



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 3, 2024 – 03:18 PM JST

PDB ID : 8KAH
Title : Crystal structure of SpyCas9-crRNA-tracrRNA complex bound to 18nt target DNA
Authors : Chen, Y.; Chen, J.; Liu, L.
Deposited on : 2023-08-03
Resolution : 3.36 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 : 2.36.2
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) : 2.36.2

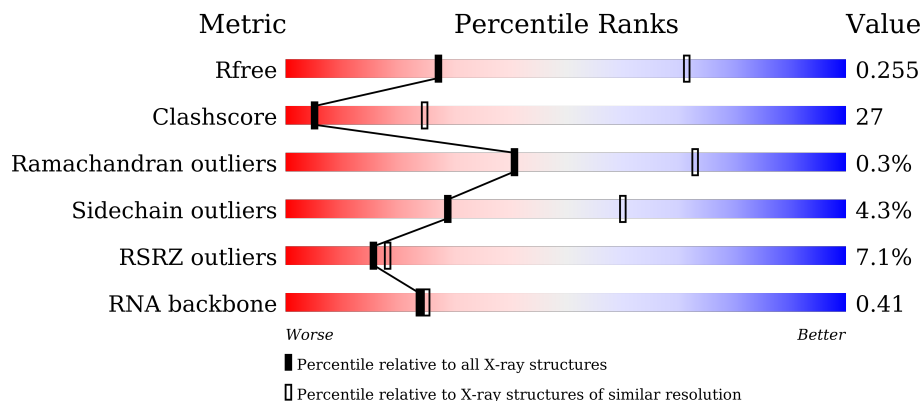
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.36 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.




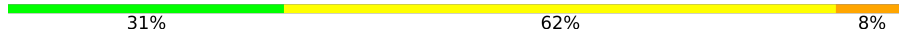



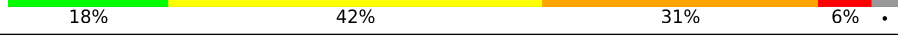
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1558 (3.42-3.30)
Clashscore	141614	1627 (3.42-3.30)
Ramachandran outliers	138981	1599 (3.42-3.30)
Sidechain outliers	138945	1598 (3.42-3.30)
RSRZ outliers	127900	1507 (3.42-3.30)
RNA backbone	3102	1023 (3.80-2.92)

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	34	
1	E	34	
2	B	1368	
2	F	1368	

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Mol	Chain	Length	Quality of chain
3	C	26	 23% 69% 8%
3	G	26	 31% 62% 8%
4	D	11	 9% 36% 55% 9%
4	H	11	 18% 36% 55% 9%
5	I	65	 20% 43% 23% 11% .
5	J	65	 2% 18% 42% 31% 6% .

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 27025 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 RNA chain called RNA (34-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A	34	Total 725	C 325	N 127	O 239	P 34	0	0	0
1	E	32	Total 685	C 307	N 123	O 223	P 32	0	0	0

- Molecule 2 is a protein called CRISPR-associated endonuclease Cas9/Csn1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	1322	Total 10732	C 6827	N 1864	O 2019	S 22	0	0	0
2	F	1327	Total 10695	C 6814	N 1845	O 2014	S 22	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	10	ALA	ASP	engineered mutation	UNP Q99ZW2
B	840	ALA	HIS	engineered mutation	UNP Q99ZW2
F	10	ALA	ASP	engineered mutation	UNP Q99ZW2
F	840	ALA	HIS	engineered mutation	UNP Q99ZW2

- Molecule 3 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	C	26	Total 521	C 254	N 85	O 157	P 25	0	0	0
3	G	26	Total 521	C 254	N 85	O 157	P 25	0	0	0

- Molecule 4 is a DNA chain called DNA (5'-D(*TP*TP*TP*AP*GP*GP*TP*AP*TP*TP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
4	D	11	Total 225	110	37	68	10	0	0	0
4	H	11	Total 225	110	37	68	10	0	0	0

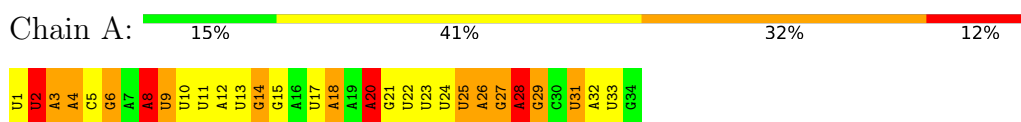
- Molecule 5 is a RNA chain called RNA (65-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
5	I	63	Total 1348	603	245	437	63	0	0	0
5	J	63	Total 1348	603	245	437	63	0	0	0

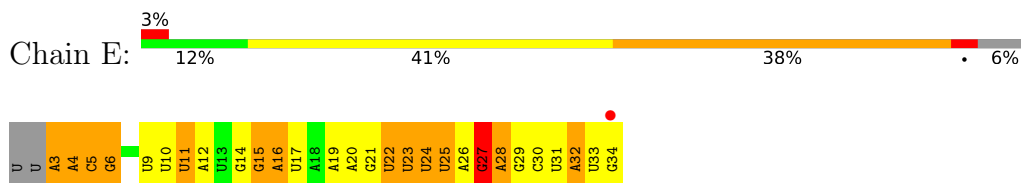
3 Residue-property plots i

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 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.

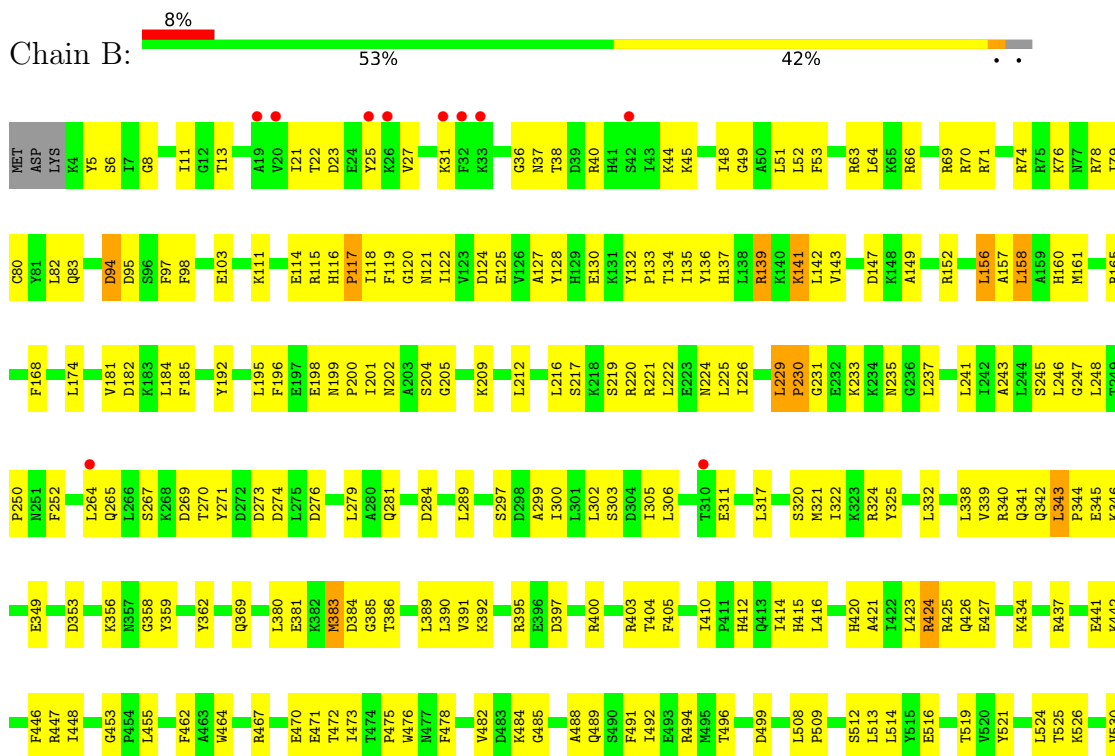
- Molecule 1: RNA (34-MER)

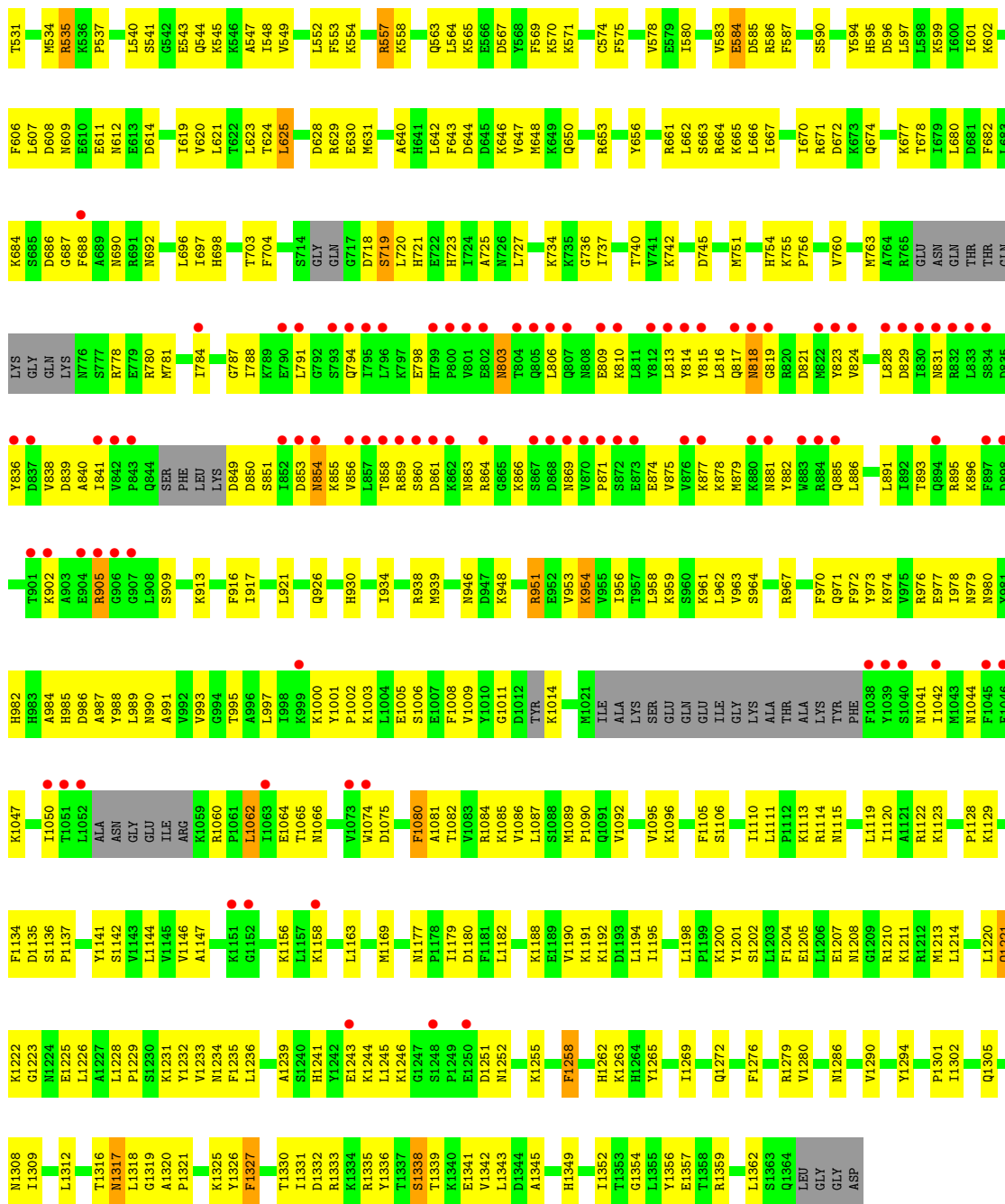


- Molecule 1: RNA (34-MER)

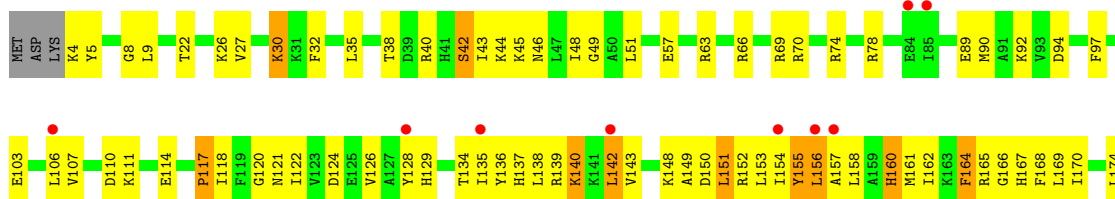


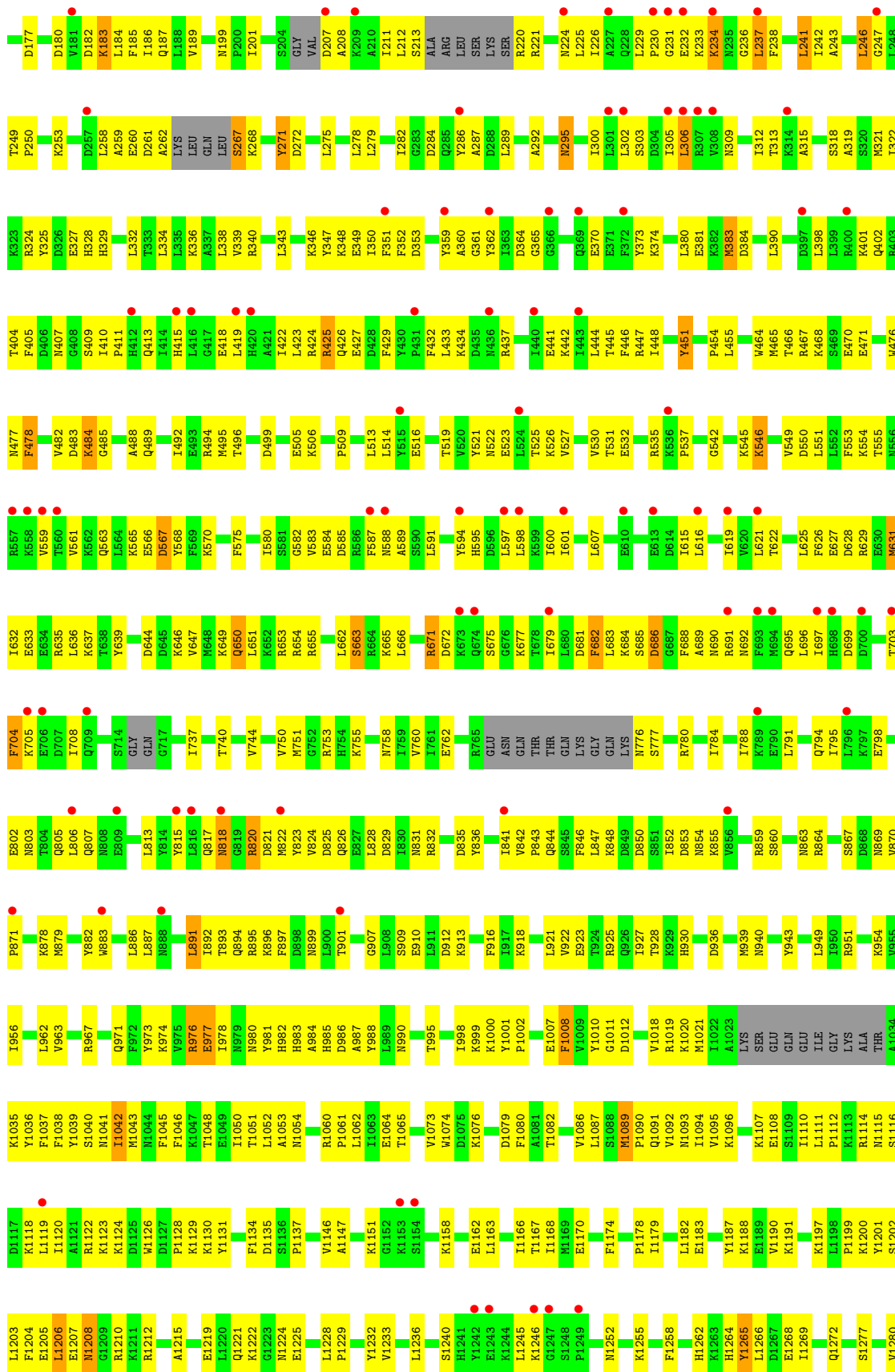
- Molecule 2: CRISPR-associated endonuclease Cas9/Csn1

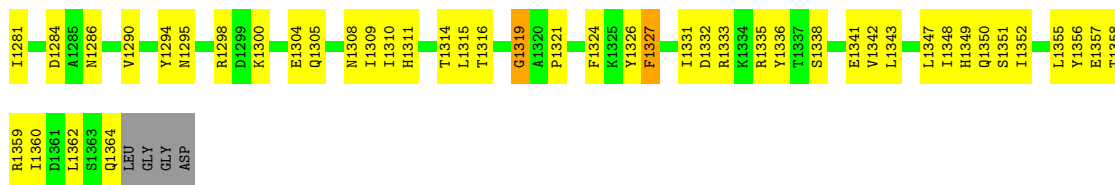




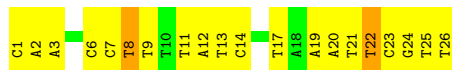
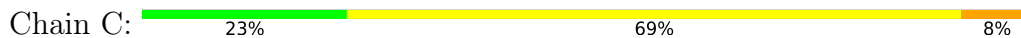
• Molecule 2: CRISPR-associated endonuclease Cas9/Csn1



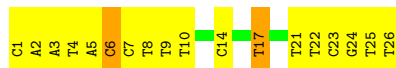




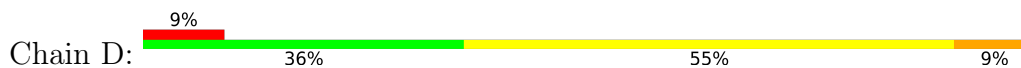
- Molecule 3: DNA (26-MER)



- Molecule 3: DNA (26-MER)



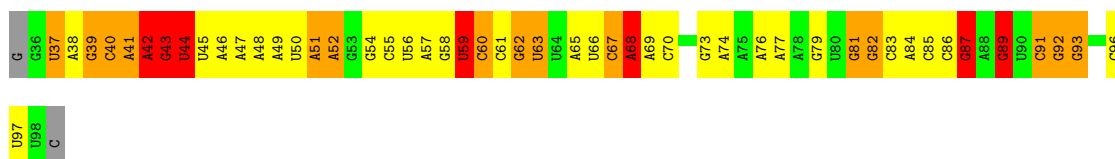
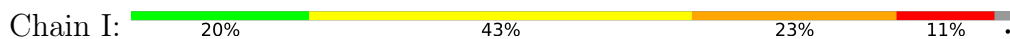
- Molecule 4: DNA (5'-D(*TP*TP*TP*AP*GP*GP*TP*AP*TP*TP*G)-3')



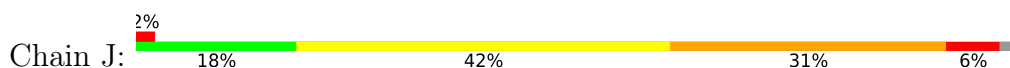
- Molecule 4: DNA (5'-D(*TP*TP*TP*AP*GP*GP*TP*AP*TP*TP*G)-3')

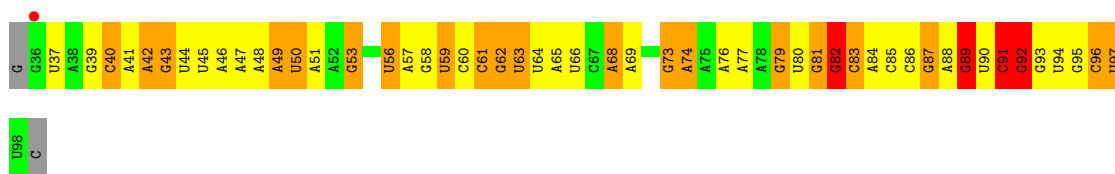


- Molecule 5: RNA (65-MER)



- Molecule 5: RNA (65-MER)





