



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:49 AM UTC

PDB ID : 4P0S / pdb_00004p0s
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:

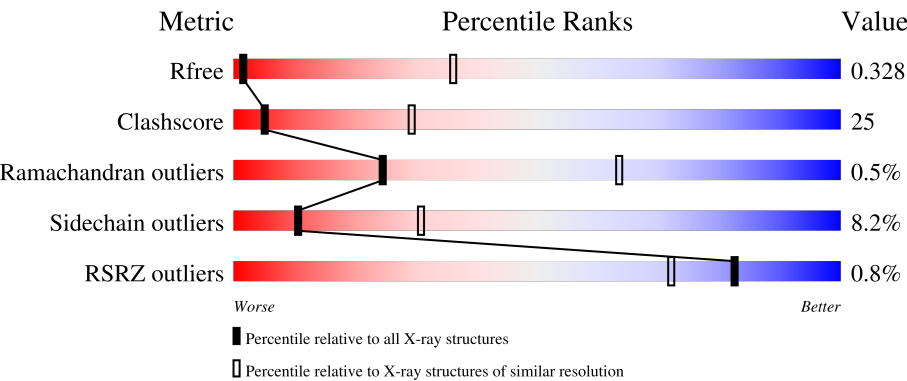
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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}	180053	1143 (8.00-4.00)
Clashscore	190562	1210 (8.00-4.00)
Ramachandran outliers	187476	1034 (8.00-4.00)
Sidechain outliers	187428	1000 (8.00-4.00)
RSRZ outliers	180081	1136 (8.00-4.00)

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 $\leq 5\%$. 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	44%35%8%•10%
1	C	306	% 47%33%9%•10%
1	E	306	% 46%35%9%•10%
1	G	306	43%35%10%•10%
2	B	393	% 32%33%7%•28%

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Mol	Chain	Length	Quality of chain
2	D	393	
2	F	393	
2	H	393	
3	I	12	
3	M	12	
3	Q	12	
3	U	12	
4	J	24	
4	N	24	
4	R	24	
4	V	24	
5	L	13	
5	P	13	
5	T	13	
5	X	13	

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			

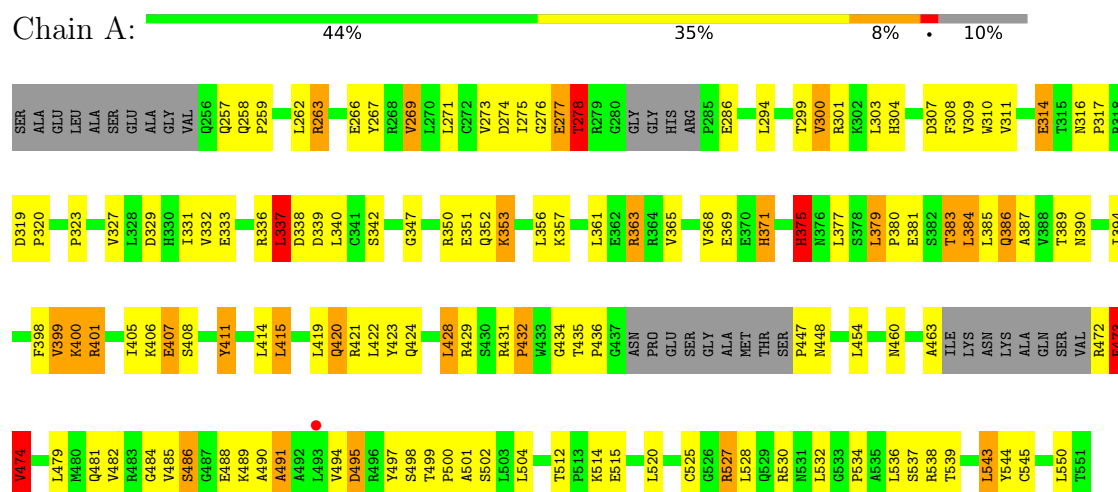
- Molecule 5 is a DNA chain called DNA TCTGCATGTCATT.

