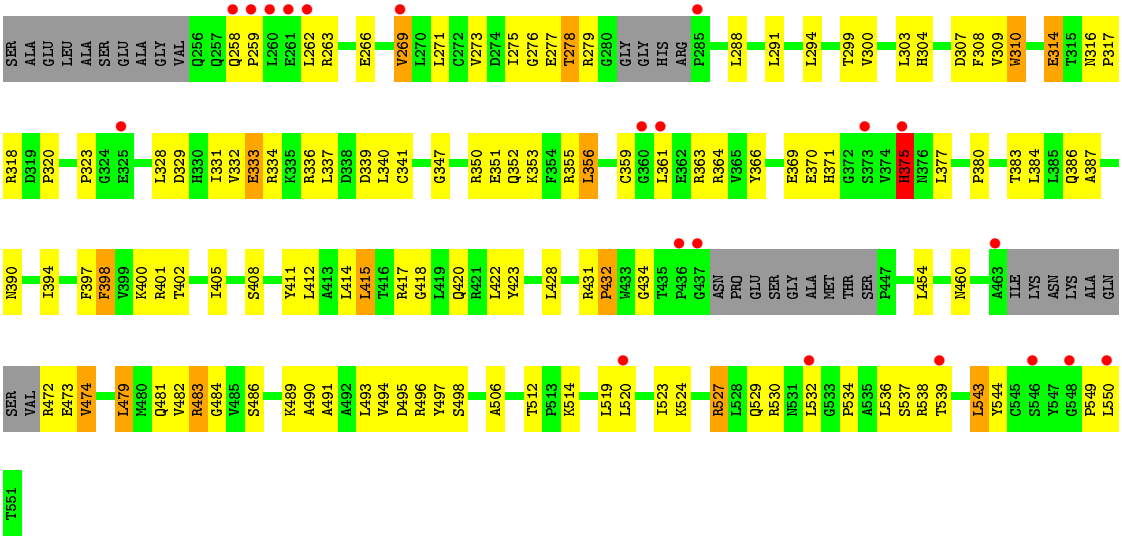
- Molecule 1: Crossover junction endonuclease MUS81

Chain E:



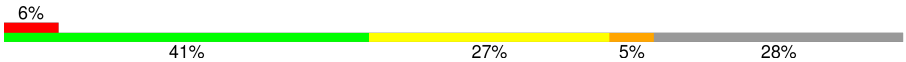
• Molecule 1: Crossover junction endonuclease MUS81

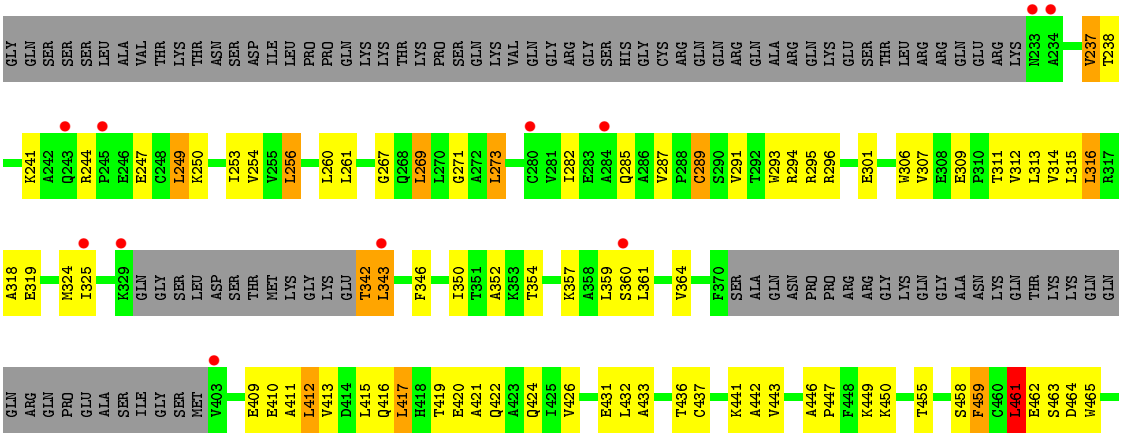
Chain G:

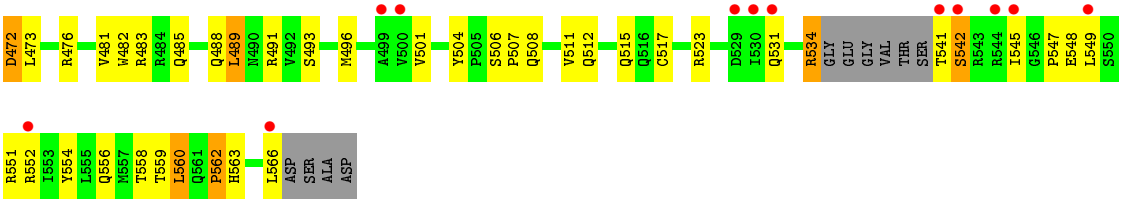


• Molecule 2: Crossover junction endonuclease EME1

Chain B:

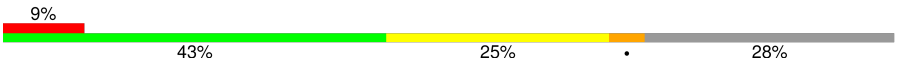


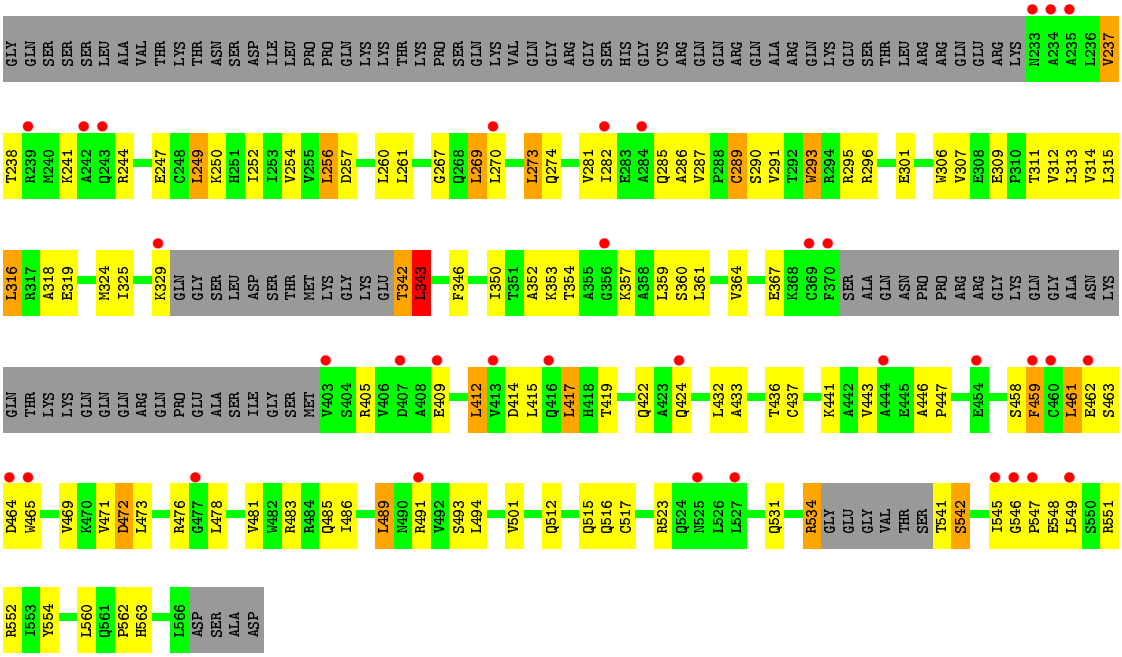




• Molecule 2: Crossover junction endonuclease EME1

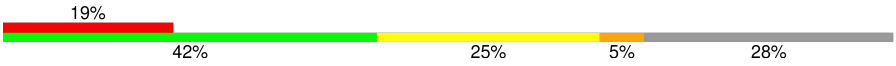
Chain D:

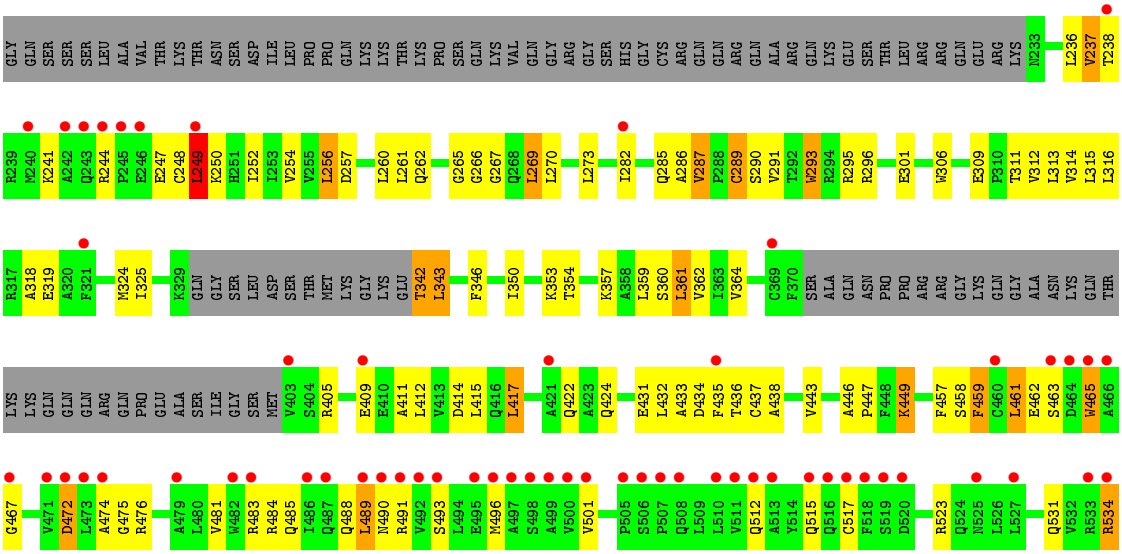


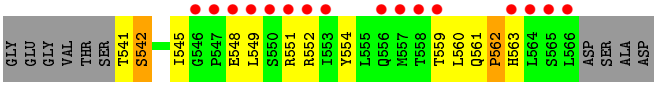


• Molecule 2: Crossover junction endonuclease EME1

Chain F:

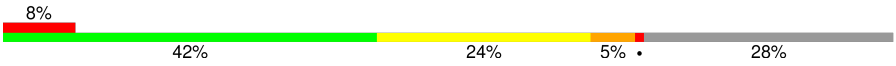


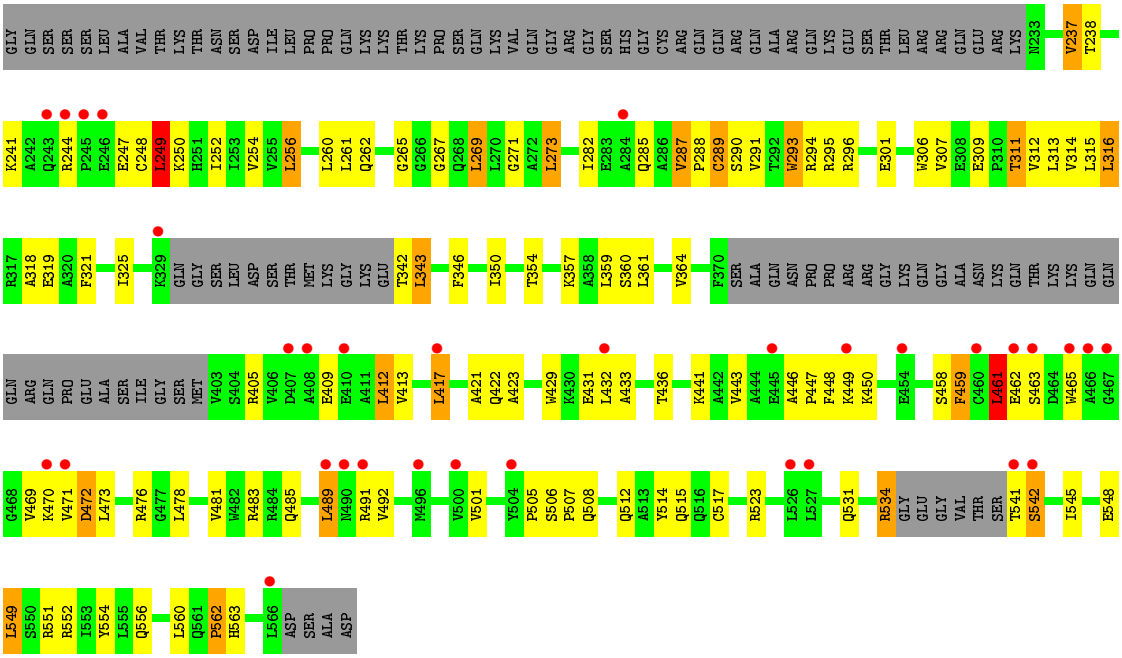




• Molecule 2: Crossover junction endonuclease EME1

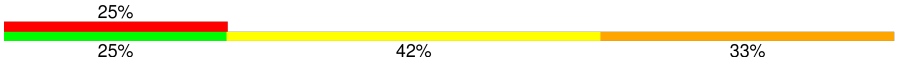
Chain H:

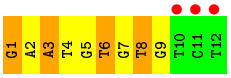




• Molecule 3: DNA GAATGTGTGTCT

Chain I:



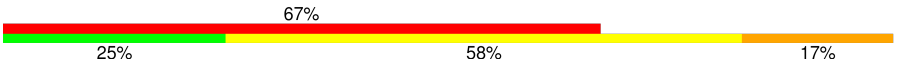


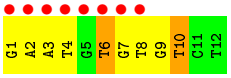
• Molecule 3: DNA GAATGTGTGTCT

Chain M:

• Molecule 3: DNA GAATGTGTGTCT

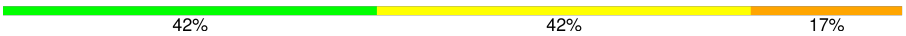
Chain Q:





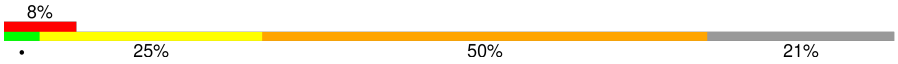
• Molecule 3: DNA GAATGTGTGTCT

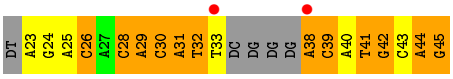
Chain U:



• Molecule 4: DNA TAGACACACATTCGGGACATGCAG

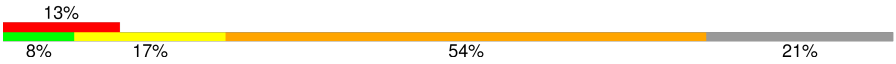
Chain J:

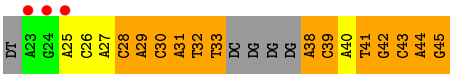




• Molecule 4: DNA TAGACACACATTCGGGACATGCAG

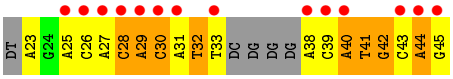
Chain N:





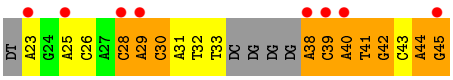
• Molecule 4: DNA TAGACACACATTCGGGACATGCAG

Chain R:



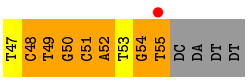
• Molecule 4: DNA TAGACACACATTCGGGACATGCAG

Chain V:



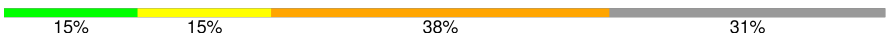
• Molecule 5: DNA TCTGCATGTCATT

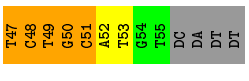
Chain L:



• Molecule 5: DNA TCTGCATGTCATT

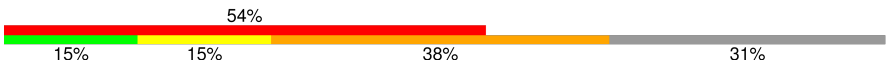
Chain P:

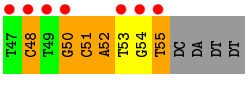




• Molecule 5: DNA TCTGCATGTCATT

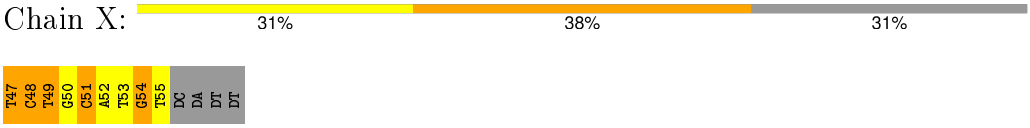
Chain T:





• Molecule 5: DNA TCTGCATGTCATT

Chain X:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	92.44Å 250.76Å 430.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.98 – 6.00 49.43 – 5.48	Depositor EDS
% Data completeness (in resolution range)	99.4 (29.98-6.00) 99.2 (49.43-5.48)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.09 (at 5.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.250 , 0.308 0.263 , 0.316	Depositor DCC
R_{free} test set	658 reflections (5.12%)	DCC
Wilson B-factor (Å^2)	323.6	Xtriage
Anisotropy	0.352	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 207.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 16835 reflections	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	20884	wwPDB-VP
Average B, all atoms (Å^2)	152.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.89	2/2211 (0.1%)	1.13	8/2989 (0.3%)
1	C	0.83	1/2211 (0.0%)	1.11	10/2989 (0.3%)
1	E	0.82	0/2211	1.13	10/2989 (0.3%)
1	G	0.93	6/2211 (0.3%)	1.13	11/2989 (0.4%)
2	B	0.85	3/2258 (0.1%)	1.13	13/3054 (0.4%)
2	D	0.88	4/2258 (0.2%)	1.13	15/3054 (0.5%)
2	F	0.83	4/2258 (0.2%)	1.10	14/3054 (0.5%)
2	H	0.87	3/2258 (0.1%)	1.13	14/3054 (0.5%)
3	I	1.10	0/278	1.82	8/428 (1.9%)
3	M	1.17	1/278 (0.4%)	1.91	12/428 (2.8%)
3	Q	0.84	0/278	1.50	4/428 (0.9%)
3	U	1.07	0/278	1.62	6/428 (1.4%)
4	J	1.46	2/436 (0.5%)	2.72	45/667 (6.7%)
4	N	1.35	3/436 (0.7%)	2.40	30/667 (4.5%)
4	R	1.05	0/436	2.05	18/667 (2.7%)
4	V	1.37	4/436 (0.9%)	2.55	35/667 (5.2%)
5	L	1.58	3/203 (1.5%)	2.93	28/311 (9.0%)
5	P	1.82	6/203 (3.0%)	2.63	19/311 (6.1%)
5	T	1.48	3/203 (1.5%)	2.43	13/311 (4.2%)
5	X	1.38	2/203 (1.0%)	2.40	15/311 (4.8%)
All	All	0.95	47/21544 (0.2%)	1.42	328/29796 (1.1%)