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4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	145.21Å 130.60Å 148.73Å 90.00° 104.08° 90.00°	Depositor
Resolution (Å)	48.23 – 3.36 48.23 – 3.29	Depositor EDS
% Data completeness (in resolution range)	59.4 (48.23-3.36) 73.5 (48.23-3.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 3.33Å)	Xtrriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.230 , 0.255 0.230 , 0.255	Depositor DCC
R_{free} test set	1990 reflections (3.44%)	wwPDB-VP
Wilson B-factor (Å ²)	56.7	Xtrriage
Anisotropy	0.207	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 17.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtrriage
Estimated twinning fraction	0.069 for l,-k,h	Xtrriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	27025	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% 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 [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	1.01	1/811 (0.1%)	1.81	32/1261 (2.5%)
1	E	0.87	0/767	1.73	23/1193 (1.9%)
2	B	0.58	1/10915 (0.0%)	0.80	11/14673 (0.1%)
2	F	0.58	2/10879 (0.0%)	0.78	4/14636 (0.0%)
3	C	1.42	6/581 (1.0%)	1.36	6/893 (0.7%)
3	G	1.25	1/581 (0.2%)	1.34	4/893 (0.4%)
4	D	1.51	1/251 (0.4%)	1.41	3/387 (0.8%)
4	H	1.49	1/251 (0.4%)	1.36	2/387 (0.5%)
5	I	1.03	1/1509 (0.1%)	1.90	61/2350 (2.6%)
5	J	0.93	0/1509	1.80	55/2350 (2.3%)
All	All	0.73	14/28054 (0.0%)	1.10	201/39023 (0.5%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	5	DA	C3'-O3'	-10.11	1.30	1.44
4	H	3	DT	C1'-N1	6.85	1.58	1.49
3	C	8	DT	C3'-O3'	-6.36	1.35	1.44
5	I	41	A	N9-C4	-6.20	1.34	1.37
2	F	1319	GLY	C-N	-5.73	1.20	1.34
3	C	19	DA	C3'-O3'	-5.61	1.36	1.44
1	A	20	A	C6-N1	-5.48	1.31	1.35
3	C	12	DA	C5'-C4'	5.46	1.57	1.51
3	C	9	DT	N1-C2	-5.35	1.33	1.38
3	C	12	DA	N3-C4	-5.16	1.31	1.34
2	B	1321	PRO	N-CD	5.14	1.55	1.47
3	G	21	DT	P-O5'	5.08	1.64	1.59
2	F	1089	MET	C-N	-5.06	1.24	1.34
3	C	6	DC	C3'-O3'	5.01	1.50	1.44

All (201) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	91	C	C4-C5-C6	-9.82	112.49	117.40
5	J	76	A	C8-N9-C4	-9.81	101.88	105.80
3	C	14	DC	O4'-C4'-C3'	-9.62	100.23	106.00
5	J	92	G	C5-C6-O6	-9.36	122.99	128.60
5	I	59	U	O5'-P-OP2	-9.32	97.31	105.70
5	J	89	G	N3-C4-N9	9.12	131.47	126.00
1	A	26	A	C8-N9-C4	9.09	109.44	105.80
5	I	49	A	C5-C6-N1	8.96	122.18	117.70
5	J	91	C	N3-C2-O2	8.75	128.03	121.90
5	I	96	C	C6-N1-C2	-8.64	116.84	120.30
5	I	45	U	C6-N1-C2	-8.63	115.82	121.00
1	A	25	U	C2-N1-C1'	-8.57	107.41	117.70
1	E	15	G	C5-C6-N1	8.56	115.78	111.50
5	I	67	C	C6-N1-C2	8.46	123.69	120.30
5	J	49	A	N1-C6-N6	-8.37	113.58	118.60
2	F	246	LEU	CA-CB-CG	8.30	134.39	115.30
5	J	89	G	C6-C5-N7	-8.27	125.44	130.40
5	I	43	G	N9-C4-C5	8.19	108.67	105.40
3	G	14	DC	O4'-C4'-C3'	-8.17	101.10	106.00
1	E	17	U	C6-N1-C2	-7.99	116.20	121.00
1	E	16	A	C8-N9-C4	7.99	109.00	105.80
5	I	62	G	C5-C6-O6	7.99	133.39	128.60
5	J	66	U	N3-C4-O4	7.93	124.95	119.40
1	A	21	G	C8-N9-C4	-7.92	103.23	106.40
5	I	45	U	C5-C6-N1	7.86	126.63	122.70
5	J	91	C	C5-C4-N4	-7.83	114.72	120.20
5	I	41	A	C2-N3-C4	-7.80	106.70	110.60
1	A	14	G	C8-N9-C4	7.80	109.52	106.40
1	A	20	A	N1-C6-N6	-7.75	113.95	118.60
5	J	97	U	C6-N1-C2	-7.65	116.41	121.00
5	J	92	G	N1-C6-O6	7.64	124.48	119.90
5	I	43	G	C4-C5-N7	-7.63	107.75	110.80
1	E	15	G	C2-N3-C4	7.60	115.70	111.90
5	J	68	A	C8-N9-C4	-7.55	102.78	105.80
3	G	10	DT	O4'-C1'-N1	7.43	113.20	108.00
2	B	82	LEU	CB-CG-CD2	-7.38	98.45	111.00
5	J	73	G	C8-N9-C4	-7.32	103.47	106.40
5	I	54	G	N1-C6-O6	7.27	124.26	119.90
1	A	2	U	C2-N1-C1'	7.20	126.34	117.70
1	E	11	U	N3-C2-O2	-7.17	117.18	122.20
5	I	48	A	C5-C6-N6	-7.09	118.03	123.70
5	I	89	G	C2-N3-C4	7.06	115.43	111.90
1	A	26	A	N1-C6-N6	7.04	122.83	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	343	LEU	CA-CB-CG	7.03	131.46	115.30
5	I	46	A	OP2-P-O3'	7.01	120.62	105.20
5	J	59	U	O5'-P-OP2	-7.01	99.39	105.70
5	J	91	C	N3-C4-C5	7.00	124.70	121.90
5	I	65	A	C8-N9-C4	-6.94	103.03	105.80
5	J	89	G	N3-C4-C5	-6.91	125.15	128.60
1	E	11	U	C5-C4-O4	6.90	130.04	125.90
5	I	58	G	N1-C6-O6	6.88	124.03	119.90
5	I	48	A	N1-C6-N6	6.87	122.72	118.60
5	I	62	G	C8-N9-C4	-6.86	103.66	106.40
1	E	24	U	C5-C6-N1	6.79	126.09	122.70
5	I	79	G	N1-C6-O6	6.77	123.96	119.90
5	I	42	A	C8-N9-C4	-6.70	103.12	105.80
5	J	62	G	C8-N9-C4	-6.62	103.75	106.40
5	J	83	C	C6-N1-C2	-6.59	117.67	120.30
5	I	42	A	N9-C4-C5	6.57	108.43	105.80
5	I	62	G	N3-C2-N2	6.57	124.50	119.90
5	I	62	G	N3-C4-C5	-6.48	125.36	128.60
5	J	76	A	N9-C4-C5	6.48	108.39	105.80
1	A	17	U	O5'-P-OP1	-6.48	99.87	105.70
1	E	15	G	O5'-P-OP1	-6.43	99.91	105.70
5	J	73	G	C6-C5-N7	-6.37	126.58	130.40
1	A	21	G	N7-C8-N9	6.37	116.28	113.10
5	I	55	C	C4-C5-C6	6.34	120.57	117.40
5	I	62	G	N1-C6-O6	-6.34	116.10	119.90
4	D	5	DA	OP1-P-OP2	6.33	129.09	119.60
5	J	86	C	N3-C4-N4	6.31	122.42	118.00
5	J	49	A	N9-C4-C5	6.31	108.32	105.80
3	C	13	DT	O4'-C4'-C3'	-6.29	101.98	104.50
4	H	11	DT	O4'-C1'-N1	6.28	112.39	108.00
5	I	87	G	C2-N3-C4	6.27	115.03	111.90
1	E	11	U	C6-N1-C2	-6.24	117.25	121.00
1	E	15	G	N1-C6-O6	-6.23	116.16	119.90
5	I	43	G	C8-N9-C4	-6.23	103.91	106.40
5	I	60	C	N3-C4-C5	-6.21	119.41	121.90
5	J	61	C	C6-N1-C2	-6.21	117.81	120.30
5	I	45	U	N3-C4-O4	6.21	123.75	119.40
1	A	13	U	O5'-P-OP2	-6.20	100.12	105.70
5	J	79	G	C8-N9-C4	6.20	108.88	106.40
5	I	96	C	C5-C6-N1	6.19	124.10	121.00
1	A	26	A	N7-C8-N9	-6.19	110.71	113.80
5	J	89	G	C8-N9-C1'	-6.17	118.97	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	45	U	O5'-P-OP1	-6.14	100.17	105.70
5	I	49	A	C2-N3-C4	6.13	113.67	110.60
1	A	23	U	N3-C4-O4	6.10	123.67	119.40
1	E	25	U	C5-C6-N1	6.09	125.75	122.70
5	I	43	G	C2-N3-C4	6.08	114.94	111.90
1	A	21	G	C2-N3-C4	6.07	114.94	111.90
5	I	43	G	C6-C5-N7	6.06	134.04	130.40
5	J	91	C	C6-N1-C2	6.06	122.72	120.30
5	J	68	A	N7-C8-N9	6.05	116.83	113.80
5	I	67	C	N3-C2-O2	6.04	126.13	121.90
5	I	87	G	N1-C2-N3	-6.04	120.27	123.90
1	E	16	A	N7-C8-N9	-6.04	110.78	113.80
2	B	1245	LEU	CB-CG-CD1	6.02	121.24	111.00
5	I	47	A	N1-C2-N3	-6.02	126.29	129.30
5	J	91	C	N1-C2-N3	-6.02	114.99	119.20
2	B	158	LEU	CB-CG-CD1	-6.01	100.79	111.00
1	A	18	A	C4-C5-C6	6.00	120.00	117.00
5	J	89	G	C4-C5-C6	5.99	122.39	118.80
1	E	22	U	N3-C2-O2	-5.98	118.01	122.20
5	J	48	A	C5-C6-N1	-5.96	114.72	117.70
5	I	68	A	OP1-P-OP2	-5.95	110.67	119.60
5	J	91	C	C5-C6-N1	5.95	123.98	121.00
1	E	10	U	C6-N1-C2	-5.94	117.43	121.00
2	B	139	ARG	NE-CZ-NH1	-5.94	117.33	120.30
5	J	66	U	N3-C2-O2	5.93	126.36	122.20
1	A	25	U	C5-C6-N1	-5.91	119.74	122.70
1	A	21	G	N3-C4-C5	-5.89	125.65	128.60
5	I	87	G	C5-C6-O6	-5.87	125.08	128.60
1	A	14	G	N7-C8-N9	-5.87	110.17	113.10
5	J	89	G	C4-N9-C1'	5.87	134.13	126.50
5	I	63	U	C2-N3-C4	-5.86	123.49	127.00
1	E	10	U	C5-C4-O4	5.83	129.40	125.90
5	I	81	G	C2-N3-C4	5.82	114.81	111.90
2	F	30	LYS	CD-CE-NZ	5.77	124.98	111.70
5	J	50	U	C6-N1-C2	5.77	124.46	121.00
2	B	1320	ALA	C-N-CD	5.77	140.52	128.40
5	I	62	G	C4-C5-N7	-5.76	108.50	110.80
5	J	66	U	N1-C2-O2	-5.75	118.78	122.80
5	I	62	G	N1-C2-N2	-5.73	111.05	116.20
5	I	54	G	C6-C5-N7	-5.72	126.97	130.40
5	J	89	G	N1-C6-O6	5.72	123.33	119.90
1	A	28	A	O4'-C1'-N9	-5.69	103.65	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	17	U	N3-C2-O2	-5.65	118.25	122.20
5	J	73	G	N1-C6-O6	5.64	123.28	119.90
5	J	89	G	C5-C6-O6	-5.64	125.22	128.60
5	I	58	G	C5-C6-O6	-5.63	125.22	128.60
5	I	59	U	N3-C2-O2	-5.62	118.27	122.20
1	A	26	A	N9-C4-C5	-5.58	103.57	105.80
5	J	49	A	C5-C6-N6	5.58	128.16	123.70
1	E	34	G	C8-N9-C4	-5.56	104.18	106.40
5	J	49	A	C4-C5-N7	-5.53	107.93	110.70
5	I	47	A	C5-C6-N1	5.52	120.46	117.70
3	C	11	DT	O4'-C4'-C3'	-5.51	102.30	104.50
5	I	96	C	N3-C4-C5	-5.49	119.70	121.90
2	B	156	LEU	CB-CG-CD2	-5.46	101.71	111.00
5	J	81	G	C5-C6-O6	-5.46	125.33	128.60
1	A	21	G	O5'-P-OP1	5.43	117.22	110.70
1	A	21	G	C4-N9-C1'	5.40	133.52	126.50
4	D	8	DT	OP1-P-OP2	-5.40	111.50	119.60
5	I	46	A	C8-N9-C4	-5.39	103.64	105.80
2	F	241	LEU	CA-CB-CG	5.38	127.66	115.30
5	J	48	A	C4-C5-C6	5.37	119.68	117.00
5	I	55	C	N1-C2-O2	-5.36	115.69	118.90
5	I	62	G	N9-C4-C5	5.35	107.54	105.40
3	G	6	DC	O4'-C1'-N1	5.35	111.74	108.00
1	E	11	U	OP2-P-O3'	5.33	116.94	105.20
1	A	23	U	N1-C2-O2	-5.33	119.07	122.80
1	A	23	U	C5-C4-O4	-5.32	122.71	125.90
5	J	77	A	C4-C5-C6	-5.32	114.34	117.00
5	J	77	A	C4-C5-N7	5.32	113.36	110.70
1	A	2	U	C6-N1-C1'	-5.31	113.76	121.20
5	J	76	A	N7-C8-N9	5.30	116.45	113.80
4	D	10	DT	OP1-P-OP2	5.30	127.55	119.60
3	G	17	DT	N3-C4-O4	5.29	123.08	119.90
2	F	306	LEU	CB-CG-CD1	5.28	119.98	111.00
5	I	79	G	N3-C2-N2	-5.26	116.22	119.90
1	A	22	U	C5-C6-N1	5.25	125.32	122.70
2	B	1245	LEU	CA-CB-CG	5.24	127.34	115.30
5	J	86	C	C5-C4-N4	-5.23	116.54	120.20
5	I	51	A	C2-N3-C4	-5.21	107.99	110.60
1	E	17	U	C5-C6-N1	5.21	125.31	122.70
1	A	25	U	C6-N1-C1'	5.20	128.48	121.20
5	J	81	G	N3-C4-N9	5.20	129.12	126.00
5	J	82	G	N9-C4-C5	-5.20	103.32	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	229	LEU	CA-CB-CG	5.20	127.25	115.30
3	C	22	DT	O4'-C1'-N1	5.20	111.64	108.00
5	J	48	A	N1-C2-N3	5.19	131.89	129.30
5	J	89	G	N9-C4-C5	-5.17	103.33	105.40
1	E	22	U	C6-N1-C2	-5.17	117.90	121.00
5	I	42	A	C2'-C3'-O3'	5.17	121.97	113.70
2	B	52	LEU	CA-CB-CG	-5.16	103.43	115.30
5	J	90	U	C2-N1-C1'	-5.16	111.50	117.70
1	A	25	U	C6-N1-C2	5.16	124.10	121.00
1	A	31	U	N1-C2-O2	5.16	126.41	122.80
1	A	26	A	C5-C6-N6	-5.15	119.58	123.70
2	B	625	LEU	CA-CB-CG	5.14	127.12	115.30
1	A	8	A	P-O3'-C3'	5.13	125.86	119.70
5	J	64	U	N3-C2-O2	-5.13	118.61	122.20
5	J	96	C	N3-C4-N4	5.12	121.59	118.00
1	A	25	U	N1-C2-O2	-5.12	119.22	122.80
1	E	15	G	OP2-P-O3'	5.12	116.46	105.20
5	I	44	U	OP2-P-O3'	5.11	116.44	105.20
5	I	52	A	N1-C6-N6	-5.10	115.54	118.60
5	I	89	G	N1-C6-O6	-5.10	116.84	119.90
1	E	27	G	P-O3'-C3'	5.09	125.81	119.70
5	I	66	U	N3-C2-O2	5.09	125.77	122.20
5	J	53	G	O5'-P-OP1	-5.08	101.12	105.70
5	I	55	C	N3-C4-N4	5.07	121.55	118.00
5	I	91	C	N3-C2-O2	5.06	125.44	121.90
1	E	23	U	OP2-P-O3'	5.06	116.33	105.20
4	H	11	DT	N3-C4-O4	5.05	122.93	119.90
1	A	25	U	N3-C2-O2	5.05	125.73	122.20
5	I	93	G	C8-N9-C4	-5.04	104.38	106.40
3	C	13	DT	OP2-P-O3'	5.04	116.28	105.20
5	J	92	G	C4-C5-N7	5.02	112.81	110.80
3	C	17	DT	N3-C4-O4	5.02	122.91	119.90

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	725	0	362	40	0
1	E	685	0	342	44	0
2	B	10732	0	10828	517	1
2	F	10695	0	10736	702	0
3	C	521	0	299	19	0
3	G	521	0	299	20	0
4	D	225	0	129	3	0
4	H	225	0	129	10	0
5	I	1348	0	678	38	0
5	J	1348	0	678	61	0
All	All	27025	0	24480	1373	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 27.