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			

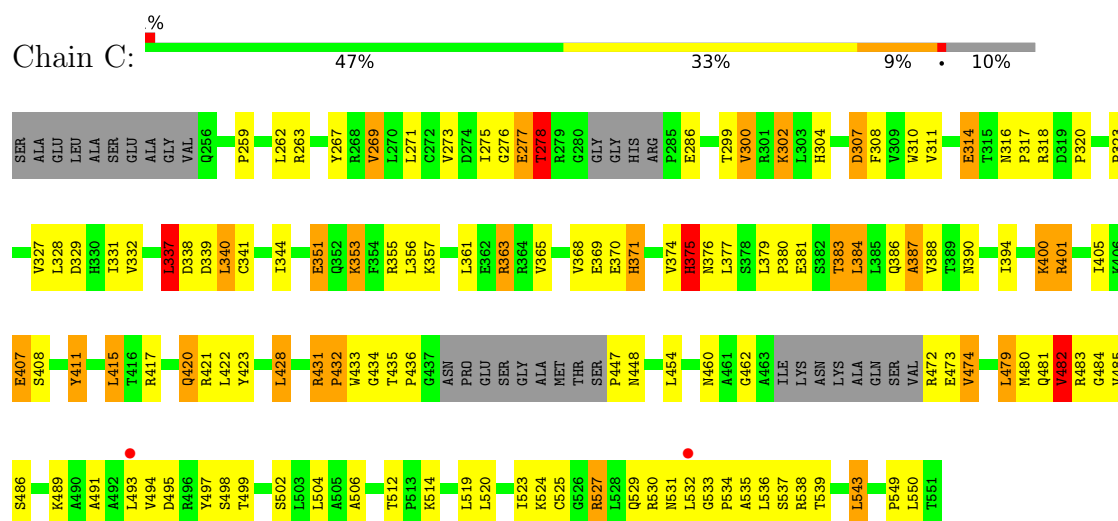
3 Residue-property plots

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

• Molecule 1: Crossover junction endonuclease MUS81

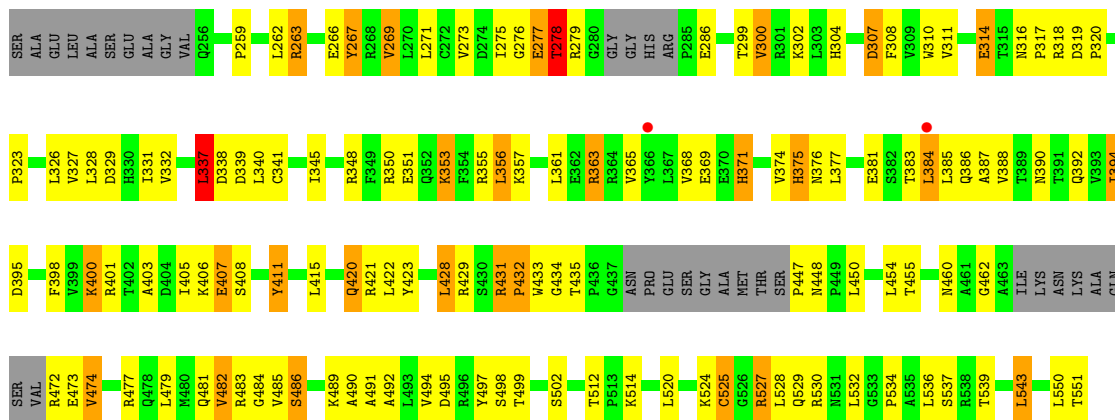


• Molecule 1: Crossover junction endonuclease MUS81

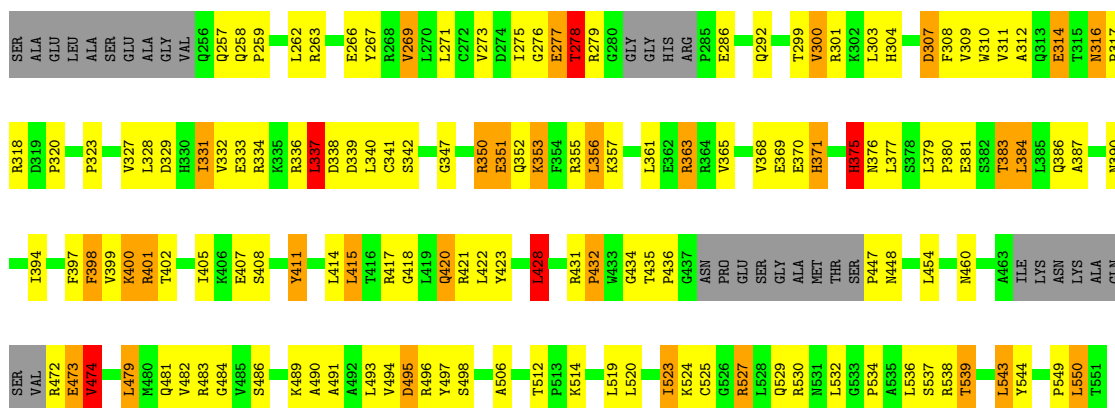


• Molecule 1: Crossover junction endonuclease MUS81

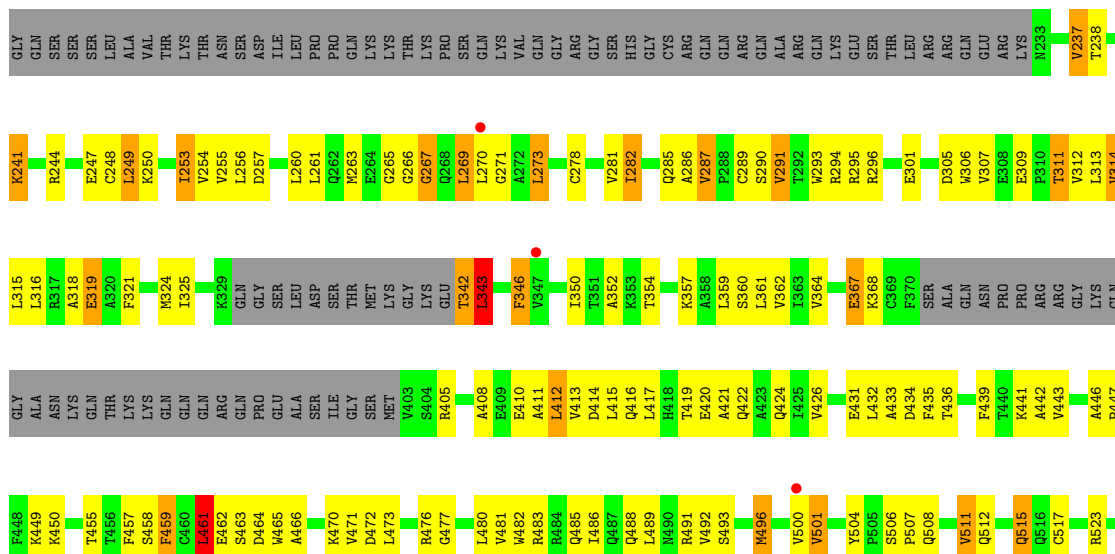




• Molecule 1: Crossover junction endonuclease MUS81

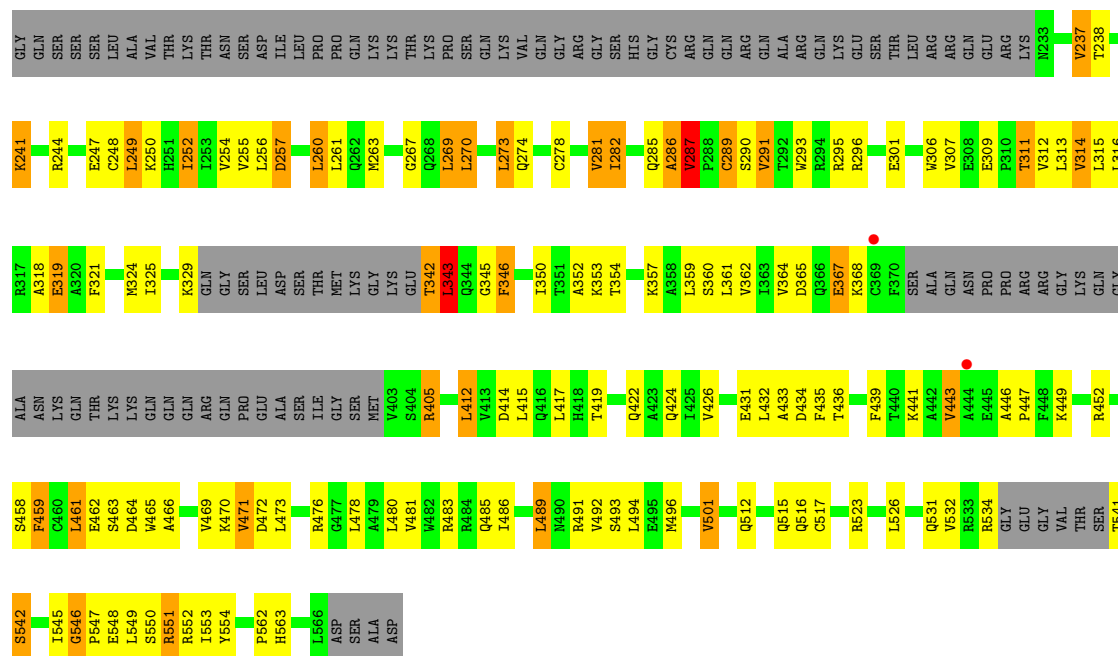


• Molecule 2: Crossover junction endonuclease EME1

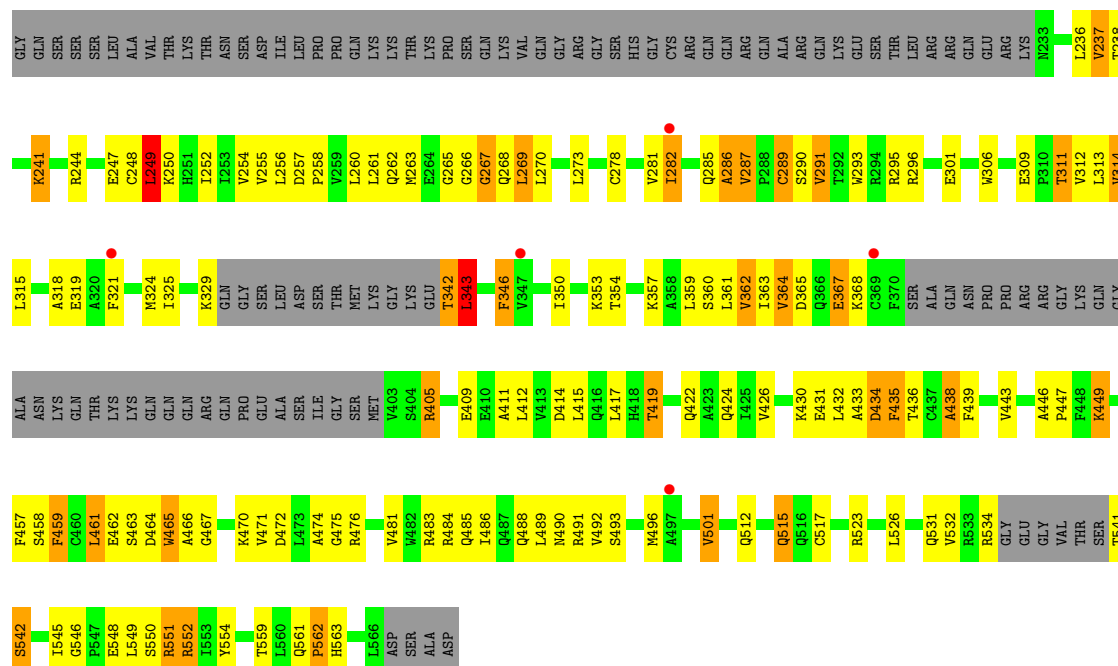




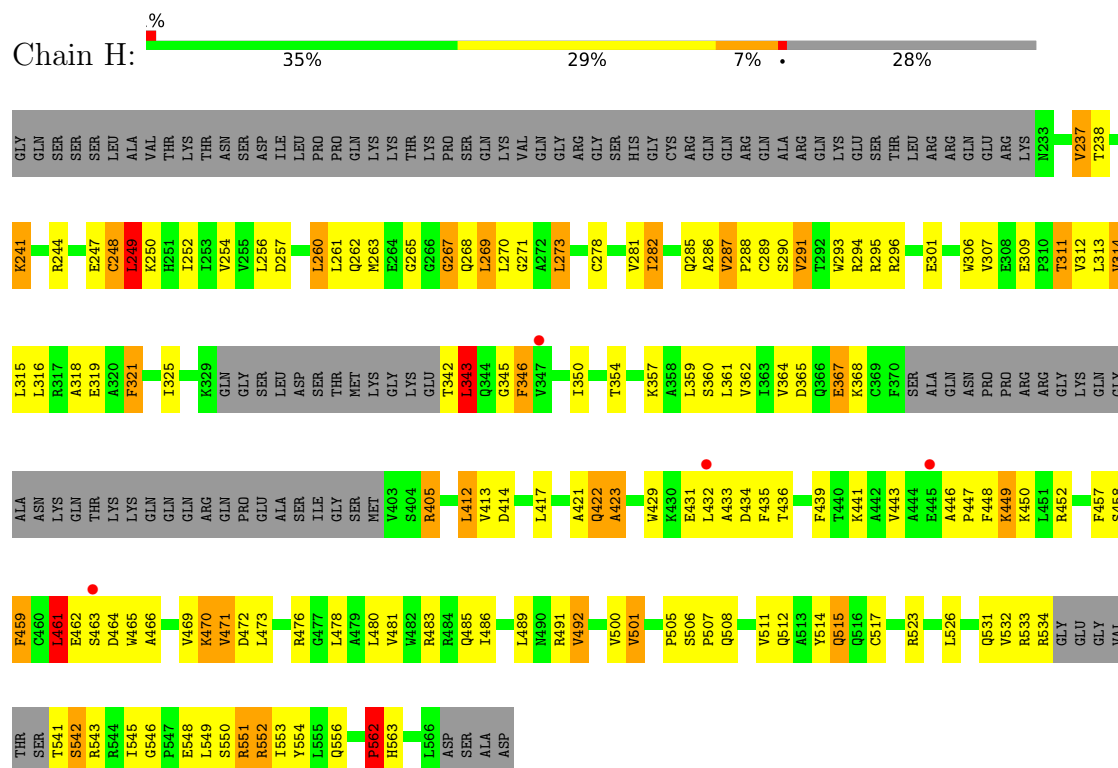
• Molecule 2: Crossover junction endonuclease EME1



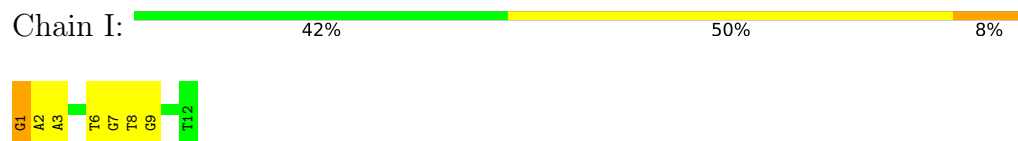
• Molecule 2: Crossover junction endonuclease EME1



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- Molecule 3: DNA GAATGTGTGTCT