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	359	CYS	CB-SG	-8.35	1.68	1.82
2	F	409	GLU	CB-CG	8.26	1.67	1.52
5	X	47	DT	C1'-N1	8.22	1.59	1.49
5	T	55	DT	C1'-N1	7.82	1.59	1.49
5	P	49	DT	C5-C7	7.78	1.54	1.50
2	H	409	GLU	CG-CD	7.74	1.63	1.51
2	F	409	GLU	CG-CD	7.73	1.63	1.51
5	P	49	DT	C5-C6	7.64	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	T	48	DC	C1'-N1	7.53	1.59	1.49
2	D	486	ILE	CA-CB	7.53	1.72	1.54
4	V	38	DA	N9-C4	7.46	1.42	1.37
2	B	409	GLU	CG-CD	7.37	1.62	1.51
5	L	47	DT	C3'-O3'	7.21	1.53	1.44
5	L	48	DC	C1'-N1	7.18	1.58	1.49
2	D	293	TRP	CB-CG	-7.04	1.37	1.50
4	J	40	DA	C3'-O3'	6.99	1.53	1.44
5	T	50	DG	C3'-O3'	6.94	1.52	1.44
5	P	47	DT	C1'-N1	6.82	1.58	1.49
1	G	366	TYR	CB-CG	6.79	1.61	1.51
5	P	49	DT	N3-C4	6.74	1.44	1.38
5	P	49	DT	N1-C6	6.69	1.43	1.38
2	F	293	TRP	CB-CG	-6.45	1.38	1.50
2	B	409	GLU	CB-CG	6.31	1.64	1.52
2	H	293	TRP	CB-CG	-6.18	1.39	1.50
5	L	50	DG	C3'-O3'	6.13	1.51	1.44
1	G	398	PHE	CB-CG	6.11	1.61	1.51
2	H	409	GLU	CB-CG	6.09	1.63	1.52
2	F	431	GLU	CG-CD	6.08	1.61	1.51
2	D	409	GLU	CB-CG	5.90	1.63	1.52
4	N	44	DA	C3'-O3'	5.90	1.51	1.44
2	D	409	GLU	CG-CD	5.89	1.60	1.51
4	N	44	DA	N9-C4	-5.86	1.34	1.37
5	P	47	DT	C3'-O3'	5.81	1.51	1.44
2	B	426	VAL	CA-CB	-5.65	1.42	1.54
1	G	333	GLU	CB-CG	5.52	1.62	1.52
3	M	10	DT	N3-C4	5.49	1.43	1.38
4	J	28	DC	C3'-O3'	5.43	1.51	1.44
4	V	44	DA	C3'-O3'	5.39	1.50	1.44
4	V	40	DA	C3'-O3'	-5.36	1.36	1.44
4	N	39	DC	C1'-N1	5.34	1.56	1.49
5	X	48	DC	C1'-N1	5.33	1.56	1.49
1	G	314	GLU	CG-CD	5.27	1.59	1.51
1	A	333	GLU	CB-CG	5.26	1.62	1.52
1	G	310	TRP	CB-CG	-5.26	1.40	1.50
1	C	307	ASP	CB-CG	5.23	1.62	1.51
1	A	411	TYR	CD1-CE1	-5.22	1.31	1.39
4	V	28	DC	C3'-O3'	5.15	1.50	1.44

All (328) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	V	38	DA	O4'-C1'-N9	22.46	123.72	108.00
4	V	45	DG	O4'-C4'-C3'	-19.19	94.49	106.00
4	J	44	DA	O4'-C1'-N9	18.59	121.01	108.00
4	N	45	DG	O4'-C4'-C3'	-16.41	96.16	106.00
5	L	48	DC	O4'-C1'-N1	14.54	118.18	108.00
4	R	41	DT	C4-C5-C7	13.42	127.05	119.00
4	R	42	DG	O4'-C4'-C3'	-12.72	98.37	106.00
4	J	41	DT	N3-C4-O4	12.68	127.51	119.90
5	L	48	DC	C6-N1-C2	-12.15	115.44	120.30
4	N	42	DG	O4'-C1'-N9	11.99	116.39	108.00
2	H	249	LEU	CA-CB-CG	11.85	142.55	115.30
5	L	48	DC	N3-C4-C5	-11.80	117.18	121.90
4	N	30	DC	O4'-C1'-N1	11.67	116.17	108.00
2	B	249	LEU	CA-CB-CG	11.54	141.85	115.30
5	T	51	DC	O4'-C1'-N1	11.52	116.06	108.00
5	P	51	DC	O4'-C4'-C3'	-11.45	99.13	106.00
5	X	55	DT	O4'-C4'-C3'	-11.31	99.21	106.00
4	V	41	DT	O4'-C1'-N1	11.27	115.89	108.00
5	L	50	DG	C4'-C3'-C2'	-10.88	93.31	103.10
4	J	38	DA	C5-C6-N1	10.78	123.09	117.70
4	R	32	DT	O4'-C1'-N1	10.77	115.54	108.00
5	T	48	DC	C6-N1-C2	-10.77	115.99	120.30
4	N	43	DC	O4'-C1'-N1	10.49	115.35	108.00
4	J	30	DC	O4'-C1'-N1	10.41	115.29	108.00
2	D	249	LEU	CA-CB-CG	10.36	139.13	115.30
4	V	32	DT	O4'-C1'-N1	10.09	115.06	108.00
5	T	52	DA	O4'-C4'-C3'	-10.01	100.00	106.00
2	F	249	LEU	CA-CB-CG	10.00	138.31	115.30
5	X	49	DT	N3-C4-O4	9.93	125.86	119.90
4	J	38	DA	C5-C6-N6	-9.66	115.97	123.70
5	P	49	DT	N3-C4-O4	9.64	125.69	119.90
4	R	41	DT	C6-C5-C7	-9.55	117.17	122.90
4	N	32	DT	O4'-C1'-N1	9.40	114.58	108.00
4	V	45	DG	C3'-C2'-C1'	-9.32	91.32	102.50
5	X	47	DT	C6-N1-C2	-9.25	116.67	121.30
4	R	44	DA	O4'-C1'-N9	9.24	114.47	108.00
4	J	41	DT	C5-C4-O4	-9.22	118.45	124.90
4	J	41	DT	C4-C5-C7	-9.15	113.51	119.00
4	V	30	DC	O4'-C1'-N1	9.15	114.40	108.00
5	X	49	DT	C5-C4-O4	-9.10	118.53	124.90
4	R	30	DC	O4'-C1'-N1	9.00	114.30	108.00
4	J	45	DG	O4'-C4'-C3'	-8.98	100.61	106.00
1	G	356	LEU	CB-CG-CD2	8.93	126.18	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	J	45	DG	C3'-C2'-C1'	-8.86	91.87	102.50
4	J	38	DA	N9-C1'-C2'	8.82	129.36	112.60
3	I	8	DT	C6-C5-C7	-8.74	117.66	122.90
4	J	44	DA	C4'-C3'-C2'	-8.70	95.27	103.10
4	R	42	DG	O4'-C1'-N9	-8.69	101.92	108.00
4	J	42	DG	C3'-C2'-C1'	-8.62	92.15	102.50
5	L	51	DC	O4'-C1'-C2'	-8.59	99.03	105.90
4	V	44	DA	O4'-C1'-N9	8.53	113.97	108.00
5	P	50	DG	O4'-C4'-C3'	8.48	111.09	106.00
4	V	38	DA	O4'-C1'-C2'	-8.44	99.15	105.90
4	N	41	DT	C4-C5-C7	8.41	124.04	119.00
2	D	489	LEU	CA-CB-CG	-8.40	95.99	115.30
5	P	48	DC	O4'-C1'-N1	8.36	113.86	108.00
4	V	45	DG	N1-C6-O6	-8.36	114.89	119.90
4	J	32	DT	N3-C4-O4	8.34	124.90	119.90
4	N	32	DT	N3-C4-O4	8.28	124.87	119.90
5	P	49	DT	N3-C2-O2	8.27	127.26	122.30
4	N	38	DA	O4'-C1'-C2'	-8.27	99.28	105.90
4	R	33	DT	C5-C4-O4	-8.27	119.11	124.90
4	J	45	DG	O4'-C1'-N9	-8.25	102.23	108.00
3	M	7	DG	N1-C6-O6	8.19	124.81	119.90
4	N	41	DT	C4'-C3'-C2'	-8.19	95.73	103.10
4	N	41	DT	C6-C5-C7	-8.18	117.99	122.90
1	C	356	LEU	CB-CG-CD2	8.15	124.86	111.00
5	L	51	DC	C3'-C2'-C1'	-8.15	92.71	102.50
5	X	49	DT	C4-C5-C7	-8.03	114.18	119.00
3	M	3	DA	N1-C6-N6	7.90	123.34	118.60
5	T	48	DC	N3-C4-C5	-7.86	118.75	121.90
5	P	49	DT	C6-C5-C7	7.80	127.58	122.90
4	V	38	DA	C8-N9-C4	-7.79	102.68	105.80
5	X	48	DC	O4'-C1'-N1	7.79	113.45	108.00
4	V	45	DG	C4-C5-N7	-7.74	107.70	110.80
4	J	40	DA	O4'-C1'-N9	7.68	113.38	108.00
4	J	32	DT	O4'-C1'-N1	7.63	113.34	108.00
4	V	41	DT	C4-C5-C7	7.61	123.57	119.00
4	N	45	DG	N3-C4-C5	-7.61	124.80	128.60
4	N	42	DG	N3-C2-N2	-7.59	114.58	119.90
5	P	49	DT	C5-C4-O4	-7.57	119.60	124.90
4	N	42	DG	N1-C6-O6	7.55	124.43	119.90
4	N	44	DA	C8-N9-C4	7.52	108.81	105.80
5	L	48	DC	C2-N3-C4	7.52	123.66	119.90
4	J	45	DG	P-O5'-C5'	-7.50	108.90	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	542	SER	N-CA-C	-7.47	90.84	111.00
4	J	42	DG	O4'-C1'-N9	7.47	113.23	108.00
5	L	52	DA	C1'-O4'-C4'	-7.44	102.66	110.10
5	L	52	DA	C4'-C3'-C2'	-7.43	96.41	103.10
5	T	48	DC	O4'-C4'-C3'	-7.43	101.53	104.50
5	L	54	DG	O4'-C1'-N9	7.42	113.20	108.00
1	E	356	LEU	CB-CG-CD2	7.42	123.61	111.00
2	B	461	LEU	CA-CB-CG	7.30	132.09	115.30
2	H	542	SER	N-CA-C	-7.26	91.40	111.00
3	I	8	DT	C4-C5-C7	7.25	123.35	119.00
4	J	45	DG	N9-C4-C5	-7.24	102.50	105.40
5	T	55	DT	C6-N1-C2	-7.22	117.69	121.30
5	L	50	DG	C1'-O4'-C4'	-7.21	102.89	110.10
5	T	55	DT	N3-C4-O4	7.20	124.22	119.90
5	T	48	DC	O4'-C1'-N1	7.18	113.03	108.00
4	V	44	DA	C4'-C3'-C2'	-7.18	96.64	103.10
2	B	542	SER	N-CA-C	-7.15	91.70	111.00
5	L	48	DC	C5-C6-N1	7.11	124.56	121.00
5	L	52	DA	O4'-C4'-C3'	-7.07	101.67	104.50
4	J	45	DG	C5-C6-O6	-7.06	124.37	128.60
4	J	44	DA	N1-C6-N6	7.05	122.83	118.60
5	T	50	DG	O4'-C4'-C3'	7.05	110.23	106.00
4	J	41	DT	C6-C5-C7	7.04	127.12	122.90
2	D	289	CYS	CA-CB-SG	7.02	126.64	114.00
3	M	1	DG	O5'-P-OP1	7.02	119.12	110.70
5	X	51	DC	O4'-C1'-N1	7.02	112.91	108.00
3	M	7	DG	C5-C6-O6	-7.02	124.39	128.60
4	V	32	DT	N3-C4-O4	7.00	124.10	119.90
2	H	461	LEU	CA-CB-CG	6.99	131.37	115.30
5	X	49	DT	O4'-C1'-N1	6.99	112.89	108.00
2	B	560	LEU	CA-CB-CG	6.98	131.36	115.30
4	N	42	DG	C5-C6-N1	-6.97	108.02	111.50
4	R	44	DA	O4'-C1'-C2'	-6.96	100.33	105.90
2	F	542	SER	N-CA-C	-6.92	92.32	111.00
5	X	54	DG	O4'-C1'-N9	6.90	112.83	108.00
5	X	48	DC	C6-N1-C2	-6.87	117.55	120.30
2	F	289	CYS	CA-CB-SG	6.85	126.33	114.00
5	P	53	DT	N3-C4-O4	6.85	124.01	119.90
4	N	31	DA	O4'-C1'-N9	6.84	112.79	108.00
2	D	560	LEU	CA-CB-CG	6.82	130.98	115.30
4	V	42	DG	C8-N9-C4	-6.81	103.67	106.40
4	N	44	DA	C4'-C3'-C2'	-6.77	97.01	103.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	415	LEU	CA-CB-CG	6.76	130.84	115.30
2	D	461	LEU	CA-CB-CG	6.73	130.78	115.30
2	H	461	LEU	CB-CG-CD2	6.70	122.38	111.00
5	P	49	DT	C4'-C3'-C2'	6.69	109.12	103.10
4	J	38	DA	C4-C5-N7	6.67	114.03	110.70
4	V	33	DT	C5-C4-O4	-6.67	120.23	124.90
5	X	49	DT	C6-C5-C7	6.65	126.89	122.90
3	I	3	DA	N1-C6-N6	6.64	122.58	118.60
4	R	33	DT	N3-C4-O4	6.64	123.88	119.90
1	E	412	LEU	CA-CB-CG	6.63	130.55	115.30
1	E	415	LEU	CA-CB-CG	6.61	130.50	115.30
2	H	489	LEU	CA-CB-CG	-6.57	100.19	115.30
2	F	417	LEU	CA-CB-CG	-6.57	100.19	115.30
2	F	461	LEU	CA-CB-CG	6.57	130.41	115.30
4	J	41	DT	O4'-C1'-N1	6.57	112.60	108.00
2	F	489	LEU	CA-CB-CG	-6.55	100.23	115.30
1	A	288	LEU	CA-CB-CG	6.54	130.34	115.30
4	N	42	DG	N3-C4-N9	-6.52	122.09	126.00
4	N	39	DC	O4'-C1'-N1	6.52	112.56	108.00
3	U	4	DT	N3-C4-O4	6.52	123.81	119.90
4	J	38	DA	C2-N3-C4	6.51	113.85	110.60
1	A	294	LEU	CA-CB-CG	-6.50	100.36	115.30
4	V	42	DG	O4'-C1'-N9	6.49	112.55	108.00
3	M	6	DT	N3-C4-O4	6.49	123.80	119.90
2	B	489	LEU	CA-CB-CG	-6.47	100.43	115.30
1	E	288	LEU	CA-CB-CG	6.46	130.17	115.30
4	V	28	DC	O4'-C1'-N1	6.45	112.52	108.00
4	R	29	DA	C3'-C2'-C1'	-6.45	94.76	102.50
1	C	288	LEU	CA-CB-CG	6.40	130.01	115.30
1	E	294	LEU	CA-CB-CG	-6.35	100.70	115.30
4	J	31	DA	O5'-P-OP1	-6.34	99.99	105.70
4	J	32	DT	C5-C4-O4	-6.34	120.46	124.90
4	N	45	DG	N3-C4-N9	6.34	129.80	126.00
4	V	39	DC	O4'-C1'-N1	6.33	112.44	108.00
3	I	4	DT	N3-C4-O4	6.33	123.70	119.90
3	U	4	DT	O4'-C1'-N1	6.31	112.42	108.00
5	P	53	DT	O4'-C1'-N1	6.30	112.41	108.00
4	V	41	DT	C1'-O4'-C4'	-6.30	103.80	110.10
4	V	45	DG	O4'-C1'-N9	-6.26	103.62	108.00
1	C	294	LEU	CA-CB-CG	-6.25	100.92	115.30
4	J	42	DG	C1'-O4'-C4'	-6.24	103.86	110.10
4	J	39	DC	C1'-O4'-C4'	-6.23	103.87	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	560	LEU	CA-CB-CG	6.20	129.56	115.30
5	T	53	DT	N3-C4-O4	6.19	123.61	119.90
5	P	48	DC	C6-N1-C2	-6.17	117.83	120.30
5	L	47	DT	C5-C4-O4	-6.16	120.59	124.90
2	F	431	GLU	CA-CB-CG	6.15	126.93	113.40
4	J	45	DG	N3-C4-N9	6.15	129.69	126.00
4	N	39	DC	C6-N1-C2	-6.12	117.85	120.30
4	J	38	DA	N9-C4-C5	-6.09	103.36	105.80
4	V	40	DA	O4'-C1'-N9	6.09	112.26	108.00
5	P	47	DT	C6-N1-C2	-6.05	118.28	121.30
2	D	417	LEU	CA-CB-CG	-6.04	101.42	115.30
3	M	3	DA	C5-C6-N6	-6.03	118.87	123.70
4	N	33	DT	C5-C4-O4	-6.03	120.68	124.90
3	M	7	DG	C6-C5-N7	-6.01	126.79	130.40
1	C	415	LEU	CA-CB-CG	5.99	129.07	115.30
4	J	38	DA	C4-C5-C6	-5.99	114.01	117.00
2	F	316	LEU	CA-CB-CG	-5.98	101.54	115.30
1	G	340	LEU	CA-CB-CG	-5.98	101.56	115.30
5	P	47	DT	N1-C1'-C2'	5.95	123.91	112.60
2	D	316	LEU	CA-CB-CG	-5.94	101.64	115.30
3	M	8	DT	C6-C5-C7	-5.94	119.34	122.90
2	H	256	LEU	CA-CB-CG	-5.93	101.66	115.30
5	L	54	DG	N9-C4-C5	5.92	107.77	105.40
1	G	294	LEU	CA-CB-CG	-5.92	101.69	115.30
1	G	288	LEU	CA-CB-CG	5.91	128.89	115.30
2	F	560	LEU	CA-CB-CG	5.90	128.86	115.30
4	V	38	DA	N7-C8-N9	5.89	116.75	113.80
4	R	28	DC	O4'-C1'-N1	5.88	112.11	108.00
4	J	26	DC	N3-C4-C5	-5.86	119.56	121.90
3	U	10	DT	C5-C4-O4	-5.85	120.80	124.90
2	H	289	CYS	CA-CB-SG	5.85	124.52	114.00
5	L	55	DT	C6-C5-C7	-5.84	119.39	122.90
1	G	258	GLN	N-CA-C	-5.84	95.23	111.00
4	R	32	DT	N3-C4-O4	5.83	123.40	119.90
4	J	26	DC	C6-N1-C2	-5.82	117.97	120.30
1	C	412	LEU	CA-CB-CG	5.81	128.67	115.30
3	U	8	DT	C6-C5-C7	-5.81	119.42	122.90
1	A	412	LEU	CA-CB-CG	5.81	128.65	115.30
5	L	47	DT	O4'-C4'-C3'	5.79	109.47	106.00
2	F	437	CYS	CA-CB-SG	5.79	124.42	114.00
4	N	29	DA	C3'-C2'-C1'	-5.79	95.55	102.50
5	P	53	DT	C5-C4-O4	-5.78	120.86	124.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	L	55	DT	C4-C5-C7	5.77	122.46	119.00
1	A	258	GLN	N-CA-C	-5.76	95.46	111.00
5	X	47	DT	N3-C4-O4	5.75	123.35	119.90
2	B	256	LEU	CA-CB-CG	-5.75	102.08	115.30
5	L	54	DG	C4-C5-N7	-5.72	108.51	110.80
1	G	415	LEU	CA-CB-CG	5.71	128.44	115.30
4	V	45	DG	C5-C6-O6	5.68	132.01	128.60
4	J	45	DG	C8-N9-C4	5.67	108.67	106.40
4	R	42	DG	C4'-C3'-C2'	-5.67	98.00	103.10
5	X	47	DT	O4'-C1'-C2'	-5.66	101.37	105.90
3	I	6	DT	O4'-C4'-C3'	5.66	109.40	106.00
3	M	4	DT	N3-C4-O4	5.66	123.29	119.90
3	M	3	DA	N1-C2-N3	-5.65	126.47	129.30
4	N	45	DG	C4-N9-C1'	5.65	133.84	126.50
4	V	41	DT	C3'-C2'-C1'	-5.63	95.75	102.50
1	C	340	LEU	CA-CB-CG	-5.62	102.36	115.30
4	R	29	DA	P-O5'-C5'	-5.62	111.91	120.90
1	E	340	LEU	CA-CB-CG	-5.62	102.38	115.30
4	V	29	DA	C3'-C2'-C1'	-5.62	95.76	102.50
3	I	4	DT	O4'-C1'-N1	5.61	111.93	108.00
4	J	29	DA	P-O5'-C5'	-5.61	111.92	120.90
4	J	29	DA	C3'-C2'-C1'	-5.61	95.77	102.50
2	B	431	GLU	CA-CB-CG	5.60	125.73	113.40
2	H	417	LEU	CA-CB-CG	-5.59	102.44	115.30
2	F	361	LEU	CA-CB-CG	-5.58	102.46	115.30
3	Q	10	DT	C5-C4-O4	-5.55	121.01	124.90
1	A	340	LEU	CA-CB-CG	-5.55	102.54	115.30
3	Q	6	DT	O4'-C1'-N1	5.54	111.87	108.00
3	U	8	DT	C4-C5-C7	5.53	122.31	119.00
3	I	1	DG	C5-C6-N1	5.52	114.26	111.50
5	L	54	DG	C8-N9-C4	-5.51	104.19	106.40
4	N	33	DT	N3-C4-O4	5.50	123.20	119.90
5	T	55	DT	O4'-C1'-N1	5.50	111.85	108.00
1	G	412	LEU	CA-CB-CG	5.48	127.91	115.30
4	V	38	DA	C4-N9-C1'	5.47	136.14	126.30
3	Q	4	DT	N3-C4-O4	5.46	123.18	119.90
4	V	33	DT	N3-C4-C5	5.46	118.48	115.20
1	G	366	TYR	CB-CG-CD1	5.46	124.27	121.00
3	M	3	DA	N9-C4-C5	-5.45	103.62	105.80
2	D	256	LEU	CA-CB-CG	-5.45	102.77	115.30
4	N	32	DT	C2-N3-C4	5.45	130.47	127.20
5	P	51	DC	N3-C4-C5	-5.44	119.72	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	465	TRP	CA-C-N	-5.43	105.24	117.20
4	R	40	DA	P-O5'-C5'	-5.43	112.21	120.90
3	I	5	DG	C4'-C3'-C2'	5.43	107.98	103.10
1	E	357	LYS	CA-CB-CG	5.42	125.31	113.40
2	H	316	LEU	CA-CB-CG	-5.42	102.84	115.30
2	B	464	ASP	C-N-CA	-5.41	108.19	121.70
4	V	41	DT	C6-C5-C7	-5.40	119.66	122.90
2	B	465	TRP	CA-C-N	-5.39	105.33	117.20
4	N	28	DC	O4'-C1'-N1	5.39	111.78	108.00
4	V	42	DG	N3-C2-N2	-5.39	116.12	119.90
4	R	29	DA	O4'-C4'-C3'	-5.35	102.36	104.50
4	V	33	DT	C6-N1-C2	5.35	123.97	121.30
1	A	357	LYS	CA-CB-CG	5.34	125.15	113.40
3	Q	10	DT	N3-C4-O4	5.34	123.10	119.90
4	V	42	DG	N9-C4-C5	5.34	107.54	105.40
5	L	49	DT	C3'-C2'-C1'	-5.34	96.09	102.50
2	B	316	LEU	CA-CB-CG	-5.33	103.04	115.30
2	D	489	LEU	CB-CG-CD1	5.33	120.06	111.00
5	L	47	DT	N3-C4-O4	5.33	123.10	119.90
4	J	39	DC	C3'-C2'-C1'	-5.32	96.11	102.50
4	J	44	DA	C5-N7-C8	-5.30	101.25	103.90
2	H	465	TRP	CA-C-N	-5.30	105.54	117.20
3	U	10	DT	N3-C4-O4	5.28	123.07	119.90
2	F	449	LYS	CA-CB-CG	-5.27	101.80	113.40
5	P	50	DG	O4'-C1'-N9	5.27	111.69	108.00
1	C	375	HIS	N-CA-C	-5.26	96.81	111.00
5	X	47	DT	N1-C1'-C2'	5.26	122.59	112.60
2	B	289	CYS	CA-CB-SG	5.24	123.42	114.00
1	C	540	LEU	CA-CB-CG	5.23	127.33	115.30
5	L	52	DA	N1-C6-N6	5.23	121.74	118.60
1	G	291	LEU	CA-CB-CG	5.23	127.33	115.30
4	J	38	DA	C5'-C4'-C3'	5.22	123.50	114.10
1	E	540	LEU	CA-CB-CG	5.22	127.30	115.30
5	T	55	DT	C4-C5-C7	-5.22	115.87	119.00
5	P	49	DT	C4-C5-C6	-5.22	114.87	118.00
2	F	256	LEU	CA-CB-CG	-5.21	103.32	115.30
4	J	45	DG	C8-N9-C1'	-5.20	120.24	127.00
4	R	31	DA	O4'-C1'-N9	5.20	111.64	108.00
1	G	314	GLU	CA-CB-CG	5.19	124.82	113.40
1	G	375	HIS	N-CA-C	-5.19	97.00	111.00
1	A	366	TYR	CB-CG-CD1	5.18	124.11	121.00
5	T	51	DC	O4'-C1'-C2'	-5.18	101.75	105.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	X	55	DT	N3-C4-O4	5.18	123.01	119.90
2	H	431	GLU	CA-CB-CG	5.18	124.79	113.40
4	N	44	DA	O4'-C1'-N9	-5.17	104.38	108.00
4	V	32	DT	C5-C4-O4	-5.17	121.28	124.90
2	F	465	TRP	CA-C-N	-5.15	105.87	117.20
4	J	31	DA	C8-N9-C4	-5.15	103.74	105.80
5	L	47	DT	N1-C2-O2	5.15	127.22	123.10
4	J	31	DA	P-O5'-C5'	-5.13	112.69	120.90
5	L	51	DC	P-O5'-C5'	-5.12	112.71	120.90
1	C	357	LYS	CA-CB-CG	5.12	124.66	113.40
2	H	489	LEU	CB-CG-CD1	5.12	119.70	111.00
1	E	314	GLU	CA-CB-CG	5.11	124.64	113.40
4	N	42	DG	N1-C2-N2	5.11	120.80	116.20
5	L	51	DC	O4'-C4'-C3'	-5.09	102.46	104.50
2	D	367	GLU	N-CA-C	5.09	124.74	111.00
4	N	42	DG	N9-C4-C5	5.09	107.44	105.40
2	B	437	CYS	CA-CB-SG	5.08	123.14	114.00
1	C	314	GLU	CA-CB-CG	5.08	124.57	113.40
5	P	47	DT	N3-C2-O2	-5.08	119.25	122.30
2	B	417	LEU	CA-CB-CG	-5.07	103.64	115.30
4	V	38	DA	N3-C4-C5	-5.06	123.26	126.80
5	L	52	DA	OP2-P-O3'	5.06	116.33	105.20
2	D	343	LEU	N-CA-C	5.05	124.64	111.00
1	E	368	VAL	N-CA-C	5.04	124.61	111.00
4	J	45	DG	N1-C6-O6	5.04	122.92	119.90
5	L	52	DA	O4'-C1'-C2'	5.04	109.93	105.90
4	J	33	DT	C5-C4-O4	-5.03	121.38	124.90
2	D	437	CYS	CA-CB-SG	5.03	123.05	114.00
4	V	45	DG	C5-N7-C8	5.03	106.81	104.30
5	P	48	DC	C1'-O4'-C4'	-5.02	105.08	110.10
2	H	549	LEU	CA-CB-CG	5.01	126.83	115.30
2	D	464	ASP	C-N-CA	-5.01	109.18	121.70
3	M	1	DG	C5-C6-N1	5.00	114.00	111.50