All (1373) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:142:LEU:CD1	2:F:154:ILE:HG12	1.37	1.54
2:F:142:LEU:HD11	2:F:154:ILE:CG1	1.39	1.51
2:F:142:LEU:CD2	2:F:154:ILE:HD11	1.41	1.48
2:F:142:LEU:CD2	2:F:154:ILE:CD1	1.94	1.45
2:B:1222:LYS:O	2:B:1318:LEU:CD2	1.66	1.42
2:F:142:LEU:HD21	2:F:154:ILE:CD1	1.49	1.38
2:F:212:LEU:CD1	2:F:300:ILE:HG12	1.55	1.35
2:F:139:ARG:CG	2:F:157:ALA:HB1	1.56	1.34
2:F:138:LEU:CD1	2:F:153:LEU:HD21	1.58	1.32
2:F:165:ARG:HD2	2:F:168:PHE:CE1	1.65	1.31
2:F:138:LEU:CD1	2:F:153:LEU:CD2	2.10	1.30
1:E:4:A:C2	1:E:5:C:C5	2.20	1.27
2:F:139:ARG:HG2	2:F:157:ALA:CB	1.63	1.27
2:F:208:ALA:CA	2:F:211:ILE:HD12	1.63	1.26
2:F:138:LEU:HD11	2:F:153:LEU:CD2	1.66	1.25
2:F:921:LEU:HD12	2:F:1008:PHE:CE2	1.71	1.22
2:F:208:ALA:HA	2:F:211:ILE:CD1	1.71	1.21
2:F:142:LEU:HD21	2:F:154:ILE:CG1	1.72	1.19
2:F:249:THR:HG1	2:F:267:SER:N	1.43	1.17
2:B:392:LYS:HG2	2:B:395:ARG:NH1	1.61	1.14
2:F:207:ASP:O	2:F:211:ILE:HG13	1.49	1.12
2:F:142:LEU:HD13	2:F:154:ILE:HG23	1.21	1.11
2:F:142:LEU:HD22	2:F:154:ILE:CD1	1.71	1.11
2:F:90:MET:CE	2:F:151:LEU:HD21	1.80	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:138:LEU:CD2	2:F:153:LEU:HD21	1.80	1.10
2:F:142:LEU:HD11	2:F:154:ILE:CB	1.81	1.10
2:F:164:PHE:O	2:F:415:HIS:CD2	2.03	1.10
2:F:165:ARG:HD2	2:F:168:PHE:CZ	1.90	1.06
2:B:392:LYS:HG2	2:B:395:ARG:HH12	0.91	1.05
2:F:212:LEU:HD12	2:F:300:ILE:HG12	1.29	1.05
2:F:142:LEU:CG	2:F:154:ILE:HG12	1.86	1.05
3:G:24:DG:H2'	3:G:25:DT:H5'	1.10	1.04
2:B:545:LYS:NZ	2:B:690:ASN:OD1	1.92	1.03
2:B:558:LYS:HE3	2:B:590:SER:HB3	1.36	1.03
2:F:142:LEU:CD1	2:F:154:ILE:CG1	2.11	1.03
2:B:1221:GLN:HG2	2:B:1319:GLY:O	1.59	1.02
2:F:151:LEU:HD13	2:F:152:ARG:H	1.22	1.02
2:F:180:ASP:HB3	2:F:183:LYS:HB2	1.39	1.02
2:B:1222:LYS:O	2:B:1318:LEU:HD21	1.60	1.00
2:F:138:LEU:CG	2:F:153:LEU:HD21	1.93	0.99
2:F:139:ARG:HD3	2:F:157:ALA:O	1.63	0.99
2:F:1210:ARG:NH2	2:F:1341:GLU:OE1	1.95	0.99
2:F:138:LEU:HD13	2:F:153:LEU:HD21	1.42	0.99
2:B:1222:LYS:O	2:B:1318:LEU:HD23	1.59	0.99
2:B:381:GLU:HG2	2:B:390:LEU:HD11	1.43	0.98
2:F:139:ARG:HD3	2:F:157:ALA:C	1.84	0.98
2:F:138:LEU:CD2	2:F:153:LEU:CD2	2.42	0.98
2:B:951:ARG:NH2	2:B:1011:GLY:HA2	1.80	0.97
2:F:90:MET:CE	2:F:151:LEU:CD2	2.42	0.97
2:F:142:LEU:HD22	2:F:154:ILE:HD13	1.45	0.97
2:F:142:LEU:CD2	2:F:154:ILE:CG1	2.39	0.96
3:G:24:DG:C2'	3:G:25:DT:H5'	1.96	0.96
2:B:1211:LYS:O	2:B:1223:GLY:HA3	1.65	0.95
2:B:137:HIS:HA	2:B:322:ILE:HD11	1.47	0.95
2:F:212:LEU:CD1	2:F:300:ILE:CG1	2.44	0.95
2:B:1222:LYS:O	2:B:1318:LEU:HD22	1.67	0.94
2:F:921:LEU:HD12	2:F:1008:PHE:HE2	1.15	0.94
1:A:4:A:O2'	1:A:5:C:O5'	1.83	0.94
3:G:24:DG:H2'	3:G:25:DT:C5'	1.97	0.94
2:B:220:ARG:O	2:B:224:ASN:ND2	2.00	0.94
2:F:142:LEU:HD13	2:F:154:ILE:CG2	1.97	0.94
2:F:212:LEU:HD11	2:F:300:ILE:HG12	1.48	0.94
2:F:165:ARG:HD2	2:F:168:PHE:HE1	1.15	0.93
2:F:142:LEU:CD1	2:F:154:ILE:HG23	1.98	0.93
1:A:3:A:O2'	1:A:4:A:O5'	1.85	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:142:LEU:HD22	2:F:154:ILE:HD11	1.38	0.93
2:F:626:PHE:O	2:F:655:ARG:NH1	2.01	0.93
1:E:4:A:N3	1:E:5:C:C6	2.38	0.92
2:F:149:ALA:HB3	2:F:154:ILE:CD1	2.00	0.92
2:F:138:LEU:HD13	2:F:153:LEU:CD2	1.97	0.91
2:F:90:MET:HE1	2:F:151:LEU:HD21	1.53	0.91
2:F:777:SER:HA	2:F:807:GLN:HE21	1.35	0.91
2:F:138:LEU:HD11	2:F:153:LEU:HD22	1.51	0.91
2:F:485:GLY:HA3	2:F:631:MET:HG3	1.52	0.91
2:F:90:MET:HE1	2:F:151:LEU:CD2	2.00	0.90
2:F:142:LEU:HD21	2:F:154:ILE:HD11	1.00	0.90
2:F:686:ASP:CG	2:F:690:ASN:HA	1.91	0.90
2:B:601:ILE:HD11	2:B:607:LEU:HD21	1.53	0.90
2:F:142:LEU:HD11	2:F:154:ILE:CA	2.02	0.90
2:F:978:ILE:HD12	2:F:1233:VAL:HG22	1.53	0.90
2:F:686:ASP:CB	2:F:690:ASN:HA	2.02	0.89
2:F:138:LEU:HD21	2:F:153:LEU:CD2	2.03	0.89
2:F:142:LEU:HD11	2:F:154:ILE:HA	1.54	0.89
2:F:138:LEU:CD1	2:F:153:LEU:HD22	2.02	0.88
1:E:4:A:N3	1:E:5:C:C5	2.40	0.88
2:F:380:LEU:HD11	2:F:390:LEU:HG	1.53	0.88
2:F:328:HIS:HE2	2:F:359:TYR:HH	1.20	0.88
2:B:392:LYS:CG	2:B:395:ARG:HH12	1.84	0.87
1:E:4:A:C2	1:E:5:C:C6	2.63	0.87
2:F:142:LEU:CD2	2:F:154:ILE:HG12	2.04	0.87
2:F:467:ARG:HA	2:F:482:VAL:HG22	1.57	0.87
2:F:249:THR:OG1	2:F:267:SER:N	2.08	0.86
2:F:142:LEU:CD1	2:F:154:ILE:HA	2.06	0.85
2:B:921:LEU:HD21	2:B:1042:ILE:HG21	1.57	0.85
2:B:967:ARG:HE	2:B:974:LYS:HB2	1.42	0.85
2:F:893:THR:HG23	2:F:896:LYS:H	1.40	0.84
2:F:279:LEU:HD21	2:F:287:ALA:HB2	1.59	0.84
2:F:226:ILE:HG13	2:F:232:GLU:HG2	1.59	0.84
2:F:139:ARG:HH21	2:F:160:HIS:CD2	1.95	0.84
2:F:208:ALA:HA	2:F:211:ILE:HD12	0.88	0.84
2:B:455:LEU:HD23	2:B:473:ILE:HD12	1.60	0.84
2:F:451:TYR:O	2:F:464:TRP:NE1	2.10	0.84
5:J:46:A:H2'	5:J:47:A:C8	2.13	0.83
1:A:2:U:H3	1:A:4:A:H3'	1.42	0.83
3:G:1:DC:N4	4:H:12:DG:O6	2.11	0.83
2:F:1045:PHE:HA	2:F:1060:ARG:HH11	1.43	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1110:ILE:HD12	2:B:1122:ARG:HD2	1.60	0.83
2:F:151:LEU:HD13	2:F:152:ARG:N	1.93	0.82
1:A:14:G:OP2	2:B:63:ARG:NH1	2.12	0.82
2:B:1236:LEU:HD11	2:B:1269:ILE:HD13	1.62	0.82
2:B:384:ASP:OD1	2:B:385:GLY:N	2.12	0.82
2:F:1045:PHE:HB2	2:F:1064:GLU:HG2	1.62	0.82
3:G:25:DT:H2''	3:G:26:DT:OP2	1.80	0.81
2:F:138:LEU:HD21	2:F:153:LEU:HD23	1.59	0.81
2:F:151:LEU:HD22	2:F:152:ARG:N	1.95	0.81
2:F:164:PHE:O	2:F:415:HIS:HD2	1.58	0.81
1:E:4:A:C2	1:E:5:C:C4	2.68	0.81
2:F:1120:ILE:HD11	2:F:1137:PRO:HD3	1.62	0.81
2:B:212:LEU:O	2:B:221:ARG:NH1	2.14	0.81
2:F:165:ARG:CD	2:F:168:PHE:CE1	2.56	0.81
2:F:1212:ARG:NH2	2:F:1280:VAL:O	2.15	0.80
2:F:142:LEU:CD1	2:F:154:ILE:CB	2.52	0.80
2:F:1041:ASN:O	2:F:1043:MET:N	2.13	0.80
2:F:425:ARG:HG3	2:F:426:GLN:HG2	1.63	0.79
2:F:139:ARG:CD	2:F:157:ALA:O	2.29	0.79
2:F:165:ARG:CD	2:F:168:PHE:HE1	1.92	0.79
2:F:135:ILE:HD11	2:F:156:LEU:HB3	1.64	0.79
2:F:686:ASP:HB3	2:F:690:ASN:HA	1.63	0.79
2:B:823:TYR:HA	2:B:875:VAL:HG11	1.64	0.79
2:F:89:GLU:OE2	2:F:92:LYS:NZ	2.15	0.79
2:F:90:MET:SD	2:F:151:LEU:HD21	2.22	0.79
2:B:116:HIS:CE1	2:B:122:ILE:HG12	2.17	0.78
2:F:166:GLY:HA3	2:F:410:ILE:HG22	1.64	0.78
2:B:404:THR:HG22	2:B:405:PHE:CD1	2.19	0.78
2:F:886:LEU:HA	2:F:891:LEU:HD21	1.64	0.78
2:F:142:LEU:CD1	2:F:154:ILE:CG2	2.59	0.78
2:B:442:LYS:HE3	2:B:476:TRP:HA	1.65	0.78
2:B:725:ALA:O	2:B:734:LYS:NZ	2.17	0.77
2:F:522:ASN:OD1	2:F:692:ASN:ND2	2.16	0.77
2:B:1222:LYS:HE3	2:B:1317:ASN:O	1.85	0.77
2:F:94:ASP:HB3	2:F:97:PHE:HB2	1.65	0.77
2:F:846:PHE:O	2:F:1040:SER:OG	2.02	0.77
2:F:70:ARG:NH2	5:J:61:C:OP1	2.16	0.77
2:F:63:ARG:HA	2:F:66:ARG:HG3	1.65	0.77
1:A:27:G:H5'	1:A:28:A:H5''	1.67	0.77
2:F:649:LYS:O	2:F:653:ARG:NE	2.17	0.77
2:B:1147:ALA:HB2	2:B:1190:VAL:HA	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:6:DC:N4	4:H:7:DG:O6	2.18	0.77
2:B:279:LEU:HD11	2:B:284:ASP:HA	1.68	0.76
2:F:142:LEU:HD11	2:F:154:ILE:HG12	0.76	0.76
2:B:913:LYS:HA	2:B:916:PHE:HD2	1.50	0.76
2:B:201:ILE:HG22	2:B:202:ASN:H	1.51	0.76
2:B:524:LEU:HD12	2:B:587:PHE:HE2	1.50	0.76
1:E:15:G:OP1	2:F:66:ARG:NH2	2.19	0.76
2:F:921:LEU:HD21	2:F:1042:ILE:HG21	1.67	0.76
2:B:586:ARG:NH1	3:C:26:DT:O2	2.19	0.76
2:F:128:TYR:CE1	2:F:153:LEU:HD11	2.21	0.76
2:F:1045:PHE:HA	2:F:1060:ARG:NH1	2.01	0.76
2:F:999:LYS:HB3	2:F:1073:VAL:HG12	1.66	0.75
2:F:139:ARG:HG2	2:F:157:ALA:HB1	0.79	0.75
2:F:139:ARG:CG	2:F:157:ALA:CB	2.40	0.75
2:F:149:ALA:CB	2:F:154:ILE:CD1	2.65	0.74
2:F:446:PHE:HZ	2:F:478:PHE:HD1	1.34	0.74
2:B:45:LYS:NZ	2:B:1357:GLU:OE2	2.15	0.74
2:B:864:ARG:NH2	2:B:869:ASN:O	2.19	0.74
2:F:1215:ALA:HB2	2:F:1221:GLN:HG3	1.68	0.74
2:F:168:PHE:HB2	2:F:447:ARG:HH11	1.52	0.74
2:F:844:GLN:OE1	2:F:848:LYS:NZ	2.15	0.74
2:B:74:ARG:HH21	5:I:60:C:P	2.10	0.74
2:B:1211:LYS:O	2:B:1223:GLY:CA	2.34	0.74
2:F:842:VAL:HG12	2:F:854:ASN:OD1	1.87	0.74
2:F:148:LYS:CB	2:F:429:PHE:CD2	2.70	0.73
2:F:446:PHE:CZ	2:F:478:PHE:HD1	2.06	0.73
1:A:20:A:OP2	2:B:403:ARG:NH1	2.21	0.73
2:F:199:ASN:O	2:F:201:ILE:HD11	1.87	0.73
2:F:138:LEU:HD22	2:F:153:LEU:HD21	1.69	0.73
2:F:142:LEU:HD21	2:F:149:ALA:CB	2.17	0.73
2:F:149:ALA:CB	2:F:154:ILE:HG13	2.18	0.73
2:F:913:LYS:HG3	2:F:1040:SER:HB3	1.69	0.73
3:C:25:DT:C2	3:C:26:DT:H72	2.24	0.73
1:E:27:G:N2	5:J:44:U:OP2	2.22	0.73
2:F:149:ALA:CB	2:F:154:ILE:HD11	2.18	0.73
2:F:370:GLU:OE2	2:F:374:LYS:NZ	2.22	0.72
2:B:279:LEU:CD1	2:B:284:ASP:HA	2.19	0.72
2:B:1210:ARG:NH2	2:B:1341:GLU:OE1	2.22	0.72
2:F:923:GLU:HG2	2:F:928:THR:HG21	1.72	0.72
2:B:619:ILE:O	2:B:623:LEU:HB2	1.90	0.72
2:F:530:VAL:HG22	2:F:537:PRO:HB3	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:19:A:O2'	2:F:405:PHE:O	2.07	0.72
2:F:253:LYS:HG3	2:F:261:ASP:HA	1.72	0.72
2:B:1210:ARG:HB2	2:B:1280:VAL:HG13	1.72	0.71
2:F:90:MET:HE2	2:F:151:LEU:CD2	2.20	0.71
2:F:1205:GLU:OE1	2:F:1359:ARG:NH2	2.22	0.71
2:B:21:ILE:HD11	2:B:995:THR:HG21	1.71	0.71
2:B:217:SER:HB2	2:B:220:ARG:H	1.56	0.71
2:B:1220:LEU:HD11	2:B:1339:THR:HA	1.70	0.71
2:F:128:TYR:HE1	2:F:153:LEU:HD11	1.55	0.71
2:B:165:ARG:NH2	2:B:446:PHE:O	2.24	0.71
2:B:787:GLY:HA3	2:B:891:LEU:HD21	1.71	0.71
2:B:299:ALA:O	2:B:303:SER:OG	2.07	0.71
2:F:527:VAL:HA	2:F:582:GLY:HA3	1.73	0.71
3:C:25:DT:N3	3:C:26:DT:C4	2.59	0.70
2:F:505:GLU:HG3	2:F:665:LYS:HB2	1.72	0.70
2:F:1207:GLU:OE2	2:F:1210:ARG:NH1	2.24	0.70
2:B:530:VAL:HG22	2:B:537:PRO:HB3	1.72	0.70
2:F:139:ARG:CD	2:F:157:ALA:HB1	2.21	0.70
2:F:921:LEU:HD21	2:F:1042:ILE:HD13	1.73	0.70
2:B:874:GLU:HA	2:B:877:LYS:HE3	1.74	0.70
2:B:1135:ASP:OD1	2:B:1136:SER:N	2.24	0.70
2:B:650:GLN:OE1	2:B:653:ARG:NH2	2.25	0.70
2:B:951:ARG:CZ	2:B:1011:GLY:HA2	2.21	0.70
2:F:128:TYR:CE1	2:F:153:LEU:CD1	2.75	0.70
3:G:24:DG:C2'	3:G:25:DT:C5'	2.65	0.70
2:B:69:ARG:HD3	5:I:62:G:N7	2.07	0.70
2:F:936:ASP:OD1	2:F:940:ASN:ND2	2.24	0.70
2:B:1119:LEU:HD23	2:B:1128:PRO:HB2	1.73	0.69
2:B:1333:ARG:NH1	2:B:1335:ARG:HD2	2.06	0.69
2:F:921:LEU:HD12	2:F:1008:PHE:CZ	2.25	0.69
2:F:1206:LEU:HD11	2:F:1210:ARG:CZ	2.21	0.69
2:B:51:LEU:HD13	2:B:1095:VAL:HG23	1.74	0.69
2:F:199:ASN:O	2:F:201:ILE:CD1	2.41	0.69
2:F:446:PHE:HZ	2:F:478:PHE:CD1	2.11	0.69
2:F:892:ILE:HB	2:F:896:LYS:HE3	1.74	0.69
2:B:345:GLU:N	2:B:345:GLU:OE1	2.26	0.69
5:J:40:C:H2'	5:J:41:A:C8	2.28	0.68
2:B:243:ALA:O	2:B:248:LEU:HB2	1.93	0.68
2:F:471:GLU:OE1	2:F:477:ASN:ND2	2.26	0.68
2:F:1091:GLN:HG3	5:J:91:C:H5''	1.76	0.68
2:F:1219:GLU:OE1	2:F:1335:ARG:NH2	2.22	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:745:ASP:OD2	2:B:938:ARG:NH2	2.27	0.68
2:F:151:LEU:HD22	2:F:151:LEU:C	2.14	0.68
2:B:369:GLN:HE22	2:B:400:ARG:HD2	1.57	0.68
2:F:697:ILE:HD11	2:F:708:ILE:HG13	1.76	0.67
5:J:40:C:H2'	5:J:41:A:H8	1.59	0.67
2:B:557:ARG:NH2	2:B:596:ASP:OD1	2.27	0.67
2:F:686:ASP:OD2	2:F:690:ASN:HA	1.93	0.67
2:B:565:LYS:HE2	2:B:580:ILE:HG12	1.77	0.67
2:B:818:ASN:O	2:B:818:ASN:ND2	2.28	0.67
2:B:860:SER:OG	2:B:863:ASN:OD1	2.11	0.67
2:F:208:ALA:HA	2:F:211:ILE:CG1	2.24	0.67
2:F:148:LYS:HB3	2:F:429:PHE:CD2	2.30	0.67
2:B:229:LEU:HB2	2:B:230:PRO:HD2	1.76	0.67
2:B:1241:HIS:CE1	2:B:1244:LYS:HA	2.29	0.67
2:F:870:VAL:HG12	2:F:871:PRO:HD2	1.77	0.67
2:B:1318:LEU:HD13	2:B:1319:GLY:N	2.09	0.67
2:F:153:LEU:HD23	2:F:153:LEU:C	2.16	0.67
2:F:791:LEU:HD23	2:F:818:ASN:OD1	1.94	0.67
2:F:826:GLN:OE1	2:F:859:ARG:NH1	2.28	0.67
1:A:27:G:H5'	1:A:28:A:C5'	2.25	0.66
2:B:70:ARG:NH2	5:I:61:C:OP1	2.28	0.66
2:F:70:ARG:NE	5:J:61:C:OP2	2.19	0.66
2:F:967:ARG:NH1	2:F:986:ASP:OD1	2.27	0.66
2:B:585:ASP:OD1	2:B:586:ARG:N	2.28	0.66
2:F:672:ASP:OD1	2:F:703:THR:HG22	1.95	0.66
2:B:5:TYR:CE2	2:B:756:PRO:HB3	2.30	0.66
2:F:139:ARG:NE	2:F:157:ALA:O	2.28	0.66
2:F:165:ARG:CD	2:F:168:PHE:CZ	2.73	0.66
2:B:967:ARG:NE	2:B:974:LYS:HB2	2.09	0.66
2:F:46:ASN:HD21	5:J:88:A:H61	1.44	0.66
2:F:892:ILE:HB	2:F:896:LYS:CE	2.25	0.66
2:F:40:ARG:NE	2:F:43:ILE:HD11	2.11	0.66
2:F:633:GLU:O	2:F:637:LYS:N	2.27	0.66
2:B:317:LEU:HD22	2:B:414:ILE:HD11	1.78	0.66
2:F:1206:LEU:HD11	2:F:1210:ARG:NH2	2.11	0.66
2:B:5:TYR:OH	2:B:754:HIS:O	2.13	0.66
2:F:340:ARG:HG3	2:F:347:TYR:CE1	2.31	0.66
2:F:686:ASP:HB3	2:F:690:ASN:OD1	1.96	0.66
2:B:544:GLN:O	2:B:548:ILE:N	2.18	0.65
2:F:90:MET:HE2	2:F:151:LEU:HD23	1.79	0.65
2:F:142:LEU:HD21	2:F:154:ILE:HG12	1.64	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:524:LEU:HD12	2:B:587:PHE:CE2	2.30	0.65
2:B:549:VAL:HA	2:B:553:PHE:HD2	1.61	0.65
2:B:989:LEU:HD21	2:B:1087:LEU:HD21	1.78	0.65
2:B:404:THR:HG22	2:B:405:PHE:H	1.61	0.65
2:F:853:ASP:HB3	2:F:895:ARG:HH11	1.61	0.65
2:B:823:TYR:HD2	2:B:858:THR:HG21	1.61	0.65
2:F:212:LEU:O	2:F:221:ARG:CB	2.45	0.65
2:F:686:ASP:HB3	2:F:690:ASN:CA	2.26	0.65
2:F:867:SER:HB2	2:F:1054:ASN:N	2.11	0.65
2:B:181:VAL:O	2:B:185:PHE:N	2.28	0.65
3:C:22:DT:H2''	3:C:23:DC:O5'	1.95	0.65
2:F:986:ASP:O	2:F:990:ASN:ND2	2.30	0.65
2:B:939:MET:HE2	2:B:953:VAL:HG21	1.79	0.65
3:C:25:DT:N3	3:C:26:DT:O4	2.29	0.65
2:F:153:LEU:HD23	2:F:153:LEU:O	1.96	0.65
2:F:422:ILE:O	2:F:425:ARG:HG2	1.97	0.65
2:F:978:ILE:CD1	2:F:1233:VAL:HG22	2.25	0.65
2:F:1197:LYS:O	2:F:1199:PRO:HD3	1.97	0.65
2:F:1304:GLU:O	2:F:1308:ASN:ND2	2.29	0.65
2:B:516:GLU:O	2:B:519:THR:HG22	1.98	0.64
2:B:824:VAL:HG22	2:B:863:ASN:HD22	1.61	0.64
2:F:167:HIS:HD2	2:F:169:LEU:HB2	1.60	0.64
2:F:221:ARG:O	2:F:225:LEU:N	2.22	0.64
1:A:5:C:O2'	1:A:6:G:O5'	2.16	0.64
2:B:879:MET:HG3	2:B:882:TYR:HB3	1.78	0.64
2:F:887:LEU:HD21	2:F:894:GLN:HG2	1.80	0.64
2:F:1357:GLU:O	5:J:81:G:N2	2.29	0.64
2:F:923:GLU:OE2	2:F:925:ARG:NH1	2.29	0.64
1:E:3:A:C4	1:E:4:A:N7	2.66	0.64
2:F:149:ALA:HB3	2:F:154:ILE:HG13	1.80	0.64
2:F:760:VAL:HG22	2:F:956:ILE:HD12	1.79	0.64
2:B:1120:ILE:HD11	2:B:1137:PRO:HG3	1.79	0.64
2:F:149:ALA:HB3	2:F:154:ILE:CG1	2.28	0.64
2:F:1110:ILE:HD13	2:F:1122:ARG:CZ	2.28	0.64
2:F:1286:ASN:ND2	2:F:1332:ASP:O	2.31	0.64
2:F:89:GLU:HG3	2:F:432:PHE:HD2	1.62	0.63
2:F:165:ARG:HG2	2:F:166:GLY:O	1.98	0.63
2:F:184:LEU:HD13	2:F:295:ASN:HB3	1.79	0.63
2:F:853:ASP:HB3	2:F:895:ARG:NH1	2.12	0.63
2:F:1147:ALA:HB2	2:F:1190:VAL:HA	1.79	0.63
2:B:1312:LEU:HD21	2:B:1326:TYR:HD1	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:U:O2	1:A:3:A:H2'	1.97	0.63
2:F:135:ILE:HG21	5:J:46:A:H5'	1.80	0.63
2:F:189:VAL:HG13	2:F:201:ILE:HG22	1.80	0.63
1:A:2:U:O2	1:A:3:A:C2'	2.46	0.63
2:F:168:PHE:HB2	2:F:447:ARG:NH1	2.14	0.63
2:F:373:TYR:OH	2:F:398:LEU:N	2.30	0.63
2:B:121:ASN:OD1	2:B:124:ASP:HB2	1.99	0.63
2:B:270:THR:O	2:B:274:ASP:HB2	1.98	0.63
1:E:19:A:OP1	2:F:164:PHE:HD1	1.82	0.63
2:B:103:GLU:OE2	2:B:111:LYS:HG2	1.99	0.62
2:F:121:ASN:OD1	2:F:124:ASP:N	2.31	0.62
2:F:601:ILE:CD1	2:F:607:LEU:HD21	2.28	0.62
2:F:646:LYS:O	2:F:650:GLN:NE2	2.22	0.62
2:F:921:LEU:CD1	2:F:1008:PHE:HE2	2.02	0.62
2:F:963:VAL:HG21	2:F:990:ASN:OD1	1.99	0.62
2:B:70:ARG:HH22	2:B:462:PHE:HD2	1.47	0.62
2:F:89:GLU:HG3	2:F:432:PHE:CD2	2.34	0.62
2:F:139:ARG:HH21	2:F:160:HIS:HD2	1.45	0.62
2:F:168:PHE:CB	2:F:447:ARG:HH11	2.12	0.62
2:F:182:ASP:O	2:F:186:ILE:HD12	1.99	0.62
1:E:3:A:H2'	1:E:4:A:H8	1.64	0.62
2:F:918:LYS:O	2:F:922:VAL:HG22	2.00	0.62
2:F:1266:LEU:HB3	2:F:1294:TYR:OH	1.99	0.62
2:F:1294:TYR:HE1	2:F:1305:GLN:HE21	1.45	0.62
2:F:1311:HIS:O	2:F:1314:THR:HG22	2.00	0.62
1:A:5:C:H2'	1:A:6:G:H8	1.64	0.62
2:F:114:GLU:HG2	2:F:120:GLY:HA2	1.81	0.62
2:B:893:THR:HG23	2:B:896:LYS:H	1.63	0.62
2:F:841:ILE:HD12	2:F:854:ASN:HA	1.82	0.62
