Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 04:23 am BST

PDB ID	:	4LD9
Title	:	Crystal structure of the N-terminally acetylated BAH domain of Sir3 bound to the nucleosome core particle
Authors	:	Arnaudo, N.; Fernandez, I.S.; McLaughlin, S.H.; Peak-Chew, S.Y.; Rhodes, D.; Martino, F.
Deposited on	:	2013-06-24
Resolution	:	3.31 Å(reported)

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

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

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

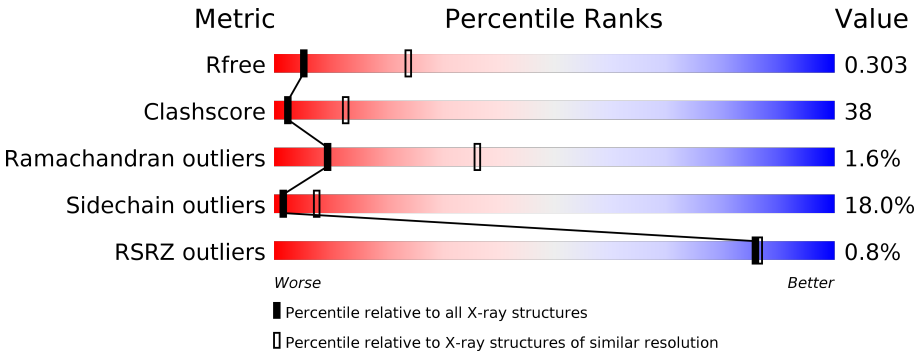
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.31 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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

Mol	Chain	Length	Quality of chain
1	A	136	40% 26% • 29%
1	E	136	37% 22% 5% • 34%
2	B	103	5% 42% 38% 7% 14%
2	F	103	28% 36% 11% 6% 19%
3	C	130	2% 27% 40% 8% 25%
3	G	130	23% 44% 8% • 23%

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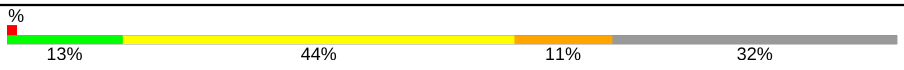
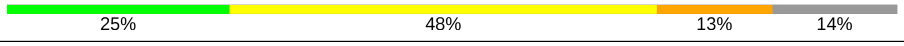
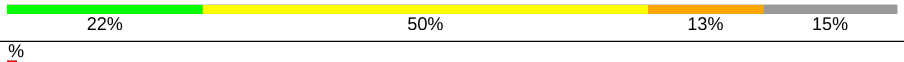
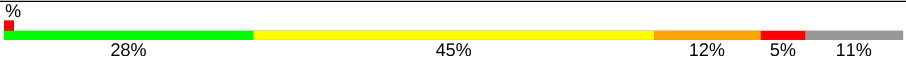
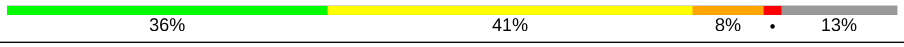
Mol	Chain	Length	Quality of chain
4	D	126	
4	H	126	
5	I	167	
6	J	167	
7	K	236	
7	L	236	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 15140 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Histone H3.2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	97	Total	C	N	O	S	0	0	0
			799	505	153	138	3			
1	E	90	Total	C	N	O	S	0	0	0
			729	459	137	130	3			

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	89	Total	C	N	O	S	0	0	0
			716	451	145	119	1			
2	F	83	Total	C	N	O	S	0	0	0
			674	426	134	113	1			

- Molecule 3 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	98	Total	C	N	O	0	0	0
			753	476	146	131			
3	G	100	Total	C	N	O	0	0	0
			768	485	148	135			

- Molecule 4 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	86	Total	C	N	O	S	0	0	0
			673	427	119	125	2			
4	H	88	Total	C	N	O	S	0	0	0
			690	437	122	129	2			

- Molecule 5 is a DNA chain called Widom 601 sequence reverse.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	143	Total	C	N	O	P	0	0	0
			2946	1396	551	857	142			

- Molecule 6 is a DNA chain called Widom 601 sequence forward.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	J	142	Total	C	N	O	P	0	0	0
			2895	1375	527	851	142			

- Molecule 7 is a protein called Regulatory protein SIR3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	K	211	Total	C	N	O	S	0	0	0
			1761	1136	295	328	2			
7	L	206	Total	C	N	O	S	0	0	0
			1736	1122	284	328	2			

There are 16 discrepancies between the modelled and reference sequences:

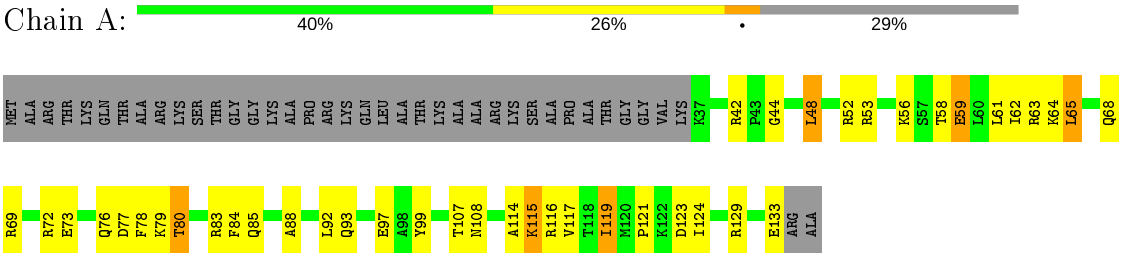
Chain	Residue	Modelled	Actual	Comment	Reference
K	1	ACE	-	ACETYLATION	UNP P06701
K	230	LYS	-	EXPRESSION TAG	UNP P06701
K	231	HIS	-	EXPRESSION TAG	UNP P06701
K	232	HIS	-	EXPRESSION TAG	UNP P06701
K	233	HIS	-	EXPRESSION TAG	UNP P06701
K	234	HIS	-	EXPRESSION TAG	UNP P06701
K	235	HIS	-	EXPRESSION TAG	UNP P06701
K	236	HIS	-	EXPRESSION TAG	UNP P06701
L	1	ACE	-	ACETYLATION	UNP P06701
L	230	LYS	-	EXPRESSION TAG	UNP P06701
L	231	HIS	-	EXPRESSION TAG	UNP P06701
L	232	HIS	-	EXPRESSION TAG	UNP P06701
L	233	HIS	-	EXPRESSION TAG	UNP P06701
L	234	HIS	-	EXPRESSION TAG	UNP P06701
L	235	HIS	-	EXPRESSION TAG	UNP P06701
L	236	HIS	-	EXPRESSION TAG	UNP P06701

3 Residue-property plots (i)

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

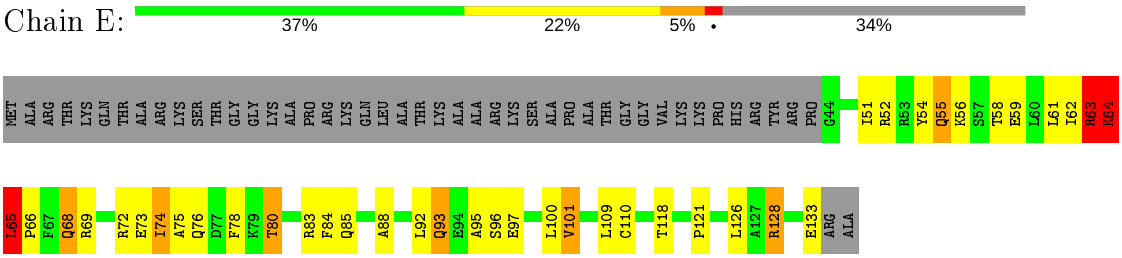
- Molecule 1: Histone H3.2

Chain A:



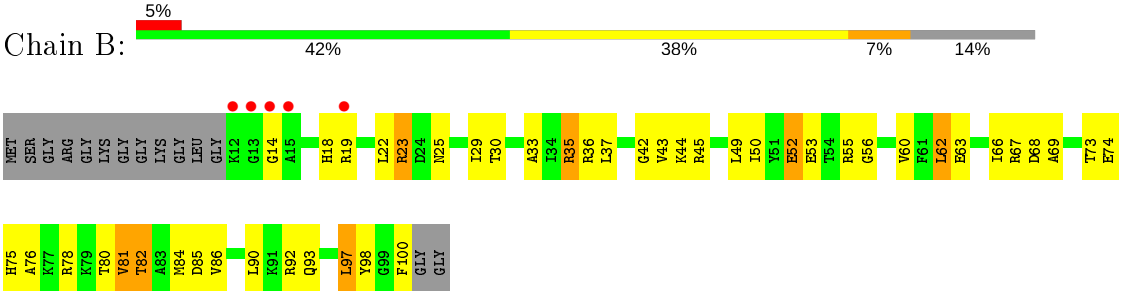
- Molecule 1: Histone H3.2

Chain E:



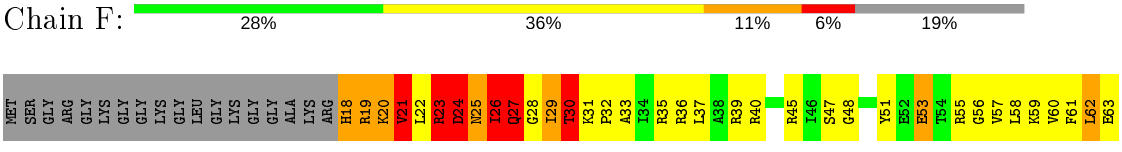
- Molecule 2: Histone H4

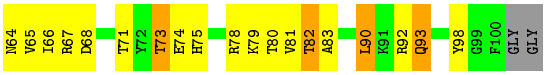
Chain B:



- Molecule 2: Histone H4

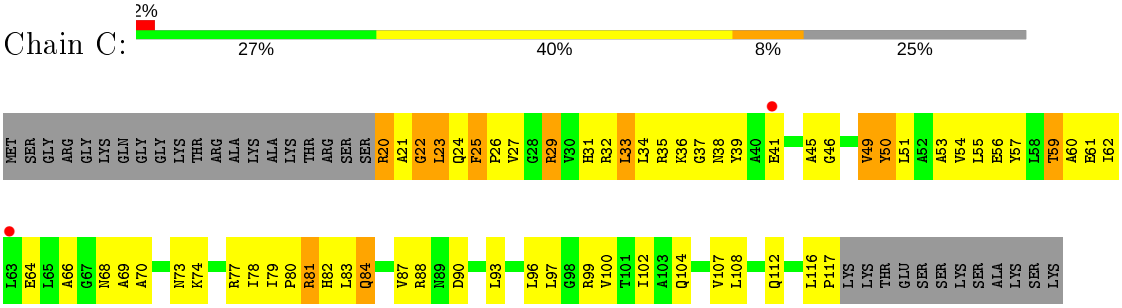
Chain F:





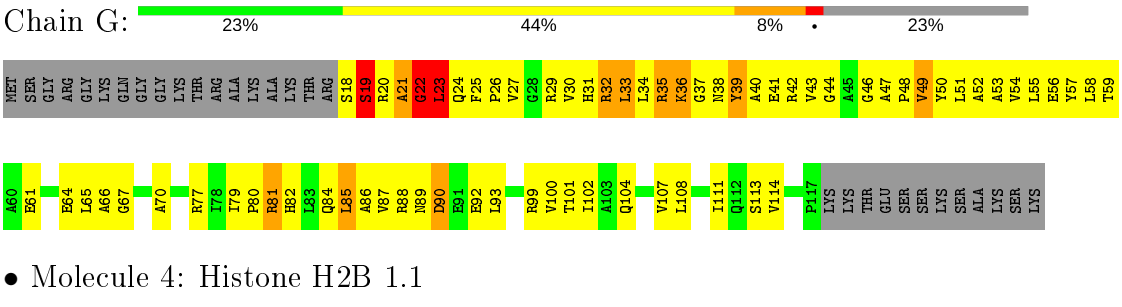
- Molecule 3: Histone H2A

Chain C:



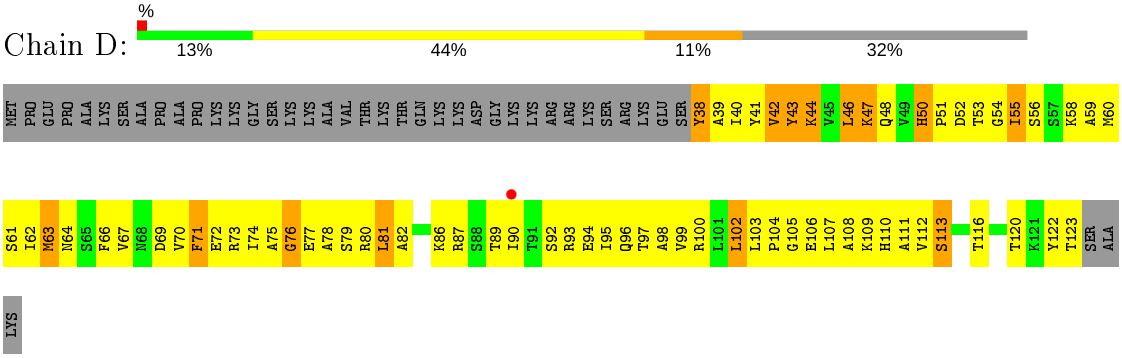
- Molecule 3: Histone H2A

Chain G:



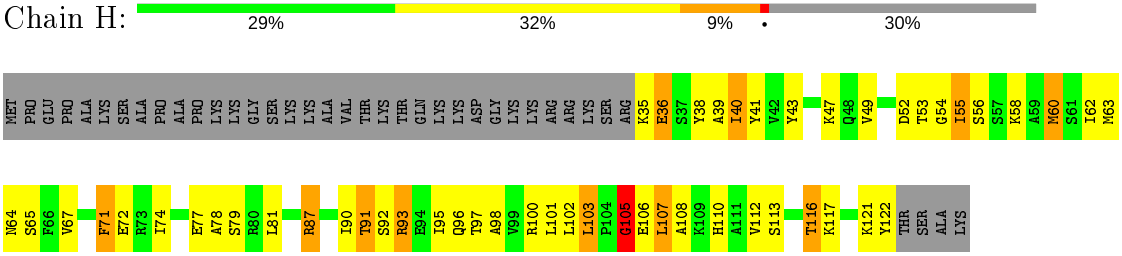
- Molecule 4: Histone H2B 1.1

Chain D:



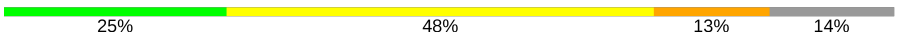
- Molecule 4: Histone H2B 1.1

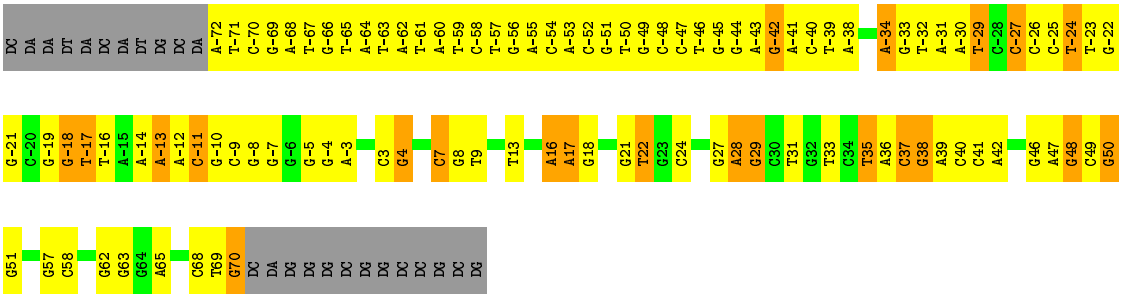
Chain H:



- Molecule 5: Widom 601 sequence reverse

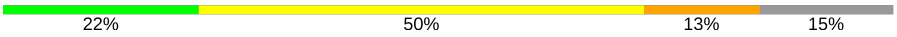
Chain I:

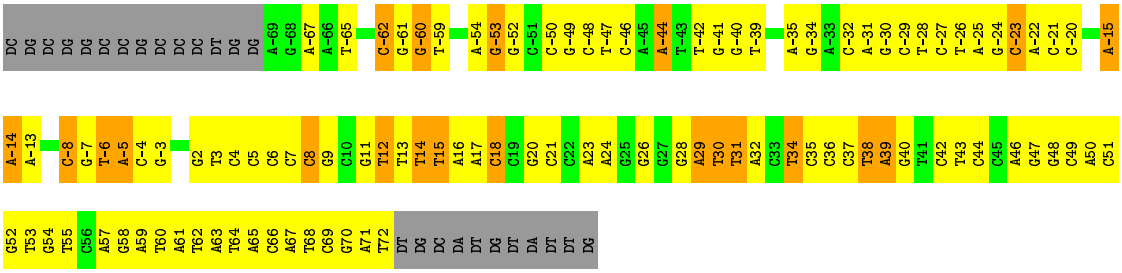




• Molecule 6: Widom 601 sequence forward

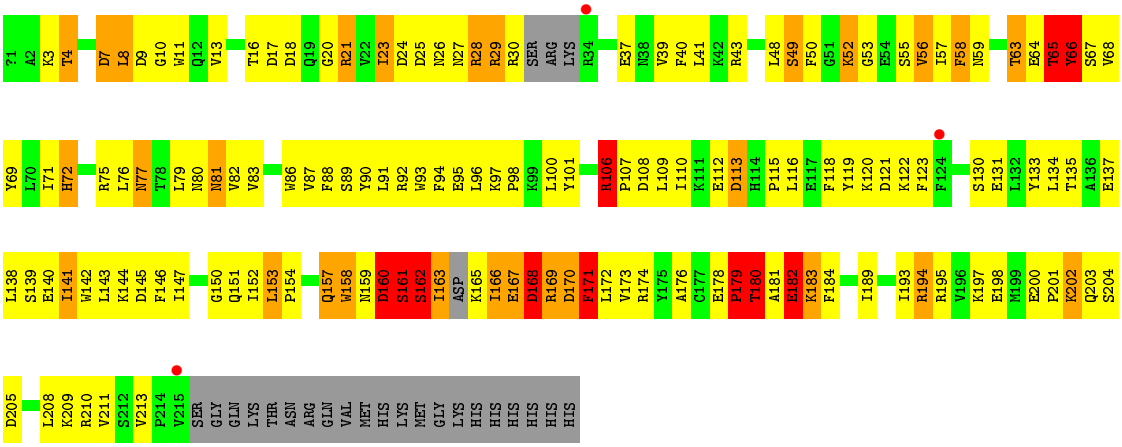
Chain J:





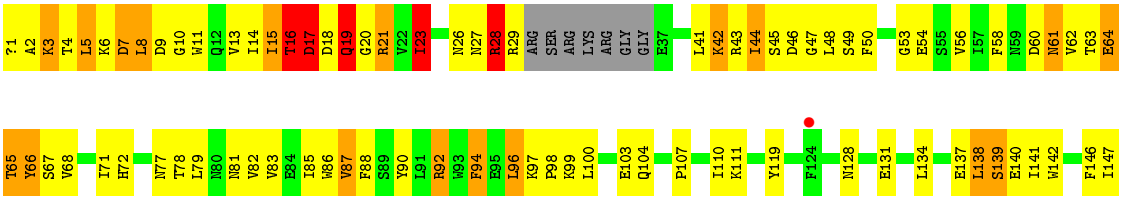
• Molecule 7: Regulatory protein SIR3

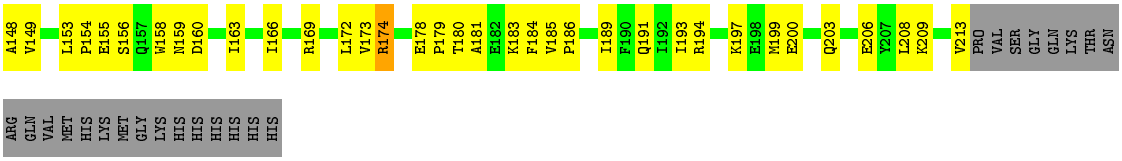
Chain K:



• Molecule 7: Regulatory protein SIR3

Chain L:




A148 V149 L153 P154 E155 S156 Q157 W158 N159 D160 I163 I166 R169 L172 V173 R174 E178 P179 T180 A181 E182 K183 F184 V185 P186 I189 F190 Q191 I192 I193 R194 K197 E198 M199 E200 Q203 E206 Y207 L208 K209 V213 PRO VAL SER GLY GLN LYS THR ASN
ARG GLN VAL MET HIS LYS MET GLY LYS HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	105.51Å 105.51Å 488.23Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.31 20.00 – 3.31	Depositor EDS
% Data completeness (in resolution range)	97.5 (20.00-3.31) 97.5 (20.00-3.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.31 (at 3.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.238 , 0.295 0.255 , 0.303	Depositor DCC
R_{free} test set	2217 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	118.4	Xtriage
Anisotropy	0.164	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 10.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.098 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	15140	wwPDB-VP
Average B, all atoms (Å^2)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACE

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.62	0/811	0.77	0/1088
1	E	0.71	2/737 (0.3%)	0.91	4/988 (0.4%)
2	B	0.67	0/724	0.87	1/966 (0.1%)
2	F	0.99	4/682 (0.6%)	1.07	5/913 (0.5%)
3	C	0.59	0/763	0.84	1/1033 (0.1%)
3	G	0.61	0/778	0.93	4/1053 (0.4%)
4	D	0.62	0/684	0.85	0/923
4	H	0.66	0/701	0.81	1/944 (0.1%)
5	I	0.76	3/3308 (0.1%)	1.45	64/5109 (1.3%)
6	J	0.75	1/3244 (0.0%)	1.42	55/5000 (1.1%)
7	K	0.95	8/1797 (0.4%)	1.05	17/2428 (0.7%)
7	L	0.84	6/1773 (0.3%)	0.90	10/2398 (0.4%)
All	All	0.77	24/16002 (0.1%)	1.18	162/22843 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	2
2	F	0	6
3	G	0	6
7	K	0	9
7	L	0	3
All	All	0	26

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	K	153	LEU	C-N	17.69	1.67	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	27	GLN	C-N	14.93	1.59	1.33
7	L	19	GLN	C-N	14.50	1.59	1.33
7	K	182	GLU	C-N	13.21	1.64	1.34
7	L	18	ASP	C-N	12.34	1.62	1.34
1	E	65	LEU	C-N	10.62	1.54	1.34
7	K	180	THR	C-N	9.17	1.55	1.34
2	F	21	VAL	C-N	9.15	1.55	1.34
2	F	26	ILE	C-N	9.04	1.54	1.34
7	K	179	PRO	C-N	8.15	1.52	1.34
2	F	25	ASN	C-N	8.12	1.52	1.34
7	K	183	LYS	C-N	7.97	1.52	1.34
7	K	162	SER	C-N	7.75	1.51	1.34
7	K	65	THR	C-N	7.42	1.51	1.34
7	K	66	TYR	C-N	7.41	1.51	1.34
7	L	16	THR	C-N	6.95	1.50	1.34
5	I	-24	DT	C1'-N1	6.16	1.57	1.49
7	L	17	ASP	C-N	6.05	1.48	1.34
6	J	38	DT	C1'-N1	5.82	1.56	1.49
1	E	64	LYS	C-N	5.66	1.47	1.34
7	L	23	ILE	C-N	-5.46	1.21	1.34
5	I	-39	DT	C1'-N1	5.37	1.56	1.49
5	I	-25	DC	C1'-N1	5.16	1.55	1.49
7	L	186	PRO	N-CD	5.11	1.55	1.47