There are no chirality outliers.

There are no planarity outliers.

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	2173	0	2203	143	1
1	C	2173	0	2203	87	0
1	E	2173	0	2203	101	0
1	G	2173	0	2203	122	0
2	B	2227	0	2265	160	0
2	D	2227	0	2265	112	1
2	F	2227	0	2265	121	0
2	H	2227	0	2265	144	0
3	I	249	0	138	14	0
3	M	249	0	138	19	0
3	Q	249	0	138	17	0
3	U	249	0	138	10	0
4	J	389	0	214	33	0
4	N	389	0	214	34	0
4	R	389	0	214	33	0
4	V	389	0	214	31	0
5	L	183	0	104	26	0
5	P	183	0	104	12	0
5	T	183	0	104	21	0
5	X	183	0	104	28	0
All	All	20884	0	19696	971	1

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 24.

All (971) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:538:ARG:NH2	2:H:473:LEU:O	1.87	1.05
1:A:499:THR:HG21	2:B:560:LEU:HA	1.33	1.05
1:E:401:ARG:NH1	2:F:424:GLN:OE1	1.91	1.03
2:H:269:LEU:HD21	2:H:436:THR:HG21	1.41	1.02
1:C:276:GLY:H	1:C:278:THR:HG22	1.19	1.02
1:E:276:GLY:H	1:E:278:THR:HG22	1.23	1.01
1:C:401:ARG:NH1	2:D:424:GLN:OE1	1.93	1.01
2:F:269:LEU:HD21	2:F:436:THR:HG21	1.43	1.00
2:B:547:PRO:HD2	4:J:45:DG:H3'	1.42	0.99
1:E:486:SER:HB3	4:R:30:DC:P	2.04	0.98
1:E:477:ARG:NH2	2:F:488:GLN:OE1	1.97	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:276:GLY:H	1:G:278:THR:HG22	1.27	0.97
1:E:431:ARG:NH1	1:E:434:GLY:O	1.98	0.96
2:B:534:ARG:NH1	5:L:50:DG:OP1	1.97	0.96
1:G:275:ILE:HD12	1:G:278:THR:HG21	1.46	0.96
2:F:491:ARG:NH2	4:R:45:DG:OP1	1.99	0.96
2:F:449:LYS:NZ	3:Q:2:DA:OP2	1.99	0.94
1:C:275:ILE:HD12	1:C:278:THR:HG21	1.45	0.94
2:B:269:LEU:HD21	2:B:436:THR:HG21	1.50	0.93
1:G:347:GLY:HA3	2:H:461:LEU:HD22	1.50	0.93
4:V:44:DA:N6	5:X:49:DT:O4	2.00	0.93
2:D:269:LEU:HD21	2:D:436:THR:HG21	1.49	0.93
1:A:276:GLY:H	1:A:278:THR:HG22	1.33	0.92
1:A:275:ILE:HD12	1:A:278:THR:HG21	1.48	0.92
2:B:309:GLU:O	2:B:357:LYS:NZ	2.03	0.92
1:E:275:ILE:HD12	1:E:278:THR:HG21	1.52	0.92
2:D:274:GLN:NE2	2:H:267:GLY:H	1.68	0.91
1:C:276:GLY:H	1:C:278:THR:CG2	1.83	0.90
2:H:309:GLU:O	2:H:357:LYS:NZ	2.04	0.90
1:E:385:LEU:HD21	2:F:434:ASP:HB3	1.51	0.90
1:E:276:GLY:H	1:E:278:THR:CG2	1.84	0.90
3:Q:3:DA:H61	4:R:32:DT:H3	1.13	0.88
1:G:474:VAL:HB	2:H:556:GLN:NE2	1.90	0.87
1:A:486:SER:HB3	4:J:30:DC:H3'	1.55	0.87
1:A:353:LYS:HA	1:A:356:LEU:HD12	1.57	0.87
1:G:530:ARG:CZ	4:N:29:DA:H5"	2.05	0.86
2:D:281:VAL:HA	2:H:262:GLN:HG2	1.56	0.86
1:C:483:ARG:HD3	4:V:31:DA:H4'	1.57	0.86
1:A:534:PRO:HD2	3:I:9:DG:OP1	1.74	0.86
1:E:386:GLN:HE22	2:F:438:ALA:HA	1.41	0.86
2:D:309:GLU:O	2:D:357:LYS:NZ	2.10	0.85
1:C:353:LYS:HA	1:C:356:LEU:HD12	1.57	0.85
1:C:431:ARG:NH1	1:C:434:GLY:O	2.10	0.84
1:A:431:ARG:NH1	1:A:434:GLY:O	2.11	0.84
2:F:449:LYS:NZ	3:Q:1:DG:H3'	1.93	0.84
1:G:489:LYS:NZ	4:N:30:DC:OP1	2.10	0.83
4:N:28:DC:H2"	4:N:29:DA:H5'	1.59	0.83
1:G:353:LYS:HA	1:G:356:LEU:HD12	1.57	0.83
1:A:394:ILE:HG23	2:B:450:LYS:HE3	1.61	0.83
1:A:489:LYS:NZ	4:J:30:DC:OP1	2.11	0.83
1:E:353:LYS:HA	1:E:356:LEU:HD12	1.59	0.83
1:G:276:GLY:H	1:G:278:THR:CG2	1.91	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:493:SER:HB3	5:X:51:DC:H3'	1.61	0.81
2:B:360:SER:HA	2:B:422:GLN:HB3	1.61	0.81
3:U:6:DT:H2"	3:U:7:DG:C8	2.13	0.81
1:A:472:ARG:HD3	2:B:562:PRO:HB2	1.63	0.81
1:A:474:VAL:HB	2:B:556:GLN:NE2	1.95	0.81
1:C:531:ASN:ND2	3:U:10:DT:OP2	2.13	0.81
2:D:534:ARG:HH12	5:X:50:DG:P	2.04	0.81
2:H:541:THR:OG1	5:P:50:DG:O5'	1.99	0.81
1:A:398:PHE:HE2	2:B:421:ALA:O	1.64	0.80
1:A:386:GLN:HG2	3:I:2:DA:OP1	1.80	0.80
5:L:50:DG:H5'	5:L:50:DG:C8	2.16	0.80
2:D:274:GLN:HE22	2:H:267:GLY:H	1.27	0.80
1:A:276:GLY:H	1:A:278:THR:CG2	1.94	0.80
1:G:269:VAL:HG13	1:G:420:GLN:HG2	1.64	0.80
1:G:347:GLY:CA	2:H:461:LEU:HD22	2.12	0.80
1:C:269:VAL:HG13	1:C:420:GLN:HG2	1.64	0.79
1:G:483:ARG:HB2	2:H:470:LYS:HA	1.65	0.79
3:M:3:DA:H61	4:N:32:DT:H3	1.30	0.79
5:P:47:DT:H2"	5:P:48:DC:H6	1.47	0.79
2:D:267:GLY:HA3	2:H:271:GLY:HA2	1.64	0.79
1:G:279:ARG:NH2	4:N:41:DT:H4'	1.98	0.78
4:R:42:DG:C8	4:R:42:DG:H5'	2.19	0.78
1:A:269:VAL:HG13	1:A:420:GLN:HG2	1.65	0.77
3:M:6:DT:H2"	3:M:7:DG:C8	2.19	0.77
3:M:9:DG:O6	4:N:25:DA:N6	2.17	0.77
1:E:269:VAL:HG13	1:E:420:GLN:HG2	1.67	0.77
1:A:472:ARG:N	2:B:562:PRO:O	2.17	0.77
2:B:548:GLU:HB2	4:J:45:DG:OP1	1.85	0.77
1:E:390:ASN:ND2	3:Q:2:DA:OP1	2.18	0.77
2:F:548:GLU:HB3	4:R:45:DG:H3'	1.68	0.76
3:Q:6:DT:H2"	3:Q:7:DG:C8	2.21	0.76
1:E:331:ILE:HB	1:E:361:LEU:HD23	1.67	0.76
2:H:360:SER:HA	2:H:422:GLN:HB3	1.66	0.75
4:N:45:DG:N2	5:P:49:DT:O2	2.19	0.75
2:B:483:ARG:HA	2:B:501:VAL:HG21	1.69	0.75
2:H:534:ARG:NH1	5:P:50:DG:OP1	2.14	0.74
2:D:360:SER:HA	2:D:422:GLN:HB3	1.68	0.74
4:J:43:DC:O2	5:L:50:DG:N2	2.19	0.74
2:H:562:PRO:HG2	2:H:563:HIS:CD2	2.23	0.74
2:H:241:LYS:HB3	2:H:244:ARG:HH11	1.51	0.73
1:C:276:GLY:N	1:C:278:THR:HG22	2.00	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:279:ARG:HH21	4:N:41:DT:H4'	1.51	0.73
2:F:360:SER:HA	2:F:422:GLN:HB3	1.68	0.73
2:F:354:THR:HB	2:F:357:LYS:HD2	1.69	0.73
2:F:309:GLU:O	2:F:357:LYS:NZ	2.21	0.73
3:M:3:DA:N6	4:N:32:DT:H3	1.86	0.73
2:B:562:PRO:HG2	2:B:563:HIS:CD2	2.22	0.72
2:H:325:ILE:HG22	2:H:343:LEU:HD12	1.69	0.72
2:F:562:PRO:HG2	2:F:563:HIS:CD2	2.24	0.72
2:B:325:ILE:HG22	2:B:343:LEU:HD12	1.72	0.72
1:A:398:PHE:CE2	2:B:421:ALA:O	2.43	0.72
2:D:562:PRO:HG2	2:D:563:HIS:CD2	2.25	0.72
2:B:271:GLY:HA2	2:F:267:GLY:HA3	1.71	0.72
2:H:449:LYS:NZ	3:M:1:DG:H5"	2.05	0.72
2:D:241:LYS:HB3	2:D:244:ARG:HH11	1.51	0.72
2:F:314:VAL:O	2:F:361:LEU:HD12	1.90	0.71
5:T:50:DG:H2"	5:T:51:DC:H5'	1.73	0.71
1:A:394:ILE:CG2	2:B:450:LYS:HE3	2.20	0.71
1:C:543:LEU:HD23	2:D:478:LEU:HD22	1.71	0.71
2:D:534:ARG:NH1	5:X:50:DG:OP1	2.23	0.71
2:H:449:LYS:NZ	3:M:1:DG:P	2.64	0.71
1:G:481:GLN:HB2	2:H:481:VAL:HG13	1.72	0.71
3:I:6:DT:H2"	3:I:7:DG:C8	2.26	0.71
2:B:548:GLU:O	2:B:551:ARG:HB3	1.90	0.71
1:G:483:ARG:CB	2:H:470:LYS:HA	2.21	0.70
2:B:241:LYS:HB3	2:B:244:ARG:HH11	1.54	0.70
2:F:548:GLU:CB	4:R:45:DG:H3'	2.20	0.70
5:L:54:DG:H2"	5:L:55:DT:H71	1.73	0.70
2:B:547:PRO:HD2	4:J:45:DG:C3'	2.21	0.70
2:F:241:LYS:HB3	2:F:244:ARG:HH11	1.55	0.70
1:E:276:GLY:N	1:E:278:THR:HG22	2.03	0.70
2:B:548:GLU:HB2	4:J:45:DG:P	2.31	0.70
1:A:488:GLU:HG2	2:B:455:THR:HG22	1.73	0.69
2:F:296:ARG:NH2	2:F:301:GLU:HB2	2.06	0.69
2:B:296:ARG:NH2	2:B:301:GLU:HB2	2.07	0.69
1:E:472:ARG:NH2	2:F:457:PHE:HZ	1.89	0.69
1:G:331:ILE:HB	1:G:361:LEU:HD23	1.75	0.69
2:D:548:GLU:O	2:D:551:ARG:HB3	1.93	0.69
2:D:512:GLN:HA	2:D:515:GLN:HE21	1.57	0.69
2:F:541:THR:N	5:T:50:DG:O5'	2.25	0.69
1:C:486:SER:OG	4:V:30:DC:OP1	2.10	0.69
1:A:474:VAL:HG22	2:B:566:LEU:HD11	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:355:ARG:NH1	5:T:55:DT:OP1	2.25	0.69
1:G:534:PRO:HD2	3:M:9:DG:OP1	1.93	0.68
1:A:474:VAL:CG2	2:B:566:LEU:HD11	2.24	0.68
5:P:50:DG:H2"	5:P:51:DC:H5"	1.74	0.68
5:X:48:DC:H2"	5:X:49:DT:H5'	1.75	0.68
2:B:312:VAL:HG11	2:B:354:THR:HG21	1.74	0.68
1:G:474:VAL:HG21	2:H:556:GLN:OE1	1.92	0.68
2:D:296:ARG:NH2	2:D:301:GLU:HB2	2.08	0.68
2:D:325:ILE:HG22	2:D:343:LEU:HD12	1.75	0.68
2:F:325:ILE:HG22	2:F:343:LEU:HD12	1.75	0.68
2:H:548:GLU:O	2:H:551:ARG:HB3	1.94	0.68
2:H:483:ARG:HA	2:H:501:VAL:HG21	1.75	0.68
2:B:493:SER:HB3	5:L:51:DC:H3'	1.75	0.68
2:H:354:THR:HB	2:H:357:LYS:HD2	1.76	0.68
2:B:267:GLY:CA	2:F:270:LEU:HD23	2.24	0.68
1:A:472:ARG:HB2	2:B:562:PRO:CB	2.23	0.67
2:B:491:ARG:HA	5:L:52:DA:H4'	1.77	0.67
2:B:267:GLY:HA2	2:F:270:LEU:HD23	1.75	0.67
1:C:331:ILE:HB	1:C:361:LEU:HD23	1.77	0.67
1:A:386:GLN:HE22	2:B:441:LYS:HB3	1.60	0.67
1:G:530:ARG:NH1	4:N:29:DA:H5"	2.09	0.66
1:A:472:ARG:HB2	2:B:562:PRO:HB2	1.76	0.66
2:F:312:VAL:HG11	2:F:354:THR:HG21	1.77	0.66
1:A:545:CYS:HA	2:B:508:GLN:HE21	1.60	0.66
2:B:534:ARG:HE	2:B:534:ARG:HA	1.60	0.66
1:G:530:ARG:NE	4:N:29:DA:H5"	2.10	0.66
1:G:483:ARG:N	2:H:469:VAL:O	2.25	0.66
2:B:282:ILE:HG12	2:F:262:GLN:HE21	1.60	0.66
4:R:38:DA:H2"	4:R:39:DC:H5'	1.76	0.66
1:G:276:GLY:N	1:G:278:THR:HG22	2.08	0.66
1:A:390:ASN:HB3	1:A:394:ILE:HD12	1.75	0.66
2:H:541:THR:HG22	2:H:542:SER:O	1.95	0.66
1:E:304:HIS:ND1	1:E:460:ASN:O	2.29	0.66
1:G:481:GLN:O	2:H:481:VAL:HG22	1.96	0.66
1:E:551:THR:C	2:F:475:GLY:H	1.99	0.66
2:B:541:THR:N	5:L:50:DG:H5"	2.11	0.65
2:H:296:ARG:NH2	2:H:301:GLU:HB2	2.10	0.65
2:F:541:THR:HG22	2:F:542:SER:O	1.96	0.65
2:D:314:VAL:O	2:D:361:LEU:HD12	1.95	0.65
1:E:385:LEU:CD2	2:F:434:ASP:HB3	2.25	0.65
2:F:483:ARG:HA	2:F:501:VAL:HG21	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:534:ARG:HE	2:F:534:ARG:HA	1.60	0.65
1:G:550:LEU:HB2	2:H:505:PRO:O	1.97	0.65
4:N:28:DC:H5'	4:N:28:DC:H6	1.62	0.65
1:E:350:ARG:HE	3:Q:1:DG:P	2.20	0.64
1:G:350:ARG:HD3	2:H:461:LEU:HD13	1.79	0.64
1:E:348:ARG:HG2	5:T:55:DT:H72	1.79	0.64
1:E:486:SER:HB3	4:R:30:DC:OP1	1.95	0.64
2:D:534:ARG:HA	2:D:534:ARG:HE	1.63	0.64
1:E:277:GLU:HG3	1:E:307:ASP:HB3	1.80	0.64
2:B:541:THR:HG22	2:B:542:SER:O	1.97	0.64
1:A:386:GLN:NE2	2:B:441:LYS:HB3	2.12	0.64
3:Q:7:DG:O6	4:R:27:DA:N6	2.18	0.64
1:A:331:ILE:HB	1:A:361:LEU:HD23	1.77	0.64
2:D:489:LEU:N	2:D:489:LEU:HD12	2.13	0.64
1:G:310:TRP:O	1:G:328:LEU:N	2.27	0.64
2:D:459:PHE:HA	2:D:462:GLU:HB3	1.80	0.64
5:P:47:DT:H2"	5:P:48:DC:C6	2.32	0.64
2:H:523:ARG:HB3	2:H:554:TYR:CE1	2.33	0.64
4:J:42:DG:O6	5:L:51:DC:N4	2.27	0.64
1:E:279:ARG:HH21	4:R:40:DA:C5'	2.11	0.64
1:G:431:ARG:NH1	1:G:434:GLY:O	2.31	0.63
2:B:459:PHE:HA	2:B:462:GLU:HB3	1.81	0.63
2:D:523:ARG:HB3	2:D:554:TYR:CE1	2.33	0.63
2:H:459:PHE:HA	2:H:462:GLU:HB3	1.79	0.63
2:H:314:VAL:O	2:H:361:LEU:HD12	1.97	0.63
2:F:548:GLU:O	2:F:551:ARG:HB3	1.98	0.63
5:P:49:DT:H2"	5:P:50:DG:H5'	1.79	0.63
4:R:28:DC:H5'	4:R:28:DC:H6	1.64	0.63
2:F:449:LYS:HZ2	3:Q:1:DG:H3'	1.64	0.63
1:A:304:HIS:ND1	1:A:460:ASN:O	2.31	0.63
1:A:534:PRO:HA	1:A:537:SER:HB3	1.81	0.63
2:D:241:LYS:HB3	2:D:244:ARG:NH1	2.14	0.62
2:D:483:ARG:HA	2:D:501:VAL:HG21	1.80	0.62
1:E:486:SER:HB3	4:R:30:DC:OP2	1.99	0.62
1:A:398:PHE:CE2	2:B:422:GLN:HA	2.33	0.62
1:G:304:HIS:ND1	1:G:460:ASN:O	2.33	0.62
1:A:415:LEU:HD22	2:B:417:LEU:HD21	1.81	0.62
1:C:543:LEU:HD23	2:D:478:LEU:HB3	1.82	0.62
1:A:545:CYS:O	2:B:508:GLN:HG3	1.99	0.62
1:A:369:GLU:OE1	1:A:405:ILE:HG12	2.00	0.62
2:H:449:LYS:NZ	3:M:1:DG:OP2	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:ARG:HB3	2:B:562:PRO:O	1.99	0.62
3:I:3:DA:H61	4:J:32:DT:H3	1.48	0.62
2:D:354:THR:HB	2:D:357:LYS:HD2	1.80	0.62
2:B:271:GLY:CA	2:F:267:GLY:HA3	2.30	0.62
3:U:9:DG:H8	3:U:9:DG:OP2	1.83	0.62
4:N:39:DC:H2"	4:N:40:DA:C8	2.35	0.62
2:H:512:GLN:HA	2:H:515:GLN:HE21	1.64	0.61
2:F:491:ARG:HH21	2:F:552:ARG:NH1	1.98	0.61
1:A:394:ILE:HG12	2:B:446:ALA:HA	1.80	0.61
1:C:269:VAL:HG11	1:C:420:GLN:HA	1.82	0.61
4:V:44:DA:N1	5:X:49:DT:C4	2.69	0.61
2:H:238:THR:HA	2:H:241:LYS:HG3	1.81	0.61
2:B:318:ALA:HB2	2:B:364:VAL:O	2.01	0.61
1:E:477:ARG:CZ	2:F:488:GLN:OE1	2.47	0.61
