Full wwPDB X-ray Structure Validation Report ⓘ

Dec 16, 2023 – 10:28 AM EST

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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

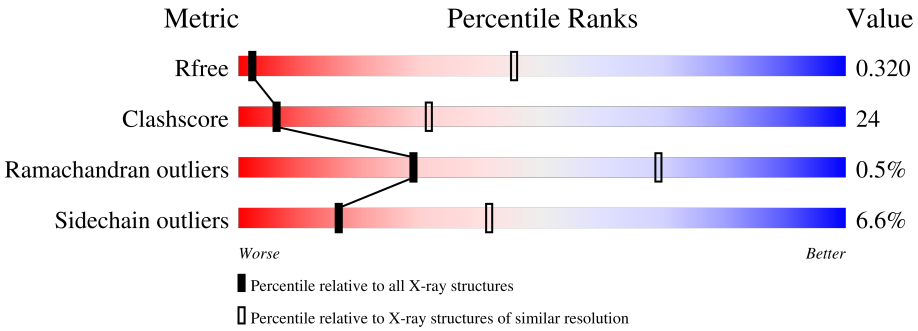
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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}	130704	1000 (8.00-3.88)
Clashscore	141614	1049 (8.00-3.90)
Ramachandran outliers	138981	1016 (8.00-3.86)
Sidechain outliers	138945	1017 (8.00-3.82)

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

Mol	Chain	Length	Quality of chain
1	A	306	52% 34% · 10%
1	C	306	53% 32% · 10%
1	E	306	53% 35% · 10%
1	G	306	49% 36% 5% 10%
2	B	393	41% 27% 5% 28%
2	D	393	43% 25% · 28%
2	F	393	42% 25% 5% 28%

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

2 Entry composition (i)

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.

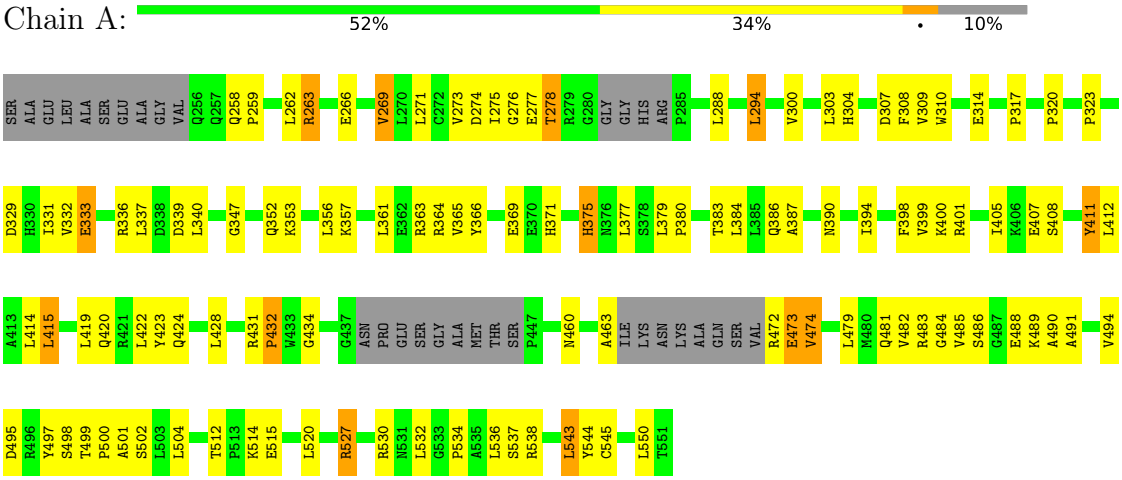
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	L	9	Total	C	N	O	P	0	0	0
			183	88	29	57	9			
5	P	9	Total	C	N	O	P	0	0	0
			183	88	29	57	9			
5	T	9	Total	C	N	O	P	0	0	0
			183	88	29	57	9			
5	X	9	Total	C	N	O	P	0	0	0
			183	88	29	57	9			

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

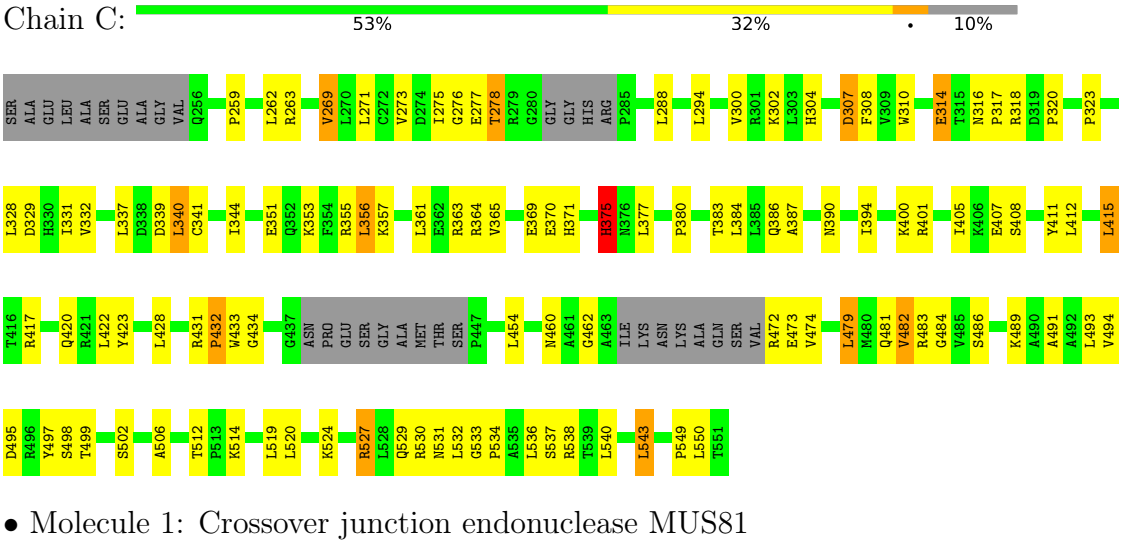
• Molecule 1: Crossover junction endonuclease MUS81

Chain A:



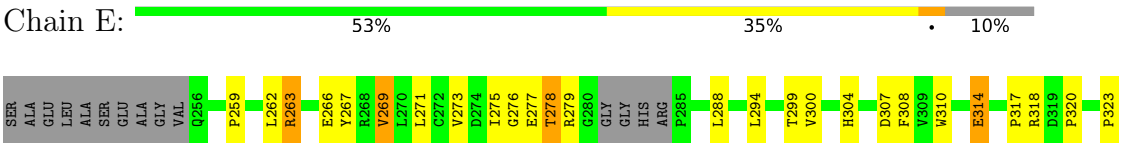
• Molecule 1: Crossover junction endonuclease MUS81

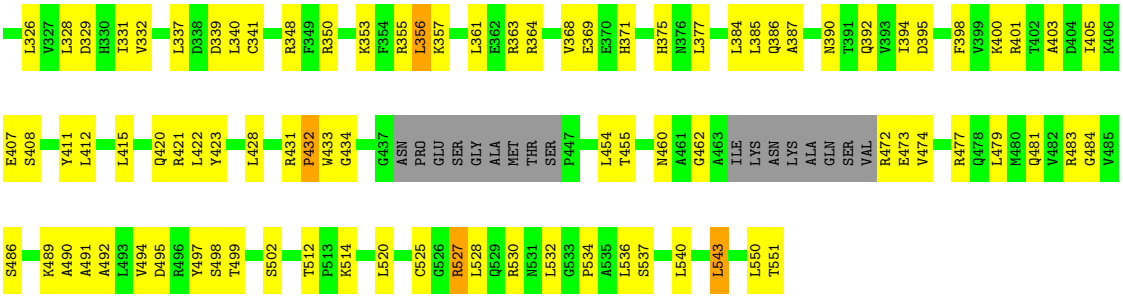
Chain C:



• Molecule 1: Crossover junction endonuclease MUS81

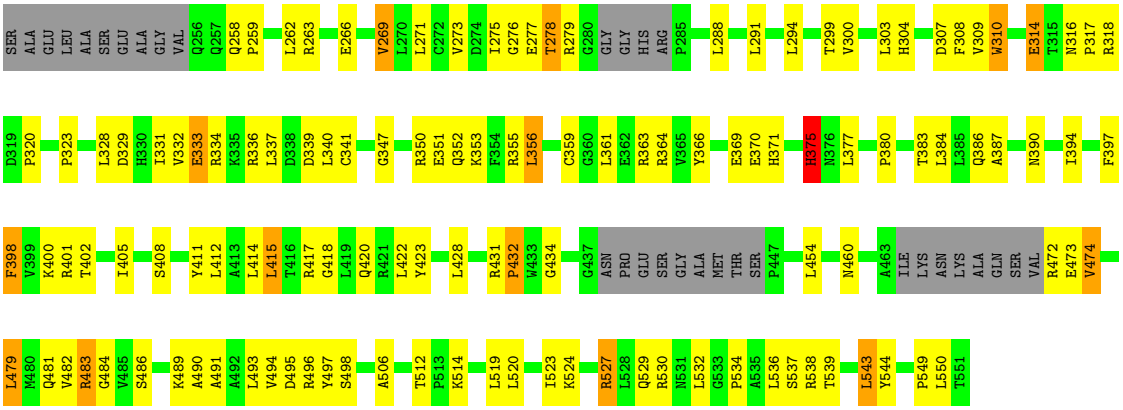
Chain E:





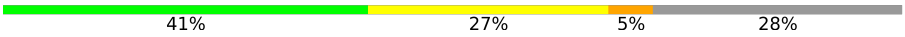
• Molecule 1: Crossover junction endonuclease MUS81

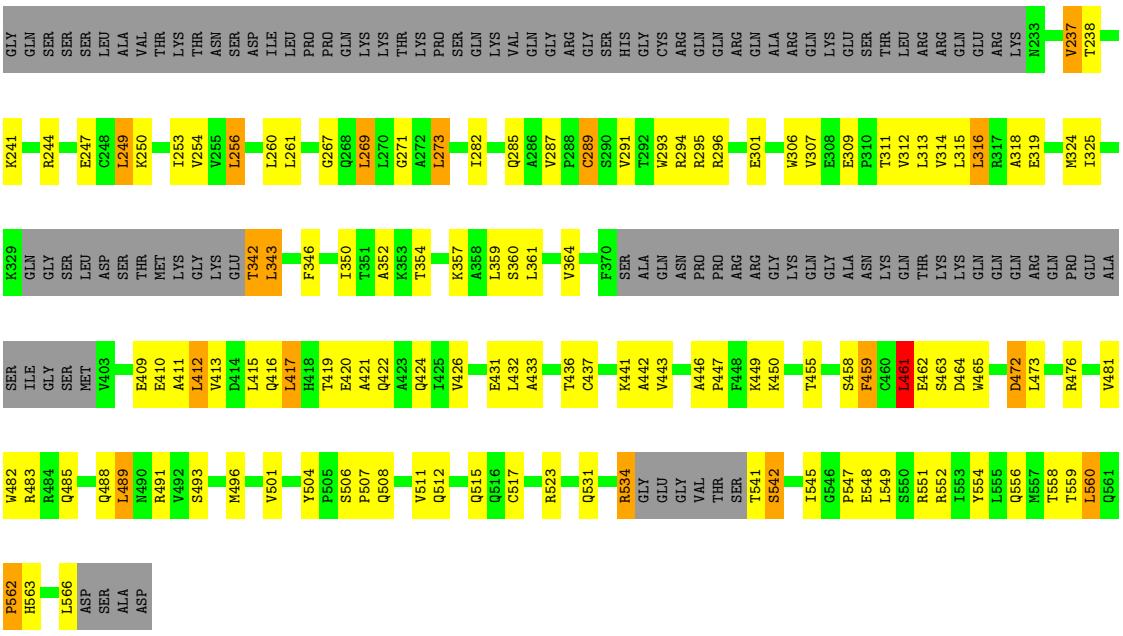
Chain G:



• Molecule 2: Crossover junction endonuclease EME1

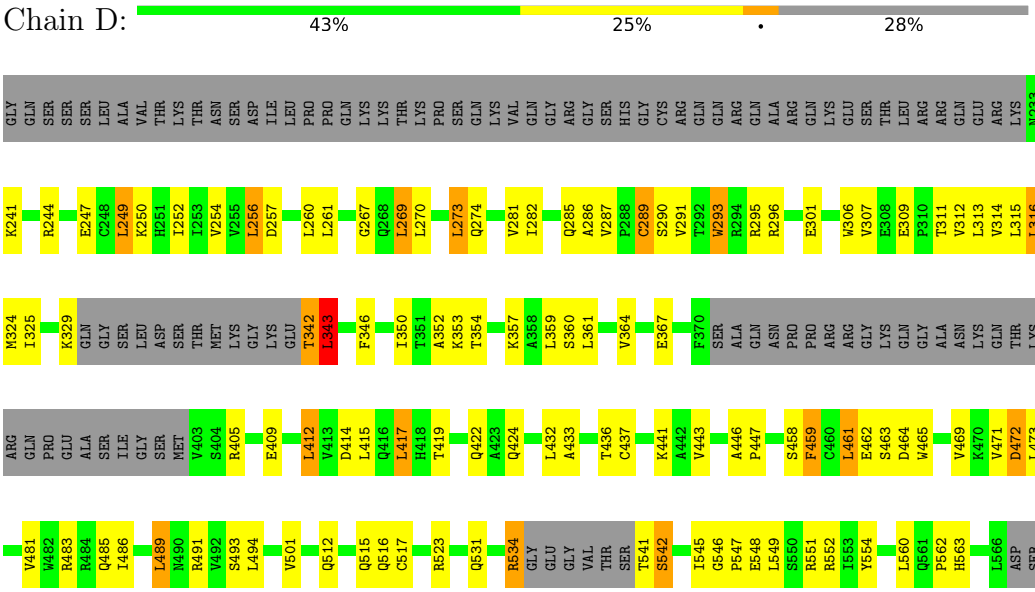
Chain B:





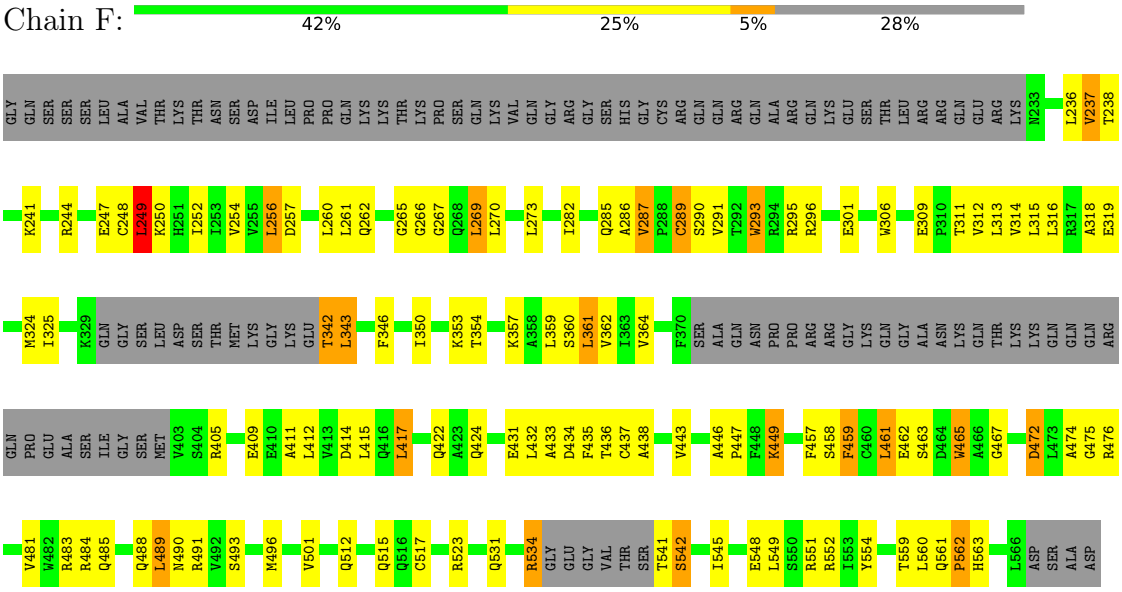
• Molecule 2: Crossover junction endonuclease EME1

Chain D:



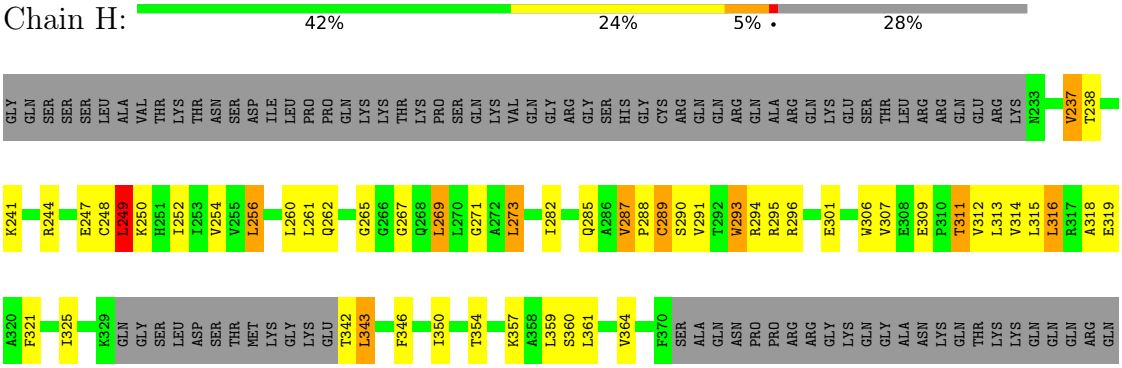
• Molecule 2: Crossover junction endonuclease EME1