2:B:823:TYR:HA	2:B:875:VAL:CG1	2.30	0.62
2:F:189:VAL:HG13	2:F:201:ILE:CG2	2.30	0.62
2:F:207:ASP:O	2:F:211:ILE:CG1	2.39	0.62
2:F:977:GLU:HG3	2:F:1310:ILE:CG2	2.30	0.62
2:F:1300:LYS:NZ	2:F:1304:GLU:OE1	2.33	0.62
2:B:118:ILE:HD13	2:B:128:TYR:CD2	2.35	0.62
2:F:184:LEU:O	2:F:187:GLN:OE1	2.18	0.62
2:B:233:LYS:HG2	2:B:235:ASN:H	1.65	0.61
2:B:247:GLY:O	2:B:248:LEU:HG	2.00	0.61
2:B:810:LYS:HG2	2:B:838:VAL:HG23	1.82	0.61
2:B:184:LEU:HD12	2:B:299:ALA:HB2	1.82	0.61
2:F:183:LYS:H	2:F:183:LYS:HD2	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:174:LEU:HD23	2:B:302:LEU:HD23	1.81	0.61
1:E:19:A:H4'	2:F:407:ASN:C	2.20	0.61
2:F:208:ALA:N	2:F:211:ILE:HD12	2.15	0.61
2:B:332:LEU:HD13	2:B:359:TYR:CE1	2.35	0.61
2:F:212:LEU:HD11	2:F:300:ILE:CG1	2.19	0.61
5:J:83:C:H2'	5:J:84:A:H8	1.65	0.61
5:I:83:C:H2'	5:I:84:A:H8	1.64	0.61
2:B:1318:LEU:HD13	2:B:1318:LEU:C	2.20	0.61
2:F:1064:GLU:OE1	2:F:1065:THR:N	2.31	0.61
2:B:525:THR:HA	2:B:545:LYS:HE2	1.83	0.61
2:B:1000:LYS:HE2	2:B:1066:ASN:HA	1.83	0.61
2:F:35:LEU:HB2	2:F:1358:THR:HG22	1.83	0.61
2:F:841:ILE:CD1	2:F:896:LYS:HG3	2.30	0.61
2:F:275:LEU:O	2:F:279:LEU:N	2.34	0.61
2:F:818:ASN:ND2	2:F:818:ASN:O	2.32	0.61
5:J:44:U:O2'	5:J:45:U:H5'	1.99	0.61
2:B:168:PHE:CD2	2:B:447:ARG:HD3	2.35	0.61
2:B:114:GLU:HG2	2:B:120:GLY:HA2	1.83	0.60
1:A:31:U:H1'	5:I:39:G:N2	2.15	0.60
2:F:1062:LEU:O	2:F:1062:LEU:HG	2.01	0.60
2:F:1206:LEU:CD1	2:F:1210:ARG:NH1	2.64	0.60
2:B:1123:LYS:NZ	5:I:52:A:OP1	2.34	0.60
2:F:70:ARG:HH21	5:J:61:C:P	2.24	0.60
2:F:149:ALA:CB	2:F:154:ILE:CG1	2.79	0.60
1:A:2:U:O2	1:A:4:A:H8	1.83	0.60
2:B:917:ILE:HD11	2:B:1042:ILE:HG22	1.82	0.60
2:F:692:ASN:O	2:F:696:LEU:HG	2.01	0.60
2:B:909:SER:O	2:B:913:LYS:N	2.26	0.60
2:F:737:ILE:O	2:F:740:THR:HG22	2.01	0.60
2:F:1120:ILE:HB	2:F:1134:PHE:HB2	1.84	0.60
2:B:27:VAL:HG12	2:B:1086:VAL:HG22	1.83	0.60
2:B:250:PRO:HD2	2:B:264:LEU:O	2.01	0.60
2:B:420:HIS:ND1	2:B:441:GLU:OE2	2.35	0.60
2:F:69:ARG:NH2	5:J:63:U:OP2	2.35	0.60
2:F:545:LYS:NZ	2:F:683:LEU:O	2.35	0.60
2:F:142:LEU:HD21	2:F:149:ALA:HB2	1.83	0.60
2:B:541:SER:N	2:B:544:GLN:OE1	2.34	0.59
2:B:670:ILE:HG22	2:B:704:PHE:HE1	1.67	0.59
2:B:1305:GLN:O	2:B:1309:ILE:HG13	2.02	0.59
2:F:821:ASP:HB2	2:F:828:LEU:HD21	1.83	0.59
2:B:902:LYS:HA	2:B:905:ARG:HE	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:138:LEU:HD11	2:F:153:LEU:HD23	1.74	0.59
2:B:158:LEU:HD11	2:B:423:LEU:HD21	1.84	0.59
2:B:386:THR:O	2:B:386:THR:HG22	2.01	0.59
2:B:1062:LEU:HD23	2:B:1062:LEU:H	1.67	0.59
2:F:137:HIS:HA	2:F:322:ILE:HD11	1.83	0.59
2:F:138:LEU:HD21	2:F:153:LEU:O	2.01	0.59
2:F:149:ALA:HB2	2:F:154:ILE:HD11	1.82	0.59
2:F:677:LYS:HB3	2:F:682:PHE:CD2	2.36	0.59
1:A:10:U:H2'	1:A:11:U:C6	2.37	0.59
3:C:25:DT:H2'	3:C:25:DT:O2	2.01	0.59
2:B:979:ASN:OD1	2:B:980:ASN:N	2.35	0.59
2:B:358:GLY:O	2:B:362:TYR:N	2.33	0.59
2:B:644:ASP:HB3	2:B:647:VAL:HG23	1.85	0.59
2:F:253:LYS:HB2	2:F:262:ALA:H	1.66	0.59
2:F:686:ASP:OD2	2:F:691:ARG:N	2.35	0.59
2:B:1252:ASN:HD22	2:B:1255:LYS:HD2	1.66	0.59
2:F:531:THR:HG21	2:F:575:PHE:CE1	2.38	0.59
2:B:828:LEU:HD22	2:B:836:TYR:CE2	2.37	0.59
2:F:943:TYR:CE2	2:F:949:LEU:HD13	2.38	0.59
2:B:971:GLN:O	2:B:971:GLN:HG2	2.01	0.59
2:B:1308:ASN:HD22	2:B:1327:PHE:H	1.51	0.59
2:F:601:ILE:HD11	2:F:607:LEU:HD21	1.83	0.59
2:B:1258:PHE:HE1	2:B:1262:HIS:CD2	2.21	0.59
2:B:1290:VAL:HG22	2:B:1331:ILE:HD13	1.85	0.59
2:F:1326:TYR:CE2	2:F:1327:PHE:HD2	2.21	0.58
2:B:565:LYS:HA	2:B:569:PHE:HB2	1.84	0.58
2:F:1206:LEU:HD11	2:F:1210:ARG:NH1	2.16	0.58
2:B:563:GLN:O	2:B:567:ASP:HB2	2.03	0.58
2:B:971:GLN:O	2:B:1234:ASN:ND2	2.35	0.58
2:B:671:ARG:HG3	2:B:678:THR:HG22	1.84	0.58
2:B:1146:VAL:HG11	2:B:1194:LEU:HD12	1.86	0.58
2:F:466:THR:O	2:F:482:VAL:HG13	2.04	0.58
2:B:135:ILE:HG21	2:B:160:HIS:CD2	2.39	0.58
5:J:53:G:C4	5:J:62:G:N2	2.72	0.58
2:F:208:ALA:O	2:F:211:ILE:HB	2.04	0.58
2:F:448:ILE:HD12	2:F:455:LEU:HD11	1.86	0.58
2:F:135:ILE:HD13	2:F:156:LEU:HD23	1.85	0.58
2:F:139:ARG:NH1	2:F:418:GLU:OE2	2.37	0.58
2:B:243:ALA:O	2:B:246:LEU:O	2.21	0.58
2:F:844:GLN:HA	2:F:847:LEU:O	2.04	0.58
2:B:119:PHE:HD1	2:B:152:ARG:NH1	2.01	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1041:ASN:O	2:B:1044:ASN:ND2	2.36	0.58
2:F:149:ALA:HB3	2:F:154:ILE:HD12	1.82	0.58
2:F:226:ILE:CG1	2:F:232:GLU:HG2	2.30	0.58
2:B:544:GLN:HA	2:B:547:ALA:HB3	1.86	0.57
2:F:305:ILE:HG13	2:F:306:LEU:HD13	1.86	0.57
2:F:499:ASP:HB2	2:F:663:SER:HB3	1.85	0.57
2:B:245:SER:HA	2:B:297:SER:HB2	1.85	0.57
2:B:687:GLY:O	2:B:690:ASN:ND2	2.38	0.57
2:F:677:LYS:HB3	2:F:682:PHE:CE2	2.39	0.57
1:E:3:A:N6	1:E:4:A:H62	2.01	0.57
2:F:78:ARG:CZ	2:F:165:ARG:NH2	2.67	0.57
2:F:1286:ASN:O	2:F:1290:VAL:HG23	2.04	0.57
2:F:135:ILE:CG2	5:J:46:A:H5'	2.33	0.57
2:F:962:LEU:HB3	2:F:1043:MET:CE	2.35	0.57
2:F:1019:ARG:O	2:F:1021:MET:N	2.31	0.57
2:B:76:LYS:HE3	2:B:80:CYS:SG	2.44	0.57
2:B:229:LEU:O	2:B:231:GLY:N	2.38	0.57
2:B:485:GLY:HA3	2:B:631:MET:SD	2.44	0.57
2:B:954:LYS:HG3	2:B:1009:VAL:HG11	1.86	0.57
1:E:14:G:OP2	2:F:63:ARG:HD3	2.04	0.57
1:E:4:A:O2'	1:E:5:C:O5'	2.21	0.57
2:F:886:LEU:HD22	2:F:891:LEU:HD11	1.87	0.57
2:B:11:ILE:HB	2:B:763:MET:HG2	1.87	0.57
2:B:70:ARG:HH21	5:I:61:C:P	2.27	0.57
2:B:51:LEU:CD1	2:B:1095:VAL:HG23	2.35	0.57
2:B:338:LEU:O	2:B:383:MET:CE	2.53	0.57
2:B:816:LEU:HD12	2:B:891:LEU:HA	1.86	0.57
4:H:11:DT:H2''	4:H:12:DG:C8	2.39	0.57
2:F:212:LEU:HA	2:F:221:ARG:CB	2.35	0.57
2:F:921:LEU:HD21	2:F:1042:ILE:CD1	2.35	0.57
2:F:1179:ILE:O	2:F:1183:GLU:HG3	2.05	0.57
2:B:22:THR:HG22	2:B:23:ASP:H	1.69	0.56
2:B:45:LYS:NZ	2:B:1354:GLY:O	2.34	0.56
2:B:756:PRO:O	2:B:953:VAL:HG22	2.05	0.56
2:F:514:LEU:H	2:F:514:LEU:HD12	1.70	0.56
2:B:40:ARG:NH2	5:I:92:G:OP1	2.37	0.56
2:B:127:ALA:HA	2:B:130:GLU:HB2	1.87	0.56
2:B:1220:LEU:CD1	2:B:1338:SER:O	2.53	0.56
2:F:272:ASP:HA	2:F:275:LEU:HB3	1.86	0.56
2:F:1114:ARG:HD2	2:F:1116:SER:HB2	1.88	0.56
2:B:139:ARG:O	2:B:143:VAL:HG23	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:583:VAL:HG22	2:B:584:GLU:N	2.19	0.56
2:B:1000:LYS:O	2:B:1000:LYS:HD3	2.05	0.56
2:B:1349:HIS:HB3	5:I:68:A:N3	2.20	0.56
2:F:149:ALA:HB1	2:F:154:ILE:HG13	1.86	0.56
2:F:167:HIS:CD2	2:F:169:LEU:HB2	2.40	0.56
2:F:258:LEU:HD22	2:F:260:GLU:H	1.69	0.56
2:F:925:ARG:HB3	2:F:928:THR:HG22	1.87	0.56
5:J:94:U:H2'	5:J:95:G:C8	2.40	0.56
2:B:6:SER:HB2	2:B:21:ILE:HG13	1.86	0.56
2:B:1228:LEU:HD12	2:B:1229:PRO:HD2	1.86	0.56
2:F:94:ASP:CB	2:F:97:PHE:HB2	2.36	0.56
2:F:551:LEU:O	2:F:555:THR:OG1	2.14	0.56
2:F:870:VAL:HG11	2:F:899:ASN:O	2.05	0.56
2:F:1326:TYR:HE2	2:F:1327:PHE:HD2	1.54	0.56
5:J:91:C:O2'	5:J:92:G:P	2.64	0.56
2:B:114:GLU:HG3	2:B:116:HIS:H	1.70	0.56
2:B:489:GLN:HG3	2:B:625:LEU:HD21	1.88	0.56
2:F:135:ILE:HG21	2:F:160:HIS:ND1	2.21	0.56
2:F:332:LEU:HD21	2:F:336:LYS:HE3	1.85	0.56
2:F:681:ASP:HA	2:F:684:LYS:NZ	2.20	0.56
2:B:543:GLU:O	2:B:547:ALA:N	2.38	0.56
2:B:956:ILE:HG12	2:B:1009:VAL:HG22	1.88	0.56
2:F:820:ARG:HG3	2:F:826:GLN:O	2.06	0.56
2:B:369:GLN:NE2	2:B:400:ARG:HD2	2.21	0.56
2:B:755:LYS:NZ	2:B:939:MET:O	2.19	0.56
2:F:829:ASP:OD1	2:F:831:ASN:N	2.39	0.56
2:F:1114:ARG:NH1	4:H:9:DA:OP1	2.38	0.56
1:A:5:C:C2'	1:A:6:G:O5'	2.54	0.56
2:B:321:MET:O	2:B:324:ARG:N	2.39	0.56
2:B:8:GLY:HA3	2:B:991:ALA:HB2	1.88	0.55
2:B:38:THR:HG22	2:B:40:ARG:H	1.71	0.55
2:B:395:ARG:NH2	2:B:397:ASP:OD2	2.38	0.55
2:F:185:PHE:O	2:F:189:VAL:HG23	2.07	0.55
2:F:1266:LEU:HG	2:F:1309:ILE:CD1	2.36	0.55
2:B:620:VAL:O	2:B:624:THR:HG22	2.06	0.55
2:B:875:VAL:HA	2:B:878:LYS:HD2	1.88	0.55
4:D:5:DA:H1'	4:D:6:DG:C8	2.41	0.55
2:F:51:LEU:HD13	2:F:1352:ILE:HG13	1.87	0.55
2:F:162:ILE:HG12	2:F:444:LEU:HD12	1.88	0.55
2:F:516:GLU:O	2:F:519:THR:HG22	2.06	0.55
2:B:1041:ASN:HB2	2:B:1044:ASN:HD21	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:25:U:H5'	2:F:107:VAL:HG12	1.87	0.55
2:F:478:PHE:HE2	2:F:482:VAL:HB	1.71	0.55
2:F:336:LYS:HE2	2:F:351:PHE:CE1	2.41	0.55
2:F:243:ALA:HB3	2:F:250:PRO:HG3	1.88	0.55
2:F:671:ARG:HD3	2:F:671:ARG:N	2.21	0.55
2:B:1207:GLU:HG2	2:B:1210:ARG:HH11	1.72	0.55
2:F:122:ILE:O	2:F:126:VAL:HG23	2.05	0.55
2:F:1224:ASN:HB2	2:F:1280:VAL:HG11	1.87	0.55
2:F:106:LEU:HD22	2:F:1131:TYR:OH	2.06	0.55
2:F:46:ASN:HD22	2:F:1089:MET:CE	2.20	0.55
2:F:151:LEU:HD13	2:F:151:LEU:N	2.21	0.55
2:F:853:ASP:CG	2:F:893:THR:HG21	2.27	0.55
2:B:325:TYR:HD1	5:I:44:U:C2	2.24	0.55
2:B:595:HIS:HB3	2:B:599:LYS:NZ	2.22	0.55
2:F:234:LYS:H	2:F:234:LYS:HD3	1.71	0.55
2:F:309:ASN:OD1	2:F:312:ILE:HG23	2.07	0.55
2:F:1349:HIS:CE1	5:J:69:A:H5'	2.41	0.55
2:B:824:VAL:HG11	2:B:859:ARG:HH12	1.72	0.55
2:B:1120:ILE:HB	2:B:1134:PHE:HB2	1.89	0.55
2:F:427:GLU:HA	2:F:433:LEU:HB2	1.87	0.55
2:F:523:GLU:OE1	2:F:589:ALA:N	2.38	0.55
2:F:672:ASP:HB3	2:F:675:SER:HB2	1.89	0.55
2:F:921:LEU:HD11	2:F:1042:ILE:HD13	1.89	0.55
2:F:1262:HIS:HB3	2:F:1265:TYR:CD2	2.41	0.55
2:B:971:GLN:HA	2:B:973:TYR:CE2	2.42	0.54
2:F:583:VAL:HG22	2:F:584:GLU:H	1.72	0.54
2:B:212:LEU:HD21	2:B:225:LEU:HD12	1.90	0.54
2:B:1318:LEU:HD22	2:B:1319:GLY:H	1.72	0.54
2:F:328:HIS:NE2	2:F:359:TYR:OH	2.24	0.54
3:G:3:DA:N6	4:H:9:DA:H61	2.04	0.54
4:H:11:DT:H2''	4:H:12:DG:H8	1.72	0.54
2:B:117:PRO:HD2	2:B:125:GLU:OE2	2.07	0.54
2:B:930:HIS:O	2:B:934:ILE:HG13	2.06	0.54
2:B:217:SER:O	2:B:221:ARG:HG3	2.08	0.54
2:B:545:LYS:CE	2:B:690:ASN:OD1	2.55	0.54
2:B:212:LEU:O	2:B:221:ARG:HD2	2.08	0.54
2:F:662:LEU:HD22	2:F:666:LEU:HD23	1.89	0.54
2:F:962:LEU:HB3	2:F:1043:MET:HE1	1.89	0.54
2:B:824:VAL:HG22	2:B:863:ASN:ND2	2.23	0.54
2:F:140:LYS:HD3	2:F:319:ALA:HB2	1.90	0.54
2:F:1108:GLU:HB2	3:G:9:DT:H5''	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:265:GLN:HG2	2:B:267:SER:H	1.72	0.54
2:B:980:ASN:HB2	2:B:1225:GLU:CD	2.28	0.54
5:J:96:C:C4	5:J:97:U:C4	2.96	0.54
2:B:219:SER:O	2:B:222:LEU:HB3	2.08	0.54
2:B:302:LEU:HA	2:B:305:ILE:HG12	1.90	0.54
2:F:869:ASN:HD21	2:F:907:GLY:HA3	1.72	0.54
2:F:922:VAL:CG1	2:F:1007:GLU:HG3	2.38	0.54
2:B:339:VAL:HA	2:B:383:MET:HE1	1.90	0.54
2:F:750:VAL:HG21	2:F:1355:LEU:HD12	1.90	0.54
2:B:137:HIS:HE1	2:B:325:TYR:CD2	2.25	0.54
2:B:521:TYR:CE2	2:B:549:VAL:HG21	2.43	0.54
2:B:621:LEU:O	2:B:625:LEU:HB2	2.08	0.54
1:E:27:G:H5'	1:E:28:A:O5'	2.07	0.54
2:F:343:LEU:HD11	2:F:383:MET:HB2	1.90	0.54
2:F:489:GLN:HG3	2:F:625:LEU:HD21	1.89	0.54
2:F:1019:ARG:C	2:F:1021:MET:H	2.11	0.54
2:B:464:TRP:CZ2	2:B:491:PHE:HD1	2.26	0.53
2:F:362:TYR:OH	2:F:401:LYS:HG3	2.08	0.53
1:A:3:A:H2'	1:A:3:A:N3	2.23	0.53
2:B:94:ASP:OD2	2:B:152:ARG:HD3	2.08	0.53
2:B:1207:GLU:HG3	2:B:1208:ASN:N	2.22	0.53
1:E:27:G:H5'	1:E:28:A:C5'	2.39	0.53
2:F:5:TYR:CE2	2:F:751:MET:HG3	2.44	0.53
2:F:212:LEU:CD1	2:F:300:ILE:CD1	2.87	0.53
5:I:37:U:H2'	5:I:38:A:C8	2.43	0.53
5:J:45:U:C2	5:J:46:A:C8	2.97	0.53
2:B:742:LYS:NZ	5:I:67:C:OP1	2.21	0.53
2:F:32:PHE:O	2:F:42:SER:HA	2.08	0.53
2:F:220:ARG:O	2:F:224:ASN:N	2.37	0.53
2:F:841:ILE:HD11	2:F:896:LYS:HG3	1.89	0.53
2:F:1124:LYS:N	5:J:53:G:OP1	2.33	0.53
3:G:3:DA:H61	4:H:9:DA:N6	2.07	0.53
2:B:1147:ALA:HB1	2:B:1188:LYS:O	2.08	0.53
2:B:1207:GLU:HG3	2:B:1208:ASN:H	1.74	0.53
1:E:27:G:H1'	2:F:129:HIS:CD2	2.44	0.53
2:F:1295:ASN:HA	2:F:1298:ARG:NH1	2.24	0.53
1:A:2:U:N3	1:A:4:A:H3'	2.19	0.53
2:B:1232:TYR:HA	2:B:1235:PHE:HB3	1.89	0.53
2:F:468:LYS:HE3	2:F:483:ASP:HB3	1.91	0.53
2:F:976:ARG:HA	2:F:982:HIS:CD2	2.43	0.53
2:B:642:LEU:HB2	2:B:643:PHE:CD2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:972:PHE:HE1	2:B:1084:ARG:HB2	1.73	0.53
2:F:48:ILE:HG12	2:F:984:ALA:HB1	1.90	0.53
2:F:137:HIS:HA	2:F:322:ILE:CD1	2.39	0.53
2:F:271:TYR:O	2:F:275:LEU:N	2.34	0.53
2:B:118:ILE:HD13	2:B:128:TYR:HD2	1.71	0.53
2:B:672:ASP:HA	2:B:703:THR:HG22	1.91	0.53
2:B:849:ASP:OD2	2:B:895:ARG:NH1	2.40	0.53
3:C:25:DT:C2	3:C:26:DT:C5	2.96	0.53
2:F:649:LYS:HB3	2:F:653:ARG:HH21	1.74	0.53
5:I:69:A:H2'	5:I:70:C:C6	2.44	0.53
2:B:273:ASP:N	2:B:273:ASP:OD1	2.36	0.53
2:F:226:ILE:HD11	2:F:232:GLU:CD	2.30	0.53
2:F:312:ILE:HG13	2:F:313:THR:N	2.24	0.53
2:F:1048:THR:HA	2:F:1076:LYS:HD3	1.91	0.53
2:B:672:ASP:HA	2:B:703:THR:CG2	2.39	0.53
2:F:164:PHE:O	2:F:415:HIS:NE2	2.41	0.53
2:F:860:SER:OG	2:F:863:ASN:OD1	2.27	0.53
2:B:380:LEU:O	2:B:386:THR:HG21	2.07	0.52
2:B:1211:LYS:C	2:B:1223:GLY:HA3	2.28	0.52
2:F:66:ARG:HA	2:F:69:ARG:NH1	2.24	0.52
2:B:1047:LYS:HB2	2:B:1050:ILE:HG22	1.90	0.52
2:B:1106:SER:HB2	2:B:1135:ASP:O	2.09	0.52
2:B:1241:HIS:ND1	2:B:1244:LYS:HA	2.25	0.52
2:F:139:ARG:O	2:F:143:VAL:HG23	2.09	0.52
2:F:977:GLU:HG3	2:F:1310:ILE:HG21	1.90	0.52
2:F:1351:SER:OG	2:F:1356:TYR:HB2	2.09	0.52
3:G:3:DA:H61	4:H:9:DA:H61	1.57	0.52
2:B:233:LYS:HG2	2:B:235:ASN:N	2.25	0.52
2:B:1002:PRO:HA	2:B:1005:GLU:HG3	1.90	0.52
2:F:167:HIS:HD2	2:F:169:LEU:CB	2.23	0.52
2:F:1050:ILE:HG13	2:F:1050:ILE:O	2.09	0.52
1:A:2:U:O2	1:A:3:A:O2'	2.27	0.52
1:A:10:U:H2'	1:A:11:U:H6	1.75	0.52
2:F:38:THR:HG22	2:F:40:ARG:H	1.74	0.52
2:F:140:LYS:HB3	2:F:322:ILE:CD1	2.40	0.52
2:F:922:VAL:HG11	2:F:1007:GLU:HG3	1.90	0.52
2:B:391:VAL:O	2:B:395:ARG:HG3	2.09	0.52
2:B:427:GLU:OE1	2:B:437:ARG:NH1	2.42	0.52
2:F:151:LEU:HD22	2:F:152:ARG:CA	2.40	0.52
4:H:6:DG:H2''	4:H:7:DG:H5''	1.91	0.52
2:B:1231:LYS:HD2	2:B:1265:TYR:OH	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:844:GLN:HG3	2:F:848:LYS:HD2	1.91	0.52
2:F:867:SER:HB2	2:F:1053:ALA:C	2.30	0.52
2:F:151:LEU:N	2:F:151:LEU:CD1	2.73	0.52
2:F:531:THR:HG1	2:F:575:PHE:HD1	1.57	0.52
2:F:776:ASN:O	2:F:780:ARG:HG2	2.08	0.52
2:F:980:ASN:HB2	2:F:1225:GLU:OE2	2.10	0.52
5:I:39:G:H5'	5:I:40:C:OP2	2.10	0.52
2:B:737:ILE:O	2:B:740:THR:HG22	2.09	0.51
2:B:1074:TRP:HZ2	2:B:1080:PHE:CD2	2.28	0.51
2:B:1243:GLU:HG3	2:B:1246:LYS:NZ	2.26	0.51
2:F:262:ALA:HB1	2:F:278:LEU:HG	1.91	0.51
2:F:867:SER:HB2	2:F:1054:ASN:CA	2.40	0.51
2:F:1000:LYS:HG3	2:F:1001:TYR:CD2	2.46	0.51
1:A:5:C:O2'	1:A:6:G:C5'	2.58	0.51
2:B:201:ILE:HG22	2:B:202:ASN:N	2.22	0.51
2:B:849:ASP:OD1	2:B:851:SER:OG	2.25	0.51
2:F:40:ARG:HE	2:F:43:ILE:HD11	1.75	0.51
2:F:542:GLY:HA3	2:F:685:SER:HA	1.92	0.51
2:F:878:LYS:HB3	2:F:879:MET:SD	2.51	0.51
2:F:1167:THR:HG23	2:F:1170:GLU:H	1.74	0.51
5:J:45:U:H2'	5:J:46:A:C8	2.45	0.51
2:F:551:LEU:HD23	2:F:568:TYR:HD1	1.75	0.51
1:A:29:G:N3	5:I:41:A:C2	2.78	0.51
2:F:134:THR:O	2:F:137:HIS:HB2	2.11	0.51
2:F:650:GLN:O	2:F:653:ARG:HG2	2.11	0.51
2:B:686:ASP:HB3	2:B:690:ASN:HA	1.92	0.51
2:B:921:LEU:HB3	2:B:1008:PHE:CZ	2.45	0.51
2:F:349:GLU:O	2:F:353:ASP:HB3	2.11	0.51
3:G:22:DT:H2''	3:G:23:DC:O5'	2.09	0.51
2:B:492:ILE:O	2:B:496:THR:HG23	2.10	0.51
2:B:1060:ARG:NH1	2:B:1064:GLU:OE2	2.42	0.51
2:B:1074:TRP:HZ2	2:B:1080:PHE:CE2	2.28	0.51
2:F:142:LEU:CD1	2:F:154:ILE:CD1	2.85	0.51
2:B:338:LEU:O	2:B:383:MET:HE1	2.10	0.51
2:B:353:ASP:CG	2:B:356:LYS:HG2	2.30	0.51
2:F:44:LYS:NZ	5:J:92:G:O6	2.21	0.51
2:F:410:ILE:HG21	2:F:415:HIS:NE2	2.26	0.51
2:F:755:LYS:HD3	2:F:939:MET:HE3	1.93	0.51
1:A:25:U:H2'	1:A:26:A:C8	2.46	0.51
2:B:325:TYR:CD1	5:I:44:U:C2	2.99	0.51
2:B:677:LYS:HD3	2:B:682:PHE:CZ	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1232:TYR:O	2:B:1236:LEU:N	2.29	0.51
2:B:1308:ASN:HD22	2:B:1327:PHE:N	2.07	0.51
2:F:167:HIS:N	2:F:410:ILE:O	2.41	0.51
2:F:1051:THR:HG22	2:F:1053:ALA:H	1.76	0.51
2:B:66:ARG:HD2	2:B:462:PHE:CE2	2.46	0.51