1:C:273:VAL:HG13	1:C:308:PHE:CE1	2.36	0.61
1:G:371:HIS:NE2	1:G:401:ARG:HB3	2.15	0.61
2:F:493:SER:HB3	5:T:51:DC:H3'	1.83	0.61
2:F:523:ARG:HB3	2:F:554:TYR:CE1	2.36	0.61
3:I:9:DG:H8	3:I:9:DG:OP2	1.84	0.61
1:A:375:HIS:C	1:A:377:LEU:H	2.01	0.61
1:G:347:GLY:HA3	2:H:461:LEU:CD2	2.26	0.61
1:A:488:GLU:OE1	2:B:455:THR:HG21	2.01	0.61
1:A:474:VAL:HG21	2:B:556:GLN:OE1	2.01	0.61
2:D:261:LEU:HD11	2:D:282:ILE:HD12	1.83	0.60
1:G:486:SER:HB3	4:N:31:DA:OP2	2.01	0.60
2:H:491:ARG:HH21	2:H:552:ARG:NH1	1.98	0.60
2:D:541:THR:HG22	2:D:542:SER:O	2.01	0.60
1:A:337:LEU:HD23	1:A:377:LEU:HD11	1.83	0.60
1:E:329:ASP:O	1:E:363:ARG:HB2	2.02	0.60
1:G:269:VAL:HG11	1:G:420:GLN:HA	1.83	0.60
1:E:473:GLU:HG3	2:F:459:PHE:CZ	2.37	0.60
1:A:544:TYR:O	2:B:508:GLN:NE2	2.33	0.60
1:C:329:ASP:O	1:C:363:ARG:HB2	2.02	0.60
2:B:491:ARG:HH21	2:B:552:ARG:NH1	1.99	0.60
1:E:551:THR:C	2:F:475:GLY:N	2.55	0.60
1:G:543:LEU:HD23	2:H:478:LEU:HB3	1.82	0.60
1:C:481:GLN:O	2:D:469:VAL:N	2.35	0.60
2:D:547:PRO:HD2	4:V:45:DG:H3'	1.83	0.60
5:X:47:DT:H2"	5:X:48:DC:C6	2.37	0.60
3:Q:3:DA:N6	4:R:32:DT:H3	1.92	0.60
1:C:543:LEU:CD2	2:D:478:LEU:HB3	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:39:DC:H2"	4:R:40:DA:C8	2.36	0.60
5:L:52:DA:H2"	5:L:53:DT:OP2	2.01	0.59
1:G:474:VAL:HB	2:H:556:GLN:HE22	1.65	0.59
1:E:273:VAL:HG13	1:E:308:PHE:CE1	2.37	0.59
1:G:550:LEU:HD13	2:H:506:SER:CB	2.31	0.59
1:A:276:GLY:N	1:A:278:THR:HG22	2.13	0.59
5:T:54:DG:H2"	5:T:55:DT:H71	1.85	0.59
1:C:486:SER:HG	4:V:30:DC:P	2.25	0.59
1:C:337:LEU:HD23	1:C:377:LEU:HD11	1.85	0.59
1:G:329:ASP:O	1:G:363:ARG:HB2	2.02	0.59
4:R:38:DA:H8	4:R:38:DA:H5"	1.68	0.59
2:F:350:ILE:HG21	2:F:359:LEU:HD22	1.85	0.59
2:B:314:VAL:O	2:B:361:LEU:HD12	2.03	0.59
1:C:276:GLY:C	1:C:278:THR:H	2.05	0.59
1:G:534:PRO:HA	1:G:537:SER:HB3	1.84	0.59
1:A:527:ARG:NE	1:A:530:ARG:HB2	2.18	0.59
5:L:50:DG:H1'	5:L:51:DC:C2	2.38	0.58
2:D:301:GLU:HG2	2:D:306:TRP:HZ2	1.68	0.58
1:E:273:VAL:HG22	1:E:308:PHE:CD1	2.37	0.58
1:A:277:GLU:HG3	1:A:307:ASP:HB3	1.85	0.58
1:E:276:GLY:C	1:E:278:THR:H	2.07	0.58
2:B:354:THR:HB	2:B:357:LYS:HD2	1.85	0.58
2:D:491:ARG:HH21	2:D:552:ARG:NH1	2.00	0.58
2:F:512:GLN:HA	2:F:515:GLN:HE21	1.67	0.58
2:H:241:LYS:HB3	2:H:244:ARG:NH1	2.16	0.58
2:B:261:LEU:HD11	2:B:282:ILE:HD12	1.85	0.58
1:C:277:GLU:HG3	1:C:307:ASP:HB3	1.85	0.58
1:G:394:ILE:HG12	2:H:446:ALA:HA	1.84	0.58
1:E:390:ASN:HB3	1:E:394:ILE:HD12	1.86	0.58
2:F:238:THR:HA	2:F:241:LYS:HG3	1.84	0.58
1:A:371:HIS:NE2	1:A:401:ARG:HB3	2.19	0.58
1:A:380:PRO:O	1:A:383:THR:HB	2.03	0.58
1:C:390:ASN:HB3	1:C:394:ILE:HD12	1.86	0.58
4:R:43:DC:H2"	4:R:44:DA:C8	2.39	0.58
2:D:274:GLN:HE22	2:H:267:GLY:N	2.00	0.58
2:H:312:VAL:HG11	2:H:354:THR:HG21	1.85	0.58
1:A:488:GLU:HG2	2:B:455:THR:CG2	2.34	0.58
2:F:459:PHE:HA	2:F:462:GLU:HB3	1.86	0.58
1:C:371:HIS:NE2	1:C:401:ARG:HB3	2.18	0.58
1:A:489:LYS:NZ	4:J:30:DC:P	2.77	0.58
2:H:534:ARG:HA	2:H:534:ARG:HE	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:241:LYS:HB3	2:F:244:ARG:NH1	2.18	0.58
1:A:363:ARG:NH1	2:B:420:GLU:OE1	2.37	0.58
1:E:398:PHE:HA	2:F:422:GLN:OE1	2.03	0.58
1:A:499:THR:HG23	1:A:502:SER:H	1.69	0.58
2:F:301:GLU:HG2	2:F:306:TRP:HZ2	1.67	0.58
1:A:329:ASP:O	1:A:363:ARG:HB2	2.04	0.58
2:D:274:GLN:CD	2:H:267:GLY:H	2.06	0.58
1:C:407:GLU:CD	2:D:405:ARG:HH12	2.06	0.58
4:V:28:DC:H5'	4:V:28:DC:H6	1.67	0.57
5:X:52:DA:H2"	5:X:53:DT:C6	2.40	0.57
1:A:472:ARG:NH2	2:B:563:HIS:HE1	2.01	0.57
2:B:238:THR:HA	2:B:241:LYS:HG3	1.87	0.57
1:A:501:ALA:HB2	2:B:558:THR:HA	1.85	0.57
4:V:42:DG:N2	5:X:52:DA:C2	2.73	0.57
4:J:41:DT:H2"	4:J:42:DG:H8	1.68	0.57
4:V:43:DC:H2"	4:V:44:DA:H8	1.69	0.57
1:E:355:ARG:NH1	5:T:54:DG:H3'	2.20	0.57
4:N:38:DA:P	4:N:38:DA:O4'	2.63	0.57
1:E:371:HIS:NE2	1:E:401:ARG:HB3	2.20	0.57
2:B:491:ARG:HA	5:L:52:DA:O5'	2.05	0.57
2:D:541:THR:OG1	5:X:50:DG:H4'	2.04	0.57
2:D:315:LEU:HD12	2:D:432:LEU:HD21	1.87	0.57
3:Q:9:DG:OP2	3:Q:9:DG:H8	1.88	0.57
1:G:491:ALA:O	1:G:495:ASP:HB2	2.05	0.57
4:V:44:DA:C6	5:X:49:DT:O4	2.58	0.56
1:A:472:ARG:HG3	1:A:494:VAL:HG11	1.86	0.56
2:H:448:PHE:CD2	2:H:449:LYS:HE3	2.40	0.56
2:H:449:LYS:HZ2	3:M:1:DG:P	2.26	0.56
2:B:241:LYS:NZ	4:J:28:DC:OP1	2.27	0.56
1:A:472:ARG:O	1:A:473:GLU:C	2.43	0.56
2:B:241:LYS:HB3	2:B:244:ARG:NH1	2.18	0.56
3:M:5:DG:O6	4:N:29:DA:N6	2.38	0.56
2:D:286:ALA:O	2:D:353:LYS:HD3	2.05	0.56
2:B:491:ARG:HA	5:L:52:DA:C4'	2.34	0.56
2:H:314:VAL:HB	2:H:359:LEU:HD11	1.87	0.56
2:D:293:TRP:CD2	2:D:443:VAL:HG11	2.41	0.56
1:C:369:GLU:OE1	1:C:405:ILE:HG12	2.06	0.56
3:Q:9:DG:C6	4:R:25:DA:N6	2.74	0.56
2:F:287:VAL:HG13	2:F:290:SER:OG	2.05	0.56
1:G:277:GLU:HG3	1:G:307:ASP:HB3	1.87	0.56
2:F:318:ALA:HB2	2:F:364:VAL:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:9:DG:OP2	3:M:9:DG:H8	1.89	0.56
2:D:238:THR:HA	2:D:241:LYS:HG3	1.87	0.56
1:G:337:LEU:HD23	1:G:377:LEU:HD11	1.87	0.56
1:C:527:ARG:NE	1:C:530:ARG:HB2	2.21	0.56
1:G:390:ASN:HB3	1:G:394:ILE:HD12	1.88	0.55
1:E:421:ARG:HH21	2:F:414:ASP:CG	2.10	0.55
1:G:273:VAL:HG13	1:G:308:PHE:CE1	2.41	0.55
1:G:486:SER:O	1:G:490:ALA:N	2.37	0.55
2:F:489:LEU:N	2:F:489:LEU:HD12	2.22	0.55
1:G:472:ARG:N	2:H:562:PRO:O	2.40	0.55
2:F:449:LYS:HZ3	3:Q:1:DG:H3'	1.68	0.55
1:C:310:TRP:O	1:C:328:LEU:N	2.36	0.55
5:L:50:DG:H2"	5:L:51:DC:C6	2.42	0.55
1:C:304:HIS:ND1	1:C:460:ASN:O	2.40	0.55
4:R:39:DC:H2'	4:R:39:DC:OP2	2.07	0.55
1:A:273:VAL:HG13	1:A:308:PHE:CE1	2.41	0.55
2:H:459:PHE:HA	2:H:462:GLU:CB	2.37	0.55
1:E:273:VAL:HG22	1:E:308:PHE:HD1	1.72	0.55
1:A:489:LYS:HD2	1:A:532:LEU:CD1	2.37	0.55
1:E:269:VAL:HG11	1:E:420:GLN:HA	1.88	0.55
1:C:423:TYR:HD2	1:C:428:LEU:HD11	1.72	0.55
1:A:363:ARG:CZ	2:B:420:GLU:OE1	2.55	0.54
2:B:482:TRP:CZ3	2:B:507:PRO:HG3	2.42	0.54
1:E:534:PRO:HA	1:E:537:SER:HB3	1.88	0.54
2:F:261:LEU:HD11	2:F:282:ILE:HD12	1.88	0.54
2:F:433:ALA:O	2:F:436:THR:HB	2.07	0.54
2:D:312:VAL:HG11	2:D:354:THR:HG21	1.88	0.54
1:G:489:LYS:NZ	4:N:30:DC:P	2.80	0.54
2:H:293:TRP:CD2	2:H:443:VAL:HG11	2.41	0.54
1:A:472:ARG:CB	2:B:562:PRO:HB2	2.37	0.54
1:C:534:PRO:HA	1:C:537:SER:HB3	1.90	0.54
2:D:282:ILE:H	2:H:262:GLN:HE21	1.55	0.54
1:A:504:LEU:HD13	2:B:511:VAL:HG21	1.90	0.54
4:N:41:DT:H2"	4:N:42:DG:N7	2.22	0.54
4:V:28:DC:H2"	4:V:29:DA:H5'	1.90	0.54
2:B:512:GLN:HA	2:B:515:GLN:HE21	1.73	0.54
1:E:369:GLU:OE1	1:E:405:ILE:HG12	2.07	0.54
2:B:432:LEU:O	2:B:436:THR:OG1	2.14	0.54
2:B:446:ALA:HB3	2:B:447:PRO:HD3	1.89	0.54
1:C:534:PRO:HD2	3:U:9:DG:OP1	2.08	0.54
1:A:491:ALA:O	1:A:495:ASP:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:48:DC:H2"	5:L:49:DT:H72	1.89	0.54
1:C:302:LYS:NZ	5:X:54:DG:H4'	2.23	0.54
1:A:394:ILE:O	2:B:450:LYS:HE2	2.08	0.54
1:C:384:LEU:O	1:C:387:ALA:HB3	2.08	0.54
1:A:499:THR:HG22	1:A:502:SER:HB2	1.89	0.53
1:G:394:ILE:O	2:H:450:LYS:HE2	2.09	0.53
2:B:301:GLU:HG2	2:B:306:TRP:HZ2	1.73	0.53
2:H:301:GLU:HG2	2:H:306:TRP:HZ2	1.74	0.53
5:X:48:DC:H2'	5:X:49:DT:H71	1.91	0.53
1:C:538:ARG:NH2	2:D:473:LEU:O	2.41	0.53
1:C:484:GLY:C	4:V:30:DC:H4'	2.29	0.53
2:F:296:ARG:HB3	2:F:306:TRP:CZ3	2.43	0.53
1:E:386:GLN:NE2	2:F:438:ALA:HA	2.17	0.53
1:G:489:LYS:HZ1	4:N:30:DC:P	2.30	0.53
1:A:269:VAL:HG11	1:A:420:GLN:HA	1.91	0.53
2:D:459:PHE:HA	2:D:462:GLU:CB	2.39	0.53
2:H:313:LEU:HD23	2:H:314:VAL:N	2.23	0.53
1:G:262:LEU:HD22	1:G:314:GLU:HB3	1.90	0.53
1:C:489:LYS:NZ	4:V:30:DC:OP1	2.39	0.52
2:D:314:VAL:HB	2:D:359:LEU:HD11	1.91	0.52
2:B:433:ALA:O	2:B:436:THR:HB	2.09	0.52
1:G:398:PHE:HE2	2:H:421:ALA:O	1.92	0.52
2:F:446:ALA:HB3	2:F:447:PRO:HD3	1.91	0.52
2:B:491:ARG:HA	5:L:52:DA:C5'	2.39	0.52
4:J:41:DT:H2"	4:J:42:DG:C8	2.44	0.52
2:B:309:GLU:C	2:B:311:THR:H	2.13	0.52
4:J:28:DC:H6	4:J:28:DC:H5'	1.73	0.52
2:B:482:TRP:CE3	2:B:507:PRO:HG3	2.45	0.52
1:C:491:ALA:O	1:C:495:ASP:HB2	2.08	0.52
2:D:547:PRO:HD2	4:V:45:DG:C3'	2.39	0.52
1:A:472:ARG:CB	2:B:562:PRO:O	2.57	0.52
1:C:472:ARG:HG3	1:C:494:VAL:HG11	1.92	0.52
1:E:407:GLU:CD	2:F:405:ARG:HH12	2.12	0.52
1:C:483:ARG:HD3	4:V:31:DA:C4'	2.37	0.52
2:B:296:ARG:HH22	2:B:301:GLU:HB2	1.75	0.52
2:B:459:PHE:HA	2:B:462:GLU:CB	2.39	0.52
2:H:433:ALA:O	2:H:436:THR:HB	2.10	0.52
4:N:45:DG:C8	4:N:45:DG:H5'	2.44	0.52
5:P:48:DC:H2"	5:P:49:DT:O5'	2.09	0.52
2:D:296:ARG:HB3	2:D:306:TRP:CZ3	2.45	0.52
1:G:271:LEU:HA	1:G:310:TRP:CD1	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:293:TRP:CZ2	2:H:443:VAL:HG21	2.44	0.52
2:B:346:PHE:CE2	2:B:350:ILE:HD11	2.44	0.52
1:C:380:PRO:O	1:C:383:THR:HB	2.09	0.52
4:R:28:DC:H2"	4:R:29:DA:H5'	1.92	0.52
5:X:50:DG:H8	5:X:50:DG:H5"	1.74	0.52
1:G:472:ARG:CB	2:H:562:PRO:HB2	2.40	0.52
2:F:346:PHE:CE2	2:F:350:ILE:HD11	2.45	0.52
1:E:491:ALA:O	1:E:495:ASP:HB2	2.09	0.52
2:H:545:ILE:HG23	2:H:549:LEU:HD23	1.92	0.52
1:C:275:ILE:CD1	1:C:278:THR:HG21	2.31	0.52
4:R:45:DG:N2	5:T:48:DC:O2	2.43	0.52
5:X:47:DT:H2"	5:X:48:DC:C5	2.45	0.52
1:A:499:THR:OG1	2:B:559:THR:O	2.15	0.51
2:H:517:CYS:HB2	2:H:523:ARG:HG3	1.90	0.51
2:H:261:LEU:HD11	2:H:282:ILE:HD12	1.92	0.51
4:V:40:DA:H2"	4:V:41:DT:C6	2.45	0.51
4:N:28:DC:H5'	4:N:28:DC:C6	2.42	0.51
3:I:3:DA:N6	4:J:32:DT:H3	2.06	0.51
2:D:350:ILE:HG21	2:D:359:LEU:HD22	1.93	0.51
1:C:317:PRO:HB3	1:C:323:PRO:HA	1.92	0.51
1:E:337:LEU:HD23	1:E:377:LEU:HD11	1.92	0.51
1:G:276:GLY:C	1:G:278:THR:H	2.12	0.51
2:D:296:ARG:HH22	2:D:301:GLU:HB2	1.74	0.51
2:D:318:ALA:HB2	2:D:364:VAL:O	2.11	0.51
2:D:237:VAL:O	2:D:241:LYS:HG3	2.11	0.51
2:F:296:ARG:HB3	2:F:306:TRP:CH2	2.45	0.51
1:C:524:LYS:HG3	1:C:529:GLN:CD	2.31	0.51
1:A:347:GLY:CA	2:B:461:LEU:HD22	2.41	0.51
1:G:512:THR:HG22	1:G:514:LYS:H	1.75	0.51
2:B:548:GLU:OE1	2:B:552:ARG:HD3	2.11	0.51
1:G:472:ARG:HG3	1:G:494:VAL:HG11	1.92	0.51
4:R:40:DA:H3'	4:R:40:DA:P	2.50	0.51
1:A:273:VAL:HG22	1:A:308:PHE:CD1	2.46	0.51
1:E:310:TRP:O	1:E:328:LEU:N	2.36	0.51
1:G:527:ARG:NE	1:G:530:ARG:HB2	2.25	0.51
2:D:548:GLU:OE1	2:D:552:ARG:HD3	2.10	0.51
1:A:411:TYR:HH	2:B:416:GLN:CD	2.10	0.51
1:C:375:HIS:HA	1:C:377:LEU:HG	1.93	0.51
2:B:260:LEU:HB2	2:B:289:CYS:HA	1.93	0.51
3:Q:10:DT:O4	4:R:23:DA:N6	2.43	0.51
1:E:489:LYS:HD2	1:E:532:LEU:CD1	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:432:LEU:O	2:D:436:THR:OG1	2.24	0.51
1:A:512:THR:HG22	1:A:514:LYS:H	1.75	0.51
2:H:541:THR:OG1	5:P:50:DG:P	2.69	0.51
2:H:296:ARG:HB3	2:H:306:TRP:CZ3	2.46	0.51
1:A:474:VAL:HB	2:B:556:GLN:CD	2.31	0.51
1:C:494:VAL:O	1:C:498:SER:HA	2.11	0.51
1:E:473:GLU:HG3	2:F:459:PHE:CE2	2.46	0.51
1:E:355:ARG:HH22	5:T:54:DG:H5"	1.76	0.51
2:F:548:GLU:OE1	2:F:552:ARG:HD3	2.11	0.50
4:N:28:DC:C2'	4:N:29:DA:H5'	2.35	0.50
3:I:1:DG:N2	3:I:2:DA:N3	2.58	0.50
2:H:548:GLU:OE1	2:H:552:ARG:HD3	2.11	0.50
1:A:545:CYS:HA	2:B:508:GLN:NE2	2.25	0.50
2:F:517:CYS:HB2	2:F:523:ARG:HG3	1.93	0.50
2:F:432:LEU:O	2:F:436:THR:OG1	2.15	0.50