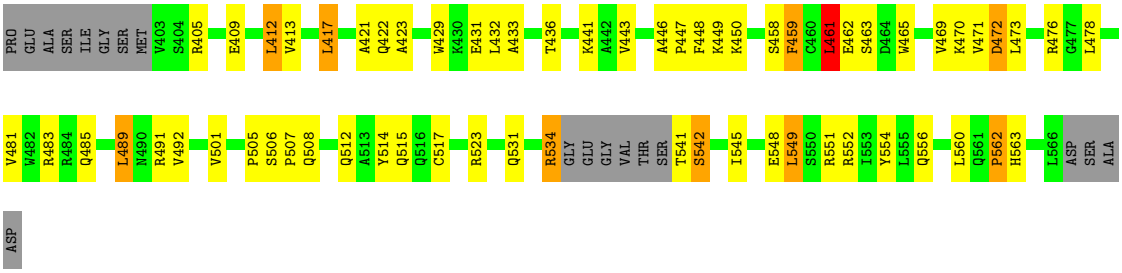
Chain F:



• Molecule 2: Crossover junction endonuclease EME1

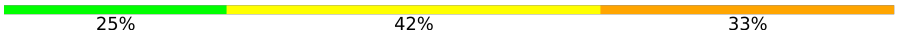
Chain H:

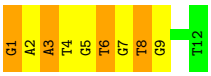




• Molecule 3: DNA GAATGTGTGTCT

Chain I:



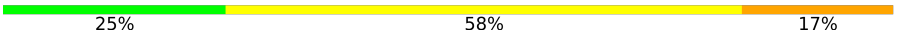


• Molecule 3: DNA GAATGTGTGTCT

Chain M:

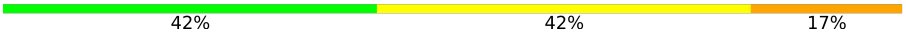
• Molecule 3: DNA GAATGTGTGTCT

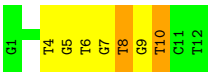
Chain Q:



• 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

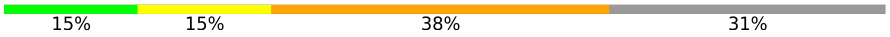
Chain V:

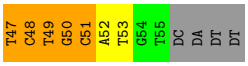
• Molecule 5: DNA TCTGCATGTCATT

Chain L:

• Molecule 5: DNA TCTGCATGTCATT

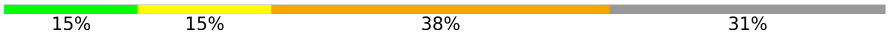
Chain P:





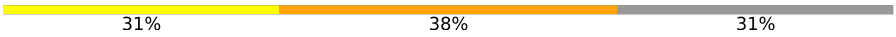
• Molecule 5: DNA TCTGCATGTCATT

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 0.268 , 0.320	Depositor DCC
R_{free} test set	853 reflections (5.07%)	wwPDB-VP
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 , 207.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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
2:D:269:LEU:HD21	2:D:436:THR:HG21	1.49	0.93
4:V:44:DA:N6	5:X:49:DT:O4	2.00	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:A:394:ILE:HG23	2:B:450:LYS:HE3	1.61	0.83
1:G:353:LYS:HA	1:G:356:LEU:HD12	1.57	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:B:360:SER:HA	2:B:422:GLN:HB3	1.61	0.81
2:D:493:SER:HB3	5:X:51:DC:H3'	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
2:D:274:GLN:HE22	2:H:267:GLY:H	1.27	0.80
5:L:50:DG:H5'	5:L:50:DG:C8	2.16	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
2:D:267:GLY:HA3	2:H:271:GLY:HA2	1.64	0.79
5:P:47:DT:H2"	5:P:48:DC:H6	1.47	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
1:E:331:ILE:HB	1:E:361:LEU:HD23	1.67	0.76
3:Q:6:DT:H2"	3:Q:7:DG:C8	2.21	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
2:H:562:PRO:HG2	2:H:563:HIS:CD2	2.23	0.74
4:J:43:DC:O2	5:L:50:DG:N2	2.19	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:B:271:GLY:HA2	2:F:267:GLY:HA3	1.71	0.72
2:D:562:PRO:HG2	2:D:563:HIS:CD2	2.25	0.72
2:D:241:LYS:HB3	2:D:244:ARG:HH11	1.51	0.72
2:H:449:LYS:NZ	3:M:1:DG:H5"	2.05	0.72
2:F:314:VAL:O	2:F:361:LEU:HD12	1.90	0.71
1:A:394:ILE:CG2	2:B:450:LYS:HE3	2.20	0.71
5:T:50:DG:H2"	5:T:51:DC:H5'	1.73	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
1:G:481:GLN:HB2	2:H:481:VAL:HG13	1.72	0.71
2:H:449:LYS:NZ	3:M:1:DG:P	2.64	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
2:B:241:LYS:HB3	2:B:244:ARG:HH11	1.54	0.70
1:G:483:ARG:CB	2:H:470:LYS:HA	2.21	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:B:296:ARG:NH2	2:B:301:GLU:HB2	2.07	0.69
2:F:296:ARG:NH2	2:F:301:GLU:HB2	2.06	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
1:A:474:VAL:HG22	2:B:566:LEU:HD11	1.74	0.69
1:C:486:SER:OG	4:V:30:DC:OP1	2.10	0.69
2:F:541:THR:N	5:T:50:DG:O5'	2.25	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
2:B:312:VAL:HG11	2:B:354:THR:HG21	1.74	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
1:G:474:VAL:HG21	2:H:556:GLN:OE1	1.92	0.68
2:H:548:GLU:O	2:H:551:ARG:HB3	1.94	0.68
5:X:48:DC:H2"	5:X:49:DT:H5'	1.75	0.68
2:H:483:ARG:HA	2:H:501:VAL:HG21	1.75	0.68
2:B:267:GLY:CA	2:F:270:LEU:HD23	2.24	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
1:A:472:ARG:HB2	2:B:562:PRO:CB	2.23	0.67
2:B:267:GLY:HA2	2:F:270:LEU:HD23	1.75	0.67
2:B:491:ARG:HA	5:L:52:DA:H4'	1.77	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:A:472:ARG:HB2	2:B:562:PRO:HB2	1.76	0.66
1:A:545:CYS:HA	2:B:508:GLN:HE21	1.60	0.66
2:F:312:VAL:HG11	2:F:354:THR:HG21	1.77	0.66
1:G:530:ARG:NH1	4:N:29:DA:H5"	2.09	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
2:B:282:ILE:HG12	2:F:262:GLN:HE21	1.60	0.66
1:G:483:ARG:N	2:H:469:VAL:O	2.25	0.66
4:R:38:DA:H2"	4:R:39:DC:H5'	1.76	0.66
1:A:390:ASN:HB3	1:A:394:ILE:HD12	1.75	0.66
1:G:276:GLY:N	1:G:278:THR:HG22	2.08	0.66
1:E:304:HIS:ND1	1:E:460:ASN:O	2.29	0.66
2:H:541:THR:HG22	2:H:542:SER:O	1.95	0.66
1:E:551:THR:C	2:F:475:GLY:H	1.99	0.66
1:G:481:GLN:O	2:H:481:VAL:HG22	1.96	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:D:314:VAL:O	2:D:361:LEU:HD12	1.95	0.65
2:F:541:THR:HG22	2:F:542:SER:O	1.96	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:H6	4:N:28:DC:H5'	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
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
1:E:486:SER:HB3	4:R:30:DC:OP1	1.95	0.64
1:A:386:GLN:NE2	2:B:441:LYS:HB3	2.12	0.64
2:B:541:THR:HG22	2:B:542:SER:O	1.97	0.64
1:A:331:ILE:HB	1:A:361:LEU:HD23	1.77	0.64
2:D:459:PHE:HA	2:D:462:GLU:HB3	1.80	0.64
2:D:489:LEU:HD12	2:D:489:LEU:N	2.13	0.64
1:G:310:TRP:O	1:G:328:LEU:N	2.27	0.64
3:Q:7:DG:O6	4:R:27:DA:N6	2.18	0.64
2:H:523:ARG:HB3	2:H:554:TYR:CE1	2.33	0.64
5:P:47:DT:H2"	5:P:48:DC:C6	2.32	0.64
1:E:279:ARG:HH21	4:R:40:DA:C5'	2.11	0.64
4:J:42:DG:O6	5:L:51:DC:N4	2.27	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:314:VAL:O	2:H:361:LEU:HD12	1.97	0.63
2:H:459:PHE:HA	2:H:462:GLU:HB3	1.79	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:H6	4:R:28:DC:H5'	1.64	0.63
1:A:304:HIS:ND1	1:A:460:ASN:O	2.31	0.63
2:F:449:LYS:HZ2	3:Q:1:DG:H3'	1.64	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:A:398:PHE:CE2	2:B:422:GLN:HA	2.33	0.62
1:A:415:LEU:HD22	2:B:417:LEU:HD21	1.81	0.62
1:E:486:SER:HB3	4:R:30:DC:OP2	1.99	0.62
1:G:304:HIS:ND1	1:G:460:ASN:O	2.33	0.62
1:A:369:GLU:OE1	1:A:405:ILE:HG12	2.00	0.62
1:A:545:CYS:O	2:B:508:GLN:HG3	1.99	0.62
1:C:543:LEU:HD23	2:D:478:LEU:HB3	1.82	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:B:271:GLY:CA	2:F:267:GLY:HA3	2.30	0.62
2:D:354:THR:HB	2:D:357:LYS:HD2	1.80	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
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
2:F:491:ARG:HH21	2:F:552:ARG:NH1	1.98	0.61
4:V:44:DA:N1	5:X:49:DT:C4	2.69	0.61
2:B:318:ALA:HB2	2:B:364:VAL:O	2.01	0.61
2:H:238:THR:HA	2:H:241:LYS:HG3	1.81	0.61
1:C:273:VAL:HG13	1:C:308:PHE:CE1	2.36	0.61
1:E:477:ARG:CZ	2:F:488:GLN:OE1	2.47	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
1:A:375:HIS:C	1:A:377:LEU:H	2.01	0.61
3:I:9:DG:H8	3:I:9:DG:OP2	1.84	0.61
1:A:488:GLU:OE1	2:B:455:THR:HG21	2.01	0.61
1:G:347:GLY:HA3	2:H:461:LEU:CD2	2.26	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
1:A:337:LEU:HD23	1:A:377:LEU:HD11	1.83	0.60
2:D:541:THR:HG22	2:D:542:SER:O	2.01	0.60
1:E:329:ASP:O	1:E:363:ARG:HB2	2.02	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
1:E:473:GLU:HG3	2:F:459:PHE:CZ	2.37	0.60
1:G:269:VAL:HG11	1:G:420:GLN:HA	1.83	0.60
2:B:491:ARG:HH21	2:B:552:ARG:NH1	1.99	0.60
1:C:481:GLN:O	2:D:469:VAL:N	2.35	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:543:LEU:CD2	2:D:478:LEU:HB3	2.32	0.60
2:D:547:PRO:HD2	4:V:45:DG:H3'	1.83	0.60
3:Q:3:DA:N6	4:R:32:DT:H3	1.92	0.60
5:X:47:DT:H2"	5:X:48:DC:C6	2.37	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