2:F:465:MET:SD	2:F:482:VAL:HG21	2.51	0.51
5:J:83:C:H2'	5:J:84:A:C8	2.46	0.51
2:F:137:HIS:HA	2:F:322:ILE:CG1	2.41	0.51
2:F:226:ILE:CG2	2:F:231:GLY:H	2.24	0.51
2:F:971:GLN:HG2	2:F:973:TYR:CE2	2.47	0.51
2:B:509:PRO:HB3	2:B:624:THR:HG21	1.93	0.50
2:B:977:GLU:N	2:B:977:GLU:OE1	2.44	0.50
1:A:1:U:H5	2:B:661:ARG:HH12	1.59	0.50
2:B:823:TYR:CD2	2:B:858:THR:HG21	2.45	0.50
2:B:1081:ALA:O	2:B:1085:LYS:HG3	2.11	0.50
2:F:148:LYS:HB2	2:F:429:PHE:CD2	2.46	0.50
2:F:1205:GLU:CD	2:F:1359:ARG:HH22	2.13	0.50
2:B:281:GLN:OE1	2:B:281:GLN:N	2.38	0.50
2:B:1356:TYR:HB3	5:I:81:G:N1	2.27	0.50
2:F:128:TYR:CE1	2:F:153:LEU:HD12	2.45	0.50
2:F:601:ILE:HD11	2:F:607:LEU:HD11	1.93	0.50
2:F:1045:PHE:CA	2:F:1060:ARG:NH1	2.73	0.50
2:F:1046:PHE:O	2:F:1076:LYS:NZ	2.45	0.50
2:B:448:ILE:HD13	2:B:455:LEU:HD13	1.93	0.50
2:B:1105:PHE:CG	2:B:1169:MET:HG3	2.46	0.50
3:C:24:DG:H5''	3:C:25:DT:OP2	2.11	0.50
2:F:43:ILE:HG22	2:F:45:LYS:HG3	1.91	0.50
2:B:69:ARG:HD3	5:I:62:G:C8	2.47	0.50
2:B:1047:LYS:CB	2:B:1050:ILE:HG22	2.42	0.50
1:E:23:U:H5''	2:F:1112:PRO:HG3	1.93	0.50
2:F:762:GLU:OE1	2:F:990:ASN:ND2	2.39	0.50
5:J:95:G:C6	5:J:96:C:N4	2.79	0.50
2:B:670:ILE:HG22	2:B:704:PHE:CE1	2.45	0.50
2:F:1333:ARG:CZ	2:F:1335:ARG:HD2	2.41	0.50
2:B:195:LEU:HB3	2:B:196:PHE:HD1	1.77	0.50
2:B:813:LEU:O	2:B:817:GLN:HG3	2.11	0.50
2:B:1207:GLU:CG	2:B:1208:ASN:H	2.25	0.50
2:F:8:GLY:O	2:F:987:ALA:HB1	2.11	0.50
2:F:74:ARG:O	2:F:78:ARG:HG3	2.12	0.50
2:F:160:HIS:CD2	2:F:160:HIS:C	2.85	0.50
2:B:595:HIS:HB3	2:B:599:LYS:HZ2	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:606:PHE:O	2:B:612:ASN:ND2	2.44	0.50
2:B:913:LYS:O	2:B:916:PHE:HB2	2.12	0.50
2:B:1226:LEU:HB2	2:B:1276:PHE:CE2	2.47	0.50
2:F:155:TYR:C	2:F:155:TYR:CD1	2.84	0.50
2:F:237:LEU:HD12	2:F:238:PHE:N	2.27	0.50
2:B:1220:LEU:HD12	2:B:1338:SER:O	2.12	0.50
2:F:27:VAL:HG12	2:F:1086:VAL:HG22	1.92	0.50
2:F:616:LEU:HA	2:F:619:ILE:HG22	1.93	0.50
2:B:74:ARG:NH2	5:I:60:C:OP1	2.44	0.49
2:B:514:LEU:HD11	2:B:667:ILE:HG21	1.94	0.49
2:B:1096:LYS:HG2	2:B:1201:TYR:CD2	2.47	0.49
2:F:427:GLU:OE1	2:F:434:LYS:HA	2.12	0.49
2:F:981:TYR:O	2:F:983:HIS:N	2.45	0.49
2:B:1235:PHE:O	2:B:1239:ALA:N	2.33	0.49
2:F:410:ILE:HD13	2:F:415:HIS:NE2	2.27	0.49
2:F:695:GLN:O	2:F:699:ASP:HB2	2.12	0.49
2:F:985:HIS:CD2	2:F:1087:LEU:HD22	2.47	0.49
2:F:1147:ALA:HB1	2:F:1188:LYS:O	2.11	0.49
2:F:1206:LEU:HD12	2:F:1210:ARG:HH12	1.76	0.49
2:F:1228:LEU:HD12	2:F:1229:PRO:HD2	1.94	0.49
2:B:961:LYS:HA	2:B:964:SER:HB3	1.94	0.49
2:F:628:ASP:O	2:F:632:ILE:HG13	2.12	0.49
2:F:918:LYS:CE	2:F:1018:VAL:HG11	2.43	0.49
2:B:784:ILE:HG21	2:B:815:TYR:HD2	1.77	0.49
2:F:139:ARG:HD3	2:F:157:ALA:CA	2.43	0.49
2:F:334:LEU:O	2:F:338:LEU:HG	2.12	0.49
2:F:566:GLU:O	2:F:570:LYS:HB3	2.11	0.49
2:F:583:VAL:HG22	2:F:584:GLU:N	2.26	0.49
2:B:809:GLU:OE1	2:B:855:LYS:HE2	2.12	0.49
2:B:850:ASP:HB3	2:B:855:LYS:NZ	2.27	0.49
2:F:433:LEU:O	2:F:437:ARG:HB2	2.12	0.49
2:F:795:ILE:HA	2:F:798:GLU:HB2	1.94	0.49
2:F:1114:ARG:HG2	2:F:1115:ASN:N	2.28	0.49
5:J:88:A:C6	5:J:91:C:N4	2.76	0.49
2:F:253:LYS:CG	2:F:261:ASP:HA	2.43	0.49
2:F:268:LYS:O	2:F:271:TYR:HD2	1.95	0.49
2:F:794:GLN:H	2:F:794:GLN:CD	2.15	0.49
2:F:850:ASP:O	2:F:855:LYS:HD2	2.11	0.49
2:F:1300:LYS:HG3	2:F:1327:PHE:CZ	2.48	0.49
2:B:1111:LEU:HD12	2:B:1135:ASP:HB2	1.95	0.49
2:B:1252:ASN:ND2	2:B:1255:LYS:HD2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:158:LEU:O	2:F:161:MET:N	2.46	0.49
2:F:324:ARG:O	2:F:327:GLU:HB2	2.12	0.49
2:F:981:TYR:O	2:F:984:ALA:N	2.45	0.49
2:F:1206:LEU:CD1	2:F:1210:ARG:HH12	2.25	0.49
2:B:252:PHE:CE1	2:B:264:LEU:HD13	2.47	0.49
2:F:784:ILE:HG21	2:F:815:TYR:HD1	1.78	0.49
2:F:791:LEU:CD2	2:F:818:ASN:OD1	2.59	0.49
2:B:149:ALA:H	2:B:426:GLN:HE22	1.59	0.49
2:B:455:LEU:HD12	2:B:455:LEU:N	2.28	0.49
2:B:512:SER:O	2:B:516:GLU:HG2	2.13	0.49
2:B:1204:PHE:CG	2:B:1342:VAL:HG13	2.48	0.49
2:B:1357:GLU:O	5:I:81:G:N2	2.46	0.49
2:F:758:ASN:HD22	2:F:995:THR:HG22	1.78	0.49
5:J:79:G:C2'	5:J:80:U:H5'	2.43	0.49
2:B:478:PHE:HE2	2:B:484:LYS:HE2	1.78	0.49
1:E:3:A:N6	1:E:4:A:N6	2.60	0.49
2:F:411:PRO:HB2	2:F:413:GLN:OE1	2.13	0.49
2:F:632:ILE:O	2:F:636:LEU:HD13	2.13	0.49
2:F:843:PRO:HG3	2:F:864:ARG:HH22	1.77	0.49
2:F:1002:PRO:HD2	2:F:1036:TYR:OH	2.13	0.49
2:F:1314:THR:HG21	2:F:1324:PHE:HB3	1.94	0.49
5:J:94:U:H2'	5:J:95:G:H8	1.77	0.49
2:B:83:GLN:HG2	2:B:98:PHE:CE1	2.48	0.48
2:B:850:ASP:O	2:B:855:LYS:HD2	2.13	0.48
2:B:1062:LEU:O	2:B:1075:ASP:HA	2.13	0.48
3:C:25:DT:C2	3:C:26:DT:C7	2.94	0.48
2:F:923:GLU:CG	2:F:928:THR:HG21	2.40	0.48
2:B:241:LEU:HD11	2:B:289:LEU:HD11	1.96	0.48
2:B:531:THR:HG21	2:B:575:PHE:HE2	1.78	0.48
2:F:140:LYS:HB3	2:F:322:ILE:HD12	1.96	0.48
2:B:736:GLY:O	2:B:740:THR:HB	2.14	0.48
2:F:346:LYS:O	2:F:350:ILE:N	2.42	0.48
1:A:3:A:H2'	1:A:4:A:H8	1.78	0.48
2:B:83:GLN:HG2	2:B:98:PHE:CZ	2.49	0.48
2:B:525:THR:CG2	2:B:690:ASN:HB3	2.43	0.48
2:B:540:LEU:HD12	2:B:540:LEU:HA	1.52	0.48
2:F:844:GLN:HG3	2:F:848:LYS:HA	1.95	0.48
2:F:1162:GLU:OE2	2:F:1187:TYR:OH	2.16	0.48
2:B:157:ALA:O	2:B:161:MET:HG3	2.14	0.48
2:F:138:LEU:HD22	2:F:153:LEU:CD2	2.34	0.48
2:F:142:LEU:HD12	2:F:154:ILE:HA	1.93	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:563:GLN:O	2:F:567:ASP:HB2	2.14	0.48
5:J:95:G:H2'	5:J:96:C:C6	2.49	0.48
2:B:472:THR:HG23	5:I:59:U:OP2	2.14	0.48
2:B:697:ILE:HG22	2:B:698:HIS:ND1	2.29	0.48
2:B:985:HIS:O	2:B:989:LEU:HG	2.13	0.48
2:F:208:ALA:CA	2:F:211:ILE:CD1	2.53	0.48
2:F:373:TYR:HE1	2:F:398:LEU:HB3	1.77	0.48
2:F:780:ARG:HB2	2:F:806:LEU:HD12	1.95	0.48
5:J:49:A:O5'	5:J:49:A:H8	1.96	0.48
2:B:525:THR:HG23	2:B:690:ASN:HB3	1.95	0.48
2:B:531:THR:HG1	2:B:575:PHE:HD2	1.59	0.48
2:F:361:GLY:HA2	2:F:365:GLY:HA3	1.96	0.48
2:F:446:PHE:CZ	2:F:478:PHE:CD1	2.92	0.48
2:F:467:ARG:HD3	2:F:470:GLU:HA	1.95	0.48
2:F:1038:PHE:CD2	2:F:1039:TYR:HE1	2.31	0.48
1:A:2:U:O2	1:A:4:A:C8	2.67	0.48
2:F:44:LYS:HD3	5:J:92:G:N7	2.29	0.48
2:F:151:LEU:CD1	2:F:151:LEU:H	2.27	0.48
2:F:404:THR:HG22	2:F:405:PHE:CD1	2.48	0.48
2:F:1119:LEU:HD23	2:F:1128:PRO:HB2	1.94	0.48
2:F:1205:GLU:CB	2:F:1348:ILE:HD11	2.44	0.48
2:F:1272:GLN:CD	5:J:89:G:H1	2.18	0.48
2:B:63:ARG:O	2:B:66:ARG:N	2.47	0.48
2:B:181:VAL:HG21	2:B:209:LYS:HA	1.96	0.48
2:B:597:LEU:O	2:B:601:ILE:HG12	2.14	0.48
2:B:980:ASN:HB2	2:B:1225:GLU:OE1	2.14	0.48
2:F:143:VAL:HG21	2:F:315:ALA:HB2	1.96	0.48
2:F:1115:ASN:OD1	2:F:1129:LYS:HE3	2.14	0.48
2:F:1200:LYS:HG2	2:F:1201:TYR:CD1	2.49	0.48
2:B:530:VAL:CG2	2:B:537:PRO:HB3	2.42	0.47
1:E:19:A:O3'	2:F:407:ASN:HB2	2.14	0.47
2:F:137:HIS:HA	2:F:322:ILE:HG12	1.95	0.47
2:F:373:TYR:CE1	2:F:398:LEU:HB3	2.49	0.47
2:F:1266:LEU:HG	2:F:1309:ILE:HD12	1.96	0.47
2:B:66:ARG:HD2	2:B:462:PHE:HE2	1.78	0.47
2:B:269:ASP:O	2:B:271:TYR:N	2.41	0.47
2:B:531:THR:HG23	2:B:534:MET:HG3	1.96	0.47
2:B:644:ASP:OD2	2:B:646:LYS:HB2	2.14	0.47
2:B:1179:ILE:HD11	2:B:1192:LYS:HD2	1.94	0.47
2:B:1208:ASN:OD1	2:B:1279:ARG:HG3	2.14	0.47
2:B:1333:ARG:CZ	2:B:1335:ARG:HD2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:6:G:C2	3:G:24:DG:N2	2.82	0.47
2:F:282:ILE:HG22	2:F:286:TYR:CD1	2.49	0.47
2:F:795:ILE:HG13	2:F:795:ILE:O	2.15	0.47
2:B:1006:SER:HG	2:B:1014:LYS:N	2.12	0.47
3:G:6:DC:H2''	3:G:7:DC:O5'	2.14	0.47
2:B:1122:ARG:O	5:I:52:A:H5''	2.14	0.47
2:B:1251:ASP:O	2:B:1255:LYS:HG3	2.13	0.47
2:F:853:ASP:OD1	2:F:893:THR:HG21	2.14	0.47
1:A:25:U:H2'	1:A:26:A:H8	1.78	0.47
2:B:136:TYR:CG	2:B:321:MET:HG3	2.49	0.47
2:B:217:SER:HB2	2:B:220:ARG:HG2	1.96	0.47
2:B:985:HIS:ND1	2:B:1087:LEU:HD13	2.29	0.47
2:B:1235:PHE:CE1	2:B:1239:ALA:HB2	2.50	0.47
1:E:31:U:N3	1:E:32:A:N7	2.62	0.47
2:F:167:HIS:ND1	2:F:410:ILE:O	2.39	0.47
2:F:455:LEU:O	5:J:60:C:H5'	2.15	0.47
2:F:671:ARG:HD3	2:F:671:ARG:H	1.78	0.47
2:F:1326:TYR:CE2	2:F:1327:PHE:CD2	3.03	0.47
2:B:48:ILE:HG12	2:B:984:ALA:HB1	1.97	0.47
2:B:121:ASN:H	2:B:121:ASN:ND2	2.12	0.47
2:B:570:LYS:NZ	2:B:571:LYS:HG2	2.30	0.47
2:B:620:VAL:HG13	2:B:656:TYR:HD2	1.80	0.47
2:B:1000:LYS:HB3	2:B:1001:TYR:CE2	2.50	0.47
2:B:1110:ILE:HD13	2:B:1134:PHE:HE1	1.79	0.47
2:B:1286:ASN:ND2	2:B:1332:ASP:O	2.47	0.47
1:E:3:A:C5	1:E:4:A:N7	2.83	0.47
1:E:15:G:P	2:F:66:ARG:HH22	2.37	0.47
2:F:180:ASP:CB	2:F:183:LYS:HB2	2.28	0.47
2:F:258:LEU:HD23	2:F:259:ALA:H	1.80	0.47
2:B:49:GLY:HA2	2:B:1092:VAL:CG1	2.45	0.47
2:B:114:GLU:HG2	2:B:120:GLY:CA	2.45	0.47
2:B:939:MET:HG3	2:B:953:VAL:HG11	1.97	0.47
1:E:21:G:H2'	1:E:22:U:O4'	2.15	0.47
2:B:721:HIS:O	2:B:725:ALA:N	2.39	0.47
2:B:1114:ARG:O	2:B:1129:LYS:HA	2.15	0.47
2:B:1177:ASN:ND2	2:B:1180:ASP:OD2	2.47	0.47
2:F:424:ARG:HH12	2:F:437:ARG:NE	2.13	0.47
2:F:103:GLU:OE2	2:F:111:LYS:HG2	2.14	0.47
2:F:237:LEU:HD12	2:F:238:PHE:H	1.80	0.47
2:F:1205:GLU:HB2	2:F:1348:ILE:HD11	1.96	0.47
5:J:73:G:H5'	5:J:74:A:OP2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:343:LEU:HD21	2:B:346:LYS:HG3	1.98	0.46
2:B:478:PHE:CE1	2:B:482:VAL:HG21	2.51	0.46
2:B:1089:MET:HA	2:B:1090:PRO:HD3	1.64	0.46
2:B:1163:LEU:HG	2:B:1343:LEU:HD21	1.97	0.46
2:F:832:ARG:HD2	2:F:835:ASP:OD2	2.15	0.46
2:B:74:ARG:O	2:B:78:ARG:HG3	2.15	0.46
2:B:143:VAL:HG13	2:B:421:ALA:HB1	1.97	0.46
2:B:970:PHE:HZ	2:B:1047:LYS:HG2	1.80	0.46
5:I:37:U:H2'	5:I:38:A:H8	1.79	0.46
2:B:133:PRO:HD2	2:B:137:HIS:CG	2.50	0.46
2:B:453:GLY:O	2:B:455:LEU:HD12	2.15	0.46
3:C:7:DC:H2'	3:C:8:DT:C6	2.50	0.46
2:F:553:PHE:HZ	2:F:587:PHE:CD2	2.34	0.46
1:A:11:U:C2	1:A:12:A:C8	3.03	0.46
1:E:16:A:H5''	2:F:74:ARG:HH12	1.79	0.46
2:F:521:TYR:CE2	2:F:549:VAL:HG21	2.49	0.46
2:F:1232:TYR:CE1	2:F:1265:TYR:CD1	3.04	0.46
2:B:1294:TYR:HE1	2:B:1305:GLN:HE21	1.62	0.46
1:E:27:G:H5'	1:E:28:A:H5''	1.97	0.46
2:F:142:LEU:CD1	2:F:154:ILE:CA	2.72	0.46
2:F:142:LEU:CD2	2:F:149:ALA:HB2	2.46	0.46
2:F:258:LEU:HB3	2:F:260:GLU:O	2.16	0.46
2:F:404:THR:HG22	2:F:405:PHE:H	1.80	0.46
2:F:842:VAL:CG1	2:F:854:ASN:OD1	2.61	0.46
2:F:1038:PHE:CD2	2:F:1039:TYR:CE1	3.04	0.46
2:F:1045:PHE:O	2:F:1076:LYS:NZ	2.49	0.46
3:G:25:DT:C2'	3:G:26:DT:OP2	2.55	0.46
2:B:221:ARG:NH1	2:B:246:LEU:HD22	2.30	0.46
1:E:3:A:H8	1:E:3:A:O5'	1.99	0.46
2:F:22:THR:HG23	2:F:26:LYS:O	2.15	0.46
2:F:468:LYS:HD2	2:F:483:ASP:N	2.29	0.46
2:F:1232:TYR:HE1	2:F:1265:TYR:CD1	2.33	0.46
2:B:718:ASP:H	2:B:723:HIS:HE1	1.64	0.46
2:F:151:LEU:CD1	2:F:152:ARG:N	2.73	0.46
2:F:600:ILE:HD13	2:F:651:LEU:HA	1.97	0.46
5:I:42:A:O3'	5:I:43:G:C8	2.69	0.46
1:A:3:A:H2'	1:A:4:A:C8	2.51	0.46
1:A:11:U:N3	1:A:12:A:N7	2.63	0.46
2:B:448:ILE:HD13	2:B:455:LEU:CD1	2.46	0.46
2:B:780:ARG:HB2	2:B:806:LEU:HD12	1.97	0.46
2:B:963:VAL:HG21	2:B:990:ASN:OD1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1:DC:H2'	3:C:2:DA:C8	2.51	0.46
2:F:828:LEU:HD22	2:F:836:TYR:CE2	2.51	0.46
5:J:79:G:O2'	5:J:80:U:H5'	2.15	0.46
2:B:128:TYR:CE1	2:B:132:TYR:HB2	2.50	0.46
2:B:139:ARG:HH12	2:B:415:HIS:CD2	2.34	0.46
2:B:143:VAL:HG13	2:B:421:ALA:CB	2.46	0.46
2:B:343:LEU:HD13	2:B:383:MET:SD	2.56	0.46
2:B:818:ASN:HB3	2:B:882:TYR:OH	2.16	0.46
2:F:241:LEU:HD23	2:F:241:LEU:H	1.81	0.46
2:F:971:GLN:OE1	2:F:1255:LYS:HE3	2.16	0.46
2:F:978:ILE:HD13	2:F:1228:LEU:HD23	1.98	0.46
1:A:20:A:P	2:B:403:ARG:NH1	2.89	0.46
2:B:317:LEU:O	2:B:320:SER:HB3	2.16	0.46
2:B:692:ASN:O	2:B:696:LEU:HD23	2.16	0.46
2:B:978:ILE:HD12	2:B:1233:VAL:HG22	1.98	0.46
2:B:1115:ASN:HA	2:B:1129:LYS:HG2	1.98	0.46
2:F:1151:LYS:HD2	2:F:1158:LYS:HB3	1.97	0.46
2:B:548:ILE:HG23	2:B:552:LEU:CD1	2.46	0.45
2:B:1357:GLU:OE1	2:B:1359:ARG:NH1	2.49	0.45
2:F:238:PHE:O	2:F:242:ILE:HG12	2.15	0.45
2:F:1245:LEU:HD23	2:F:1245:LEU:HA	1.63	0.45
2:B:513:LEU:HD11	2:B:597:LEU:HD12	1.97	0.45
2:B:881:ASN:OD1	2:B:885:GLN:NE2	2.48	0.45
2:B:1146:VAL:HG13	2:B:1191:LYS:HB2	1.97	0.45
2:F:138:LEU:HD13	2:F:153:LEU:HD22	1.82	0.45
2:F:166:GLY:HA3	2:F:410:ILE:CG2	2.41	0.45
2:F:1096:LYS:HG2	2:F:1201:TYR:CD2	2.51	0.45
2:B:340:ARG:HA	2:B:344:PRO:HB3	1.97	0.45
2:B:640:ALA:HA	2:B:648:MET:CE	2.47	0.45
2:B:976:ARG:HB2	2:B:977:GLU:OE1	2.17	0.45
2:F:554:LYS:HB3	2:F:594:TYR:CE2	2.51	0.45
2:F:615:ILE:HG23	2:F:639:TYR:CD1	2.51	0.45
2:B:204:SER:HB2	2:B:205:GLY:H	1.47	0.45
2:B:392:LYS:CG	2:B:395:ARG:NH1	2.54	0.45
2:F:177:ASP:OD1	2:F:177:ASP:N	2.50	0.45
2:F:328:HIS:ND1	5:J:44:U:C2	2.85	0.45
5:J:82:G:N7	5:J:97:U:O2	2.50	0.45
2:B:853:ASP:CG	2:B:893:THR:HG21	2.36	0.45
2:B:1144:LEU:O	2:B:1195:ILE:HA	2.17	0.45
2:B:1204:PHE:HE2	2:B:1214:LEU:HB2	1.80	0.45
3:C:25:DT:N1	3:C:26:DT:H72	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:90:MET:CE	2:F:151:LEU:HD23	2.33	0.45
2:F:151:LEU:CD2	2:F:152:ARG:N	2.75	0.45
2:F:506:LYS:H	2:F:506:LYS:HG2	1.52	0.45
2:F:795:ILE:HA	2:F:798:GLU:OE1	2.15	0.45
2:F:855:LYS:NZ	2:F:1246:LYS:O	2.32	0.45
5:J:87:G:N3	5:J:87:G:H2'	2.31	0.45
2:B:1308:ASN:ND2	2:B:1327:PHE:H	2.15	0.45
3:C:25:DT:N3	3:C:26:DT:C5	2.85	0.45
3:C:25:DT:N3	3:C:26:DT:C7	2.80	0.45
2:F:139:ARG:HD3	2:F:157:ALA:HB1	1.97	0.45
2:F:1079:ASP:HA	2:F:1082:THR:HG23	1.98	0.45
5:J:91:C:O2'	5:J:92:G:O5'	2.34	0.45
5:J:92:G:H2'	5:J:93:G:C8	2.51	0.45
2:B:269:ASP:OD1	2:B:270:THR:N	2.50	0.45
2:B:760:VAL:HG11	2:B:958:LEU:HD12	1.99	0.45
2:B:1243:GLU:HG3	2:B:1246:LYS:HZ1	1.80	0.45
2:F:247:GLY:O	2:F:267:SER:HB3	2.16	0.45
2:F:551:LEU:HD12	2:F:551:LEU:HA	1.80	0.45
2:F:565:LYS:HD2	2:F:580:ILE:HG12	1.99	0.45
2:F:622:THR:HG21	2:F:635:ARG:CB	2.46	0.45
2:F:844:GLN:CG	2:F:848:LYS:HD2	2.47	0.45
2:B:36:GLY:HA3	2:B:1359:ARG:O	2.17	0.45
2:B:226:ILE:HA	2:B:229:LEU:HG	1.99	0.45
2:B:317:LEU:HD21	2:B:410:ILE:HD13	1.99	0.45
2:B:525:THR:HA	2:B:545:LYS:CE	2.47	0.45
2:F:137:HIS:HE1	2:F:325:TYR:CG	2.34	0.45
2:F:329:HIS:HB2	5:J:44:U:O4	2.17	0.45
2:F:913:LYS:O	2:F:916:PHE:HB2	2.17	0.45
2:F:1349:HIS:ND1	5:J:69:A:H5'	2.31	0.45
5:J:45:U:H2'	5:J:46:A:O4'	2.17	0.45
2:B:6:SER:HB2	2:B:21:ILE:CG1	2.47	0.45
2:B:94:ASP:HB3	2:B:97:PHE:HB2	1.99	0.45
2:B:116:HIS:NE2	2:B:122:ILE:HG23	2.32	0.45
2:B:165:ARG:O	2:B:412:HIS:HA	2.17	0.45
2:B:414:ILE:HG21	2:B:414:ILE:HD13	1.74	0.45
2:B:531:THR:HG21	2:B:575:PHE:CE2	2.52	0.45
2:F:328:HIS:CG	5:J:44:U:C2	3.05	0.45
2:F:909:SER:N	2:F:912:ASP:HB2	2.32	0.45
5:I:83:C:H2'	5:I:84:A:C8	2.49	0.45
2:B:467:ARG:NH2	2:B:471:GLU:O	2.50	0.45
2:B:1111:LEU:HD23	2:B:1111:LEU:HA	1.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:546:LYS:HE3	2:F:546:LYS:HB3	1.79	0.45
1:A:3:A:C2'	1:A:4:A:H8	2.30	0.44
2:B:719:SER:OG	2:B:720:LEU:N	2.49	0.44
2:B:864:ARG:HB2	2:B:871:PRO:HA	1.97	0.44
2:B:1113:LYS:HB2	2:B:1129:LYS:O	2.17	0.44
2:F:681:ASP:HA	2:F:684:LYS:HZ3	1.81	0.44
2:F:788:ILE:HA	2:F:791:LEU:HB2	1.98	0.44
2:F:879:MET:HB3	2:F:882:TYR:HB3	1.99	0.44
2:F:954:LYS:NZ	2:F:998:ILE:HD13	2.32	0.44
2:F:1284:ASP:OD1	2:F:1284:ASP:N	2.43	0.44
2:B:115:ARG:HG3	2:B:116:HIS:CE1	2.53	0.44
2:B:118:ILE:HD12	2:B:125:GLU:OE2	2.17	0.44
2:B:662:LEU:HD23	2:B:666:LEU:HD22	1.98	0.44
2:B:958:LEU:HD22	2:B:962:LEU:HD12	1.99	0.44
2:B:1272:GLN:NE2	5:I:89:G:O6	2.31	0.44
1:E:3:A:O5'	1:E:3:A:C8	2.70	0.44
2:F:151:LEU:CD2	2:F:151:LEU:C	2.86	0.44
2:F:208:ALA:N	2:F:211:ILE:CD1	2.78	0.44
2:F:410:ILE:HD13	2:F:415:HIS:HE2	1.82	0.44
2:F:509:PRO:HG2	2:F:621:LEU:HA	1.98	0.44
2:F:615:ILE:HG23	2:F:639:TYR:CE1	2.52	0.44
2:F:1290:VAL:HG22	2:F:1331:ILE:HD13	2.00	0.44