2:H:462:GLU:HG2	2:H:463:SER:N	2.26	0.50
2:D:346:PHE:CE2	2:D:350:ILE:HD11	2.46	0.50
1:A:400:LYS:HG3	1:A:411:TYR:CZ	2.47	0.50
1:A:274:ASP:HB2	1:A:303:LEU:HB2	1.93	0.50
5:X:50:DG:H2"	5:X:51:DC:O4'	2.10	0.50
1:G:369:GLU:OE1	1:G:405:ILE:HG12	2.11	0.50
4:N:25:DA:H2"	4:N:26:DC:O4'	2.11	0.50
2:H:491:ARG:NH2	2:H:552:ARG:NH1	2.59	0.50
1:C:423:TYR:CD2	1:C:428:LEU:HD11	2.47	0.50
2:H:247:GLU:HG2	2:H:250:LYS:HB2	1.93	0.50
2:H:287:VAL:O	2:H:290:SER:OG	2.19	0.50
3:U:10:DT:O4	4:V:23:DA:N6	2.44	0.50
2:F:313:LEU:HD23	2:F:314:VAL:N	2.27	0.50
2:H:315:LEU:HD12	2:H:432:LEU:HD21	1.93	0.50
2:F:296:ARG:HH22	2:F:301:GLU:HB2	1.75	0.50
2:D:458:SER:O	2:D:462:GLU:HB2	2.12	0.50
2:D:517:CYS:HB2	2:D:523:ARG:HG3	1.94	0.50
4:R:28:DC:H5'	4:R:28:DC:C6	2.45	0.50
1:E:421:ARG:NH2	2:F:414:ASP:OD1	2.36	0.50
1:G:308:PHE:HB2	1:G:332:VAL:HB	1.94	0.50
1:A:400:LYS:HG3	1:A:411:TYR:CE1	2.47	0.50
1:A:303:LEU:HD11	1:A:309:VAL:HG22	1.93	0.50
4:J:38:DA:H2"	4:J:39:DC:C6	2.47	0.50
2:D:446:ALA:HB3	2:D:447:PRO:HD3	1.93	0.50
2:D:313:LEU:HD23	2:D:314:VAL:N	2.27	0.50
2:D:472:ASP:OD1	2:D:476:ARG:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:324:MET:HG2	2:B:342:THR:N	2.26	0.49
1:C:472:ARG:N	2:D:562:PRO:O	2.45	0.49
2:D:346:PHE:O	2:D:350:ILE:HG13	2.11	0.49
1:G:375:HIS:HA	1:G:377:LEU:HG	1.94	0.49
2:B:315:LEU:HD12	2:B:432:LEU:HD21	1.94	0.49
1:A:414:LEU:C	2:B:413:VAL:HG11	2.33	0.49
2:F:472:ASP:OD1	2:F:476:ARG:HB2	2.12	0.49
2:H:318:ALA:HB2	2:H:364:VAL:O	2.12	0.49
1:A:276:GLY:C	1:A:278:THR:H	2.15	0.49
1:A:333:GLU:OE1	1:A:352:GLN:NE2	2.45	0.49
3:M:8:DT:H2'	3:M:9:DG:C8	2.48	0.49
1:C:499:THR:HG23	1:C:502:SER:H	1.77	0.49
1:A:308:PHE:HB2	1:A:332:VAL:HB	1.95	0.49
1:E:407:GLU:O	1:E:411:TYR:N	2.40	0.49
4:J:38:DA:H2"	4:J:39:DC:H6	1.77	0.49
2:D:260:LEU:HB2	2:D:289:CYS:HA	1.94	0.49
2:F:496:MET:CE	5:T:51:DC:H5"	2.43	0.49
5:T:51:DC:H2"	5:T:52:DA:OP2	2.12	0.49
2:F:346:PHE:O	2:F:350:ILE:HG13	2.12	0.49
1:C:482:VAL:HA	2:D:469:VAL:O	2.13	0.49
2:H:472:ASP:OD1	2:H:476:ARG:HB2	2.13	0.49
1:E:350:ARG:NE	3:Q:1:DG:P	2.86	0.49
1:A:485:VAL:O	4:J:31:DA:OP1	2.31	0.49
2:H:293:TRP:CG	2:H:443:VAL:HG11	2.47	0.49
2:B:489:LEU:HD12	2:B:489:LEU:N	2.28	0.49
5:T:54:DG:H2"	5:T:55:DT:C7	2.43	0.49
1:C:341:CYS:SG	1:C:384:LEU:HD21	2.53	0.49
1:A:431:ARG:HG2	1:A:432:PRO:HD2	1.95	0.48
4:N:42:DG:OP2	4:N:42:DG:H8	1.96	0.48
1:A:375:HIS:HA	1:A:377:LEU:HG	1.94	0.48
2:B:293:TRP:CZ2	2:B:443:VAL:HG21	2.48	0.48
1:E:279:ARG:NH2	4:R:40:DA:O5'	2.46	0.48
2:D:489:LEU:N	2:D:489:LEU:CD1	2.75	0.48
2:H:458:SER:O	2:H:462:GLU:HB2	2.12	0.48
1:A:271:LEU:HA	1:A:310:TRP:CD1	2.48	0.48
2:D:545:ILE:HG23	2:D:549:LEU:HD23	1.95	0.48
1:G:423:TYR:HD2	1:G:428:LEU:HD11	1.78	0.48
1:A:472:ARG:HG3	1:A:494:VAL:CG1	2.43	0.48
2:D:491:ARG:NH2	2:D:552:ARG:NH1	2.61	0.48
4:R:40:DA:C5	4:R:41:DT:C2	3.01	0.48
1:A:304:HIS:HB3	1:A:463:ALA:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:308:PHE:HB2	1:E:332:VAL:HB	1.94	0.48
2:D:433:ALA:O	2:D:436:THR:HB	2.13	0.48
1:G:398:PHE:CE2	2:H:422:GLN:HA	2.49	0.48
2:B:296:ARG:HB3	2:B:306:TRP:CZ3	2.48	0.48
2:H:517:CYS:CB	2:H:523:ARG:HG3	2.42	0.48
1:A:414:LEU:HB3	2:B:413:VAL:HG21	1.94	0.48
1:G:384:LEU:O	1:G:387:ALA:HB3	2.13	0.48
2:H:489:LEU:HD12	2:H:489:LEU:N	2.27	0.48
2:F:293:TRP:CD2	2:F:443:VAL:HG11	2.48	0.48
2:F:491:ARG:HA	5:T:52:DA:H5'	1.94	0.48
1:E:392:GLN:NE2	2:F:435:PHE:HZ	2.11	0.48
2:B:491:ARG:NH2	2:B:552:ARG:NH1	2.62	0.48
5:L:52:DA:H1'	5:L:53:DT:C6	2.49	0.48
2:D:546:GLY:HA3	4:V:45:DG:H3'	1.95	0.48
2:F:459:PHE:HA	2:F:462:GLU:CB	2.44	0.48
1:C:273:VAL:HG22	1:C:308:PHE:CD1	2.48	0.48
2:B:458:SER:O	2:B:462:GLU:HB2	2.13	0.48
2:B:449:LYS:NZ	3:I:1:DG:H3'	2.28	0.48
1:A:494:VAL:O	1:A:498:SER:HA	2.14	0.48
1:A:472:ARG:HB2	2:B:562:PRO:CA	2.44	0.48
2:H:449:LYS:NZ	3:M:1:DG:C5'	2.75	0.48
2:D:256:LEU:HD23	2:D:260:LEU:HD23	1.95	0.48
2:F:237:VAL:O	2:F:241:LYS:HG3	2.13	0.48
2:H:296:ARG:HB3	2:H:306:TRP:CH2	2.48	0.48
4:J:28:DC:C6	4:J:28:DC:H5'	2.49	0.48
2:B:346:PHE:O	2:B:350:ILE:HG13	2.13	0.48
5:L:50:DG:H5'	5:L:50:DG:N9	2.26	0.48
1:G:489:LYS:HD2	1:G:532:LEU:CD1	2.44	0.48
2:D:512:GLN:HA	2:D:515:GLN:NE2	2.28	0.48
2:B:462:GLU:HG2	2:B:463:SER:N	2.29	0.48
2:F:545:ILE:HG23	2:F:549:LEU:HD23	1.95	0.48
2:H:252:ILE:HD11	2:H:295:ARG:NH1	2.28	0.48
1:E:494:VAL:O	1:E:498:SER:HA	2.14	0.47
2:F:493:SER:HB3	5:T:51:DC:C3'	2.44	0.47
2:F:491:ARG:NH2	2:F:552:ARG:NH1	2.63	0.47
3:I:9:DG:C6	4:J:25:DA:N6	2.82	0.47
2:H:296:ARG:HH22	2:H:301:GLU:HB2	1.78	0.47
4:V:28:DC:C6	4:V:28:DC:H5'	2.49	0.47
2:D:417:LEU:HD23	2:D:417:LEU:HA	1.63	0.47
1:E:384:LEU:O	1:E:387:ALA:HB3	2.14	0.47
5:L:48:DC:H2"	5:L:49:DT:C7	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:28:DC:H2"	4:J:29:DA:H5'	1.95	0.47
1:C:512:THR:HG22	1:C:514:LYS:H	1.78	0.47
2:B:412:LEU:HA	2:B:412:LEU:HD12	1.72	0.47
2:B:295:ARG:HB3	2:B:307:VAL:HG12	1.96	0.47
5:X:52:DA:C4	5:X:53:DT:C2	3.02	0.47
1:A:486:SER:CB	4:J:30:DC:H3'	2.34	0.47
1:E:386:GLN:HE22	2:F:438:ALA:CA	2.20	0.47
1:C:405:ILE:O	1:C:408:SER:HB2	2.15	0.47
2:B:523:ARG:HB3	2:B:554:TYR:CE1	2.50	0.47
2:F:248:CYS:SG	2:F:249:LEU:N	2.87	0.47
1:E:477:ARG:HH21	2:F:488:GLN:CD	2.18	0.47
2:H:309:GLU:C	2:H:311:THR:H	2.16	0.47
1:A:500:PRO:HG2	2:B:556:GLN:O	2.14	0.47
4:R:25:DA:H2"	4:R:26:DC:O4'	2.14	0.47
1:G:308:PHE:HE2	1:G:334:ARG:HB2	1.79	0.47
2:B:256:LEU:HD23	2:B:260:LEU:HD23	1.95	0.47
1:G:544:TYR:O	2:H:508:GLN:NE2	2.28	0.47
2:B:237:VAL:O	2:B:241:LYS:HG3	2.15	0.47
1:G:550:LEU:HD13	2:H:506:SER:HB2	1.94	0.47
1:E:271:LEU:HA	1:E:310:TRP:CD1	2.49	0.47
1:G:484:GLY:HA3	1:G:536:LEU:HD21	1.97	0.47
1:A:317:PRO:HB3	1:A:323:PRO:HA	1.95	0.47
2:F:491:ARG:NH1	4:R:44:DA:H4'	2.30	0.47
1:C:484:GLY:HA3	1:C:536:LEU:HD21	1.96	0.47
1:G:486:SER:H	1:G:489:LYS:HB2	1.80	0.47
1:G:539:THR:HG21	2:H:471:VAL:HG11	1.96	0.47
2:D:247:GLU:HG2	2:D:250:LYS:HB2	1.97	0.47
2:F:490:ASN:O	2:F:552:ARG:NH2	2.46	0.47
3:U:5:DG:C2	4:V:31:DA:C2	3.03	0.47
2:F:458:SER:O	2:F:462:GLU:HB2	2.13	0.47
1:A:262:LEU:HB2	1:A:428:LEU:HB2	1.97	0.47
1:C:351:GLU:O	1:C:355:ARG:HG3	2.15	0.47
1:G:318:ARG:O	1:G:320:PRO:HD3	2.14	0.47
2:B:296:ARG:HB3	2:B:306:TRP:CH2	2.49	0.47
4:V:25:DA:H2"	4:V:26:DC:O4'	2.15	0.47
1:A:347:GLY:HA3	2:B:461:LEU:HD22	1.97	0.47
2:D:329:LYS:NZ	2:D:414:ASP:OD2	2.34	0.47
1:E:353:LYS:NZ	1:E:395:ASP:OD2	2.42	0.47
1:A:273:VAL:HG22	1:A:308:PHE:HD1	1.79	0.47
2:D:517:CYS:CB	2:D:523:ARG:HG3	2.45	0.47
1:G:380:PRO:O	1:G:383:THR:HB	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:315:LEU:HD12	2:F:432:LEU:HD21	1.96	0.46
1:A:394:ILE:O	2:B:450:LYS:CE	2.63	0.46
1:C:308:PHE:O	1:C:331:ILE:HG13	2.15	0.46
1:E:551:THR:O	2:F:474:ALA:HB1	2.15	0.46
1:G:550:LEU:HD13	2:H:506:SER:HB3	1.96	0.46
2:H:446:ALA:HB3	2:H:447:PRO:HD3	1.96	0.46
2:B:472:ASP:OD1	2:B:476:ARG:HB2	2.15	0.46
2:B:352:ALA:HB1	2:D:352:ALA:O	2.14	0.46
2:H:492:VAL:N	5:P:52:DA:OP1	2.48	0.46
4:V:39:DC:H2"	4:V:40:DA:C8	2.50	0.46
4:J:30:DC:C2	4:J:31:DA:C8	3.02	0.46
2:D:483:ARG:NH1	2:D:494:LEU:HD12	2.30	0.46
2:H:346:PHE:CE2	2:H:350:ILE:HD11	2.49	0.46
1:C:499:THR:HG22	1:C:502:SER:HB2	1.97	0.46
2:D:295:ARG:HB3	2:D:307:VAL:HG12	1.98	0.46
2:F:541:THR:OG1	5:T:50:DG:H4'	2.15	0.46
2:D:296:ARG:HB3	2:D:306:TRP:CH2	2.50	0.46
2:B:313:LEU:HD23	2:B:314:VAL:N	2.31	0.46
1:G:317:PRO:HG2	1:G:320:PRO:HA	1.98	0.46
2:H:260:LEU:HB2	2:H:289:CYS:HA	1.96	0.46
4:V:38:DA:H2"	4:V:39:DC:OP2	2.16	0.46
2:H:241:LYS:HA	2:H:244:ARG:CD	2.45	0.46
2:F:314:VAL:HB	2:F:359:LEU:HD11	1.97	0.46
2:H:481:VAL:O	2:H:485:GLN:HG3	2.16	0.46
1:C:308:PHE:HB2	1:C:332:VAL:HB	1.97	0.46
1:C:262:LEU:HD22	1:C:314:GLU:HB3	1.97	0.46
1:E:318:ARG:O	1:E:320:PRO:HD3	2.16	0.46
1:E:371:HIS:HB2	1:E:403:ALA:HA	1.97	0.46
1:C:431:ARG:HG2	1:C:432:PRO:HD2	1.97	0.46
2:H:241:LYS:HA	2:H:244:ARG:HD2	1.98	0.46
1:A:545:CYS:C	2:B:508:GLN:HG3	2.35	0.46
2:B:417:LEU:HA	2:B:417:LEU:HD23	1.68	0.46
4:V:28:DC:C2'	4:V:29:DA:H5'	2.46	0.46
2:D:481:VAL:O	2:D:485:GLN:HG3	2.16	0.46
1:G:350:ARG:CD	2:H:461:LEU:HD13	2.44	0.46
1:A:486:SER:O	1:A:490:ALA:N	2.41	0.46
1:A:405:ILE:O	1:A:408:SER:HB2	2.14	0.46
1:A:543:LEU:O	2:B:507:PRO:HG2	2.15	0.46
1:A:414:LEU:HB3	2:B:413:VAL:HG11	1.97	0.46
2:H:405:ARG:O	2:H:405:ARG:HG3	2.16	0.46
1:G:400:LYS:HG3	1:G:411:TYR:CZ	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:541:THR:C	2:H:542:SER:O	2.47	0.46
1:A:415:LEU:CD2	2:B:417:LEU:HD21	2.45	0.46
2:D:293:TRP:CG	2:D:443:VAL:HG11	2.51	0.46
1:E:486:SER:O	1:E:490:ALA:N	2.38	0.46
2:H:346:PHE:O	2:H:350:ILE:HG13	2.15	0.46
2:B:541:THR:C	2:B:542:SER:O	2.49	0.46
2:H:237:VAL:O	2:H:241:LYS:HG3	2.16	0.46
2:H:448:PHE:HD2	2:H:449:LYS:HE3	1.79	0.46
2:D:462:GLU:HG2	2:D:463:SER:N	2.29	0.46
2:D:287:VAL:HG13	2:D:290:SER:OG	2.16	0.46
5:X:52:DA:C2	5:X:53:DT:O2	2.69	0.45
2:D:270:LEU:HG	2:H:267:GLY:HA3	1.98	0.45
3:I:1:DG:N2	3:I:2:DA:C2	2.84	0.45
2:F:517:CYS:CB	2:F:523:ARG:HG3	2.46	0.45
2:B:293:TRP:CD2	2:B:443:VAL:HG11	2.51	0.45
1:E:484:GLY:HA3	1:E:536:LEU:HD21	1.97	0.45
1:C:486:SER:HB3	4:V:30:DC:O5'	2.15	0.45
1:E:421:ARG:NH2	2:F:414:ASP:CG	2.69	0.45
1:C:317:PRO:HG2	1:C:320:PRO:HA	1.99	0.45
2:D:541:THR:OG1	5:X:50:DG:C4'	2.64	0.45
1:A:474:VAL:HG21	2:B:566:LEU:HD11	1.97	0.45
1:C:337:LEU:HD22	1:C:370:GLU:O	2.16	0.45
1:C:310:TRP:HH2	1:C:415:LEU:HD13	1.80	0.45
2:D:324:MET:HG2	2:D:342:THR:N	2.31	0.45
1:A:481:GLN:OE1	2:B:488:GLN:NE2	2.49	0.45
1:A:497:TYR:HE2	1:A:520:LEU:CD2	2.28	0.45
1:A:499:THR:CG2	2:B:560:LEU:HA	2.23	0.45
1:C:302:LYS:NZ	5:X:54:DG:O3'	2.42	0.45
3:M:7:DG:O6	4:N:27:DA:N1	2.49	0.45
2:H:541:THR:OG1	5:P:50:DG:OP1	2.34	0.45
2:F:462:GLU:HG2	2:F:463:SER:N	2.31	0.45
4:R:28:DC:C2'	4:R:29:DA:H5'	2.46	0.45
2:B:517:CYS:HB2	2:B:523:ARG:HG3	1.97	0.45
1:G:333:GLU:OE1	1:G:352:GLN:NE2	2.50	0.45
2:F:324:MET:HG2	2:F:342:THR:N	2.31	0.45
2:D:534:ARG:NH1	5:X:50:DG:P	2.80	0.45
1:A:278:THR:OG1	1:A:278:THR:O	2.33	0.45
2:H:312:VAL:HG12	2:H:357:LYS:CB	2.47	0.45
1:G:472:ARG:HB2	2:H:562:PRO:HB2	1.98	0.45
1:E:317:PRO:HG2	1:E:320:PRO:HA	1.98	0.45
1:G:400:LYS:HG3	1:G:411:TYR:CE1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:418:GLY:HA3	2:H:417:LEU:CD1	2.47	0.45
1:G:524:LYS:HG3	1:G:529:GLN:CD	2.36	0.45
1:G:489:LYS:HZ3	4:N:30:DC:C5'	2.30	0.45
5:L:54:DG:C2'	5:L:55:DT:H71	2.44	0.45
3:U:8:DT:H2'	3:U:9:DG:C8	2.51	0.45
1:C:479:LEU:HG	1:C:493:LEU:HD13	1.99	0.45
2:D:309:GLU:C	2:D:311:THR:H	2.18	0.45
2:H:449:LYS:HZ2	3:M:1:DG:H5"	1.81	0.45
2:D:293:TRP:CZ2	2:D:443:VAL:HG21	2.51	0.45
2:B:342:THR:O	2:B:342:THR:OG1	2.35	0.45
2:F:256:LEU:HD23	2:F:260:LEU:HD23	1.99	0.45
1:E:499:THR:HG22	1:E:502:SER:HB2	1.98	0.45
4:J:23:DA:H2'	4:J:24:DG:C8	2.52	0.45
1:A:489:LYS:HZ3	4:J:30:DC:C5'	2.30	0.45
1:C:273:VAL:HG22	1:C:308:PHE:HD1	1.82	0.45
1:A:310:TRP:HH2	1:A:415:LEU:HD13	1.82	0.45