1:E:273:VAL:HG13	1:E:308:PHE:CE1	2.37	0.59
1:G:474:VAL:HB	2:H:556:GLN:HE22	1.65	0.59
5:L:52:DA:H2"	5:L:53:DT:OP2	2.01	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:337:LEU:HD23	1:C:377:LEU:HD11	1.85	0.59
1:C:486:SER:HG	4:V:30:DC:P	2.25	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:A:527:ARG:NE	1:A:530:ARG:HB2	2.18	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:277:GLU:HG3	1:A:307:ASP:HB3	1.85	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
5:L:50:DG:H1'	5:L:51:DC:C2	2.38	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
1:E:276:GLY:C	1:E:278:THR:H	2.07	0.58
2:F:512:GLN:HA	2:F:515:GLN:HE21	1.67	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
2:H:241:LYS:HB3	2:H:244:ARG:NH1	2.16	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
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:488:GLU:HG2	2:B:455:THR:CG2	2.34	0.58
2:D:274:GLN:HE22	2:H:267:GLY:N	2.00	0.58
2:F:459:PHE:HA	2:F:462:GLU:HB3	1.86	0.58
2:H:312:VAL:HG11	2:H:354:THR:HG21	1.85	0.58
4:R:43:DC:H2"	4:R:44:DA:C8	2.39	0.58
1:A:363:ARG:NH1	2:B:420:GLU:OE1	2.37	0.58
1:A:489:LYS:NZ	4:J:30:DC:P	2.77	0.58
1:C:371:HIS:NE2	1:C:401:ARG:HB3	2.18	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
2:H:534:ARG:HE	2:H:534:ARG:HA	1.68	0.58
1:E:398:PHE:HA	2:F:422:GLN:OE1	2.03	0.58
1:A:329:ASP:O	1:A:363:ARG:HB2	2.04	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:C:407:GLU:CD	2:D:405:ARG:HH12	2.06	0.58
2:D:274:GLN:CD	2:H:267:GLY:H	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
1:E:355:ARG:NH1	5:T:54:DG:H3'	2.20	0.57
4:J:41:DT:H2"	4:J:42:DG:H8	1.68	0.57
4:N:38:DA:O4'	4:N:38:DA:P	2.63	0.57
4:V:43:DC:H2"	4:V:44:DA:H8	1.69	0.57
2:B:491:ARG:HA	5:L:52:DA:O5'	2.05	0.57
1:E:371:HIS:NE2	1:E:401:ARG:HB3	2.20	0.57
2:D:315:LEU:HD12	2:D:432:LEU:HD21	1.87	0.57
2:D:541:THR:OG1	5:X:50:DG:H4'	2.04	0.57
1:G:491:ALA:O	1:G:495:ASP:HB2	2.05	0.57
3:Q:9:DG:H8	3:Q:9:DG:OP2	1.88	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:B:241:LYS:NZ	4:J:28:DC:OP1	2.27	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
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
2:D:286:ALA:O	2:D:353:LYS:HD3	2.05	0.56
3:M:5:DG:O6	4:N:29:DA:N6	2.38	0.56
2:B:491:ARG:HA	5:L:52:DA:C4'	2.34	0.56
2:D:293:TRP:CD2	2:D:443:VAL:HG11	2.41	0.56
2:H:314:VAL:HB	2:H:359:LEU:HD11	1.87	0.56
1:C:369:GLU:OE1	1:C:405:ILE:HG12	2.06	0.56
2:F:287:VAL:HG13	2:F:290:SER:OG	2.05	0.56
3:Q:9:DG:C6	4:R:25:DA:N6	2.74	0.56
2:F:318:ALA:HB2	2:F:364:VAL:O	2.05	0.56
1:G:277:GLU:HG3	1:G:307:ASP:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:527:ARG:NE	1:C:530:ARG:HB2	2.21	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
3:M:9:DG:OP2	3:M:9:DG:H8	1.89	0.56
1:E:421:ARG:HH21	2:F:414:ASP:CG	2.10	0.55
1:G:390:ASN:HB3	1:G:394:ILE:HD12	1.88	0.55
1:G:273:VAL:HG13	1:G:308:PHE:CE1	2.41	0.55
2:F:489:LEU:HD12	2:F:489:LEU:N	2.22	0.55
1:G:486:SER:O	1:G:490:ALA:N	2.37	0.55
1:G:472:ARG:N	2:H:562:PRO:O	2.40	0.55
1:C:310:TRP:O	1:C:328:LEU:N	2.36	0.55
2:F:449:LYS:HZ3	3:Q:1:DG:H3'	1.68	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
1:A:273:VAL:HG13	1:A:308:PHE:CE1	2.41	0.55
1:E:273:VAL:HG22	1:E:308:PHE:HD1	1.72	0.55
2:H:459:PHE:HA	2:H:462:GLU:CB	2.37	0.55
4:R:39:DC:OP2	4:R:39:DC:H2'	2.07	0.55
1:A:489:LYS:HD2	1:A:532:LEU:CD1	2.37	0.55
1:C:423:TYR:HD2	1:C:428:LEU:HD11	1.72	0.55
1:E:269:VAL:HG11	1:E:420:GLN:HA	1.88	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:D:312:VAL:HG11	2:D:354:THR:HG21	1.88	0.54
2:F:433:ALA:O	2:F:436:THR:HB	2.07	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
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
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
1:A:491:ALA:O	1:A:495:ASP:HB2	2.08	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:ILE:O	2:B:450:LYS:HE2	2.08	0.54
1:C:302:LYS:NZ	5:X:54:DG:H4'	2.23	0.54
1:C:384:LEU:O	1:C:387:ALA:HB3	2.08	0.54
5:L:48:DC:H2"	5:L:49:DT:H72	1.89	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
1:C:538:ARG:NH2	2:D:473:LEU:O	2.41	0.53
5:X:48:DC:H2'	5:X:49:DT:H71	1.91	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
1:G:262:LEU:HD22	1:G:314:GLU:HB3	1.90	0.53
2:H:313:LEU:HD23	2:H:314:VAL:N	2.23	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
2:F:446:ALA:HB3	2:F:447:PRO:HD3	1.91	0.52
1:G:398:PHE:HE2	2:H:421:ALA:O	1.92	0.52
2:B:309:GLU:C	2:B:311:THR:H	2.13	0.52
2:B:482:TRP:CE3	2:B:507:PRO:HG3	2.45	0.52
2:B:491:ARG:HA	5:L:52:DA:C5'	2.39	0.52
1:C:491:ALA:O	1:C:495:ASP:HB2	2.08	0.52
4:J:28:DC:H5'	4:J:28:DC:H6	1.73	0.52
4:J:41:DT:H2"	4:J:42:DG:C8	2.44	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
2:D:547:PRO:HD2	4:V:45:DG:C3'	2.39	0.52
1:E:407:GLU:CD	2:F:405:ARG:HH12	2.12	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
1:C:483:ARG:HD3	4:V:31:DA:C4'	2.37	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
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
2:D:296:ARG:HB3	2:D:306:TRP:CZ3	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:271:LEU:HA	1:G:310:TRP:CD1	2.44	0.52
2:H:293:TRP:CZ2	2:H:443:VAL:HG21	2.44	0.52
5:P:48:DC:H2"	5:P:49:DT:O5'	2.09	0.52
4:R:28:DC:H2"	4:R:29:DA:H5'	1.92	0.52
1:E:491:ALA:O	1:E:495:ASP:HB2	2.09	0.52
2:F:346:PHE:CE2	2:F:350:ILE:HD11	2.45	0.52
1:G:472:ARG:CB	2:H:562:PRO:HB2	2.40	0.52
2:H:545:ILE:HG23	2:H:549:LEU:HD23	1.92	0.52
5:X:50:DG:H5"	5:X:50:DG:H8	1.74	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:261:LEU:HD11	2:H:282:ILE:HD12	1.92	0.51
2:H:517:CYS:HB2	2:H:523:ARG:HG3	1.90	0.51
3:I:3:DA:N6	4:J:32:DT:H3	2.06	0.51
4:N:28:DC:H5'	4:N:28:DC:C6	2.42	0.51
4:V:40:DA:H2"	4:V:41:DT:C6	2.45	0.51
1:C:317:PRO:HB3	1:C:323:PRO:HA	1.92	0.51
2:D:350:ILE:HG21	2:D:359:LEU:HD22	1.93	0.51
1:E:337:LEU:HD23	1:E:377:LEU:HD11	1.92	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
1:G:276:GLY:C	1:G:278:THR:H	2.12	0.51
1:A:347:GLY:CA	2:B:461:LEU:HD22	2.41	0.51
1:C:524:LYS:HG3	1:C:529:GLN:CD	2.31	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:G:512:THR:HG22	1:G:514:LYS:H	1.75	0.51
1:A:273:VAL:HG22	1:A:308:PHE:CD1	2.46	0.51
2:B:548:GLU:OE1	2:B:552:ARG:HD3	2.11	0.51
1:E:310:TRP:O	1:E:328:LEU:N	2.36	0.51