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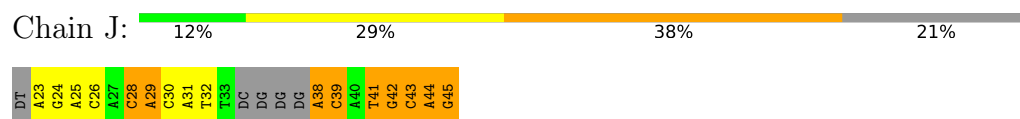
- Molecule 3: DNA GAATGTGTGTCT



- Molecule 3: DNA GAATGTGTGTCT



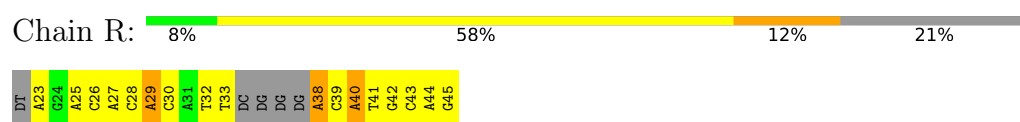
• Molecule 4: DNA TAGACACACATTCGGGACATGCAG



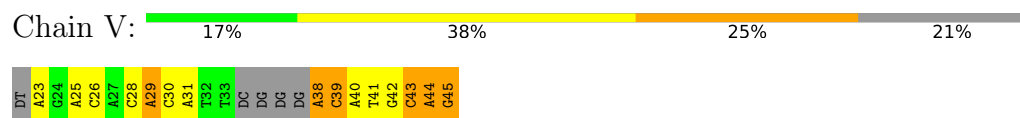
• Molecule 4: DNA TAGACACACATTCGGGACATGCAG



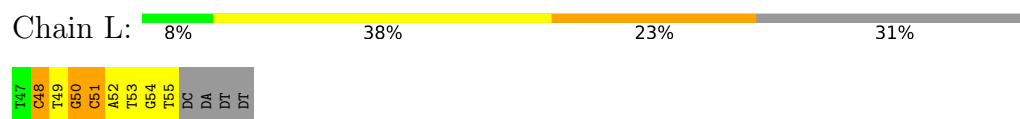
• Molecule 4: DNA TAGACACACATTCGGGACATGCAG



• Molecule 4: DNA TAGACACACATTCGGGACATGCAG



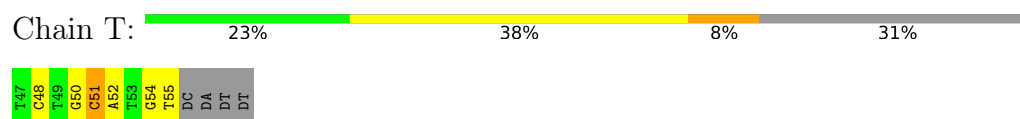
• Molecule 5: DNA TCTGCATGTCATT



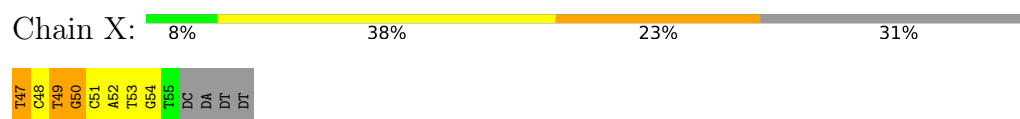
• Molecule 5: DNA TCTGCATGTCATT



• Molecule 5: DNA TCTGCATGTCATT



• Molecule 5: DNA TCTGCATGTCATT



4 Data and refinement statistics

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 29.98 – 6.00	Depositor EDS
% Data completeness (in resolution range)	99.4 (29.98-6.00) 98.5 (29.98-6.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.09 (at 5.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.250 , 0.308 0.276 , 0.328	Depositor DCC
R_{free} test set	853 reflections (5.02%)	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)	0.28 , 165.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.17	6/2211 (0.3%)	1.62	53/2989 (1.8%)
1	C	1.11	4/2211 (0.2%)	1.60	47/2989 (1.6%)
1	E	1.12	7/2211 (0.3%)	1.63	51/2989 (1.7%)
1	G	1.21	9/2211 (0.4%)	1.62	53/2989 (1.8%)
2	B	1.12	5/2258 (0.2%)	1.62	51/3054 (1.7%)
2	D	1.17	11/2258 (0.5%)	1.64	51/3054 (1.7%)
2	F	1.09	6/2258 (0.3%)	1.61	52/3054 (1.7%)
2	H	1.13	5/2258 (0.2%)	1.65	63/3054 (2.1%)
3	I	0.49	0/278	1.11	1/428 (0.2%)
3	M	0.49	0/278	1.07	1/428 (0.2%)
3	Q	0.31	0/278	0.92	0/428
3	U	0.42	0/278	0.96	1/428 (0.2%)
4	J	0.68	0/436	1.75	15/667 (2.2%)
4	N	0.62	0/436	1.52	11/667 (1.6%)
4	R	0.45	0/436	1.30	4/667 (0.6%)
4	V	0.65	0/436	1.62	11/667 (1.6%)
5	L	0.74	0/203	1.79	4/311 (1.3%)
5	P	0.77	0/203	1.84	6/311 (1.9%)
5	T	0.66	0/203	1.49	1/311 (0.3%)
5	X	0.60	0/203	1.50	3/311 (1.0%)
All	All	1.07	53/21544 (0.2%)	1.59	479/29796 (1.6%)

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	486	ILE	CA-CB	12.75	1.72	1.54
2	B	426	VAL	CA-CB	-8.86	1.42	1.54
1	G	307	ASP	CA-C	8.79	1.64	1.52
1	E	307	ASP	CA-C	8.61	1.64	1.52
2	H	486	ILE	CA-CB	7.35	1.64	1.54
1	C	307	ASP	CA-C	7.31	1.62	1.52
1	E	448	ASN	CA-C	7.18	1.60	1.53
2	F	486	ILE	CA-CB	7.14	1.64	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	389	THR	N-CA	-7.13	1.37	1.46
2	F	362	VAL	CA-CB	-7.04	1.45	1.54
1	G	435	THR	CA-C	7.02	1.59	1.52
2	B	362	VAL	CA-CB	-6.95	1.45	1.54
1	G	435	THR	N-CA	6.64	1.51	1.45
2	F	363	ILE	CA-CB	-6.59	1.46	1.54
2	H	362	VAL	CA-CB	-6.36	1.46	1.54
1	E	345	ILE	CA-CB	6.19	1.61	1.54
2	D	367	GLU	CA-C	6.18	1.61	1.52
2	D	291	VAL	CA-CB	-6.17	1.46	1.54
1	E	388	VAL	CA-C	-6.16	1.45	1.52
1	G	331	ILE	CA-CB	-6.07	1.46	1.54
2	H	367	GLU	CA-C	6.07	1.60	1.52
2	F	426	VAL	CA-CB	-6.06	1.46	1.54
1	A	491	ALA	CA-C	-6.05	1.44	1.52
1	A	448	ASN	CA-C	5.95	1.60	1.53
1	G	398	PHE	CA-CB	5.94	1.61	1.53
1	G	448	ASN	CA-C	5.84	1.60	1.53
1	G	399	VAL	CA-CB	-5.84	1.47	1.54
2	D	314	VAL	CA-C	5.61	1.60	1.52
1	A	386	GLN	N-CA	-5.60	1.39	1.46
1	C	388	VAL	CA-C	-5.60	1.45	1.52
2	B	253	ILE	CA-CB	-5.59	1.47	1.54
1	E	448	ASN	N-CA	5.56	1.53	1.45
1	E	429	ARG	CA-C	5.51	1.59	1.52
2	D	281	VAL	CA-CB	-5.47	1.46	1.54
1	A	399	VAL	CA-CB	-5.41	1.47	1.54
2	D	443	VAL	CA-CB	5.41	1.61	1.54
1	E	356	LEU	CA-C	5.38	1.60	1.52
2	D	252	ILE	CA-CB	-5.37	1.47	1.54
1	A	385	LEU	CA-C	-5.35	1.45	1.52
2	B	367	GLU	CA-C	5.28	1.59	1.52
2	B	486	ILE	CA-CB	5.26	1.61	1.54
2	D	282	ILE	CA-CB	5.23	1.59	1.53
1	G	356	LEU	CA-C	5.21	1.59	1.52
1	C	535	ALA	CA-CB	-5.18	1.45	1.53
2	F	364	VAL	CA-CB	-5.17	1.48	1.54
1	C	480	MET	N-CA	-5.17	1.40	1.46
2	D	362	VAL	CA-CB	-5.15	1.48	1.54
2	H	291	VAL	CA-CB	-5.13	1.48	1.54
2	F	409	GLU	CB-CG	5.13	1.67	1.52
2	D	426	VAL	CA-CB	-5.09	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	287	VAL	CA-CB	-5.06	1.50	1.54
2	H	422	GLN	CA-C	-5.01	1.46	1.52
1	G	428	LEU	CA-C	5.01	1.58	1.52