2:H:295:ARG:HB3	2:H:307:VAL:HG12	1.98	0.45
1:G:317:PRO:HB3	1:G:323:PRO:HA	1.98	0.45
1:A:474:VAL:HB	2:B:556:GLN:HE22	1.80	0.45
2:H:541:THR:HG1	5:P:50:DG:C5'	2.28	0.45
5:T:50:DG:C2'	5:T:51:DC:H5'	2.43	0.45
2:H:449:LYS:HZ3	3:M:1:DG:P	2.40	0.45
1:E:528:LEU:HD22	2:F:236:LEU:CD2	2.47	0.45
4:R:40:DA:N7	4:R:41:DT:N3	2.64	0.44
1:G:351:GLU:O	1:G:355:ARG:HG3	2.17	0.44
2:B:273:LEU:HD12	2:B:273:LEU:HA	1.63	0.44
3:I:7:DG:H2'	3:I:8:DT:H6	1.82	0.44
1:C:533:GLY:HA3	3:U:9:DG:O5'	2.16	0.44
2:F:260:LEU:HB2	2:F:289:CYS:HA	1.98	0.44
1:E:499:THR:HG23	1:E:502:SER:H	1.81	0.44
4:J:25:DA:H2"	4:J:26:DC:O4'	2.17	0.44
3:U:9:DG:C6	4:V:25:DA:N6	2.85	0.44
1:G:394:ILE:O	2:H:450:LYS:CE	2.66	0.44
1:E:267:TYR:OH	1:E:423:TYR:O	2.34	0.44
4:J:43:DC:N3	5:L:50:DG:N1	2.59	0.44
3:I:8:DT:H2'	3:I:9:DG:C8	2.53	0.44
1:G:308:PHE:O	1:G:331:ILE:HG13	2.17	0.44
1:A:384:LEU:O	1:A:387:ALA:HB3	2.18	0.44
2:D:273:LEU:HA	2:D:273:LEU:HD12	1.64	0.44
1:A:407:GLU:O	1:A:411:TYR:N	2.44	0.44
1:C:271:LEU:HA	1:C:310:TRP:CD1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:541:THR:N	5:T:50:DG:P	2.91	0.44
4:V:40:DA:H61	5:X:52:DA:N6	2.15	0.44
4:V:42:DG:H1	5:X:51:DC:H42	1.65	0.44
1:G:472:ARG:HB3	2:H:562:PRO:HB2	1.98	0.44
2:F:309:GLU:C	2:F:311:THR:H	2.19	0.44
1:G:481:GLN:HG3	2:H:485:GLN:HA	1.99	0.44
1:A:543:LEU:HD22	1:A:550:LEU:HD21	1.99	0.44
1:E:400:LYS:HG3	1:E:411:TYR:CE1	2.53	0.44
2:F:293:TRP:CZ2	2:F:443:VAL:HG21	2.53	0.44
2:B:446:ALA:O	2:B:450:LYS:HG2	2.17	0.44
2:F:254:VAL:O	2:F:256:LEU:HD12	2.18	0.44
1:G:303:LEU:HD11	1:G:309:VAL:HG22	2.00	0.44
1:E:497:TYR:HE2	1:E:520:LEU:CD2	2.31	0.44
1:E:481:GLN:HG3	2:F:481:VAL:HG13	2.00	0.44
2:F:481:VAL:O	2:F:485:GLN:HG3	2.15	0.44
2:B:241:LYS:HA	2:B:244:ARG:CD	2.48	0.44
1:A:414:LEU:O	2:B:413:VAL:HG11	2.18	0.44
1:E:262:LEU:HB2	1:E:428:LEU:HB2	1.99	0.44
3:M:2:DA:N1	4:N:33:DT:O4	2.51	0.44
1:E:472:ARG:NH2	2:F:457:PHE:CZ	2.79	0.44
1:G:543:LEU:HD22	1:G:550:LEU:HD21	1.99	0.44
1:G:550:LEU:HD22	2:H:506:SER:HA	2.00	0.44
2:F:364:VAL:O	2:F:364:VAL:HG13	2.18	0.44
2:B:293:TRP:CG	2:B:443:VAL:HG11	2.52	0.44
1:G:341:CYS:SG	1:G:384:LEU:HD21	2.57	0.44
1:A:263:ARG:HG3	1:A:266:GLU:OE2	2.18	0.44
2:H:412:LEU:HD12	2:H:412:LEU:HA	1.79	0.44
2:H:491:ARG:NH2	2:H:552:ARG:CZ	2.81	0.43
1:A:415:LEU:HD21	2:B:416:GLN:CD	2.38	0.43
1:E:262:LEU:HD22	1:E:314:GLU:HB3	1.99	0.43
2:H:254:VAL:O	2:H:256:LEU:HD12	2.18	0.43
1:C:486:SER:OG	4:V:30:DC:P	2.74	0.43
2:B:548:GLU:HG3	4:J:44:DA:H3'	1.98	0.43
1:E:486:SER:CB	4:R:30:DC:OP2	2.66	0.43
1:G:310:TRP:HH2	1:G:415:LEU:HD13	1.84	0.43
2:B:294:ARG:HA	2:B:307:VAL:O	2.19	0.43
2:B:247:GLU:HG2	2:B:250:LYS:HB2	2.00	0.43
2:B:481:VAL:O	2:B:485:GLN:HG3	2.19	0.43
1:G:494:VAL:O	1:G:498:SER:HA	2.18	0.43
1:E:472:ARG:O	1:E:473:GLU:C	2.57	0.43
1:A:266:GLU:O	1:A:314:GLU:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:486:SER:H	1:E:489:LYS:HB2	1.82	0.43
1:A:390:ASN:HD22	3:I:1:DG:H5"	1.84	0.43
1:C:318:ARG:O	1:C:320:PRO:HD3	2.19	0.43
2:B:415:LEU:HA	2:B:415:LEU:HD12	1.78	0.43
1:G:386:GLN:NE2	2:H:441:LYS:HB3	2.34	0.43
2:B:415:LEU:O	2:B:419:THR:OG1	2.22	0.43
2:B:253:ILE:HG13	2:B:253:ILE:O	2.19	0.43
5:T:51:DC:H1'	5:T:52:DA:O5'	2.19	0.43
2:D:241:LYS:HA	2:D:244:ARG:CD	2.49	0.43
1:E:400:LYS:HG3	1:E:411:TYR:CZ	2.53	0.43
2:B:411:ALA:O	2:B:415:LEU:HB2	2.19	0.43
2:D:241:LYS:CB	2:D:244:ARG:HH11	2.28	0.43
2:H:491:ARG:HD3	4:N:44:DA:H4'	2.01	0.43
1:E:405:ILE:O	1:E:408:SER:HB2	2.19	0.43
1:C:433:TRP:CZ2	1:C:462:GLY:HA3	2.54	0.43
5:X:50:DG:H2"	5:X:51:DC:C5'	2.49	0.43
2:H:350:ILE:HG21	2:H:359:LEU:HD22	2.01	0.43
2:H:321:PHE:HZ	2:H:412:LEU:HD13	1.83	0.43
2:F:247:GLU:HG2	2:F:250:LYS:HB2	2.00	0.43
1:G:506:ALA:HB1	1:G:519:LEU:HD21	1.99	0.43
2:B:541:THR:HG1	5:L:50:DG:P	2.39	0.43
4:V:44:DA:C2	5:X:49:DT:N3	2.87	0.43
2:H:534:ARG:NH1	2:H:541:THR:HB	2.33	0.43
1:G:273:VAL:HG22	1:G:308:PHE:CD1	2.53	0.43
1:G:328:LEU:N	1:G:328:LEU:HD12	2.33	0.43
2:B:314:VAL:HB	2:B:359:LEU:HD11	2.00	0.43
1:E:528:LEU:HD22	2:F:236:LEU:HD21	2.00	0.43
2:F:411:ALA:O	2:F:415:LEU:HB2	2.19	0.43
1:E:512:THR:HG22	1:E:514:LYS:H	1.83	0.43
3:M:10:DT:H6	3:M:10:DT:H2'	1.57	0.43
1:C:497:TYR:HE2	1:C:520:LEU:CD2	2.32	0.43
2:D:534:ARG:NH2	5:X:50:DG:O5'	2.42	0.42
2:H:287:VAL:HG13	2:H:290:SER:OG	2.18	0.42
2:F:559:THR:OG1	2:F:561:GLN:HG2	2.19	0.42
2:F:417:LEU:HA	2:F:417:LEU:HD23	1.64	0.42
2:B:541:THR:N	5:L:49:DT:O3'	2.52	0.42
1:A:486:SER:HB3	4:J:30:DC:C3'	2.38	0.42
2:D:247:GLU:O	2:D:250:LYS:HB2	2.20	0.42
1:E:433:TRP:CZ2	1:E:462:GLY:HA3	2.54	0.42
2:H:273:LEU:HD12	2:H:273:LEU:HA	1.69	0.42
2:F:252:ILE:HD13	2:F:295:ARG:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:431:ARG:HG2	1:E:432:PRO:HD2	1.99	0.42
2:D:534:ARG:NH1	2:D:541:THR:HB	2.34	0.42
4:V:30:DC:C2	4:V:31:DA:C8	3.07	0.42
2:F:257:ASP:O	2:F:260:LEU:HB3	2.19	0.42
2:H:265:GLY:HA3	2:H:429:TRP:CE3	2.54	0.42
1:G:483:ARG:HB3	2:H:470:LYS:HA	2.01	0.42
3:Q:7:DG:H2'	3:Q:8:DT:H6	1.84	0.42
2:H:448:PHE:CE2	2:H:449:LYS:HE3	2.55	0.42
1:G:431:ARG:HG2	1:G:432:PRO:HD2	2.02	0.42
2:H:247:GLU:O	2:H:250:LYS:HB2	2.19	0.42
1:E:341:CYS:SG	1:E:384:LEU:HD21	2.59	0.42
1:E:543:LEU:HD22	1:E:550:LEU:HD21	2.00	0.42
4:J:43:DC:H6	4:J:43:DC:P	2.42	0.42
2:B:547:PRO:CD	4:J:45:DG:H3'	2.30	0.42
2:D:267:GLY:HA3	2:H:271:GLY:CA	2.43	0.42
2:H:422:GLN:HG3	2:H:423:ALA:N	2.34	0.42
1:A:332:VAL:HA	1:A:365:VAL:O	2.20	0.42
2:D:257:ASP:O	2:D:260:LEU:HB3	2.19	0.42
2:B:545:ILE:HG23	2:B:549:LEU:HD23	2.00	0.42
1:E:326:LEU:HD23	1:E:455:THR:HA	2.00	0.42
2:D:281:VAL:HB	2:H:262:GLN:NE2	2.35	0.42
1:A:390:ASN:OD1	2:B:442:ALA:HA	2.20	0.42
3:Q:8:DT:H2'	3:Q:9:DG:C8	2.55	0.42
2:F:241:LYS:HA	2:F:244:ARG:CD	2.50	0.42
2:B:254:VAL:O	2:B:256:LEU:HD12	2.20	0.42
4:J:43:DC:H2'	4:J:43:DC:O5'	2.19	0.42
1:G:530:ARG:HE	4:N:29:DA:H4'	1.84	0.42
1:C:489:LYS:HD2	1:C:532:LEU:CD1	2.49	0.42
2:B:517:CYS:CB	2:B:523:ARG:HG3	2.50	0.42
2:B:504:TYR:C	2:B:506:SER:H	2.23	0.42
2:B:316:LEU:HA	2:B:316:LEU:HD12	1.63	0.42
1:A:489:LYS:HD2	1:A:532:LEU:HD12	2.02	0.42
4:J:28:DC:C2'	4:J:29:DA:H5'	2.50	0.42
2:D:491:ARG:NH2	2:D:552:ARG:CZ	2.83	0.42
1:G:336:ARG:HA	1:G:369:GLU:HB3	2.02	0.42
1:A:414:LEU:HD23	2:B:410:GLU:HA	2.02	0.42
1:A:484:GLY:HA3	1:A:536:LEU:HD21	2.01	0.42
1:A:419:LEU:HD23	1:A:419:LEU:HA	1.83	0.42
1:C:417:ARG:HA	1:C:417:ARG:HD2	1.87	0.42
2:D:541:THR:N	5:X:49:DT:C4'	2.83	0.42
1:C:472:ARG:O	1:C:473:GLU:C	2.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:254:VAL:O	2:D:256:LEU:HD12	2.20	0.42
2:D:252:ILE:HD13	2:D:295:ARG:HA	2.02	0.42
4:R:41:DT:H6	4:R:41:DT:H2'	1.47	0.42
2:D:405:ARG:O	2:D:405:ARG:HG3	2.19	0.42
1:A:423:TYR:HD2	1:A:428:LEU:HD11	1.85	0.42
1:A:294:LEU:HA	1:A:294:LEU:HD23	1.83	0.42
1:G:278:THR:O	1:G:278:THR:OG1	2.36	0.41
1:C:400:LYS:HG3	1:C:411:TYR:CE1	2.55	0.41
1:G:402:THR:HG21	1:G:408:SER:OG	2.20	0.41
2:F:467:GLY:O	2:F:484:ARG:NH2	2.47	0.41
1:E:492:ALA:HB2	1:E:525:CYS:HA	2.02	0.41
2:H:316:LEU:HD12	2:H:316:LEU:HA	1.57	0.41
1:E:278:THR:OG1	1:E:278:THR:O	2.31	0.41
2:B:496:MET:SD	5:L:51:DC:H5"	2.59	0.41
1:G:543:LEU:HD13	2:H:507:PRO:HG2	2.02	0.41
1:A:336:ARG:HA	1:A:369:GLU:HB3	2.02	0.41
1:A:512:THR:O	1:A:515:GLU:HB3	2.20	0.41
1:A:497:TYR:CE2	1:A:520:LEU:CD2	3.03	0.41
2:D:541:THR:C	2:D:542:SER:O	2.46	0.41
1:A:512:THR:O	1:A:515:GLU:N	2.54	0.41
1:E:392:GLN:NE2	2:F:435:PHE:CZ	2.86	0.41
1:E:423:TYR:HD2	1:E:428:LEU:HD11	1.85	0.41
1:A:538:ARG:NH2	2:B:473:LEU:O	2.54	0.41
1:G:497:TYR:HE2	1:G:520:LEU:CD2	2.33	0.41
1:A:352:GLN:O	1:A:356:LEU:HG	2.20	0.41
1:A:375:HIS:CA	1:A:377:LEU:HG	2.50	0.41
1:A:401:ARG:NH1	2:B:424:GLN:OE1	2.53	0.41
2:D:316:LEU:HD12	2:D:316:LEU:HA	1.61	0.41
2:B:449:LYS:HD3	3:I:1:DG:P	2.61	0.41
4:N:45:DG:H5'	4:N:45:DG:N9	2.35	0.41
1:G:483:ARG:NE	2:H:470:LYS:HB2	2.35	0.41
2:F:361:LEU:HG	2:F:362:VAL:N	2.36	0.41
1:C:543:LEU:HD22	1:C:550:LEU:HD21	2.02	0.41
1:A:308:PHE:O	1:A:331:ILE:HG13	2.20	0.41
1:G:417:ARG:HD2	1:G:417:ARG:HA	1.85	0.41
1:E:317:PRO:HB3	1:E:323:PRO:HA	2.01	0.41
2:F:265:GLY:O	2:F:266:GLY:C	2.59	0.41
1:G:405:ILE:HA	1:G:408:SER:HB2	2.02	0.41
2:H:287:VAL:HA	2:H:288:PRO:HD3	1.96	0.41
2:D:471:VAL:HG22	2:D:472:ASP:O	2.20	0.41
2:H:248:CYS:SG	2:H:249:LEU:N	2.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:415:LEU:O	2:D:419:THR:OG1	2.25	0.41
2:F:496:MET:HE1	5:T:51:DC:H5"	2.03	0.41
1:A:486:SER:H	1:A:489:LYS:HB2	1.85	0.41
1:A:472:ARG:CD	2:B:562:PRO:HB2	2.43	0.41
1:G:472:ARG:O	1:G:473:GLU:C	2.59	0.41
1:A:371:HIS:CE1	1:A:401:ARG:HD3	2.56	0.41
1:G:266:GLU:O	1:G:314:GLU:HA	2.21	0.41
2:D:412:LEU:HD12	2:D:412:LEU:HA	1.75	0.41
1:E:527:ARG:NE	1:E:530:ARG:HB2	2.36	0.41
1:E:489:LYS:HD2	1:E:532:LEU:HD12	2.03	0.41
1:E:477:ARG:NH2	2:F:465:TRP:HZ3	2.19	0.41
1:A:399:VAL:N	2:B:422:GLN:OE1	2.51	0.41
1:G:472:ARG:HG3	1:G:494:VAL:CG1	2.51	0.41
1:C:407:GLU:O	1:C:411:TYR:N	2.48	0.41
2:B:473:LEU:H	2:B:473:LEU:HD12	1.85	0.41
2:D:270:LEU:HD23	2:H:267:GLY:HA2	2.03	0.41
1:G:527:ARG:NH2	4:N:29:DA:OP1	2.51	0.41
3:U:10:DT:H2'	3:U:10:DT:H6	1.55	0.41
1:G:472:ARG:HB2	2:H:562:PRO:CB	2.51	0.41
1:C:332:VAL:HA	1:C:365:VAL:O	2.21	0.41
1:E:266:GLU:O	1:E:314:GLU:HA	2.21	0.41
2:F:541:THR:C	2:F:542:SER:O	2.51	0.40
2:H:252:ILE:HD11	2:H:295:ARG:CZ	2.51	0.40
1:G:316:ASN:HA	1:G:317:PRO:HD2	1.93	0.40
1:A:379:LEU:HD23	1:A:384:LEU:HD11	2.02	0.40
1:G:414:LEU:HB3	2:H:413:VAL:HG21	2.02	0.40
1:C:340:LEU:O	1:C:344:ILE:HG13	2.21	0.40
5:L:50:DG:H2"	5:L:51:DC:N1	2.36	0.40
2:D:493:SER:HB3	5:X:51:DC:C3'	2.44	0.40
4:N:39:DC:H2"	4:N:40:DA:N7	2.36	0.40
1:E:263:ARG:HB2	1:E:266:GLU:OE2	2.21	0.40
1:E:543:LEU:HA	1:E:543:LEU:HD22	1.86	0.40
4:R:42:DG:H8	4:R:42:DG:OP2	2.03	0.40
3:M:5:DG:H2'	3:M:6:DT:H71	2.03	0.40
1:G:489:LYS:NZ	4:N:30:DC:O5'	2.52	0.40
4:N:42:DG:H2"	4:N:43:DC:C6	2.57	0.40
2:B:267:GLY:HA3	2:F:270:LEU:CG	2.51	0.40
1:C:375:HIS:C	1:C:377:LEU:H	2.25	0.40
2:H:471:VAL:HG22	2:H:472:ASP:O	2.22	0.40
1:A:262:LEU:HD22	1:A:314:GLU:HB3	2.04	0.40
1:C:386:GLN:NE2	2:D:441:LYS:HB3	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:496:ARG:HG2	1:G:523:ILE:CD1	2.52	0.40
5:L:50:DG:C4	5:L:51:DC:N3	2.90	0.40
2:B:541:THR:OG1	5:L:50:DG:H4'	2.21	0.40
4:R:42:DG:N1	5:T:52:DA:C2	2.90	0.40
2:H:514:TYR:O	2:H:523:ARG:HD3	2.20	0.40
1:G:337:LEU:HD22	1:G:370:GLU:O	2.21	0.40
3:Q:10:DT:H6	3:Q:10:DT:H2'	1.63	0.40
2:H:294:ARG:HA	2:H:307:VAL:O	2.21	0.40
1:C:506:ALA:HB1	1:C:519:LEU:HD21	2.03	0.40
1:G:397:PHE:N	1:G:397:PHE:CD1	2.88	0.40
2:F:286:ALA:O	2:F:353:LYS:HD3	2.21	0.40
2:F:493:SER:HB3	5:T:51:DC:O3'	2.21	0.40
1:G:273:VAL:HG22	1:G:308:PHE:HD1	1.87	0.40
1:C:316:ASN:HA	1:C:317:PRO:HD2	1.94	0.40
2:F:293:TRP:CG	2:F:443:VAL:HG11	2.56	0.40
1:A:317:PRO:HG2	1:A:320:PRO:HA	2.04	0.40
1:G:479:LEU:HG	1:G:493:LEU:HD13	2.02	0.40