1:G:472:ARG:HG3	1:G:494:VAL:HG11	1.92	0.51
4:R:40:DA:P	4:R:40:DA:H3'	2.50	0.51
1:A:411:TYR:HH	2:B:416:GLN:CD	2.10	0.51
2:B:260:LEU:HB2	2:B:289:CYS:HA	1.93	0.51
1:C:375:HIS:HA	1:C:377:LEU:HG	1.93	0.51
2:D:548:GLU:OE1	2:D:552:ARG:HD3	2.10	0.51
1:G:527:ARG:NE	1:G:530:ARG:HB2	2.25	0.51
3:Q:10:DT:O4	4:R:23:DA:N6	2.43	0.51
1:A:512:THR:HG22	1:A:514:LYS:H	1.75	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:E:489:LYS:HD2	1:E:532:LEU:CD1	2.41	0.51
2:H:296:ARG:HB3	2:H:306:TRP:CZ3	2.46	0.51
2:H:541:THR:OG1	5:P:50:DG:P	2.69	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:355:ARG:HH22	5:T:54:DG:H5"	1.76	0.51
1:E:473:GLU:HG3	2:F:459:PHE:CE2	2.46	0.51
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:548:GLU:OE1	2:F:552:ARG:HD3	2.11	0.50
2:H:548:GLU:OE1	2:H:552:ARG:HD3	2.11	0.50
3:I:1:DG:N2	3:I:2:DA:N3	2.58	0.50
4:N:28:DC:C2'	4:N:29:DA:H5'	2.35	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
1:A:274:ASP:HB2	1:A:303:LEU:HB2	1.93	0.50
1:A:400:LYS:HG3	1:A:411:TYR:CZ	2.47	0.50
2:D:346:PHE:CE2	2:D:350:ILE:HD11	2.46	0.50
1:G:369:GLU:OE1	1:G:405:ILE:HG12	2.11	0.50
5:X:50:DG:H2"	5:X:51:DC:O4'	2.10	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
2:H:491:ARG:NH2	2:H:552:ARG:NH1	2.59	0.50
4:N:25:DA:H2"	4:N:26:DC:O4'	2.11	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
3:U:10:DT:O4	4:V:23:DA:N6	2.44	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
1:E:421:ARG:NH2	2:F:414:ASP:OD1	2.36	0.50
2:F:296:ARG:HH22	2:F:301:GLU:HB2	1.75	0.50
4:R:28:DC:H5'	4:R:28:DC:C6	2.45	0.50
1:A:303:LEU:HD11	1:A:309:VAL:HG22	1.93	0.50
1:A:400:LYS:HG3	1:A:411:TYR:CE1	2.47	0.50
2:D:446:ALA:HB3	2:D:447:PRO:HD3	1.93	0.50
1:G:308:PHE:HB2	1:G:332:VAL:HB	1.94	0.50
4:J:38:DA:H2"	4:J:39:DC:C6	2.47	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
1:A:414:LEU:C	2:B:413:VAL:HG11	2.33	0.49
2:B:315:LEU:HD12	2:B:432:LEU:HD21	1.94	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
1:C:499:THR:HG23	1:C:502:SER:H	1.77	0.49
3:M:8:DT:H2'	3:M:9:DG:C8	2.48	0.49
1:A:308:PHE:HB2	1:A:332:VAL:HB	1.95	0.49
2:D:260:LEU:HB2	2:D:289:CYS:HA	1.94	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
1:C:482:VAL:HA	2:D:469:VAL:O	2.13	0.49
2:F:346:PHE:O	2:F:350:ILE:HG13	2.12	0.49
2:F:496:MET:CE	5:T:51:DC:H5"	2.43	0.49
2:H:472:ASP:OD1	2:H:476:ARG:HB2	2.13	0.49
5:T:51:DC:H2"	5:T:52:DA:OP2	2.12	0.49
1:A:485:VAL:O	4:J:31:DA:OP1	2.31	0.49
1:E:350:ARG:NE	3:Q:1:DG:P	2.86	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
1:C:341:CYS:SG	1:C:384:LEU:HD21	2.53	0.49
5:T:54:DG:H2"	5:T:55:DT:C7	2.43	0.49
1:A:375:HIS:HA	1:A:377:LEU:HG	1.94	0.48
1:A:431:ARG:HG2	1:A:432:PRO:HD2	1.95	0.48
2:B:293:TRP:CZ2	2:B:443:VAL:HG21	2.48	0.48
4:N:42:DG:OP2	4:N:42:DG:H8	1.96	0.48
1:A:271:LEU:HA	1:A:310:TRP:CD1	2.48	0.48
2:D:489:LEU:N	2:D:489:LEU:CD1	2.75	0.48
2:D:545:ILE:HG23	2:D:549:LEU:HD23	1.95	0.48
1:E:279:ARG:NH2	4:R:40:DA:O5'	2.46	0.48
1:G:423:TYR:HD2	1:G:428:LEU:HD11	1.78	0.48
2:H:458:SER:O	2:H:462:GLU:HB2	2.12	0.48
1:A:304:HIS:HB3	1:A:463:ALA:HB3	1.94	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
1:E:308:PHE:HB2	1:E:332:VAL:HB	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:40:DA:C5	4:R:41:DT:C2	3.01	0.48
1:A:414:LEU:HB3	2:B:413:VAL:HG21	1.94	0.48
2:B:296:ARG:HB3	2:B:306:TRP:CZ3	2.48	0.48
2:D:433:ALA:O	2:D:436:THR:HB	2.13	0.48
2:F:293:TRP:CD2	2:F:443:VAL:HG11	2.48	0.48
1:G:384:LEU:O	1:G:387:ALA:HB3	2.13	0.48
1:G:398:PHE:CE2	2:H:422:GLN:HA	2.49	0.48
2:H:489:LEU:N	2:H:489:LEU:HD12	2.27	0.48
2:H:517:CYS:CB	2:H:523:ARG:HG3	2.42	0.48
1:E:392:GLN:NE2	2:F:435:PHE:HZ	2.11	0.48
2:F:491:ARG:HA	5:T:52:DA:H5'	1.94	0.48
2:B:458:SER:O	2:B:462:GLU:HB2	2.13	0.48
2:B:491:ARG:NH2	2:B:552:ARG:NH1	2.62	0.48
1:C:273:VAL:HG22	1:C:308:PHE:CD1	2.48	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
5:L:52:DA:H1'	5:L:53:DT:C6	2.49	0.48
1:A:472:ARG:HB2	2:B:562:PRO:CA	2.44	0.48
1:A:494:VAL:O	1:A:498:SER:HA	2.14	0.48
2:B:449:LYS:NZ	3:I:1:DG:H3'	2.28	0.48
2:D:256:LEU:HD23	2:D:260:LEU:HD23	1.95	0.48
2:H:449:LYS:NZ	3:M:1:DG:C5'	2.75	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
2:B:346:PHE:O	2:B:350:ILE:HG13	2.13	0.48
4:J:28:DC:H5'	4:J:28:DC:C6	2.49	0.48
2:B:462:GLU:HG2	2:B:463:SER:N	2.29	0.48
2:D:512:GLN:HA	2:D:515:GLN:NE2	2.28	0.48
2:F:545:ILE:HG23	2:F:549:LEU:HD23	1.95	0.48
1:G:489:LYS:HD2	1:G:532:LEU:CD1	2.44	0.48
2:H:252:ILE:HD11	2:H:295:ARG:NH1	2.28	0.48
5:L:50:DG:H5'	5:L:50:DG:N9	2.26	0.48
1:E:494:VAL:O	1:E:498:SER:HA	2.14	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
2:F:491:ARG:NH2	2:F:552:ARG:NH1	2.63	0.47
2:F:493:SER:HB3	5:T:51:DC:C3'	2.44	0.47
2:H:296:ARG:HH22	2:H:301:GLU:HB2	1.78	0.47
3:I:9:DG:C6	4:J:25:DA:N6	2.82	0.47
4:V:28:DC:H5'	4:V:28:DC:C6	2.49	0.47
2:B:295:ARG:HB3	2:B:307:VAL:HG12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:412:LEU:HD12	2:B:412:LEU:HA	1.72	0.47
1:C:512:THR:HG22	1:C:514:LYS:H	1.78	0.47
4:J:28:DC:H2"	4:J:29:DA:H5'	1.95	0.47
5:L:48:DC:H2"	5:L:49:DT:C7	2.44	0.47
1:A:486:SER:CB	4:J:30:DC:H3'	2.34	0.47
2:B:523:ARG:HB3	2:B:554:TYR:CE1	2.50	0.47
1:C:405:ILE:O	1:C:408:SER:HB2	2.15	0.47
1:E:386:GLN:HE22	2:F:438:ALA:CA	2.20	0.47
2:F:248:CYS:SG	2:F:249:LEU:N	2.87	0.47
5:X:52:DA:C4	5:X:53:DT:C2	3.02	0.47
1:A:500:PRO:HG2	2:B:556:GLN:O	2.14	0.47
2:B:256:LEU:HD23	2:B:260:LEU:HD23	1.95	0.47
1:E:477:ARG:HH21	2:F:488:GLN:CD	2.18	0.47
1:G:308:PHE:HE2	1:G:334:ARG:HB2	1.79	0.47
1:G:544:TYR:O	2:H:508:GLN:NE2	2.28	0.47
2:H:309:GLU:C	2:H:311:THR:H	2.16	0.47
4:R:25:DA:H2"	4:R:26:DC:O4'	2.14	0.47
1:A:317:PRO:HB3	1:A:323:PRO:HA	1.95	0.47
2:B:237:VAL:O	2:B:241:LYS:HG3	2.15	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:G:550:LEU:HD13	2:H:506:SER:HB2	1.94	0.47
1:C:484:GLY:HA3	1:C:536:LEU:HD21	1.96	0.47
2:D:247:GLU:HG2	2:D:250:LYS:HB2	1.97	0.47
2:F:491:ARG:NH1	4:R:44:DA:H4'	2.30	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
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
2:F:458:SER:O	2:F:462:GLU:HB2	2.13	0.47
2:F:490:ASN:O	2:F:552:ARG:NH2	2.46	0.47
1:G:318:ARG:O	1:G:320:PRO:HD3	2.14	0.47
3:U:5:DG:C2	4:V:31:DA:C2	3.03	0.47
1:A:347:GLY:HA3	2:B:461:LEU:HD22	1.97	0.47