2:B:264:LEU:HD23	2:B:271:TYR:CE1	2.52	0.44
2:B:390:LEU:HD23	2:B:390:LEU:HA	1.63	0.44
2:F:164:PHE:O	2:F:164:PHE:CD1	2.70	0.44
2:F:167:HIS:HD1	2:F:167:HIS:H	1.65	0.44
5:J:88:A:C2	5:J:91:C:N3	2.85	0.44
2:B:37:ASN:OD1	2:B:37:ASN:N	2.46	0.44
2:B:51:LEU:HD22	2:B:1352:ILE:HG13	1.98	0.44
2:B:192:TYR:HE1	2:B:237:LEU:HD23	1.82	0.44
2:B:548:ILE:HD13	2:B:564:LEU:HD11	1.98	0.44
2:F:233:LYS:HB3	2:F:236:GLY:H	1.82	0.44
2:F:300:ILE:O	2:F:303:SER:OG	2.24	0.44
2:F:883:TRP:HB3	2:F:897:PHE:HD1	1.82	0.44
2:F:1167:THR:OG1	2:F:1168:ILE:N	2.50	0.44
1:A:5:C:H2'	1:A:6:G:C8	2.47	0.44
2:B:147:ASP:O	2:B:426:GLN:NE2	2.51	0.44
2:F:30:LYS:HB2	2:F:30:LYS:HE3	1.81	0.44
2:F:821:ASP:HA	2:F:828:LEU:HD11	2.00	0.44
2:F:1212:ARG:HD2	2:F:1336:TYR:HD2	1.83	0.44
1:A:8:A:H2'	1:A:9:U:C6	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:720:LEU:HD13	2:B:938:ARG:HH11	1.82	0.44
2:B:1241:HIS:HD1	2:B:1244:LYS:HA	1.83	0.44
2:F:867:SER:HB2	2:F:1054:ASN:HA	1.99	0.44
5:J:58:G:C6	5:J:60:C:C2	3.06	0.44
2:B:565:LYS:HD3	2:B:578:VAL:HG13	1.99	0.44
2:B:643:PHE:CD2	2:B:643:PHE:N	2.86	0.44
2:B:781:MET:HG3	2:B:803:ASN:ND2	2.33	0.44
1:E:4:A:C4	1:E:5:C:C5	3.05	0.44
2:F:158:LEU:HB2	2:F:419:LEU:HD12	1.99	0.44
2:F:328:HIS:CE1	2:F:359:TYR:HH	2.33	0.44
2:F:823:TYR:HB3	2:F:863:ASN:HB3	1.99	0.44
2:F:1073:VAL:HG23	2:F:1074:TRP:N	2.32	0.44
2:B:141:LYS:HD3	2:B:142:LEU:HD23	2.00	0.44
2:B:558:LYS:HA	2:B:558:LYS:HD3	1.68	0.44
2:B:601:ILE:HG21	2:B:643:PHE:HE1	1.83	0.44
2:B:628:ASP:OD1	2:B:630:GLU:HB3	2.17	0.44
2:B:829:ASP:OD1	2:B:831:ASN:N	2.50	0.44
2:B:939:MET:CE	2:B:953:VAL:HG21	2.47	0.44
2:B:1208:ASN:CG	2:B:1208:ASN:O	2.55	0.44
1:E:25:U:H6	1:E:25:U:O5'	2.01	0.44
2:F:243:ALA:O	2:F:246:LEU:HB3	2.17	0.44
2:F:671:ARG:H	2:F:671:ARG:CD	2.30	0.44
2:F:1222:LYS:NZ	2:F:1315:LEU:O	2.47	0.44
2:B:13:THR:O	2:B:53:PHE:HE1	2.00	0.44
2:B:1276:PHE:CE2	2:B:1316:THR:HB	2.53	0.44
2:F:1095:VAL:HG13	2:F:1350:GLN:OE1	2.18	0.44
2:B:51:LEU:HD13	2:B:1095:VAL:CG2	2.44	0.43
2:B:134:THR:OG1	2:B:137:HIS:N	2.49	0.43
3:C:25:DT:C4	3:C:26:DT:O4	2.71	0.43
2:F:637:LYS:HB2	2:F:637:LYS:HE3	1.68	0.43
2:F:1212:ARG:CZ	2:F:1336:TYR:HE2	2.31	0.43
2:F:1347:LEU:HD22	2:F:1349:HIS:CD2	2.53	0.43
5:J:91:C:HO2'	5:J:92:G:P	2.41	0.43
1:A:3:A:O2'	1:A:4:A:H8	2.00	0.43
2:B:921:LEU:HB3	2:B:1008:PHE:CE1	2.53	0.43
2:B:1200:LYS:HG2	2:B:1201:TYR:CD1	2.52	0.43
2:F:46:ASN:HD21	5:J:88:A:N6	2.13	0.43
2:F:63:ARG:HG3	2:F:66:ARG:NH1	2.32	0.43
2:B:156:LEU:HA	2:B:156:LEU:HD23	1.62	0.43
2:B:416:LEU:HD11	2:B:441:GLU:HG2	2.00	0.43
2:B:1345:ALA:O	2:B:1362:LEU:HG	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:57:GLU:HB2	5:J:65:A:OP1	2.18	0.43
2:F:1010:TYR:O	2:F:1012:ASP:N	2.51	0.43
2:F:1035:LYS:HD3	2:F:1035:LYS:HA	1.57	0.43
2:F:1123:LYS:HG3	5:J:53:G:OP1	2.18	0.43
5:J:84:A:C2	5:J:85:C:C2	3.06	0.43
2:B:79:ILE:HA	2:B:79:ILE:HD13	1.77	0.43
2:B:136:TYR:CD2	2:B:321:MET:HG3	2.53	0.43
2:B:220:ARG:HD3	2:B:220:ARG:HA	1.77	0.43
2:B:958:LEU:HA	2:B:958:LEU:HD23	1.63	0.43
2:B:978:ILE:CD1	2:B:1233:VAL:HG22	2.48	0.43
2:B:1325:LYS:HB3	2:B:1330:THR:HG22	2.00	0.43
2:F:631:MET:O	2:F:635:ARG:N	2.43	0.43
2:F:1126:TRP:N	2:F:1126:TRP:CD1	2.86	0.43
5:I:76:A:H2'	5:I:77:A:O4'	2.19	0.43
2:B:184:LEU:HD23	2:B:184:LEU:HA	1.78	0.43
2:F:465:MET:HE1	2:F:482:VAL:HG21	2.01	0.43
2:B:64:LEU:HD13	2:B:64:LEU:HA	1.71	0.43
2:B:305:ILE:HG13	2:B:306:LEU:N	2.33	0.43
2:B:341:GLN:HG2	2:B:342:GLN:HG3	1.99	0.43
2:B:345:GLU:H	2:B:345:GLU:CD	2.21	0.43
2:B:926:GLN:HG2	3:C:20:DA:P	2.58	0.43
2:B:1120:ILE:HG21	2:B:1120:ILE:HD13	1.61	0.43
2:F:918:LYS:HZ1	2:F:1018:VAL:HG11	1.84	0.43
2:F:1166:ILE:HG13	2:F:1174:PHE:CE2	2.54	0.43
2:F:1356:TYR:HB3	5:J:81:G:C2	2.54	0.43
2:B:122:ILE:H	2:B:122:ILE:HG13	1.66	0.43
2:B:499:ASP:OD2	2:B:663:SER:N	2.37	0.43
2:B:839:ASP:N	2:B:856:VAL:O	2.33	0.43
2:B:886:LEU:HB3	2:B:891:LEU:HB2	2.01	0.43
2:F:1277:SER:HA	2:F:1281:ILE:HG12	2.00	0.43
5:I:73:G:C2	5:I:77:A:C6	3.05	0.43
1:A:15:G:O5'	1:A:15:G:H8	2.02	0.43
2:B:508:LEU:HD21	2:B:664:ARG:HB2	2.00	0.43
2:B:524:LEU:CD2	2:B:545:LYS:HA	2.48	0.43
2:F:51:LEU:CD1	2:F:1352:ILE:HG13	2.49	0.43
2:F:777:SER:CA	2:F:807:GLN:HE21	2.18	0.43
1:E:5:C:O2	1:E:5:C:H2'	2.18	0.43
2:F:9:LEU:HD11	2:F:744:VAL:CG2	2.48	0.43
2:F:110:ASP:OD2	2:F:1130:LYS:HE3	2.18	0.43
2:F:212:LEU:HD13	2:F:300:ILE:CD1	2.49	0.43
2:F:226:ILE:CD1	2:F:232:GLU:HG2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:561:VAL:HG12	2:F:565:LYS:HG3	2.00	0.43
2:F:597:LEU:O	2:F:601:ILE:HG12	2.19	0.43
2:F:627:GLU:HA	2:F:655:ARG:NH1	2.34	0.43
2:F:1052:LEU:HD12	2:F:1052:LEU:HA	1.86	0.43
2:B:216:LEU:HA	2:B:216:LEU:HD23	1.77	0.43
2:B:570:LYS:HE3	2:B:570:LYS:HB3	1.69	0.43
2:B:623:LEU:HD12	2:B:623:LEU:HA	1.70	0.43
2:B:946:ASN:HB3	2:B:948:LYS:HD2	2.00	0.43
1:E:15:G:H4'	2:F:454:PRO:HD3	2.01	0.43
2:F:137:HIS:CD2	2:F:322:ILE:HG23	2.54	0.43
2:F:339:VAL:HG12	2:F:347:TYR:HB2	2.00	0.43
2:F:829:ASP:OD1	2:F:832:ARG:N	2.36	0.43
5:J:96:C:H2'	5:J:97:U:O4'	2.19	0.43
2:F:5:TYR:CZ	2:F:751:MET:HG3	2.54	0.42
2:F:136:TYR:CZ	2:F:160:HIS:NE2	2.85	0.42
2:F:199:ASN:O	2:F:201:ILE:HD12	2.18	0.42
2:F:684:LYS:O	2:F:685:SER:OG	2.31	0.42
2:F:686:ASP:CB	2:F:690:ASN:CA	2.85	0.42
2:F:817:GLN:HB3	2:F:820:ARG:O	2.19	0.42
2:F:843:PRO:O	2:F:846:PHE:HB2	2.19	0.42
5:I:85:C:H42	5:I:93:G:H1	1.67	0.42
5:I:85:C:H2'	5:I:86:C:C6	2.54	0.42
1:A:3:A:O2'	1:A:4:A:P	2.77	0.42
2:B:814:TYR:CE2	2:B:819:GLY:HA2	2.54	0.42
1:E:26:A:C6	1:E:27:G:N7	2.87	0.42
2:F:484:LYS:H	2:F:484:LYS:CE	2.32	0.42
2:F:686:ASP:HB3	2:F:689:ALA:O	2.19	0.42
2:F:802:GLU:H	2:F:805:GLN:HG3	1.84	0.42
2:F:1019:ARG:C	2:F:1021:MET:N	2.73	0.42
5:J:96:C:H2'	5:J:97:U:C6	2.54	0.42
2:B:594:TYR:OH	2:B:608:ASP:OD1	2.37	0.42
2:B:727:LEU:HD11	2:B:934:ILE:HD11	2.01	0.42
2:B:1163:LEU:HD23	2:B:1163:LEU:HA	1.71	0.42
2:B:1301:PRO:O	2:B:1305:GLN:HB2	2.20	0.42
2:B:1336:TYR:N	2:B:1336:TYR:CD1	2.87	0.42
1:E:19:A:OP1	2:F:164:PHE:CD1	2.68	0.42
2:F:165:ARG:CD	2:F:168:PHE:HZ	2.29	0.42
2:F:183:LYS:HD2	2:F:183:LYS:N	2.34	0.42
2:F:213:SER:O	2:F:213:SER:OG	2.32	0.42
2:F:350:ILE:O	2:F:359:TYR:N	2.52	0.42
2:F:848:LYS:HB3	2:F:848:LYS:HE3	1.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1228:LEU:HD12	2:F:1228:LEU:HA	1.82	0.42
2:B:424:ARG:NE	2:B:427:GLU:OE2	2.52	0.42
2:B:913:LYS:HA	2:B:916:PHE:CD2	2.41	0.42
2:B:1110:ILE:CD1	2:B:1134:PHE:HE1	2.31	0.42
2:B:1246:LYS:HB2	2:B:1246:LYS:HE2	1.86	0.42
4:D:3:DT:H1'	4:D:4:DT:H5'	2.00	0.42
2:F:891:LEU:H	2:F:891:LEU:HD23	1.84	0.42
2:F:1266:LEU:HG	2:F:1309:ILE:HD11	2.00	0.42
3:G:23:DC:H2'	3:G:24:DG:O4'	2.19	0.42
2:B:609:ASN:ND2	2:B:611:GLU:OE1	2.45	0.42
2:B:840:ALA:HA	2:B:854:ASN:O	2.19	0.42
2:B:1082:THR:O	2:B:1086:VAL:HG23	2.19	0.42
1:E:15:G:H2'	1:E:16:A:O4'	2.19	0.42
2:F:824:VAL:HG12	2:F:825:ASP:H	1.83	0.42
2:F:1135:ASP:OD1	4:H:8:DT:H5''	2.20	0.42
1:A:4:A:O2'	1:A:5:C:C5'	2.68	0.42
2:B:665:LYS:O	2:B:670:ILE:HG12	2.19	0.42
2:B:986:ASP:O	2:B:990:ASN:ND2	2.52	0.42
2:B:1213:MET:O	2:B:1221:GLN:N	2.48	0.42
2:B:1244:LYS:HB2	2:B:1244:LYS:HE2	1.80	0.42
2:F:381:GLU:H	2:F:381:GLU:HG2	1.72	0.42
2:F:424:ARG:HH22	2:F:437:ARG:NH1	2.17	0.42
2:F:679:ILE:HG12	2:F:704:PHE:CZ	2.54	0.42
2:F:981:TYR:HE1	2:F:1225:GLU:HG3	1.84	0.42
2:F:985:HIS:CG	2:F:1087:LEU:HD22	2.55	0.42
2:F:988:TYR:CZ	2:F:1086:VAL:HG11	2.54	0.42
2:F:1111:LEU:HD23	2:F:1111:LEU:HA	1.64	0.42
2:F:1264:HIS:ND1	2:F:1268:GLU:OE2	2.49	0.42
5:J:42:A:O2'	5:J:43:G:OP1	2.30	0.42
2:B:25:TYR:O	2:B:988:TYR:OH	2.36	0.42
2:B:997:LEU:HD23	2:B:997:LEU:HA	1.87	0.42
1:E:11:U:C2	1:E:12:A:C8	3.07	0.42
2:F:165:ARG:CG	2:F:168:PHE:HE1	2.33	0.42
2:F:1089:MET:HA	2:F:1090:PRO:HD3	1.66	0.42
2:F:1178:PRO:O	2:F:1182:LEU:HG	2.19	0.42
2:B:8:GLY:O	2:B:987:ALA:HB1	2.20	0.42
2:B:1182:LEU:HD13	2:B:1190:VAL:HG11	2.01	0.42
2:F:226:ILE:HG22	2:F:230:PRO:HA	2.01	0.42
2:F:813:LEU:O	2:F:817:GLN:HG3	2.20	0.42
2:F:1321:PRO:HG2	2:F:1335:ARG:HA	2.02	0.42
2:B:1141:TYR:C	2:B:1141:TYR:CD1	2.94	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:170:ILE:HG22	2:F:413:GLN:NE2	2.35	0.42
2:F:495:MET:HB3	3:G:17:DT:H1'	2.02	0.42
2:F:521:TYR:HE1	2:F:684:LYS:HD2	1.85	0.42
2:F:1096:LYS:HE2	2:F:1201:TYR:CE2	2.55	0.42
2:B:1142:SER:O	2:B:1198:LEU:N	2.35	0.42
2:F:441:GLU:O	2:F:445:THR:HG22	2.20	0.42
2:F:591:LEU:O	2:F:595:HIS:ND1	2.48	0.42
2:F:644:ASP:HB3	2:F:647:VAL:HG23	2.02	0.42
2:F:823:TYR:CD2	2:F:863:ASN:HB2	2.55	0.42
2:B:570:LYS:O	2:B:574:CYS:HA	2.20	0.41
2:B:794:GLN:HG2	2:B:798:GLU:HG3	2.01	0.41
2:B:1191:LYS:HD2	2:B:1194:LEU:HD12	2.01	0.41
2:B:1229:PRO:HB2	2:B:1232:TYR:CE2	2.55	0.41
2:B:1258:PHE:CE1	2:B:1262:HIS:CD2	3.06	0.41
3:C:25:DT:N3	3:C:26:DT:H72	2.35	0.41
2:F:201:ILE:HD12	2:F:201:ILE:N	2.35	0.41
2:F:522:ASN:HA	2:F:683:LEU:HD13	2.01	0.41
2:F:523:GLU:OE1	2:F:588:ASN:HB2	2.20	0.41
2:F:910:GLU:OE1	2:F:910:GLU:N	2.51	0.41
2:F:1236:LEU:HD11	2:F:1269:ILE:HD13	2.01	0.41
5:J:53:G:C2	5:J:62:G:C2	3.08	0.41
2:B:40:ARG:HH22	5:I:92:G:P	2.43	0.41
2:B:300:ILE:HA	2:B:303:SER:OG	2.20	0.41
2:B:349:GLU:HG3	2:B:356:LYS:HG3	2.01	0.41
2:B:599:LYS:O	2:B:602:LYS:HG3	2.19	0.41
1:E:5:C:C2	1:E:6:G:C8	3.08	0.41
1:E:22:U:O2	2:F:1110:ILE:HD12	2.20	0.41
2:F:164:PHE:CD1	2:F:164:PHE:C	2.94	0.41
2:F:758:ASN:ND2	2:F:995:THR:HG22	2.36	0.41
2:F:794:GLN:HE21	2:F:798:GLU:CD	2.24	0.41
2:F:1221:GLN:HB3	2:F:1319:GLY:O	2.20	0.41
1:A:18:A:OP2	2:B:71:ARG:HD2	2.20	0.41
1:A:18:A:OP1	2:B:165:ARG:HD3	2.19	0.41
2:B:325:TYR:HA	5:I:44:U:O2	2.20	0.41
2:F:143:VAL:HG22	2:F:422:ILE:CG1	2.50	0.41
2:F:174:LEU:CD2	2:F:413:GLN:HB2	2.50	0.41
2:B:31:LYS:HG3	2:B:44:LYS:HG3	2.02	0.41
2:B:212:LEU:HD21	2:B:225:LEU:CD1	2.50	0.41
2:B:742:LYS:HB3	2:B:1352:ILE:HD13	2.02	0.41
2:B:1000:LYS:HE2	2:B:1065:THR:O	2.20	0.41
2:F:268:LYS:O	2:F:271:TYR:CD2	2.71	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:918:LYS:NZ	2:F:1007:GLU:OE2	2.41	0.41
2:F:1087:LEU:HD23	2:F:1087:LEU:HA	1.76	0.41
2:F:1204:PHE:CE1	2:F:1347:LEU:HG	2.56	0.41
2:F:1245:LEU:HD13	2:F:1252:ASN:ND2	2.35	0.41
5:I:87:G:C2	5:I:92:G:C6	3.09	0.41
1:A:4:A:O2'	1:A:5:C:P	2.77	0.41
2:B:475:PRO:HG3	5:I:59:U:O4	2.21	0.41
2:B:680:LEU:HD12	2:B:680:LEU:HA	1.76	0.41
2:B:1003:LYS:H	2:B:1003:LYS:HG2	1.54	0.41
2:B:1179:ILE:HD11	2:B:1192:LYS:CE	2.50	0.41
2:B:1207:GLU:HG2	2:B:1210:ARG:NH1	2.35	0.41
2:F:49:GLY:HA2	2:F:1092:VAL:CG1	2.50	0.41
2:F:174:LEU:HD22	2:F:413:GLN:HB2	2.02	0.41
2:F:289:LEU:O	2:F:292:ALA:HB3	2.19	0.41
2:F:302:LEU:HD23	2:F:305:ILE:HD11	2.02	0.41
2:F:409:SER:O	2:F:411:PRO:HD3	2.20	0.41
2:F:442:LYS:HE3	2:F:446:PHE:CD1	2.55	0.41
2:F:1228:LEU:HD12	2:F:1229:PRO:CD	2.51	0.41
2:F:1281:ILE:HG13	2:F:1316:THR:HG22	2.02	0.41
3:G:2:DA:H2''	3:G:3:DA:OP1	2.21	0.41
2:B:554:LYS:HG2	2:B:594:TYR:CE2	2.56	0.41
2:B:784:ILE:HD13	2:B:815:TYR:CB	2.51	0.41
2:B:841:ILE:HD11	2:B:896:LYS:HG3	2.02	0.41
2:B:1084:ARG:O	2:B:1084:ARG:HG2	2.18	0.41
2:F:143:VAL:HG21	2:F:315:ALA:CB	2.50	0.41
2:F:424:ARG:O	2:F:427:GLU:HG2	2.19	0.41
2:F:662:LEU:HD22	2:F:666:LEU:CD2	2.50	0.41
2:B:25:TYR:HE2	2:B:1074:TRP:CE3	2.38	0.41
2:B:1220:LEU:HD21	2:B:1342:VAL:HG21	2.02	0.41
2:B:1318:LEU:HD22	2:B:1319:GLY:N	2.35	0.41
2:F:137:HIS:CD2	2:F:322:ILE:HG12	2.55	0.41
2:F:348:LYS:HA	2:F:352:PHE:HD2	1.85	0.41
2:F:583:VAL:HG21	2:F:587:PHE:CD1	2.54	0.41
2:F:636:LEU:HA	2:F:639:TYR:HD2	1.84	0.41
2:F:649:LYS:CB	2:F:653:ARG:HH21	2.34	0.41
3:G:4:DT:H2''	3:G:5:DA:C5'	2.51	0.41
2:B:959:LYS:HB3	2:B:962:LEU:HG	2.02	0.41
3:C:2:DA:H2'	3:C:3:DA:C8	2.55	0.41
2:F:1061:PRO:O	2:F:1076:LYS:HE2	2.21	0.41
2:F:1203:LEU:HD23	2:F:1348:ILE:HD12	2.02	0.41
2:F:1343:LEU:O	2:F:1362:LEU:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:118:ILE:HG12	2:B:156:LEU:HD11	2.03	0.41
2:B:248:LEU:HA	2:B:248:LEU:HD23	1.72	0.41
2:B:447:ARG:HD3	2:B:447:ARG:HH11	1.76	0.41
2:B:524:LEU:HD23	2:B:545:LYS:HG2	2.02	0.41
2:B:535:ARG:HE	2:B:535:ARG:HB3	1.70	0.41
2:B:544:GLN:O	2:B:548:ILE:HG13	2.21	0.41
2:B:861:ASP:O	2:B:864:ARG:HG2	2.21	0.41
2:B:1119:LEU:HD12	2:B:1119:LEU:HA	1.93	0.41
2:B:1205:GLU:O	2:B:1345:ALA:HB1	2.21	0.41
1:E:4:A:HO2'	1:E:5:C:C5'	2.33	0.41
2:F:4:LYS:HE2	2:F:4:LYS:HB2	1.54	0.41
2:F:97:PHE:CE1	2:F:118:ILE:HA	2.56	0.41
2:F:117:PRO:HD2	2:F:118:ILE:HD12	2.03	0.41
2:F:336:LYS:HG2	2:F:351:PHE:CZ	2.55	0.41
2:F:513:LEU:HA	2:F:513:LEU:HD23	1.80	0.41
2:F:525:THR:OG1	2:F:545:LYS:NZ	2.30	0.41
2:F:546:LYS:NZ	2:F:550:ASP:OD2	2.53	0.41
2:F:553:PHE:CD2	2:F:559:VAL:HG21	2.56	0.41
2:F:632:ILE:O	2:F:636:LEU:N	2.39	0.41
2:F:852:ILE:O	2:F:896:LYS:HD3	2.21	0.41
2:F:853:ASP:OD2	2:F:895:ARG:HD3	2.21	0.41
2:F:878:LYS:HE3	2:F:878:LYS:HB2	1.84	0.41
2:F:897:PHE:CZ	2:F:901:THR:HG21	2.56	0.41
2:F:949:LEU:HD23	2:F:951:ARG:HH22	1.85	0.41
2:F:1163:LEU:HD23	2:F:1163:LEU:HA	1.91	0.41
2:F:1207:GLU:CG	2:F:1208:ASN:H	2.34	0.41
5:I:52:A:OP2	5:I:62:G:N2	2.51	0.41
5:I:82:G:N7	5:I:97:U:O2	2.53	0.41
5:I:92:G:H2'	5:I:93:G:C8	2.56	0.41
5:J:45:U:H2'	5:J:46:A:H8	1.86	0.41
5:J:56:U:O2	5:J:58:G:N2	2.46	0.41
2:B:198:GLU:C	2:B:200:PRO:HD3	2.41	0.41
2:B:423:LEU:HA	2:B:423:LEU:HD23	1.70	0.41
2:B:982:HIS:HA	2:B:985:HIS:HB2	2.02	0.41
2:B:1302:ILE:H	2:B:1302:ILE:HG13	1.71	0.41
2:F:318:SER:O	2:F:321:MET:HB2	2.21	0.41
2:F:1360:ILE:HD13	2:F:1360:ILE:HA	1.92	0.41
2:B:338:LEU:C	2:B:383:MET:HE1	2.42	0.40
2:B:455:LEU:O	5:I:60:C:H5'	2.21	0.40
2:B:485:GLY:O	2:B:488:ALA:N	2.54	0.40
2:B:526:LYS:HD3	2:B:526:LYS:HA	1.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:788:ILE:HA	2:B:791:LEU:HB2	2.03	0.40
3:C:20:DA:C8	3:C:21:DT:H72	2.57	0.40
2:F:324:ARG:HB3	2:F:402:GLN:HE21	1.86	0.40
2:F:360:ALA:O	2:F:364:ASP:N	2.53	0.40
2:F:492:ILE:O	2:F:496:THR:HG23	2.21	0.40
5:J:46:A:H2'	5:J:47:A:H8	1.80	0.40
2:B:198:GLU:HG2	2:B:199:ASN:N	2.35	0.40
2:B:455:LEU:N	2:B:455:LEU:CD1	2.84	0.40
2:B:1156:LYS:HE3	2:B:1156:LYS:HB2	1.91	0.40
1:E:15:G:O5'	1:E:15:G:H8	2.04	0.40
2:F:139:ARG:CG	2:F:157:ALA:CA	2.99	0.40
2:F:148:LYS:HA	2:F:429:PHE:CD2	2.56	0.40
2:F:451:TYR:CD1	2:F:488:ALA:HB2	2.56	0.40
2:F:967:ARG:NH1	2:F:974:LYS:HE3	2.36	0.40
2:F:1093:ASN:O	2:F:1094:ILE:HD13	2.22	0.40
2:F:1114:ARG:HG2	2:F:1115:ASN:H	1.85	0.40
2:B:424:ARG:CZ	2:B:437:ARG:NH1	2.85	0.40
2:B:821:ASP:OD2	2:B:828:LEU:HG	2.22	0.40
2:F:526:LYS:HA	2:F:526:LYS:HD3	1.68	0.40
2:F:927:ILE:O	2:F:930:HIS:N	2.54	0.40
2:F:1210:ARG:HB2	2:F:1280:VAL:HA	2.03	0.40
2:F:1236:LEU:O	2:F:1240:SER:OG	2.27	0.40
4:D:6:DG:H2''	4:D:7:DG:H5''	2.03	0.40
2:F:160:HIS:HE2	2:F:164:PHE:HD2	1.68	0.40
2:F:1107:LYS:HE2	3:G:8:DT:H1'	2.03	0.40
2:F:1146:VAL:O	2:F:1191:LYS:HG3	2.21	0.40
2:F:1204:PHE:CE2	2:F:1342:VAL:HG11	2.56	0.40
2:B:514:LEU:HD11	2:B:667:ILE:CG2	2.51	0.40
2:B:558:LYS:HD2	2:B:586:ARG:HD2	2.04	0.40
2:B:642:LEU:HB2	2:B:643:PHE:HD2	1.83	0.40
2:B:967:ARG:HH11	2:B:989:LEU:HD12	1.86	0.40
2:B:989:LEU:O	2:B:993:VAL:HG23	2.22	0.40
2:B:1228:LEU:HD12	2:B:1229:PRO:CD	2.51	0.40
1:E:14:G:O2'	1:E:15:G:H5'	2.22	0.40
2:F:57:GLU:HB2	5:J:65:A:P	2.62	0.40
2:F:1206:LEU:HD12	2:F:1210:ARG:NH1	2.35	0.40
2:F:1280:VAL:HG12	2:F:1281:ILE:HD13	2.03	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)
2:B:202:ASN:OD1	2:B:541:SER:OG[2_545]	2.07	0.13