All (479) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	542	SER	N-CA-C	-15.91	90.84	110.41
2	H	542	SER	N-CA-C	-15.46	91.40	110.41
2	B	542	SER	N-CA-C	-15.21	91.70	110.41
2	F	542	SER	N-CA-C	-14.71	92.32	110.41
2	D	343	LEU	N-CA-C	12.68	124.64	111.07
1	A	474	VAL	N-CA-C	12.45	123.32	110.62
1	A	383	THR	N-CA-C	12.19	124.30	111.14
1	C	277	GLU	N-CA-C	-12.01	98.61	113.02
2	B	343	LEU	N-CA-C	11.41	123.41	110.97
1	G	277	GLU	N-CA-C	-11.40	99.34	113.02
1	E	368	VAL	N-CA-C	11.38	124.61	107.99
2	F	435	PHE	N-CA-C	-11.20	99.07	111.28
1	C	368	VAL	N-CA-C	11.13	124.24	107.99
2	H	343	LEU	N-CA-C	10.89	122.72	111.07
1	E	277	GLU	N-CA-C	-10.87	99.97	113.02
2	F	343	LEU	N-CA-C	10.84	122.79	110.97
1	A	277	GLU	N-CA-C	-10.68	100.20	113.02
4	J	38	DA	N9-C1'-C2'	10.57	129.36	113.50
1	G	383	THR	N-CA-C	10.55	122.54	111.14
1	G	351	GLU	N-CA-C	10.54	122.53	111.14
4	V	38	DA	O4'-C1'-N9	10.22	123.72	108.40
1	C	383	THR	N-CA-C	10.14	122.09	111.14
1	A	368	VAL	N-CA-C	10.13	122.78	107.99
1	G	474	VAL	N-CA-C	10.05	120.87	110.62
1	G	368	VAL	N-CA-C	9.90	122.44	107.99
2	B	464	ASP	CA-C-N	-9.83	108.19	122.44
2	B	464	ASP	C-N-CA	-9.83	108.19	122.44
1	C	474	VAL	N-CA-C	9.80	120.61	110.62
1	E	474	VAL	N-CA-C	9.57	120.39	110.62
2	H	435	PHE	N-CA-C	-9.53	100.90	111.28
2	D	346	PHE	N-CA-C	-9.39	101.13	111.36
1	C	435	THR	CA-C-N	9.26	128.91	119.56
1	C	435	THR	C-N-CA	9.26	128.91	119.56
2	D	492	VAL	N-CA-C	9.25	121.26	107.75
2	D	464	ASP	CA-C-N	-9.14	109.18	122.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	464	ASP	C-N-CA	-9.14	109.18	122.44
2	H	464	ASP	CA-C-N	-9.13	109.20	122.44
2	H	464	ASP	C-N-CA	-9.13	109.20	122.44
2	F	464	ASP	CA-C-N	-9.04	109.33	122.44
2	F	464	ASP	C-N-CA	-9.04	109.33	122.44
2	B	405	ARG	N-CA-C	9.03	122.30	111.82
1	E	383	THR	N-CA-C	9.02	120.88	111.14
2	H	492	VAL	N-CA-C	9.02	120.92	107.75
1	E	415	LEU	N-CA-C	-8.89	101.54	111.14
1	C	351	GLU	N-CA-C	8.85	120.92	111.28
1	A	435	THR	CA-C-N	8.85	128.50	119.56
1	A	435	THR	C-N-CA	8.85	128.50	119.56
1	A	539	THR	N-CA-C	-8.77	101.72	111.28
2	D	405	ARG	N-CA-C	8.74	121.96	111.82
2	B	492	VAL	N-CA-C	8.70	120.45	107.75
1	G	258	GLN	N-CA-C	-8.54	95.23	108.55
2	H	405	ARG	N-CA-C	8.53	121.72	111.82
1	E	447	PRO	CA-C-N	8.48	132.53	120.49
1	E	447	PRO	C-N-CA	8.48	132.53	120.49
1	E	381	GLU	N-CA-C	8.46	120.50	111.28
4	J	44	DA	O4'-C1'-N9	8.41	121.01	108.40
1	A	258	GLN	N-CA-C	-8.39	95.46	108.55
1	C	376	ASN	N-CA-C	-8.39	100.06	111.55
2	H	346	PHE	N-CA-C	-8.35	102.25	111.36
1	A	337	LEU	N-CA-C	8.33	120.36	111.28
2	H	434	ASP	N-CA-C	8.32	120.35	111.28
2	F	314	VAL	N-CA-C	8.30	119.87	107.75
2	D	435	PHE	N-CA-C	-8.30	102.24	111.28
1	C	447	PRO	CA-C-N	8.29	132.26	120.49
1	C	447	PRO	C-N-CA	8.29	132.26	120.49
2	F	492	VAL	N-CA-C	8.29	119.85	107.75
2	F	405	ARG	N-CA-C	8.24	121.38	111.82
1	G	337	LEU	N-CA-C	8.20	120.21	111.28
1	G	376	ASN	N-CA-C	-8.19	100.33	111.55
1	A	351	GLU	N-CA-C	8.14	120.15	111.28
2	D	278	CYS	N-CA-C	8.07	122.97	108.69
2	F	439	PHE	N-CA-C	-8.05	102.50	111.28
1	E	431	ARG	CA-C-N	8.04	129.89	119.84
1	E	431	ARG	C-N-CA	8.04	129.89	119.84
2	D	434	ASP	N-CA-C	8.01	119.64	111.07
2	F	434	ASP	N-CA-C	8.00	119.63	111.07
2	D	314	VAL	N-CA-C	7.98	119.40	107.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	435	THR	CA-C-N	7.96	128.04	119.28
1	E	435	THR	C-N-CA	7.96	128.04	119.28
1	E	376	ASN	N-CA-C	-7.94	100.68	111.55
1	G	381	GLU	N-CA-C	7.83	119.82	111.28
1	G	316	ASN	CA-C-N	7.81	127.74	119.85
1	G	316	ASN	C-N-CA	7.81	127.74	119.85
1	C	415	LEU	N-CA-C	-7.79	102.73	111.14
2	F	346	PHE	N-CA-C	-7.78	102.88	111.36
1	A	375	HIS	N-CA-C	-7.73	98.81	109.71
4	V	44	DA	C4'-C3'-O3'	7.69	121.53	110.00
2	B	278	CYS	N-CA-C	7.68	122.29	108.69
1	A	420	GLN	N-CA-C	-7.68	102.91	111.28
1	G	420	GLN	N-CA-C	-7.66	102.93	111.28
2	B	435	PHE	N-CA-C	-7.66	102.93	111.28
1	G	539	THR	N-CA-C	-7.65	102.94	111.28
1	E	337	LEU	N-CA-C	7.61	119.58	111.28
2	B	314	VAL	N-CA-C	7.61	118.86	107.75
5	L	50	DG	C2'-C3'-O3'	7.61	122.91	111.50
2	H	278	CYS	N-CA-C	7.60	122.15	108.69
2	H	465	TRP	CA-C-N	7.59	132.35	121.50
2	H	465	TRP	C-N-CA	7.59	132.35	121.50
2	B	465	TRP	CA-C-N	7.50	132.23	121.50
2	B	465	TRP	C-N-CA	7.50	132.23	121.50
2	H	249	LEU	CA-CB-CG	7.50	142.55	116.30
1	G	435	THR	CA-C-N	7.48	127.12	119.56
1	G	435	THR	C-N-CA	7.48	127.12	119.56
1	E	482	VAL	N-CA-C	7.47	118.64	108.17
1	A	407	GLU	N-CA-C	-7.45	102.84	112.23
2	B	321	PHE	N-CA-C	-7.43	103.26	111.36
1	C	539	THR	N-CA-C	-7.42	103.20	111.28
4	J	45	DG	P-O5'-C5'	-7.40	108.90	120.00
1	A	381	GLU	N-CA-C	7.38	119.32	111.28
1	G	415	LEU	N-CA-C	-7.37	103.19	111.14
2	B	249	LEU	CA-CB-CG	7.30	141.85	116.30
4	V	45	DG	O4'-C4'-C3'	-7.28	94.49	105.40
5	P	52	DA	O5'-C5'-C4'	7.25	121.67	110.80
2	F	532	VAL	N-CA-C	7.24	118.31	108.17
1	E	351	GLU	N-CA-C	7.21	119.22	111.36
2	B	346	PHE	N-CA-C	-7.17	103.55	111.36
2	F	278	CYS	N-CA-C	7.14	121.33	108.69
2	F	465	TRP	CA-C-N	7.09	131.63	121.50
2	F	465	TRP	C-N-CA	7.09	131.63	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	314	VAL	N-CA-C	7.04	118.03	107.75
1	C	337	LEU	N-CA-C	6.95	118.86	111.28
5	P	47	DT	N1-C1'-C2'	6.94	123.91	113.50
2	H	532	VAL	N-CA-C	6.91	117.84	108.17
4	N	29	DA	O5'-C5'-C4'	6.89	121.13	110.80
2	D	281	VAL	N-CA-C	6.87	119.71	108.99
4	V	45	DG	C3'-C2'-C1'	-6.86	91.32	101.60
2	B	461	LEU	N-CA-C	-6.84	103.00	112.30
2	B	267	GLY	N-CA-C	6.83	120.92	112.73
1	A	314	GLU	N-CA-C	-6.83	100.18	110.28
2	F	286	ALA	CA-C-N	-6.78	117.43	123.33
2	F	286	ALA	C-N-CA	-6.78	117.43	123.33
1	E	539	THR	N-CA-C	-6.76	103.91	111.28
2	H	553	ILE	N-CA-C	6.75	116.87	110.53
1	A	375	HIS	N-CA-CB	6.74	117.90	110.35
1	A	415	LEU	N-CA-C	-6.68	103.93	111.14
1	E	314	GLU	N-CA-C	-6.67	100.41	110.28
5	X	50	DG	C4'-C3'-O3'	-6.66	100.01	110.00
1	A	525	CYS	N-CA-C	6.63	120.21	109.40
2	H	267	GLY	N-CA-C	6.62	120.68	112.73
1	A	267	TYR	N-CA-C	6.62	119.14	109.07
1	E	267	TYR	N-CA-C	6.61	119.12	109.07
2	H	501	VAL	N-CA-C	6.58	117.37	110.72
1	G	407	GLU	N-CA-C	-6.58	103.94	112.23
2	F	362	VAL	N-CA-C	6.56	117.57	108.12
1	G	314	GLU	N-CA-C	-6.56	100.58	110.28
2	H	550	SER	N-CA-C	-6.55	104.18	111.71
2	D	367	GLU	N-CA-C	6.54	124.74	110.80
2	D	249	LEU	CA-CB-CG	6.52	139.13	116.30
5	L	48	DC	O4'-C1'-N1	6.52	118.18	108.40
1	E	406	LYS	N-CA-C	6.52	118.46	111.36
2	D	439	PHE	N-CA-C	-6.51	104.19	111.28
2	D	532	VAL	N-CA-C	6.51	117.28	108.17
2	D	465	TRP	CA-C-N	6.49	130.79	121.50
2	D	465	TRP	C-N-CA	6.49	130.79	121.50
4	J	45	DG	C3'-C2'-C1'	-6.49	91.87	101.60
2	D	550	SER	N-CA-C	-6.47	104.27	111.71
1	G	448	ASN	N-CA-C	6.46	119.00	110.08
2	B	501	VAL	N-CA-C	6.46	117.24	110.72
1	E	278	THR	N-CA-C	6.45	123.08	114.12
5	P	53	DT	O5'-C5'-C4'	6.44	120.46	110.80