2:B:296:ARG:HB3	2:B:306:TRP:CH2	2.49	0.47
2:D:329:LYS:NZ	2:D:414:ASP:OD2	2.34	0.47
4:V:25:DA:H2"	4:V:26:DC:O4'	2.15	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:E:353:LYS:NZ	1:E:395:ASP:OD2	2.42	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)
1:A:394:ILE:O	2:B:450:LYS:CE	2.63	0.46
2:B:352:ALA:HB1	2:D:352:ALA:O	2.14	0.46
2:B:472:ASP:OD1	2:B:476:ARG:HB2	2.15	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
2:F:315:LEU:HD12	2:F:432:LEU:HD21	1.96	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:H:492:VAL:N	5:P:52:DA:OP1	2.48	0.46
2:D:483:ARG:NH1	2:D:494:LEU:HD12	2.30	0.46
4:J:30:DC:C2	4:J:31:DA:C8	3.02	0.46
4:V:39:DC:H2"	4:V:40:DA:C8	2.50	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:H:346:PHE:CE2	2:H:350:ILE:HD11	2.49	0.46
2:B:313:LEU:HD23	2:B:314:VAL:N	2.31	0.46
2:D:296:ARG:HB3	2:D:306:TRP:CH2	2.50	0.46
2:F:541:THR:OG1	5:T:50:DG:H4'	2.15	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
1:C:262:LEU:HD22	1:C:314:GLU:HB3	1.97	0.46
1:C:308:PHE:HB2	1:C:332:VAL:HB	1.97	0.46
1:E:318:ARG:O	1:E:320:PRO:HD3	2.16	0.46
2:F:314:VAL:HB	2:F:359:LEU:HD11	1.97	0.46
2:H:241:LYS:HA	2:H:244:ARG:CD	2.45	0.46
2:H:481:VAL:O	2:H:485:GLN:HG3	2.16	0.46
4:V:38:DA:H2"	4:V:39:DC:OP2	2.16	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
1:C:431:ARG:HG2	1:C:432:PRO:HD2	1.97	0.46
2:D:481:VAL:O	2:D:485:GLN:HG3	2.16	0.46
1:E:371:HIS:HB2	1:E:403:ALA:HA	1.97	0.46
2:H:241:LYS:HA	2:H:244:ARG:HD2	1.98	0.46
4:V:28:DC:C2'	4:V:29:DA:H5'	2.46	0.46
1:A:405:ILE:O	1:A:408:SER:HB2	2.14	0.46
1:A:414:LEU:HB3	2:B:413:VAL:HG11	1.97	0.46
1:A:486:SER:O	1:A:490:ALA:N	2.41	0.46
1:A:543:LEU:O	2:B:507:PRO:HG2	2.15	0.46
1:G:350:ARG:CD	2:H:461:LEU:HD13	2.44	0.46
1:G:400:LYS:HG3	1:G:411:TYR:CZ	2.51	0.46
2:H:405:ARG:HG3	2:H:405:ARG:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:H:541:THR:C	2:H:542:SER:O	2.47	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:D:287:VAL:HG13	2:D:290:SER:OG	2.16	0.46
2:D:462:GLU:HG2	2:D:463:SER:N	2.29	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:B:293:TRP:CD2	2:B:443:VAL:HG11	2.51	0.45
2:D:270:LEU:HG	2:H:267:GLY:HA3	1.98	0.45
1:E:484:GLY:HA3	1:E:536:LEU:HD21	1.97	0.45
2:F:517:CYS:CB	2:F:523:ARG:HG3	2.46	0.45
3:I:1:DG:N2	3:I:2:DA:C2	2.84	0.45
5:X:52:DA:C2	5:X:53:DT:O2	2.69	0.45
1:C:317:PRO:HG2	1:C:320:PRO:HA	1.99	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:A:474:VAL:HG21	2:B:566:LEU:HD11	1.97	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:C:310:TRP:HH2	1:C:415:LEU:HD13	1.80	0.45
1:C:337:LEU:HD22	1:C:370:GLU:O	2.16	0.45
2:D:324:MET:HG2	2:D:342:THR:N	2.31	0.45
2:D:541:THR:OG1	5:X:50:DG:C4'	2.64	0.45
1:A:499:THR:CG2	2:B:560:LEU:HA	2.23	0.45
2:B:517:CYS:HB2	2:B:523:ARG:HG3	1.97	0.45
1:C:302:LYS:NZ	5:X:54:DG:O3'	2.42	0.45
2:F:324:MET:HG2	2:F:342:THR:N	2.31	0.45
2:F:462:GLU:HG2	2:F:463:SER:N	2.31	0.45
1:G:333:GLU:OE1	1:G:352:GLN:NE2	2.50	0.45
2:H:541:THR:OG1	5:P:50:DG:OP1	2.34	0.45
3:M:7:DG:O6	4:N:27:DA:N1	2.49	0.45
4:R:28:DC:C2'	4:R:29:DA:H5'	2.46	0.45
1:A:278:THR:O	1:A:278:THR:OG1	2.33	0.45
2:D:534:ARG:NH1	5:X:50:DG:P	2.80	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
1:G:418:GLY:HA3	2:H:417:LEU:CD1	2.47	0.45
1:G:472:ARG:HB2	2:H:562:PRO:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:524:LYS:HG3	1:G:529:GLN:CD	2.36	0.45
2:H:312:VAL:HG12	2:H:357:LYS:CB	2.47	0.45
1:C:479:LEU:HG	1:C:493:LEU:HD13	1.99	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
2:B:342:THR:O	2:B:342:THR:OG1	2.35	0.45
2:D:293:TRP:CZ2	2:D:443:VAL:HG21	2.51	0.45
2:D:309:GLU:C	2:D:311:THR:H	2.18	0.45
1:E:499:THR:HG22	1:E:502:SER:HB2	1.98	0.45
2:F:256:LEU:HD23	2:F:260:LEU:HD23	1.99	0.45
2:H:449:LYS:HZ2	3:M:1:DG:H5"	1.81	0.45
4:J:23:DA:H2'	4:J:24:DG:C8	2.52	0.45
1:A:310:TRP:HH2	1:A:415:LEU:HD13	1.82	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:G:317:PRO:HB3	1:G:323:PRO:HA	1.98	0.45
2:H:295:ARG:HB3	2:H:307:VAL:HG12	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
1:E:528:LEU:HD22	2:F:236:LEU:CD2	2.47	0.45
2:H:449:LYS:HZ3	3:M:1:DG:P	2.40	0.45
5:T:50:DG:C2'	5:T:51:DC:H5'	2.43	0.45
2:B:273:LEU:HD12	2:B:273:LEU:HA	1.63	0.44
1:G:351:GLU:O	1:G:355:ARG:HG3	2.17	0.44
4:R:40:DA:N7	4:R:41:DT:N3	2.64	0.44
1:C:533:GLY:HA3	3:U:9:DG:O5'	2.16	0.44
1:E:499:THR:HG23	1:E:502:SER:H	1.81	0.44
2:F:260:LEU:HB2	2:F:289:CYS:HA	1.98	0.44
3:I:7:DG:H2'	3:I:8:DT:H6	1.82	0.44
1:E:267:TYR:OH	1:E:423:TYR:O	2.34	0.44
1:G:394:ILE:O	2:H:450:LYS:CE	2.66	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:A:384:LEU:O	1:A:387:ALA:HB3	2.18	0.44
2:D:273:LEU:HD12	2:D:273:LEU:HA	1.64	0.44
1:G:308:PHE:O	1:G:331:ILE:HG13	2.17	0.44
3:I:8:DT:H2'	3:I:9:DG:C8	2.53	0.44
4:J:43:DC:N3	5:L:50:DG:N1	2.59	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)
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:F:309:GLU:C	2:F:311:THR:H	2.19	0.44
2:F:541:THR:N	5:T:50:DG:P	2.91	0.44
1:G:472:ARG:HB3	2:H:562:PRO:HB2	1.98	0.44
1:G:481:GLN:HG3	2:H:485:GLN:HA	1.99	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
2:B:446:ALA:O	2:B:450:LYS:HG2	2.17	0.44
1:E:481:GLN:HG3	2:F:481:VAL:HG13	2.00	0.44
1:E:497:TYR:HE2	1:E:520:LEU:CD2	2.31	0.44
2:F:254:VAL:O	2:F:256:LEU:HD12	2.18	0.44
2:F:481:VAL:O	2:F:485:GLN:HG3	2.15	0.44
1:G:303:LEU:HD11	1:G:309:VAL:HG22	2.00	0.44
1:A:414:LEU:O	2:B:413:VAL:HG11	2.18	0.44
2:B:241:LYS:HA	2:B:244:ARG:CD	2.48	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:A:263:ARG:HG3	1:A:266:GLU:OE2	2.18	0.44
2:B:293:TRP:CG	2:B:443:VAL:HG11	2.52	0.44
1:E:472:ARG:NH2	2:F:457:PHE:CZ	2.79	0.44
2:F:364:VAL:O	2:F:364:VAL:HG13	2.18	0.44
1:G:341:CYS:SG	1:G:384:LEU:HD21	2.57	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:H:412:LEU:HD12	2:H:412:LEU:HA	1.79	0.44
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
2:H:491:ARG:NH2	2:H:552:ARG:CZ	2.81	0.43
1:C:486:SER:OG	4:V:30:DC:P	2.74	0.43
2:B:247:GLU:HG2	2:B:250:LYS:HB2	2.00	0.43
2:B:294:ARG:HA	2:B:307:VAL:O	2.19	0.43
2:B:481:VAL:O	2:B:485:GLN:HG3	2.19	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
1:A:266:GLU:O	1:A:314:GLU:HA	2.18	0.43
1:E:472:ARG:O	1:E:473:GLU:C	2.57	0.43
1:G:494:VAL:O	1:G:498:SER:HA	2.18	0.43