All (1) 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:A:424:GLN:OE1	2:D:516:GLN:NE2[8_555]	2.11	0.09

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	267/306 (87%)	258 (97%)	6 (2%)	3 (1%)	17	63
1	C	267/306 (87%)	258 (97%)	6 (2%)	3 (1%)	17	63
1	E	267/306 (87%)	259 (97%)	6 (2%)	2 (1%)	26	71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	G	267/306 (87%)	257 (96%)	7 (3%)	3 (1%)	17 63
2	B	276/393 (70%)	265 (96%)	11 (4%)	0	100 100
2	D	276/393 (70%)	265 (96%)	11 (4%)	0	100 100
2	F	276/393 (70%)	264 (96%)	12 (4%)	0	100 100
2	H	276/393 (70%)	264 (96%)	12 (4%)	0	100 100
All	All	2172/2796 (78%)	2090 (96%)	71 (3%)	11 (0%)	34 77

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	432	PRO
1	C	432	PRO
1	E	432	PRO
1	G	432	PRO
1	C	549	PRO
1	G	549	PRO
1	A	473	GLU
1	G	259	PRO
1	A	259	PRO
1	C	259	PRO
1	E	259	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	237/259 (92%)	223 (94%)	14 (6%)	24 61
1	C	237/259 (92%)	223 (94%)	14 (6%)	24 61
1	E	237/259 (92%)	222 (94%)	15 (6%)	22 59
1	G	237/259 (92%)	221 (93%)	16 (7%)	20 57
2	B	242/334 (72%)	225 (93%)	17 (7%)	19 56
2	D	242/334 (72%)	227 (94%)	15 (6%)	23 60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	F	242/334 (72%)	225 (93%)	17 (7%)	19 56
2	H	242/334 (72%)	224 (93%)	18 (7%)	17 54
All	All	1916/2372 (81%)	1790 (93%)	126 (7%)	21 58