2	B	439	PHE	N-CA-C	-6.43	104.27	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	431	GLU	CA-CB-CG	6.42	126.93	114.10
2	H	281	VAL	N-CA-C	6.40	118.98	108.99
2	B	532	VAL	N-CA-C	6.40	117.13	108.17
2	F	368	LYS	N-CA-C	6.38	120.27	112.23
1	C	407	GLU	N-CA-C	-6.36	104.21	112.23
1	A	448	ASN	N-CA-C	6.35	118.84	110.08
4	N	42	DG	C4'-C3'-O3'	6.32	119.48	110.00
4	R	38	DA	N9-C1'-C2'	-6.32	104.02	113.50
1	C	375	HIS	N-CA-C	-6.32	96.81	108.24
1	E	420	GLN	N-CA-C	-6.32	104.40	111.28
2	H	367	GLU	N-CA-C	6.32	124.25	110.80
4	N	41	DT	O5'-C5'-C4'	6.31	120.27	110.80
1	A	436	PRO	N-CA-C	6.31	121.75	113.86
2	H	439	PHE	N-CA-C	-6.30	104.41	111.28
2	D	551	ARG	N-CA-C	6.30	117.94	111.14
4	J	42	DG	C3'-C2'-C1'	-6.30	92.15	101.60
2	F	249	LEU	CA-CB-CG	6.29	138.31	116.30
1	C	314	GLU	N-CA-C	-6.28	100.98	110.28
1	G	301	ARG	N-CA-C	6.28	116.56	108.34
2	F	367	GLU	N-CA-C	6.27	124.16	110.80
5	P	51	DC	O5'-C5'-C4'	6.25	120.18	110.80
1	C	525	CYS	N-CA-C	6.25	119.59	109.40
1	G	401	ARG	N-CA-C	-6.24	99.48	109.96
1	G	311	VAL	N-CA-C	6.21	117.72	108.46
1	G	375	HIS	N-CA-C	-6.21	97.00	108.24
1	C	267	TYR	N-CA-C	6.17	118.45	109.07
1	C	311	VAL	N-CA-C	6.17	117.65	108.46
4	N	45	DG	O4'-C4'-C3'	-6.16	96.16	105.40
1	E	448	ASN	N-CA-C	6.16	117.65	109.83
2	F	449	LYS	CA-CB-CG	-6.15	101.80	114.10
2	H	461	LEU	N-CA-C	-6.14	103.95	112.30
2	B	551	ARG	N-CA-C	6.13	117.77	111.14
2	B	368	LYS	N-CA-C	6.13	119.96	112.23
4	J	44	DA	O5'-C5'-C4'	6.13	120.00	110.80
1	C	436	PRO	N-CA-C	6.12	121.51	113.86
1	A	495	ASP	N-CA-C	6.12	117.95	111.28
2	D	319	GLU	N-CA-C	6.11	118.74	111.71
1	E	371	HIS	N-CA-C	-6.11	104.99	112.88
2	D	365	ASP	CA-C-N	-6.11	112.50	122.65
2	D	365	ASP	C-N-CA	-6.11	112.50	122.65
2	D	466	ALA	N-CA-C	-6.09	100.07	109.76
1	G	436	PRO	N-CA-C	6.08	121.47	113.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	511	VAL	N-CA-C	-6.08	104.58	110.72
5	L	50	DG	C4'-C3'-C2'	-6.06	93.31	102.40
4	V	38	DA	C4-N9-C1'	6.06	136.14	127.05
4	V	38	DA	C4'-C3'-O3'	6.06	119.09	110.00
5	X	47	DT	N1-C1'-C2'	6.06	122.59	113.50
2	B	562	PRO	CA-C-O	6.04	127.46	119.00
2	H	551	ARG	N-CA-C	6.04	117.67	111.14
1	G	338	ASP	N-CA-C	-6.03	104.79	111.36
2	H	345	GLY	N-CA-C	6.02	121.43	113.37
2	F	321	PHE	N-CA-C	-6.00	104.82	111.36
2	B	466	ALA	N-CA-C	-6.00	100.22	109.76
1	A	257	GLN	N-CA-C	5.98	118.67	108.02
2	H	466	ALA	N-CA-C	-5.98	100.25	109.76
2	H	546	GLY	CA-C-N	5.97	125.36	118.85
2	H	546	GLY	C-N-CA	5.97	125.36	118.85
1	E	353	LYS	N-CA-C	5.96	118.57	111.71
1	C	368	VAL	CB-CA-C	-5.96	102.82	110.98
1	E	300	VAL	N-CA-C	5.96	116.75	107.28
2	D	321	PHE	N-CA-C	-5.95	104.88	111.36
4	J	41	DT	C4-C5-C7	-5.93	113.51	122.40
2	D	501	VAL	N-CA-C	5.92	116.70	110.72
5	L	51	DC	C3'-C2'-C1'	-5.92	92.71	101.60
1	A	301	ARG	N-CA-C	5.91	116.08	108.34
1	C	387	ALA	N-CA-C	5.91	117.39	111.07
1	A	350	ARG	N-CA-C	-5.90	104.93	111.36
1	G	525	CYS	N-CA-C	5.90	119.02	109.40
1	E	394	ILE	N-CA-C	5.89	116.53	110.82
2	H	543	ARG	N-CA-C	-5.88	105.96	113.02
1	E	486	SER	N-CA-C	5.87	118.40	109.95
1	E	375	HIS	N-CA-C	-5.86	97.63	108.24
1	E	525	CYS	N-CA-C	5.86	118.96	109.40
4	V	38	DA	O5'-C5'-C4'	5.86	119.58	110.80
1	A	401	ARG	N-CA-C	-5.85	100.12	109.96
1	G	523	ILE	N-CA-C	-5.84	101.18	108.89
2	H	282	ILE	N-CA-C	5.84	114.77	106.53
1	A	411	TYR	N-CA-C	-5.84	104.84	111.14
2	B	281	VAL	N-CA-C	5.84	118.09	108.99
2	B	367	GLU	N-CA-C	5.83	123.22	110.80
2	H	282	ILE	CB-CA-C	-5.83	104.83	111.59
2	F	501	VAL	N-CA-C	5.82	116.60	110.72
1	E	311	VAL	N-CA-C	5.82	117.13	108.46
2	B	431	GLU	CA-CB-CG	5.81	125.73	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	546	GLY	CA-C-N	5.81	125.18	118.85
2	D	546	GLY	C-N-CA	5.81	125.18	118.85
2	D	489	LEU	CA-CB-CG	-5.80	95.99	116.30
1	G	365	VAL	CA-C-N	-5.79	114.89	123.11
1	G	365	VAL	C-N-CA	-5.79	114.89	123.11
1	G	340	LEU	N-CA-C	5.79	117.67	111.36
2	F	282	ILE	CB-CA-C	-5.78	104.88	111.59
2	H	423	ALA	N-CA-C	5.78	118.06	108.99
1	A	316	ASN	CA-C-N	5.78	125.69	119.85
1	A	316	ASN	C-N-CA	5.78	125.69	119.85
1	C	420	GLN	N-CA-C	-5.78	104.98	111.28
2	F	466	ALA	N-CA-C	-5.77	100.59	109.76
4	J	28	DC	C5'-C4'-O4'	-5.76	100.75	109.40
1	C	381	GLU	N-CA-C	5.76	117.56	111.28
2	D	362	VAL	N-CA-C	5.76	116.41	108.12
1	G	371	HIS	N-CA-C	-5.76	105.56	112.59
1	A	300	VAL	N-CA-C	5.76	116.43	107.28
1	G	363	ARG	N-CA-C	5.76	118.53	108.52
2	D	465	TRP	N-CA-C	5.75	117.75	107.80
2	F	362	VAL	CA-C-N	-5.75	115.65	123.12
2	F	362	VAL	C-N-CA	-5.75	115.65	123.12
2	B	434	ASP	N-CA-C	5.75	117.54	111.28
1	E	338	ASP	N-CA-C	-5.74	105.10	111.36
2	D	368	LYS	N-CA-C	5.74	119.46	112.23
4	J	38	DA	C5'-C4'-C3'	5.74	123.50	114.90
1	C	401	ARG	N-CA-C	-5.73	100.33	109.96
2	H	515	GLN	N-CA-C	-5.73	105.12	111.36
5	P	48	DC	C2'-C3'-O3'	5.72	120.08	111.50
1	G	267	TYR	N-CA-C	5.71	117.74	109.07
4	J	39	DC	N1-C1'-C2'	5.70	122.05	113.50
2	H	241	LYS	N-CA-C	-5.70	105.91	112.92
2	B	515	GLN	N-CA-C	-5.69	105.16	111.36
1	A	486	SER	N-CA-C	5.69	118.14	109.95
1	C	338	ASP	N-CA-C	-5.68	105.17	111.36
1	G	350	ARG	N-CA-C	-5.68	105.17	111.36
2	B	257	ASP	N-CA-C	-5.68	102.92	110.07
1	G	447	PRO	CA-C-N	5.68	129.31	120.68
1	G	447	PRO	C-N-CA	5.68	129.31	120.68
2	H	500	VAL	N-CA-C	-5.68	104.97	110.42
2	H	248	CYS	CA-C-N	5.67	128.94	120.31
2	H	248	CYS	C-N-CA	5.67	128.94	120.31
1	E	407	GLU	N-CA-C	-5.67	105.08	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	278	THR	N-CA-C	5.65	121.97	114.12
2	F	465	TRP	N-CA-C	5.65	117.58	107.80
2	B	550	SER	N-CA-C	-5.65	105.21	111.71
1	C	504	LEU	N-CA-C	5.64	117.51	111.36
2	B	552	ARG	N-CA-C	-5.64	105.22	111.36
1	C	286	GLU	N-CA-C	-5.63	101.41	110.14
1	A	473	GLU	CA-C-N	5.63	128.18	120.46
1	A	473	GLU	C-N-CA	5.63	128.18	120.46
1	E	357	LYS	CA-CB-CG	5.61	125.31	114.10
2	F	281	VAL	N-CA-C	5.60	117.73	108.99
2	F	282	ILE	N-CA-C	5.60	114.43	106.53
1	C	374	VAL	N-CA-C	-5.60	102.35	109.80
1	G	278	THR	N-CA-C	5.60	121.91	114.12
2	F	241	LYS	N-CA-C	-5.60	106.03	112.92
1	C	523	ILE	N-CA-C	-5.60	101.50	108.89
2	F	365	ASP	CA-C-N	-5.60	113.36	122.65
2	F	365	ASP	C-N-CA	-5.60	113.36	122.65
1	A	327	VAL	N-CA-C	5.59	116.36	108.36
1	C	448	ASN	N-CA-C	5.58	116.91	109.83
1	E	485	VAL	N-CA-C	5.58	115.82	107.51
4	J	45	DG	C2'-C3'-O3'	-5.58	103.14	111.50
1	E	368	VAL	CB-CA-C	-5.57	103.34	110.98
4	N	44	DA	C4'-C3'-O3'	5.57	118.36	110.00
2	B	291	VAL	N-CA-C	5.57	116.14	108.12
2	F	515	GLN	N-CA-C	-5.57	105.29	111.36
2	H	286	ALA	CA-C-N	-5.57	118.49	123.33
2	H	286	ALA	C-N-CA	-5.57	118.49	123.33
2	D	248	CYS	CA-C-N	5.56	128.76	120.31
2	D	248	CYS	C-N-CA	5.56	128.76	120.31
2	H	449	LYS	CA-CB-CG	-5.55	102.99	114.10
2	F	551	ARG	N-CA-C	5.55	117.14	111.14
4	N	38	DA	P-O5'-C5'	5.55	128.33	120.00
4	N	28	DC	C5'-C4'-O4'	-5.54	101.08	109.40