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	
2	B	1308/1368 (96%)	1268 (97%)	36 (3%)	4 (0%)	41	73
2	F	1313/1368 (96%)	1267 (96%)	41 (3%)	5 (0%)	34	68
All	All	2621/2736 (96%)	2535 (97%)	77 (3%)	9 (0%)	41	73

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	1042	ILE
2	F	585	ASP
2	F	1011	GLY
2	F	1020	LYS
2	B	1327	PHE
2	B	470	GLU
2	B	117	PRO
2	F	117	PRO
2	B	230	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	
2	B	1170/1225 (96%)	1131 (97%)	39 (3%)	38	67
2	F	1155/1225 (94%)	1093 (95%)	62 (5%)	22	54
All	All	2325/2450 (95%)	2224 (96%)	101 (4%)	29	60

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	94	ASP
2	B	95	ASP
2	B	141	LYS
2	B	182	ASP
2	B	276	ASP
2	B	311	GLU
2	B	383	MET
2	B	389	LEU
2	B	424	ARG
2	B	425	ARG
2	B	434	LYS
2	B	494	ARG
2	B	535	ARG
2	B	557	ARG
2	B	584	GLU
2	B	614	ASP
2	B	629	ARG
2	B	674	GLN
2	B	684	LYS
2	B	688	PHE
2	B	719	SER
2	B	751	MET
2	B	778	ARG
2	B	803	ASN
2	B	818	ASN
2	B	854	ASN
2	B	866	LYS
2	B	905	ARG
2	B	951	ARG
2	B	954	LYS
2	B	1062	LEU
2	B	1080	PHE
2	B	1158	LYS
2	B	1202	SER
2	B	1221	GLN