All (162) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	63	ARG	O-C-N	-13.77	100.67	122.70
2	F	27	GLN	O-C-N	-12.67	101.67	123.20
6	J	-30	DG	O4'-C1'-N9	11.54	116.07	108.00
3	G	23	LEU	O-C-N	-11.24	104.71	122.70
6	J	38	DT	O4'-C1'-N1	10.37	115.26	108.00
5	I	-27	DC	O4'-C1'-N1	10.06	115.04	108.00
5	I	17	DA	O4'-C1'-N9	10.02	115.01	108.00
5	I	-13	DA	O4'-C1'-N9	9.68	114.78	108.00
5	I	-34	DA	O4'-C1'-N9	9.63	114.74	108.00
2	F	29	ILE	O-C-N	-9.56	107.40	122.70
5	I	38	DG	O4'-C1'-N9	9.34	114.54	108.00
6	J	37	DC	O4'-C1'-N1	8.87	114.21	108.00
6	J	-23	DC	O4'-C1'-N1	8.84	114.19	108.00
7	L	23	ILE	O-C-N	-8.83	108.57	122.70
7	K	161	SER	O-C-N	-8.67	108.83	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	I	37	DC	O4'-C1'-N1	8.55	113.99	108.00
5	I	24	DC	O4'-C1'-N1	8.54	113.98	108.00
5	I	-25	DC	O4'-C1'-N1	8.49	113.94	108.00
6	J	-20	DC	O4'-C1'-N1	8.46	113.92	108.00
5	I	28	DA	O4'-C1'-N9	8.45	113.92	108.00
5	I	-24	DT	O4'-C1'-N1	8.44	113.91	108.00
6	J	-50	DC	O4'-C1'-N1	8.43	113.90	108.00
5	I	58	DC	O4'-C1'-N1	8.37	113.86	108.00
7	K	160	ASP	O-C-N	-8.04	109.84	122.70
5	I	13	DT	O4'-C1'-N1	7.99	113.59	108.00
7	L	79	LEU	N-CA-C	7.95	132.47	111.00
6	J	20	DG	O4'-C1'-N9	7.88	113.51	108.00
5	I	48	DG	O4'-C1'-N9	7.83	113.48	108.00
6	J	-8	DC	O4'-C1'-N1	7.78	113.44	108.00
6	J	-15	DA	O4'-C1'-N9	7.77	113.44	108.00
5	I	17	DA	C8-N9-C4	-7.70	102.72	105.80
6	J	-41	DG	O4'-C1'-N9	7.70	113.39	108.00
5	I	63	DG	O4'-C1'-N9	7.67	113.37	108.00
6	J	-14	DA	O4'-C1'-N9	7.59	113.31	108.00
6	J	39	DA	O4'-C1'-N9	7.56	113.30	108.00
5	I	68	DC	O4'-C1'-N1	7.56	113.29	108.00
5	I	-42	DG	O4'-C1'-N9	7.53	113.27	108.00
7	L	17	ASP	O-C-N	-7.49	110.71	122.70
6	J	-67	DA	O4'-C1'-N9	7.46	113.22	108.00
6	J	-31	DA	O4'-C1'-N9	7.46	113.22	108.00
7	L	19	GLN	O-C-N	7.44	135.85	123.20
6	J	12	DT	N3-C4-O4	7.44	124.36	119.90
5	I	70	DG	O4'-C1'-N9	7.36	113.15	108.00
7	L	19	GLN	CA-C-N	-7.25	101.70	116.20
5	I	-17	DT	N3-C4-O4	7.23	124.24	119.90
6	J	-25	DA	O4'-C1'-N9	7.21	113.05	108.00
3	G	22	GLY	O-C-N	-7.17	111.23	122.70
5	I	40	DC	O4'-C1'-N1	7.15	113.00	108.00
5	I	-19	DG	O4'-C1'-N9	7.02	112.92	108.00
7	L	15	ILE	O-C-N	-6.97	111.54	122.70
7	K	66	TYR	CA-C-N	-6.90	102.01	117.20
7	K	168	ASP	O-C-N	-6.89	111.68	122.70
6	J	21	DC	O4'-C1'-N1	6.86	112.81	108.00
2	F	21	VAL	O-C-N	-6.78	111.85	122.70
5	I	-22	DG	O4'-C1'-N9	6.76	112.73	108.00
6	J	-53	DG	O4'-C1'-N9	6.76	112.73	108.00
5	I	22	DT	O4'-C1'-N1	6.75	112.72	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	I	-25	DC	C6-N1-C2	-6.74	117.60	120.30
5	I	-24	DT	C6-N1-C2	-6.71	117.95	121.30
6	J	-44	DA	O4'-C1'-N9	6.71	112.69	108.00
7	K	106	ARG	NE-CZ-NH1	6.68	123.64	120.30
6	J	40	DG	O4'-C1'-N9	6.66	112.66	108.00
6	J	-32	DC	O4'-C1'-N1	6.61	112.63	108.00
3	G	19	SER	O-C-N	-6.59	112.16	122.70
7	K	179	PRO	C-N-CA	-6.43	105.63	121.70
6	J	-28	DT	O4'-C1'-N1	6.42	112.50	108.00
7	K	66	TYR	O-C-N	6.41	132.95	122.70
5	I	-14	DA	O4'-C1'-N9	6.40	112.48	108.00
5	I	-9	DC	O4'-C1'-N1	6.36	112.45	108.00
5	I	-16	DT	N3-C4-O4	6.35	123.71	119.90
5	I	-11	DC	O4'-C1'-C2'	-6.34	100.83	105.90
5	I	65	DA	O4'-C1'-N9	6.26	112.38	108.00
7	K	179	PRO	O-C-N	6.25	132.69	122.70
5	I	70	DG	C3'-C2'-C1'	-6.21	95.04	102.50
6	J	3	DT	N3-C4-O4	6.21	123.63	119.90
6	J	-40	DG	C8-N9-C4	-6.16	103.94	106.40
5	I	18	DG	C8-N9-C4	-6.13	103.95	106.40
7	K	65	THR	CB-CA-C	6.12	128.11	111.60
6	J	-5	DA	O4'-C1'-N9	6.11	112.28	108.00
5	I	-40	DC	O4'-C1'-N1	6.04	112.23	108.00