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:534:ARG:NH1	2:D:541:THR:HB	2.34	0.42
1:E:431:ARG:HG2	1:E:432:PRO:HD2	1.99	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
4:V:30:DC:C2	4:V:31:DA:C8	3.07	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
1:G:431:ARG:HG2	1:G:432:PRO:HD2	2.02	0.42
1:G:483:ARG:HB3	2:H:470:LYS:HA	2.01	0.42
2:H:247:GLU:O	2:H:250:LYS:HB2	2.19	0.42
2:H:448:PHE:CE2	2:H:449:LYS:HE3	2.55	0.42
3:Q:7:DG:H2'	3:Q:8:DT:H6	1.84	0.42
1:A:332:VAL:HA	1:A:365:VAL:O	2.20	0.42
2:B:545:ILE:HG23	2:B:549:LEU:HD23	2.00	0.42
2:B:547:PRO:CD	4:J:45:DG:H3'	2.30	0.42
2:D:257:ASP:O	2:D:260:LEU:HB3	2.19	0.42
2:D:267:GLY:HA3	2:H:271:GLY:CA	2.43	0.42
1:E:326:LEU:HD23	1:E:455:THR:HA	2.00	0.42
2:H:422:GLN:HG3	2:H:423:ALA:N	2.34	0.42
4:J:43:DC:H6	4:J:43:DC:P	2.42	0.42
1:A:390:ASN:OD1	2:B:442:ALA:HA	2.20	0.42
2:B:254:VAL:O	2:B:256:LEU:HD12	2.20	0.42
2:D:281:VAL:HB	2:H:262:GLN:NE2	2.35	0.42
2:F:241:LYS:HA	2:F:244:ARG:CD	2.50	0.42
3:Q:8:DT:H2'	3:Q:9:DG:C8	2.55	0.42
2:B:316:LEU:HD12	2:B:316:LEU:HA	1.63	0.42
2:B:504:TYR:C	2:B:506:SER:H	2.23	0.42
2:B:517:CYS:CB	2:B:523:ARG:HG3	2.50	0.42
1:C:489:LYS:HD2	1:C:532:LEU:CD1	2.49	0.42
1:G:530:ARG:HE	4:N:29:DA:H4'	1.84	0.42
4:J:43:DC:O5'	4:J:43:DC:H2'	2.19	0.42
1:A:414:LEU:HD23	2:B:410:GLU:HA	2.02	0.42
1:A:419:LEU:HD23	1:A:419:LEU:HA	1.83	0.42
1:A:484:GLY:HA3	1:A:536:LEU:HD21	2.01	0.42
1:A:489:LYS:HD2	1:A:532:LEU:HD12	2.02	0.42
1:C:417:ARG:HA	1:C:417:ARG:HD2	1.87	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
4:J:28:DC:C2'	4:J:29:DA:H5'	2.50	0.42
1:C:472:ARG:O	1:C:473:GLU:C	2.57	0.42
2:D:252:ILE:HD13	2:D:295:ARG:HA	2.02	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:541:THR:N	5:X:49:DT:C4'	2.83	0.42
1:A:294:LEU:HD23	1:A:294:LEU:HA	1.83	0.42
1:A:423:TYR:HD2	1:A:428:LEU:HD11	1.85	0.42
2:D:405:ARG:O	2:D:405:ARG:HG3	2.19	0.42
4:R:41:DT:H6	4:R:41:DT:H2'	1.47	0.42
1:C:400:LYS:HG3	1:C:411:TYR:CE1	2.55	0.41
1:E:492:ALA:HB2	1:E:525:CYS:HA	2.02	0.41
2:F:467:GLY:O	2:F:484:ARG:NH2	2.47	0.41
1:G:278:THR:O	1:G:278:THR:OG1	2.36	0.41
1:G:402:THR:HG21	1:G:408:SER:OG	2.20	0.41
2:H:316:LEU:HA	2:H:316:LEU:HD12	1.57	0.41
1:A:336:ARG:HA	1:A:369:GLU:HB3	2.02	0.41
1:A:497:TYR:CE2	1:A:520:LEU:CD2	3.03	0.41
1:A:512:THR:O	1:A:515:GLU:HB3	2.20	0.41
2:B:496:MET:SD	5:L:51:DC:H5"	2.59	0.41
1:E:278:THR:O	1:E:278:THR:OG1	2.31	0.41
1:G:543:LEU:HD13	2:H:507:PRO:HG2	2.02	0.41
1:A:512:THR:O	1:A:515:GLU:N	2.54	0.41
1:A:538:ARG:NH2	2:B:473:LEU:O	2.54	0.41
2:D:541:THR:C	2:D:542:SER:O	2.46	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: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:HA	2:D:316:LEU:HD12	1.61	0.41
1:A:308:PHE:O	1:A:331:ILE:HG13	2.20	0.41
2:B:449:LYS:HD3	3:I:1:DG:P	2.61	0.41
1:C:543:LEU:HD22	1:C:550:LEU:HD21	2.02	0.41
2:F:361:LEU:HG	2:F:362:VAL:N	2.36	0.41
1:G:417:ARG:HA	1:G:417:ARG:HD2	1.85	0.41
1:G:483:ARG:NE	2:H:470:LYS:HB2	2.35	0.41
4:N:45:DG:H5'	4:N:45:DG:N9	2.35	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
2:D:415:LEU:O	2:D:419:THR:OG1	2.25	0.41
2:D:471:VAL:HG22	2:D:472:ASP:O	2.20	0.41
1:G:405:ILE:HA	1:G:408:SER:HB2	2.02	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:H:287:VAL:HA	2:H:288:PRO:HD3	1.96	0.41
1:A:371:HIS:CE1	1:A:401:ARG:HD3	2.56	0.41
1:A:472:ARG:CD	2:B:562:PRO:HB2	2.43	0.41
1:A:486:SER:H	1:A:489:LYS:HB2	1.85	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
2:F:496:MET:HE1	5:T:51:DC:H5"	2.03	0.41
1:G:266:GLU:O	1:G:314:GLU:HA	2.21	0.41
1:G:472:ARG:O	1:G:473:GLU:C	2.59	0.41
1:A:399:VAL:N	2:B:422:GLN:OE1	2.51	0.41
2:B:473:LEU:H	2:B:473:LEU:HD12	1.85	0.41
1:C:407:GLU:O	1:C:411:TYR:N	2.48	0.41
1:E:477:ARG:NH2	2:F:465:TRP:HZ3	2.19	0.41
1:E:489:LYS:HD2	1:E:532:LEU:HD12	2.03	0.41
1:G:472:ARG:HG3	1:G:494:VAL:CG1	2.51	0.41
1:C:332:VAL:HA	1:C:365:VAL:O	2.21	0.41
2:D:270:LEU:HD23	2:H:267:GLY:HA2	2.03	0.41
1:E:266:GLU:O	1:E:314:GLU:HA	2.21	0.41
1:G:472:ARG:HB2	2:H:562:PRO:CB	2.51	0.41
1:G:527:ARG:NH2	4:N:29:DA:OP1	2.51	0.41
3:U:10:DT:H6	3:U:10:DT:H2'	1.55	0.41
1:A:379:LEU:HD23	1:A:384:LEU:HD11	2.02	0.40
1:C:340:LEU:O	1:C:344:ILE:HG13	2.21	0.40
2:F:541:THR:C	2:F:542:SER:O	2.51	0.40
1:G:316:ASN:HA	1:G:317:PRO:HD2	1.93	0.40
1:G:414:LEU:HB3	2:H:413:VAL:HG21	2.02	0.40
2:H:252:ILE:HD11	2:H:295:ARG:CZ	2.51	0.40
2:D:493:SER:HB3	5:X:51:DC:C3'	2.44	0.40
1:E:263:ARG:HB2	1:E:266:GLU:OE2	2.21	0.40
1:E:543:LEU:HD22	1:E:543:LEU:HA	1.86	0.40
5:L:50:DG:H2"	5:L:51:DC:N1	2.36	0.40
4:N:39:DC:H2"	4:N:40:DA:N7	2.36	0.40
1:A:262:LEU:HD22	1:A:314:GLU:HB3	2.04	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
1:C:386:GLN:NE2	2:D:441:LYS:HB3	2.36	0.40
1:G:489:LYS:NZ	4:N:30:DC:O5'	2.52	0.40
1:G:496:ARG:HG2	1:G:523:ILE:CD1	2.52	0.40
2:H:471:VAL:HG22	2:H:472:ASP:O	2.22	0.40
3:M:5:DG:H2'	3:M:6:DT:H71	2.03	0.40
4:N:42:DG:H2"	4:N:43:DC:C6	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:42:DG:H8	4:R:42:DG:OP2	2.03	0.40
2:B:541:THR:OG1	5:L:50:DG:H4'	2.21	0.40
1:C:506:ALA:HB1	1:C:519:LEU:HD21	2.03	0.40
2:F:286:ALA:O	2:F:353:LYS:HD3	2.21	0.40
1:G:337:LEU:HD22	1:G:370:GLU:O	2.21	0.40
1:G:397:PHE:N	1:G:397:PHE:CD1	2.88	0.40
2:H:294:ARG:HA	2:H:307:VAL:O	2.21	0.40
2:H:514:TYR:O	2:H:523:ARG:HD3	2.20	0.40
5:L:50:DG:C4	5:L:51:DC:N3	2.90	0.40
3:Q:10:DT:H6	3:Q:10:DT:H2'	1.63	0.40
4:R:42:DG:N1	5:T:52:DA:C2	2.90	0.40
1:A:317:PRO:HG2	1:A:320:PRO:HA	2.04	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
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: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%)	14	52
1	C	267/306 (87%)	258 (97%)	6 (2%)	3 (1%)	14	52
1	E	267/306 (87%)	259 (97%)	6 (2%)	2 (1%)	22	62

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	G	267/306 (87%)	257 (96%)	7 (3%)	3 (1%)	14 52
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%)	29 69

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%)	19 45
1	C	237/259 (92%)	223 (94%)	14 (6%)	19 45
1	E	237/259 (92%)	222 (94%)	15 (6%)	18 43
1	G	237/259 (92%)	221 (93%)	16 (7%)	16 41
2	B	242/334 (72%)	225 (93%)	17 (7%)	15 40
2	D	242/334 (72%)	227 (94%)	15 (6%)	18 43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	F	242/334 (72%)	225 (93%)	17 (7%)	15 40
2	H	242/334 (72%)	224 (93%)	18 (7%)	13 38
All	All	1916/2372 (81%)	1790 (93%)	126 (7%)	16 41

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

Sometimes 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 monosaccharides 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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.