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Mol	Chain	Res	Type
2	B	1258	PHE
2	B	1263	LYS
2	B	1317	ASN
2	B	1338	SER
2	F	42	SER
2	F	140	LYS
2	F	142	LEU
2	F	150	ASP
2	F	151	LEU
2	F	155	TYR
2	F	156	LEU
2	F	160	HIS
2	F	164	PHE
2	F	183	LYS
2	F	229	LEU
2	F	234	LYS
2	F	237	LEU
2	F	267	SER
2	F	271	TYR
2	F	284	ASP
2	F	295	ASN
2	F	383	MET
2	F	384	ASP
2	F	423	LEU
2	F	425	ARG
2	F	451	TYR
2	F	476	TRP
2	F	478	PHE
2	F	484	LYS
2	F	494	ARG
2	F	532	GLU
2	F	535	ARG
2	F	546	LYS
2	F	567	ASP
2	F	598	LEU
2	F	629	ARG
2	F	631	MET
2	F	650	GLN
2	F	654	ARG
2	F	663	SER
2	F	671	ARG
2	F	682	PHE

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Mol	Chain	Res	Type
2	F	686	ASP
2	F	688	PHE
2	F	704	PHE
2	F	705	LYS
2	F	753	ARG
2	F	803	ASN
2	F	818	ASN
2	F	820	ARG
2	F	822	MET
2	F	891	LEU
2	F	976	ARG
2	F	977	GLU
2	F	1008	PHE
2	F	1037	PHE
2	F	1080	PHE
2	F	1118	LYS
2	F	1202	SER
2	F	1206	LEU
2	F	1208	ASN
2	F	1258	PHE
2	F	1265	TYR
2	F	1327	PHE
2	F	1338	SER
2	F	1364	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	137	HIS
2	B	920	GLN
2	B	1044	ASN
2	B	1252	ASN
2	B	1262	HIS
2	B	1308	ASN
2	B	1350	GLN
2	F	46	ASN
2	F	178	ASN
2	F	295	ASN
2	F	329	HIS
2	F	758	ASN
2	F	794	GLN
2	F	807	GLN

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Mol	Chain	Res	Type
2	F	920	GLN
2	F	1252	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	33/34 (97%)	11 (33%)	4 (12%)
1	E	32/34 (94%)	11 (34%)	2 (6%)
5	I	62/65 (95%)	19 (30%)	1 (1%)
5	J	62/65 (95%)	18 (29%)	1 (1%)
All	All	189/198 (95%)	59 (31%)	8 (4%)

All (59) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	U
1	A	3	A
1	A	4	A
1	A	6	G
1	A	9	U
1	A	20	A
1	A	24	U
1	A	28	A
1	A	29	G
1	A	32	A
1	A	33	U
1	E	4	A
1	E	5	C
1	E	6	G
1	E	9	U
1	E	20	A
1	E	24	U
1	E	28	A
1	E	29	G
1	E	30	C
1	E	32	A
1	E	33	U
5	I	37	U
5	I	39	G
5	I	40	C
5	I	42	A

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Mol	Chain	Res	Type
5	I	43	G
5	I	44	U
5	I	50	U
5	I	51	A
5	I	56	U
5	I	57	A
5	I	59	U
5	I	63	U
5	I	68	A
5	I	74	A
5	I	82	G
5	I	87	G
5	I	89	G
5	I	91	C
5	I	92	G
5	J	37	U
5	J	39	G
5	J	40	C
5	J	42	A
5	J	43	G
5	J	50	U
5	J	51	A
5	J	56	U
5	J	57	A
5	J	59	U
5	J	63	U
5	J	68	A
5	J	74	A
5	J	82	G
5	J	87	G
5	J	89	G
5	J	91	C
5	J	92	G

All (8) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	3	A
1	A	8	A
1	A	27	G
1	A	28	A
1	E	3	A

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Mol	Chain	Res	Type
1	E	27	G
5	I	42	A
5	J	42	A

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 monosaccharides 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	34/34 (100%)	-0.28	0 100 100	18, 45, 134, 169	0
1	E	32/34 (94%)	-0.04	1 (3%) 49 52	38, 77, 181, 216	0
2	B	1322/1368 (96%)	0.24	103 (7%) 13 15	14, 71, 195, 218	0
2	F	1327/1368 (97%)	0.25	99 (7%) 14 16	13, 92, 149, 193	0
3	C	26/26 (100%)	-0.39	0 100 100	27, 50, 107, 115	0
3	G	26/26 (100%)	-0.54	0 100 100	45, 63, 112, 124	0
4	D	11/11 (100%)	0.05	1 (9%) 9 11	41, 53, 134, 168	0
4	H	11/11 (100%)	0.89	2 (18%) 1 1	41, 59, 110, 175	0
5	I	63/65 (96%)	-0.42	0 100 100	20, 74, 126, 157	0
5	J	63/65 (96%)	-0.38	1 (1%) 72 74	36, 56, 156, 192	0
All	All	2915/3008 (96%)	0.19	207 (7%) 16 18	13, 77, 168, 218	0

All (207) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	801	VAL	19.2
1	E	34	G	12.6
2	B	810	LYS	11.8
2	B	868	ASP	11.2
4	H	2	DT	9.8
2	B	833	LEU	9.2
2	B	872	SER	8.9
2	F	231	GLY	8.4
2	B	861	ASP	7.8
2	F	1243	GLU	7.4
2	B	842	VAL	7.4
2	B	836	TYR	7.2
2	B	841	ILE	7.2

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Mol	Chain	Res	Type	RSRZ
2	F	305	ILE	7.2
2	B	858	THR	7.2
2	F	306	LEU	7.0
2	B	867	SER	6.9
2	B	823	TYR	6.8
2	F	230	PRO	6.4
2	B	812	TYR	6.4
2	B	832	ARG	6.3
2	B	824	VAL	6.2
2	F	703	THR	6.2
2	F	557	ARG	6.2
2	B	834	SER	6.2
2	F	307	ARG	6.1
2	B	817	GLN	6.1
2	B	809	GLU	5.9
2	B	871	PRO	5.9
2	F	698	HIS	5.8
2	B	793	SER	5.8
2	F	232	GLU	5.6
2	F	1246	LYS	5.6
2	B	829	ASP	5.4
2	B	869	ASN	5.3
2	B	1046	PHE	5.3
2	B	1052	LEU	5.3
2	B	822	MET	5.1
2	F	443	ILE	5.1
2	F	135	ILE	5.0
2	B	818	ASN	4.9
2	B	830	ILE	4.9
5	J	36	G	4.9
2	F	613	GLU	4.8
2	B	864	ARG	4.8
2	F	796	LEU	4.8
2	B	1051	THR	4.7
2	F	247	GLY	4.7
2	B	791	LEU	4.7
2	B	894	GLN	4.7
2	B	856	VAL	4.5
2	F	709	GLN	4.5
2	B	859	ARG	4.5
2	F	400	ARG	4.4
2	F	1247	GLY	4.3

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Mol	Chain	Res	Type	RSRZ
2	F	308	VAL	4.3
2	B	877	LYS	4.1
2	F	301	LEU	4.1
2	F	697	ILE	4.1
2	F	362	TYR	4.1
2	B	1045	PHE	4.1
2	F	888	ASN	4.1
2	F	558	LYS	4.0
2	B	1073	VAL	4.0
2	B	843	PRO	4.0
2	B	828	LEU	4.0
2	F	209	LYS	3.9
2	B	881	ASN	3.9
2	F	700	ASP	3.9
2	B	876	VAL	3.9
2	B	853	ASP	3.8
2	F	587	PHE	3.8
4	D	2	DT	3.8
2	B	819	GLY	3.7
2	F	789	LYS	3.7
2	B	880	LYS	3.7
2	F	181	VAL	3.7
2	B	1250	GLU	3.6
2	B	901	THR	3.6
2	B	1050	ILE	3.5
2	F	369	GLN	3.5
2	B	800	PRO	3.5
2	B	854	ASN	3.4
2	F	610	GLU	3.4
2	B	795	ILE	3.4
2	F	597	LEU	3.4
2	B	42	SER	3.4
2	F	815	TYR	3.4
2	F	1242	TYR	3.3
2	F	536	LYS	3.3
2	B	310	THR	3.3
2	B	860	SER	3.3
2	B	815	TYR	3.3
2	B	1039	TYR	3.3
2	B	1248	SER	3.2
2	F	416	LEU	3.2
2	B	873	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	1151	LYS	3.2
2	F	207	ASP	3.2
2	B	1040	SER	3.2
2	F	691	ARG	3.2
2	B	31	LYS	3.1
2	B	883	TRP	3.1
2	F	679	ILE	3.1
2	F	818	ASN	3.1
2	B	897	PHE	3.1
2	F	594	TYR	3.1
2	B	831	ASN	3.1
2	F	706	GLU	3.0
2	F	705	LYS	3.0
2	B	857	LEU	3.0
2	F	234	LYS	2.9
2	F	901	THR	2.9
2	B	1038	PHE	2.9
2	B	870	VAL	2.8
2	F	1249	PRO	2.8
2	B	1074	TRP	2.8
2	B	837	ASP	2.8
2	B	805	GLN	2.8
2	B	852	ILE	2.8
2	B	25	TYR	2.8
2	F	142	LEU	2.8
2	B	804	THR	2.8
2	F	85	ILE	2.7
2	F	224	ASN	2.7
2	F	822	MET	2.7
2	B	688	PHE	2.7
2	B	898	ASP	2.7
2	F	693	PHE	2.7
2	F	883	TRP	2.7
2	B	784	ILE	2.7
2	B	264	LEU	2.6
2	F	694	MET	2.6
2	B	1152	GLY	2.6
2	B	794	GLN	2.6
2	B	813	LEU	2.5
2	B	1158	LYS	2.5
2	F	372	PHE	2.5
2	B	907	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	796	LEU	2.5
2	B	814	TYR	2.5
2	F	588	ASN	2.5
2	F	227	ALA	2.5
2	B	20	VAL	2.5
2	F	559	VAL	2.5
2	B	904	GLU	2.5
2	B	33	LYS	2.4
2	B	862	LYS	2.4
2	F	621	LEU	2.4
2	F	156	LEU	2.4
2	F	302	LEU	2.4
2	F	524	LEU	2.4
2	F	560	THR	2.4
2	B	902	LYS	2.4
2	F	420	HIS	2.4
2	F	841	ILE	2.4
2	F	1154	SER	2.4
2	B	802	GLU	2.4
2	F	286	TYR	2.4
2	F	816	LEU	2.4
2	B	806	LEU	2.3
2	B	799	HIS	2.3
2	B	884	ARG	2.3
2	F	601	ILE	2.3
2	F	154	ILE	2.3
2	B	790	GLU	2.3
2	B	1063	ILE	2.3
2	F	616	LEU	2.3
2	F	1119	LEU	2.3
2	F	515	TYR	2.3
2	B	32	PHE	2.3
2	F	856	VAL	2.3
2	F	257	ASP	2.3
4	H	3	DT	2.3
2	F	440	ILE	2.2
2	F	1153	LYS	2.2
2	F	809	GLU	2.2
2	F	415	HIS	2.2
2	F	314	LYS	2.2
2	B	1243	GLU	2.2
2	B	807	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	999	LYS	2.2
2	B	906	GLY	2.2
2	F	397	ASP	2.2
2	F	106	LEU	2.2
2	F	351	PHE	2.2
2	F	436	ASN	2.2
2	F	419	LEU	2.1
2	F	157	ALA	2.1
2	F	673	LYS	2.1
2	F	366	GLY	2.1
2	F	84	GLU	2.1
2	F	598	LEU	2.1
2	B	1042	ILE	2.1
2	F	359	TYR	2.1
2	F	674	GLN	2.1
2	F	431	PRO	2.1
2	F	128	TYR	2.1
2	B	885	GLN	2.1
2	F	806	LEU	2.1
2	B	19	ALA	2.1
2	F	237	LEU	2.0
2	F	619	ILE	2.0
2	F	412	HIS	2.0
2	F	871	PRO	2.0
2	B	26	LYS	2.0
2	B	905	ARG	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 monosaccharides 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.