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

Mol	Chain	Res	Type
1	A	263	ARG
1	A	269	VAL
1	A	278	THR
1	A	300	VAL
1	A	339	ASP
1	A	364	ARG
1	A	375	HIS
1	A	422	LEU
1	A	474	VAL
1	A	479	LEU
1	A	482	VAL
1	A	483	ARG
1	A	527	ARG
1	A	543	LEU
2	B	237	VAL
2	B	249	LEU
2	B	269	LEU
2	B	273	LEU
2	B	285	GLN
2	B	287	VAL
2	B	291	VAL
2	B	319	GLU
2	B	342	THR
2	B	343	LEU
2	B	412	LEU
2	B	459	PHE
2	B	461	LEU
2	B	472	ASP
2	B	531	GLN
2	B	534	ARG
2	B	562	PRO
1	C	263	ARG
1	C	269	VAL
1	C	278	THR

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Mol	Chain	Res	Type
1	C	300	VAL
1	C	339	ASP
1	C	364	ARG
1	C	375	HIS
1	C	422	LEU
1	C	454	LEU
1	C	474	VAL
1	C	479	LEU
1	C	482	VAL
1	C	527	ARG
1	C	543	LEU
2	D	237	VAL
2	D	249	LEU
2	D	269	LEU
2	D	273	LEU
2	D	285	GLN
2	D	291	VAL
2	D	319	GLU
2	D	342	THR
2	D	343	LEU
2	D	412	LEU
2	D	459	PHE
2	D	461	LEU
2	D	472	ASP
2	D	531	GLN
2	D	534	ARG
1	E	263	ARG
1	E	269	VAL
1	E	278	THR
1	E	299	THR
1	E	300	VAL
1	E	339	ASP
1	E	364	ARG
1	E	375	HIS
1	E	422	LEU
1	E	454	LEU
1	E	474	VAL
1	E	479	LEU
1	E	483	ARG
1	E	527	ARG
1	E	543	LEU
2	F	237	VAL

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Mol	Chain	Res	Type
2	F	249	LEU
2	F	269	LEU
2	F	273	LEU
2	F	285	GLN
2	F	287	VAL
2	F	291	VAL
2	F	319	GLU
2	F	342	THR
2	F	343	LEU
2	F	412	LEU
2	F	459	PHE
2	F	461	LEU
2	F	472	ASP
2	F	531	GLN
2	F	534	ARG
2	F	562	PRO
1	G	263	ARG
1	G	269	VAL
1	G	278	THR
1	G	299	THR
1	G	300	VAL
1	G	339	ASP
1	G	364	ARG
1	G	375	HIS
1	G	422	LEU
1	G	454	LEU
1	G	474	VAL
1	G	479	LEU
1	G	482	VAL
1	G	483	ARG
1	G	527	ARG
1	G	543	LEU
2	H	237	VAL
2	H	249	LEU
2	H	269	LEU
2	H	273	LEU
2	H	285	GLN
2	H	287	VAL
2	H	291	VAL
2	H	311	THR
2	H	319	GLU
2	H	342	THR

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Mol	Chain	Res	Type
2	H	343	LEU
2	H	412	LEU
2	H	459	PHE
2	H	461	LEU
2	H	472	ASP
2	H	531	GLN
2	H	534	ARG
2	H	562	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	257	GLN
1	A	352	GLN
1	A	386	GLN
2	B	488	GLN
2	B	515	GLN
2	B	563	HIS
1	C	316	ASN
1	C	352	GLN
1	C	448	ASN
2	D	274	GLN
2	D	515	GLN
2	D	563	HIS
1	E	257	GLN
1	E	316	ASN
1	E	352	GLN
1	E	386	GLN
1	E	392	GLN
1	E	448	ASN
2	F	262	GLN
2	F	515	GLN
2	F	563	HIS
1	G	257	GLN
1	G	316	ASN
1	G	352	GLN
1	G	386	GLN
2	H	262	GLN
2	H	488	GLN
2	H	515	GLN
2	H	563	HIS

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	275/306 (89%)	0.63	23 (8%) 14 17	21, 84, 154, 320	0
1	C	275/306 (89%)	0.36	11 (4%) 42 40	15, 99, 186, 316	0
1	E	275/306 (89%)	1.06	44 (16%) 3 8	20, 118, 367, 428	0
1	G	275/306 (89%)	0.53	21 (7%) 17 19	21, 87, 183, 265	0
2	B	284/393 (72%)	0.62	23 (8%) 15 18	41, 96, 245, 375	0
2	D	284/393 (72%)	0.72	34 (11%) 6 11	29, 113, 258, 397	0
2	F	284/393 (72%)	1.30	76 (26%) 1 5	36, 170, 498, 642	0
2	H	284/393 (72%)	0.62	33 (11%) 6 11	42, 118, 273, 403	0
3	I	12/12 (100%)	0.88	3 (25%) 1 5	94, 114, 249, 364	0
3	M	12/12 (100%)	1.21	3 (25%) 1 5	128, 153, 264, 437	0
3	Q	12/12 (100%)	4.03	8 (66%) 0 2	285, 340, 399, 455	0
3	U	12/12 (100%)	1.01	0 100 100	114, 183, 245, 282	0
4	J	19/24 (79%)	0.92	2 (10%) 8 13	80, 134, 230, 269	0
4	N	19/24 (79%)	1.17	3 (15%) 3 8	85, 183, 283, 283	0
4	R	19/24 (79%)	3.22	14 (73%) 0 2	103, 366, 471, 540	0
4	V	19/24 (79%)	1.72	8 (42%) 0 3	147, 208, 431, 438	0
5	L	9/13 (69%)	1.07	1 (11%) 7 12	109, 138, 247, 333	0
5	P	9/13 (69%)	0.00	0 100 100	98, 126, 157, 177	0
5	T	9/13 (69%)	2.68	7 (77%) 0 2	258, 344, 476, 488	0
5	X	9/13 (69%)	0.52	0 100 100	178, 245, 343, 375	0
All	All	2396/2992 (80%)	0.79	314 (13%) 5 10	15, 104, 367, 642	0

All (314) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	565	SER	9.4
3	Q	3	DA	9.2
1	A	256	GLN	8.5
2	F	492	VAL	8.2
2	F	497	ALA	8.1
2	B	329	LYS	7.9
4	N	23	DA	7.8
1	E	531	ASN	7.8
1	E	530	ARG	7.6
2	F	490	ASN	7.5
1	E	533	GLY	7.3
2	F	491	ARG	7.3
4	R	45	DG	7.0
2	F	557	MET	6.8
2	F	547	PRO	6.5
1	C	437	GLY	6.5
1	E	532	LEU	6.4
2	H	463	SER	6.3
1	A	437	GLY	6.2
3	Q	6	DT	6.2
2	F	473	LEU	6.1
1	A	261	GLU	6.0
1	E	526	GLY	6.0
2	F	533	ARG	6.0
2	D	235	ALA	5.9
1	G	437	GLY	5.9
1	E	280	GLY	5.9
1	E	483	ARG	5.8
3	M	12	DT	5.8
3	Q	2	DA	5.6
1	A	260	LEU	5.6
2	F	245	PRO	5.6
3	Q	7	DG	5.6
4	R	27	DA	5.5
4	R	29	DA	5.5
1	E	527	ARG	5.5
1	E	256	GLN	5.4
2	F	566	LEU	5.4
2	F	500	VAL	5.4
2	F	516	GLN	5.4
1	E	324	GLY	5.4
3	Q	1	DG	5.3
4	V	38	DA	5.2

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Mol	Chain	Res	Type	RSRZ
3	Q	4	DT	5.2
4	R	28	DC	5.2
2	H	245	PRO	5.0
1	E	544	TYR	5.0
2	H	246	GLU	5.0
2	F	464	ASP	5.0
1	G	260	LEU	5.0
2	B	545	ILE	5.0
2	F	474	ALA	5.0
4	N	24	DG	4.8
5	T	49	DT	4.8
2	D	369	CYS	4.8
2	F	466	ALA	4.8
2	F	548	GLU	4.8
1	E	543	LEU	4.7
2	H	467	GLY	4.7
2	F	512	GLN	4.7
2	H	542	SER	4.7
2	F	556	GLN	4.7
1	E	542	GLN	4.6
2	F	534	ARG	4.6
1	E	534	PRO	4.6
1	E	540	LEU	4.6
3	I	12	DT	4.6
3	Q	5	DG	4.4
4	R	44	DA	4.4
2	B	542	SER	4.4
2	F	486	ILE	4.4
1	G	259	PRO	4.4
2	F	552	ARG	4.4
2	D	233	ASN	4.3
1	E	312	ALA	4.3
1	E	484	GLY	4.2
2	F	483	ARG	4.2
2	D	329	LYS	4.2
2	F	499	ALA	4.2
2	D	545	ILE	4.1
5	T	55	DT	4.1
1	G	258	GLN	4.1
2	B	245	PRO	4.1
1	E	479	LEU	4.1
2	F	564	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
2	F	498	SER	4.1
1	A	269	VAL	4.0
2	D	234	ALA	4.0
2	F	465	TRP	4.0
1	E	482	VAL	3.9
1	E	536	LEU	3.9
2	F	518	PHE	3.9
1	E	525	CYS	3.8
4	R	33	DT	3.8
2	F	558	THR	3.8
4	R	38	DA	3.8
2	F	549	LEU	3.8
2	H	471	VAL	3.8
2	H	462	GLU	3.8
5	T	47	DT	3.7
2	B	566	LEU	3.7
2	H	407	ASP	3.7
2	D	242	ALA	3.7
2	B	552	ARG	3.6
2	B	530	ILE	3.6
2	F	421	ALA	3.6
2	F	321	PHE	3.6
2	F	505	PRO	3.5
2	F	551	ARG	3.5
2	F	242	ALA	3.5
2	B	233	ASN	3.4
2	D	284	ALA	3.4
2	F	511	VAL	3.4
4	V	28	DC	3.4
2	F	482	TRP	3.4
2	F	563	HIS	3.4
1	A	430	SER	3.4
2	H	445	GLU	3.4
2	F	495	GLU	3.4
4	R	26	DC	3.4
2	F	553	ILE	3.3
2	F	472	ASP	3.3
2	F	493	SER	3.3
2	F	559	THR	3.3
2	H	244	ARG	3.3
4	R	30	DC	3.3
4	J	38	DA	3.3

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Mol	Chain	Res	Type	RSRZ
4	N	25	DA	3.2
2	B	403	VAL	3.2
1	A	324	GLY	3.2
2	D	491	ARG	3.2
2	F	507	PRO	3.2
2	H	465	TRP	3.2
1	A	305	VAL	3.2
1	E	524	LYS	3.2
2	F	550	SER	3.2
2	F	489	LEU	3.2
1	A	420	GLN	3.2
1	E	500	PRO	3.2
5	L	55	DT	3.1
2	H	541	THR	3.1
1	G	262	LEU	3.1
2	D	465	TRP	3.1
1	G	375	HIS	3.1
2	F	282	ILE	3.1
2	D	547	PRO	3.1
2	F	244	ARG	3.0
1	C	401	ARG	3.0
2	F	527	LEU	3.0
1	A	360	GLY	3.0
2	D	549	LEU	3.0
4	R	31	DA	3.0
2	F	546	GLY	3.0
1	E	327	VAL	2.9
4	V	45	DG	2.9
2	F	471	VAL	2.9
1	G	261	GLU	2.9
1	E	286	GLU	2.9
2	H	410	GLU	2.9
1	E	546	SER	2.9
4	V	29	DA	2.9
1	E	328	LEU	2.9
2	B	529	ASP	2.9
2	D	243	GLN	2.9
1	G	520	LEU	2.9
1	G	360	GLY	2.8
2	B	500	VAL	2.8
2	B	541	THR	2.8
1	E	529	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	279	ARG	2.8
1	A	259	PRO	2.8
1	G	325	GLU	2.8
2	F	515	GLN	2.8
2	H	460	CYS	2.8
2	B	544	ARG	2.8
2	F	501	VAL	2.8
2	F	525	ASN	2.8
2	D	464	ASP	2.8
2	F	508	GLN	2.7
4	V	40	DA	2.7
1	A	257	GLN	2.7
2	D	239	ARG	2.7
4	V	25	DA	2.7
2	D	459	PHE	2.7
5	T	54	DG	2.7
2	B	243	GLN	2.7
1	A	280	GLY	2.7
2	F	463	SER	2.7
2	F	506	SER	2.7
3	M	11	DC	2.7
1	E	305	VAL	2.7
3	I	11	DC	2.6
2	H	466	ALA	2.6
2	H	454	GLU	2.6
1	C	256	GLN	2.6
1	G	463	ALA	2.6
4	R	43	DC	2.6
1	E	422	LEU	2.6
1	G	548	GLY	2.6
2	H	490	ASN	2.6
1	E	437	GLY	2.6
2	F	246	GLU	2.6
1	A	429	ARG	2.6
2	F	519	SER	2.6
4	V	39	DC	2.6
2	B	234	ALA	2.6
4	R	39	DC	2.6
2	F	243	GLN	2.6
1	G	269	VAL	2.6
1	A	323	PRO	2.5
2	H	496	MET	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	531	GLN	2.5
2	D	356	GLY	2.5
2	H	526	LEU	2.5
2	H	489	LEU	2.5
5	T	50	DG	2.5
1	G	539	THR	2.5
2	D	527	LEU	2.5
2	D	282	ILE	2.5
2	F	517	CYS	2.5
2	B	284	ALA	2.5
2	F	435	PHE	2.5
4	R	25	DA	2.5
1	E	276	GLY	2.5
2	F	240	MET	2.5
1	C	399	VAL	2.5
2	D	525	ASN	2.4
2	H	329	LYS	2.4
1	G	436	PRO	2.4
1	E	485	VAL	2.4
2	D	409	GLU	2.4
2	D	370	PHE	2.4
1	G	373	SER	2.4
2	H	432	LEU	2.4
4	J	33	DT	2.4
1	G	550	LEU	2.4
2	F	403	VAL	2.4
2	F	369	CYS	2.4
3	M	10	DT	2.4
2	H	284	ALA	2.4
1	A	312	ALA	2.4
1	G	285	PRO	2.4
2	F	460	CYS	2.4
1	A	326	LEU	2.4
2	H	449	LYS	2.4
2	F	513	ALA	2.3
2	F	510	LEU	2.3
2	H	243	GLN	2.3
2	B	343	LEU	2.3
2	F	467	GLY	2.3
1	A	268	ARG	2.3
2	H	566	LEU	2.3
1	E	541	SER	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	549	LEU	2.3
2	H	470	LYS	2.3
1	A	258	GLN	2.3
2	D	454	GLU	2.3
2	D	444	ALA	2.2
1	G	361	LEU	2.2
2	H	504	TYR	2.2
1	C	543	LEU	2.2
2	F	520	ASP	2.2
2	D	270	LEU	2.2
2	D	477	GLY	2.2
2	F	479	ALA	2.2
2	F	496	MET	2.2
2	D	403	VAL	2.2
1	E	279	ARG	2.2
1	A	525	CYS	2.2
4	V	23	DA	2.2
1	C	262	LEU	2.2
2	H	417	LEU	2.2
2	D	462	GLU	2.2
2	D	407	ASP	2.2
1	E	310	TRP	2.2
2	H	527	LEU	2.2
1	A	526	GLY	2.2
1	E	269	VAL	2.2
2	D	546	GLY	2.1
1	G	546	SER	2.1
1	C	269	VAL	2.1
2	F	409	GLU	2.1
2	F	249	LEU	2.1
2	B	360	SER	2.1
4	R	40	DA	2.1
1	E	257	GLN	2.1
2	H	500	VAL	2.1
2	F	487	GLN	2.1
2	B	325	ILE	2.1
1	E	522	THR	2.1
2	F	238	THR	2.1
2	H	491	ARG	2.1
2	H	408	ALA	2.1
1	E	447	PRO	2.1
1	E	278	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	523	ILE	2.1
1	A	310	TRP	2.1
3	Q	8	DT	2.1
2	B	499	ALA	2.1
5	T	48	DC	2.1
1	E	260	LEU	2.0
1	C	428	LEU	2.0
5	T	53	DT	2.0
1	A	262	LEU	2.0
2	B	280	CYS	2.0
2	D	413	VAL	2.0
2	D	416	GLN	2.0
2	D	460	CYS	2.0
1	G	532	LEU	2.0
1	E	401	ARG	2.0
2	D	424	GLN	2.0
1	C	544	TYR	2.0
3	I	10	DT	2.0
1	C	550	LEU	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.