2	D	286	ALA	CA-C-N	-5.54	118.51	123.33
2	D	286	ALA	C-N-CA	-5.54	118.51	123.33
4	V	44	DA	P-O5'-C5'	5.54	128.31	120.00
2	B	553	ILE	N-CA-C	5.54	115.73	110.53
2	H	465	TRP	N-CA-C	5.54	117.38	107.80
2	F	542	SER	O-C-N	-5.53	115.90	122.65
1	A	357	LYS	CA-CB-CG	5.53	125.15	114.10
2	D	449	LYS	CA-CB-CG	-5.52	103.06	114.10
1	G	257	GLN	N-CA-C	5.52	117.84	108.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	408	ALA	N-CA-C	5.51	117.09	111.14
4	J	43	DC	P-O5'-C5'	5.51	128.27	120.00
1	C	340	LEU	N-CA-C	5.51	117.37	111.36
1	G	495	ASP	N-CA-C	5.51	117.29	111.28
2	H	257	ASP	N-CA-C	-5.51	103.13	110.07
1	E	302	LYS	N-CA-C	5.50	117.99	107.75
2	H	542	SER	CA-C-O	-5.50	115.72	121.99
1	G	353	LYS	N-CA-C	5.48	118.01	111.71
5	X	49	DT	C4-C5-C7	-5.48	114.18	122.40
4	V	43	DC	O5'-C5'-C4'	5.47	119.01	110.80
2	B	248	CYS	CA-C-N	5.46	128.61	120.31
2	B	248	CYS	C-N-CA	5.46	128.61	120.31
3	I	1	DG	C4'-C3'-O3'	5.46	118.19	110.00
1	G	342	SER	N-CA-C	-5.45	105.33	111.28
2	D	241	LYS	N-CA-C	-5.45	106.21	112.92
2	B	319	GLU	N-CA-C	5.45	117.97	111.71
2	H	562	PRO	N-CA-C	5.44	120.66	113.86
1	G	327	VAL	N-CA-C	5.43	116.12	108.36
1	A	528	LEU	CA-C-N	5.43	131.47	121.70
1	A	528	LEU	C-N-CA	5.43	131.47	121.70
2	D	461	LEU	N-CA-C	-5.42	104.92	112.30
2	H	270	LEU	N-CA-C	-5.42	105.37	111.28
1	A	311	VAL	N-CA-C	5.42	116.53	108.46
2	B	286	ALA	CA-C-N	-5.41	118.62	123.33
2	B	286	ALA	C-N-CA	-5.41	118.62	123.33
1	C	353	LYS	N-CA-C	5.41	117.93	111.71
4	J	44	DA	N9-C1'-C2'	-5.40	105.40	113.50
1	E	374	VAL	N-CA-C	-5.39	102.62	109.80
4	R	29	DA	P-O5'-C5'	-5.39	111.91	120.00
2	H	553	ILE	CB-CA-C	-5.39	104.96	112.02
1	A	429	ARG	N-CA-C	5.38	117.58	109.23
4	J	29	DA	P-O5'-C5'	-5.38	111.92	120.00
1	E	363	ARG	N-CA-C	5.38	117.89	108.52
3	U	8	DT	C2'-C3'-O3'	-5.38	103.43	111.50
1	E	316	ASN	CA-C-N	5.38	125.28	119.85
1	E	316	ASN	C-N-CA	5.38	125.28	119.85
2	F	550	SER	N-CA-C	-5.38	105.53	111.71
4	R	33	DT	O5'-C5'-C4'	5.37	118.86	110.80
1	A	371	HIS	N-CA-C	-5.37	106.04	112.59
1	C	302	LYS	N-CA-C	5.37	117.73	107.75
1	G	314	GLU	CA-CB-CG	5.36	124.82	114.10
4	J	45	DG	N9-C1'-C2'	-5.35	105.47	113.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	319	GLU	N-CA-C	5.35	117.86	111.71
1	A	286	GLU	N-CA-C	-5.34	101.86	110.14
1	A	338	ASP	N-CA-C	-5.34	105.53	111.36
2	H	431	GLU	CA-CB-CG	5.34	124.79	114.10
1	C	300	VAL	N-CA-C	5.34	115.77	107.28
2	D	553	ILE	N-CA-C	5.33	115.55	110.53
4	N	42	DG	O4'-C1'-N9	5.33	116.39	108.40
1	C	363	ARG	N-CA-C	5.33	117.79	108.52
2	D	480	LEU	N-CA-C	-5.32	105.56	111.36
1	G	473	GLU	CA-C-N	5.32	127.75	120.46
1	G	473	GLU	C-N-CA	5.32	127.75	120.46
2	D	289	CYS	CA-CB-SG	5.32	126.64	114.40
1	E	395	ASP	N-CA-C	-5.31	106.76	113.18
2	F	461	LEU	N-CA-C	-5.30	105.09	112.30
4	V	39	DC	N1-C1'-C2'	5.30	121.46	113.50
2	H	365	ASP	CA-C-N	-5.30	113.85	122.65
2	H	365	ASP	C-N-CA	-5.30	113.85	122.65
2	H	452	ARG	N-CA-C	5.30	117.86	111.40
2	B	305	ASP	N-CA-C	-5.29	107.00	112.93
1	A	447	PRO	CA-C-N	5.29	128.72	120.68
1	A	447	PRO	C-N-CA	5.29	128.72	120.68
2	B	496	MET	N-CA-C	-5.29	105.43	111.14
1	C	357	LYS	CA-CB-CG	5.28	124.66	114.10
1	E	340	LEU	N-CA-C	5.28	117.12	111.36
2	H	321	PHE	N-CA-C	-5.28	105.20	111.69
1	C	431	ARG	CA-C-N	5.28	126.43	119.84
1	C	431	ARG	C-N-CA	5.28	126.43	119.84
1	G	292	GLN	N-CA-C	-5.27	105.59	112.23
1	E	314	GLU	CA-CB-CG	5.27	124.64	114.10
2	H	480	LEU	N-CA-C	-5.27	105.62	111.36
1	E	327	VAL	N-CA-C	5.26	115.88	108.36
2	F	319	GLU	N-CA-C	5.26	117.75	111.71
2	H	368	LYS	N-CA-C	5.26	118.85	112.23
2	B	500	VAL	N-CA-C	-5.25	105.38	110.42
2	F	255	VAL	N-CA-C	5.25	115.91	107.98
1	C	327	VAL	N-CA-C	5.25	115.87	108.36
2	H	291	VAL	N-CA-C	5.25	115.68	108.12
2	B	480	LEU	N-CA-C	-5.25	105.64	111.36
1	G	368	VAL	CB-CA-C	-5.24	103.80	110.98
2	B	543	ARG	N-CA-C	-5.24	106.73	113.02
1	C	314	GLU	CA-CB-CG	5.24	124.57	114.10
2	H	268	GLN	N-CA-C	-5.23	105.75	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	N	33	DT	O5'-C5'-C4'	5.23	118.64	110.80
4	V	29	DA	O5'-C5'-C4'	5.23	118.64	110.80
2	D	260	LEU	N-CA-C	-5.22	105.48	111.07
2	B	457	PHE	N-CA-C	5.20	117.78	110.14
1	E	286	GLU	N-CA-C	-5.20	102.09	110.14
1	E	365	VAL	CA-C-N	-5.20	115.73	123.11
1	E	365	VAL	C-N-CA	-5.20	115.73	123.11
4	R	40	DA	P-O5'-C5'	-5.20	112.21	120.00
1	A	363	ARG	N-CA-C	5.19	117.56	108.52
1	C	482	VAL	N-CA-C	5.19	115.96	108.48
1	A	319	ASP	CA-C-N	5.19	124.85	119.56
1	A	319	ASP	C-N-CA	5.19	124.85	119.56
2	F	289	CYS	CA-CB-SG	5.19	126.33	114.40
1	G	286	GLU	N-CA-C	-5.19	102.10	110.14
1	C	278	THR	CA-C-N	-5.19	115.30	123.13
1	C	278	THR	C-N-CA	-5.19	115.30	123.13
2	D	291	VAL	N-CA-C	5.18	115.58	108.12
2	B	282	ILE	CB-CA-C	-5.18	105.58	111.59
4	N	30	DC	O4'-C1'-N1	5.18	116.17	108.40
2	D	255	VAL	N-CA-C	5.17	115.79	107.98
2	H	533	ARG	N-CA-C	5.17	117.18	109.59
2	D	257	ASP	N-CA-C	-5.16	103.57	110.07
1	C	371	HIS	N-CA-C	-5.16	106.22	112.88
1	G	356	LEU	CB-CG-CD2	5.16	126.18	110.70
2	F	552	ARG	N-CA-C	-5.16	105.74	111.36
1	C	485	VAL	N-CA-C	5.16	115.19	107.51
2	D	431	GLU	CA-CB-CG	5.15	124.40	114.10
2	F	430	LYS	N-CA-C	-5.15	105.75	111.36
5	P	52	DA	C5'-C4'-C3'	5.15	122.62	114.90
1	A	368	VAL	CB-CA-C	-5.15	103.93	110.98
1	E	319	ASP	CA-C-N	5.14	124.81	119.56
1	E	319	ASP	C-N-CA	5.14	124.81	119.56
3	M	1	DG	C5'-C4'-O4'	-5.14	101.69	109.40
2	F	291	VAL	N-CA-C	5.13	115.51	108.12
2	H	362	VAL	N-CA-C	5.13	115.51	108.12
1	G	411	TYR	N-CA-C	-5.13	105.60	111.14
2	H	552	ARG	N-CA-C	-5.12	105.78	111.36
4	N	30	DC	C5'-C4'-O4'	-5.12	101.72	109.40
2	D	282	ILE	CB-CA-C	-5.11	105.66	111.59
2	D	452	ARG	N-CA-C	5.11	117.64	111.40
5	T	51	DC	O4'-C1'-N1	5.11	116.06	108.40
2	B	241	LYS	N-CA-C	-5.10	106.64	112.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	546	GLY	CA-C-N	5.10	124.41	118.85
2	F	546	GLY	C-N-CA	5.10	124.41	118.85
2	B	255	VAL	N-CA-C	5.09	115.66	107.98
2	H	457	PHE	N-CA-C	5.09	117.62	110.14
2	B	270	LEU	N-CA-C	-5.08	105.74	111.28
1	A	340	LEU	N-CA-C	5.07	116.89	111.36
1	A	353	LYS	N-CA-C	5.07	117.54	111.71
2	F	268	GLN	N-CA-C	-5.07	105.94	111.82
1	G	357	LYS	CA-CB-CG	5.06	124.23	114.10
2	B	477	GLY	N-CA-C	-5.06	108.17	113.58
1	G	312	ALA	N-CA-C	5.06	116.56	108.41
1	G	300	VAL	N-CA-C	5.05	115.32	107.28
1	A	342	SER	N-CA-C	-5.05	105.66	111.07
1	E	411	TYR	N-CA-C	-5.04	105.69	111.14
2	F	267	GLY	N-CA-C	5.04	118.78	112.73
2	D	270	LEU	N-CA-C	-5.04	105.79	111.28
2	F	419	THR	N-CA-C	5.04	117.06	109.41
2	D	345	GLY	N-CA-C	5.03	120.11	113.37
2	H	260	LEU	N-CA-C	-5.03	105.69	111.07
1	C	411	TYR	N-CA-C	-5.02	105.72	111.14
2	F	438	ALA	N-CA-C	5.02	116.75	111.28
2	H	362	VAL	CA-C-N	-5.01	116.61	123.12
2	H	362	VAL	C-N-CA	-5.01	116.61	123.12
1	A	406	LYS	N-CA-C	5.01	116.82	111.36