5	I	-21	DG	O4'-C1'-N9	6.04	112.23	108.00
6	J	14	DT	C5-C4-O4	-6.02	120.68	124.90
5	I	33	DT	C5-C4-O4	-6.02	120.69	124.90
6	J	28	DG	P-O5'-C5'	-6.01	111.29	120.90
6	J	29	DA	C3'-C2'-C1'	-5.98	95.33	102.50
6	J	-52	DG	O4'-C1'-N9	5.96	112.17	108.00
6	J	38	DT	N3-C4-O4	5.89	123.43	119.90
7	K	167	GLU	C-N-CA	5.87	136.39	121.70
1	E	63	ARG	CA-C-N	5.84	130.04	117.20
6	J	-40	DG	O4'-C1'-N9	5.81	112.07	108.00
6	J	9	DG	O4'-C1'-N9	-5.80	103.94	108.00
6	J	-65	DT	O4'-C1'-N1	5.80	112.06	108.00
6	J	2	DG	O4'-C1'-N9	5.80	112.06	108.00
6	J	30	DT	N3-C4-O4	5.79	123.37	119.90
6	J	11	DG	O4'-C1'-N9	5.78	112.05	108.00
6	J	12	DT	O4'-C1'-N1	5.78	112.05	108.00
6	J	-62	DC	O4'-C1'-N1	5.77	112.04	108.00
7	L	19	GLN	C-N-CA	-5.75	110.22	122.30
7	K	167	GLU	O-C-N	-5.75	113.50	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	I	-39	DT	O4'-C1'-N1	5.74	112.02	108.00
7	L	17	ASP	C-N-CA	-5.74	107.34	121.70
7	L	185	VAL	C-N-CD	5.72	140.41	128.40
1	E	63	ARG	C-N-CA	5.71	135.98	121.70
1	E	64	LYS	O-C-N	-5.71	113.56	122.70
6	J	28	DG	O4'-C1'-N9	5.68	111.97	108.00
6	J	-60	DG	O4'-C1'-N9	5.66	111.96	108.00
7	K	182	GLU	C-N-CA	-5.65	107.58	121.70
5	I	4	DG	O4'-C1'-N9	-5.64	104.05	108.00
6	J	-39	DT	O4'-C1'-N1	5.64	111.95	108.00
5	I	31	DT	O4'-C1'-N1	5.63	111.94	108.00
6	J	-59	DT	O4'-C1'-N1	5.63	111.94	108.00
3	G	58	LEU	CA-CB-CG	-5.61	102.41	115.30
5	I	31	DT	N3-C4-O4	5.60	123.26	119.90
5	I	38	DG	C8-N9-C4	-5.59	104.16	106.40
5	I	-27	DC	O4'-C1'-C2'	-5.58	101.44	105.90
5	I	35	DT	O4'-C1'-N1	5.57	111.90	108.00
5	I	33	DT	N3-C4-O4	5.56	123.24	119.90
5	I	-25	DC	N3-C4-C5	-5.55	119.68	121.90
7	K	182	GLU	O-C-N	-5.54	113.83	122.70
6	J	12	DT	C5-C4-O4	-5.54	121.02	124.90
5	I	9	DT	N3-C4-O4	5.52	123.21	119.90
6	J	15	DT	N3-C4-O4	5.47	123.18	119.90
5	I	29	DG	O4'-C1'-N9	5.45	111.81	108.00
6	J	-29	DC	O4'-C1'-N1	5.45	111.81	108.00
5	I	18	DG	O4'-C1'-N9	5.43	111.80	108.00
7	K	179	PRO	CA-C-N	-5.43	105.25	117.20
6	J	18	DC	C2-N1-C1'	5.43	124.77	118.80
6	J	34	DT	N3-C4-O4	5.42	123.15	119.90
3	C	36	LYS	N-CA-C	5.40	125.59	111.00
2	F	24	ASP	O-C-N	-5.39	114.07	122.70
2	B	62	LEU	CA-CB-CG	-5.39	102.91	115.30
7	K	160	ASP	C-N-CA	5.38	135.15	121.70
5	I	-29	DT	N3-C4-O4	5.38	123.13	119.90
5	I	70	DG	C1'-O4'-C4'	-5.37	104.73	110.10
5	I	-42	DG	C8-N9-C4	-5.36	104.25	106.40
5	I	17	DA	N7-C8-N9	5.36	116.48	113.80
5	I	-26	DC	O4'-C1'-N1	5.34	111.74	108.00
5	I	8	DG	C8-N9-C4	-5.34	104.26	106.40
4	H	105	GLY	N-CA-C	5.34	126.44	113.10
5	I	27	DG	O4'-C1'-N9	5.33	111.73	108.00
6	J	-42	DT	O4'-C1'-N1	5.32	111.72	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	I	16	DA	O4'-C1'-N9	5.27	111.69	108.00
7	K	180	THR	C-N-CA	-5.27	108.52	121.70
5	I	69	DT	N3-C4-O4	5.26	123.06	119.90
5	I	50	DG	O4'-C1'-N9	5.23	111.66	108.00
6	J	8	DC	C2-N1-C1'	5.21	124.53	118.80
6	J	18	DC	N3-C4-C5	-5.19	119.82	121.90
5	I	-18	DG	C8-N9-C4	-5.18	104.33	106.40
5	I	-13	DA	C8-N9-C4	-5.17	103.73	105.80
5	I	57	DG	O4'-C1'-N9	5.15	111.60	108.00
5	I	7	DC	P-O5'-C5'	-5.14	112.67	120.90
7	K	171	PHE	O-C-N	-5.12	114.50	122.70
5	I	8	DG	N3-C4-C5	-5.12	126.04	128.60
6	J	7	DC	N3-C4-C5	-5.12	119.85	121.90
7	L	23	ILE	CA-C-N	5.12	128.46	117.20
6	J	8	DC	N1-C2-O2	5.09	121.96	118.90
5	I	13	DT	N3-C4-O4	5.09	122.95	119.90
6	J	31	DT	O4'-C1'-N1	5.08	111.56	108.00
5	I	-24	DT	N3-C4-O4	5.07	122.94	119.90
2	F	23	ARG	O-C-N	-5.07	114.59	122.70
6	J	-49	DG	O4'-C1'-N9	5.02	111.51	108.00
6	J	-6	DT	O4'-C1'-C2'	-5.00	101.90	105.90