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	146	1
1	C	2173	0	2203	88	0
1	E	2173	0	2203	101	0
1	G	2173	0	2203	123	0
2	B	2227	0	2265	165	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	2227	0	2265	115	1
2	F	2227	0	2265	127	0
2	H	2227	0	2265	149	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	33	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	29	0
All	All	20884	0	19696	991	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 25.

All (991) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:551:THR:C	2:F:475:GLY:H	1.99	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:375:HIS:C	1:A:377:LEU:H	2.01	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: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:G:489:LYS:HZ1	4:N:30:DC:P	2.20	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
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
1:E:551:THR:C	2:F:475:GLY:N	2.55	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:E:276:GLY:C	1:E:278:THR:H	2.07	0.63
2:B:459:PHE:HA	2:B:462:GLU:HB3	1.81	0.63
1:C:276:GLY:C	1:C:278:THR:H	2.05	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:C:407:GLU:CD	2:D:405:ARG:HH12	2.06	0.62
2:D:274:GLN:CD	2:H:267:GLY:H	2.06	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:A:472:ARG:O	1:A:473:GLU:C	2.43	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: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:E:421:ARG:HH21	2:F:414:ASP:CG	2.10	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: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)
2:F:432:LEU:O	2:F:436:THR:OG1	2.15	0.60
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: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
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
2:F:241:LYS:HB3	2:F:244:ARG:NH1	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:484:GLY:C	4:V:30:DC:H4'	2.29	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
2:B:309:GLU:C	2:B:311:THR:H	2.13	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
2:D:329:LYS:NZ	2:D:414:ASP:OD2	2.34	0.57
1:E:371:HIS:NE2	1:E:401:ARG:HB3	2.20	0.57
1:E:407:GLU:CD	2:F:405:ARG:HH12	2.12	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
1:G:276:GLY:C	1:G:278:THR:H	2.12	0.56
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
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
1:C:524:LYS:HG3	1:C:529:GLN:CD	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:G:390:ASN:HB3	1:G:394:ILE:HD12	1.88	0.55
1:A:474:VAL:HB	2:B:556:GLN:CD	2.31	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
1:A:414:LEU:C	2:B:413:VAL:HG11	2.33	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
1:A:276:GLY:C	1:A:278:THR:H	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:D:496:MET:HE3	5:X:51:DC:OP1	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
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: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: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
2:H:309:GLU:C	2:H:311:THR:H	2.16	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
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
1:E:477:ARG:HH21	2:F:488:GLN:CD	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:A:411:TYR:HH	2:B:416:GLN:CD	2.14	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:A:545:CYS:C	2:B:508:GLN:HG3	2.35	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
2:B:263:MET:HE1	2:B:315:LEU:HD22	1.92	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:A:347:GLY:CA	2:B:461:LEU:HD22	2.41	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
2:H:432:LEU:O	2:H:436:THR:OG1	2.19	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:E:489:LYS:HD2	1:E:532:LEU:CD1	2.41	0.51
1:G:524:LYS:HG3	1:G:529:GLN:CD	2.36	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: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: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:B:541:THR:C	2:B:542:SER:O	2.49	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:D:309:GLU:C	2:D:311:THR:H	2.18	0.50
1:E:421:ARG:NH2	2:F:414:ASP:CG	2.69	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:F:329:LYS:NZ	2:F:414:ASP:OD2	2.34	0.50
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
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: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:F:309:GLU:C	2:F:311:THR:H	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:A:415:LEU:HD21	2:B:416:GLN:CD	2.38	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
1:E:472:ARG:O	1:E:473:GLU:C	2.57	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
2:H:541:THR:C	2:H:542:SER:O	2.47	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:A:375:HIS:C	1:A:377:LEU:N	2.72	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:494:VAL:O	1:E:498:SER:HA	2.14	0.47
2:B:287:VAL:O	2:B:290:SER:OG	2.28	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
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:504:TYR:C	2:B:506:SER:H	2.23	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:G:380:PRO:O	1:G:383:THR:HB	2.15	0.47
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:C:472:ARG:O	1:C:473:GLU:C	2.57	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:496:MET:HE1	5:T:51:DC:H5''	1.98	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
2:D:541:THR:C	2:D:542:SER:O	2.46	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:F:265:GLY:O	2:F:266:GLY:C	2.59	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: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
1:G:472:ARG:O	1:G:473:GLU:C	2.59	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
2:D:263:MET:HE1	2:D:315:LEU:HD22	1.98	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:287:VAL:O	2:F:290:SER:OG	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:H:312:VAL:HG12	2:H:357:LYS:CB	2.47	0.45
1:C:375:HIS:C	1:C:377:LEU:H	2.25	0.45
1:C:479:LEU:HG	1:C:493:LEU:HD13	1.99	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
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
2:F:415:LEU:O	2:F:419:THR:OG1	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:G:538:ARG:HH22	2:H:473:LEU:C	2.13	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
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: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
1:E:524:LYS:HG3	1:E:529:GLN:CD	2.41	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:263:MET:HE1	2:H:315:LEU:HD22	2.00	0.44
2:H:412:LEU:HD12	2:H:412:LEU:HA	1.79	0.44
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:494:VAL:O	1:G:498:SER:HA	2.18	0.43
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
2:F:257:ASP:CG	2:F:258:PRO:HD2	2.43	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
1:C:421:ARG:HH21	2:D:414:ASP:CG	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:541:THR:O	2:D:542:SER:C	2.61	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
1:G:421:ARG:HH21	2:H:414:ASP:CG	2.25	0.42
2:H:273:LEU:HD12	2:H:273:LEU:HA	1.69	0.42
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:F:541:THR:C	2:F:542:SER:O	2.51	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:517:CYS:CB	2:B:523:ARG:HG3	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:G:489:LYS:NZ	4:N:30:DC:O5'	2.52	0.42
4:J:28:DC:C2'	4:J:29:DA:H5'	2.50	0.42
2:D:252:ILE:HD13	2:D:295:ARG:HA	2.02	0.42
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
2:H:313:LEU:HD23	2:H:313:LEU:C	2.45	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
2:F:313:LEU:HD23	2:F:313:LEU:C	2.46	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:472:ARG:C	1:A:474:VAL:N	2.79	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: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
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
1:G:266:GLU:O	1:G:314:GLU:HA	2.21	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
2:F:260:LEU:HD12	2:F:263:MET:HE2	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
2:B:265:GLY:O	2:B:266:GLY:C	2.64	0.40
1:C:340:LEU:O	1:C:344:ILE:HG13	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:421:ARG:HH21	2:B:414:ASP:CG	2.29	0.40
2:B:267:GLY:HA3	2:F:270:LEU:CG	2.51	0.40
1:C:386:GLN:NE2	2:D:441:LYS:HB3	2.36	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
4:R:42:DG:H8	4:R:42:DG:OP2	2.03	0.40
2:B:309:GLU:C	2:B:311:THR:N	2.79	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:D:415:LEU:O	2:D:419:THR:OG1	2.25	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

5.3.1 Protein backbone

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%)	11	46
1	C	267/306 (87%)	258 (97%)	6 (2%)	3 (1%)	11	46
1	E	267/306 (87%)	259 (97%)	6 (2%)	2 (1%)	18	56
1	G	267/306 (87%)	257 (96%)	7 (3%)	3 (1%)	11	46
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%)	24	63

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

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%)	218 (92%)	19 (8%)	11	31
1	C	237/259 (92%)	218 (92%)	19 (8%)	11	31
1	E	237/259 (92%)	217 (92%)	20 (8%)	10	30
1	G	237/259 (92%)	217 (92%)	20 (8%)	10	30
2	B	242/334 (72%)	221 (91%)	21 (9%)	9	29
2	D	242/334 (72%)	223 (92%)	19 (8%)	11	32
2	F	242/334 (72%)	223 (92%)	19 (8%)	11	32
2	H	242/334 (72%)	222 (92%)	20 (8%)	10	30
All	All	1916/2372 (81%)	1759 (92%)	157 (8%)	10	31

All (157) 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	299	THR
1	A	300	VAL
1	A	337	LEU
1	A	339	ASP
1	A	375	HIS
1	A	379	LEU
1	A	384	LEU
1	A	400	LYS
1	A	422	LEU
1	A	428	LEU
1	A	454	LEU
1	A	474	VAL
1	A	479	LEU
1	A	482	VAL
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

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Mol	Chain	Res	Type
2	B	287	VAL
2	B	291	VAL
2	B	311	THR
2	B	319	GLU
2	B	342	THR
2	B	343	LEU
2	B	367	GLU
2	B	412	LEU
2	B	459	PHE
2	B	461	LEU
2	B	470	LYS
2	B	471	VAL
2	B	526	LEU
2	B	531	GLN
2	B	541	THR
2	B	562	PRO
1	C	263	ARG
1	C	269	VAL
1	C	278	THR
1	C	299	THR
1	C	300	VAL
1	C	337	LEU
1	C	339	ASP
1	C	375	HIS
1	C	379	LEU
1	C	384	LEU
1	C	400	LYS
1	C	422	LEU
1	C	428	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	287	VAL
2	D	291	VAL

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Mol	Chain	Res	Type
2	D	311	THR
2	D	319	GLU
2	D	342	THR
2	D	343	LEU
2	D	367	GLU
2	D	412	LEU
2	D	459	PHE
2	D	461	LEU
2	D	470	LYS
2	D	471	VAL
2	D	526	LEU
2	D	531	GLN
1	E	263	ARG
1	E	269	VAL
1	E	278	THR
1	E	299	THR
1	E	300	VAL
1	E	337	LEU
1	E	339	ASP
1	E	375	HIS
1	E	384	LEU
1	E	400	LYS
1	E	422	LEU
1	E	428	LEU
1	E	450	LEU
1	E	454	LEU
1	E	474	VAL
1	E	479	LEU
1	E	482	VAL
1	E	483	ARG
1	E	527	ARG
1	E	543	LEU
2	F	237	VAL
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	311	THR
2	F	342	THR
2	F	343	LEU

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Mol	Chain	Res	Type
2	F	367	GLU
2	F	412	LEU
2	F	459	PHE
2	F	461	LEU
2	F	470	LYS
2	F	471	VAL
2	F	526	LEU
2	F	531	GLN
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	337	LEU
1	G	339	ASP
1	G	375	HIS
1	G	379	LEU
1	G	384	LEU
1	G	400	LYS
1	G	422	LEU
1	G	428	LEU
1	G	454	LEU
1	G	474	VAL
1	G	479	LEU
1	G	482	VAL
1	G	527	ARG
1	G	543	LEU
1	G	550	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	342	THR
2	H	343	LEU
2	H	367	GLU
2	H	412	LEU
2	H	459	PHE

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Mol	Chain	Res	Type
2	H	461	LEU
2	H	470	LYS
2	H	471	VAL
2	H	511	VAL
2	H	526	LEU
2	H	531	GLN
2	H	562	PRO

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

Mol	Chain	Res	Type
1	A	257	GLN
1	A	386	GLN
1	A	426	HIS
1	A	448	ASN
2	B	488	GLN
2	B	515	GLN
2	B	563	HIS
1	C	257	GLN
1	C	316	ASN
1	C	352	GLN
1	C	426	HIS
1	C	448	ASN
2	D	274	GLN
2	D	285	GLN
2	D	515	GLN
2	D	563	HIS
1	E	257	GLN
1	E	316	ASN
1	E	330	HIS
1	E	352	GLN
1	E	386	GLN
1	E	392	GLN
1	E	426	HIS
1	E	448	ASN
2	F	262	GLN
2	F	285	GLN
2	F	515	GLN
2	F	563	HIS
1	G	257	GLN
1	G	316	ASN
1	G	330	HIS

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Mol	Chain	Res	Type
1	G	386	GLN
1	G	448	ASN
2	H	262	GLN
2	H	285	GLN
2	H	422	GLN
2	H	488	GLN
2	H	515	GLN
2	H	563	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	275/306 (89%)	-0.41	1 (0%) 88 79	21, 84, 154, 320	0
1	C	275/306 (89%)	-0.51	2 (0%) 84 73	15, 99, 186, 316	0
1	E	275/306 (89%)	-0.39	2 (0%) 84 73	20, 118, 367, 428	0
1	G	275/306 (89%)	-0.47	0 100 100	21, 87, 183, 265	0
2	B	284/393 (72%)	-0.40	3 (1%) 78 66	41, 96, 245, 375	0
2	D	284/393 (72%)	-0.40	2 (0%) 84 73	29, 113, 258, 397	0
2	F	284/393 (72%)	-0.25	5 (1%) 67 57	36, 170, 498, 642	0
2	H	284/393 (72%)	-0.39	4 (1%) 73 62	42, 118, 273, 403	0
3	I	12/12 (100%)	-0.56	0 100 100	94, 114, 249, 364	0
3	M	12/12 (100%)	-0.32	0 100 100	128, 153, 264, 437	0
3	Q	12/12 (100%)	-0.09	0 100 100	285, 340, 399, 455	0
3	U	12/12 (100%)	-0.29	0 100 100	114, 183, 245, 282	0
4	J	19/24 (79%)	-0.37	0 100 100	80, 134, 230, 269	0
4	N	19/24 (79%)	-0.40	0 100 100	85, 183, 283, 283	0
4	R	19/24 (79%)	-0.34	0 100 100	103, 366, 471, 540	0
4	V	19/24 (79%)	-0.28	0 100 100	147, 208, 431, 438	0
5	L	9/13 (69%)	-0.37	0 100 100	109, 138, 247, 333	0
5	P	9/13 (69%)	-0.52	0 100 100	98, 126, 157, 177	0
5	T	9/13 (69%)	-0.11	0 100 100	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%)	-0.40	19 (0%) 82 72	15, 104, 367, 642	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	321	PHE	5.6
1	C	532	LEU	4.3
2	B	347	VAL	3.7
2	F	282	ILE	3.4
2	F	497	ALA	3.3
1	E	384	LEU	3.3
2	D	369	CYS	3.1
2	H	347	VAL	3.0
2	B	270	LEU	2.8
2	H	463	SER	2.7
1	C	493	LEU	2.6
2	B	500	VAL	2.5
2	F	369	CYS	2.4
2	H	432	LEU	2.3
2	H	445	GLU	2.2
2	D	444	ALA	2.2
1	E	366	TYR	2.2
2	F	347	VAL	2.2
1	A	493	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 oligosaccharides 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.