There are no chirality outliers.

All (26) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	63	ARG	Mainchain
1	E	65	LEU	Mainchain
2	F	19	ARG	Peptide
2	F	21	VAL	Mainchain
2	F	23	ARG	Mainchain
2	F	24	ASP	Mainchain
2	F	27	GLN	Mainchain
2	F	29	ILE	Mainchain
3	G	18	SER	Mainchain
3	G	19	SER	Mainchain
3	G	21	ALA	Mainchain
3	G	22	GLY	Mainchain
3	G	23	LEU	Mainchain
3	G	24	GLN	Mainchain
7	K	158	TRP	Mainchain
7	K	159	ASN	Mainchain

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Mol	Chain	Res	Type	Group
7	K	161	SER	Mainchain
7	K	168	ASP	Mainchain
7	K	169	ARG	Mainchain
7	K	170	ASP	Mainchain
7	K	171	PHE	Mainchain
7	K	182	GLU	Mainchain
7	K	65	THR	Peptide
7	L	16	THR	Mainchain
7	L	17	ASP	Mainchain
7	L	23	ILE	Mainchain

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	799	0	837	41	0
1	E	729	0	760	44	0
2	B	716	0	773	44	0
2	F	674	0	723	87	0
3	C	753	0	793	99	0
3	G	768	0	812	98	0
4	D	673	0	693	121	0
4	H	690	0	710	81	0
5	I	2946	0	1607	139	0
6	J	2895	0	1594	136	0
7	K	1761	0	1737	177	1
7	L	1736	0	1707	182	1
All	All	15140	0	12746	1027	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 38.

All (1027) 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)
4:D:39:ALA:HB1	4:D:60:MET:CE	1.20	1.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:39:ALA:CB	4:D:60:MET:CE	1.74	1.55
7:L:1:ACE:CH3	7:L:142:TRP:CD1	1.89	1.53
7:L:10:GLY:C	7:L:44:ILE:CD1	1.77	1.50
7:L:1:ACE:H3	7:L:142:TRP:CD1	0.95	1.47
7:K:153:LEU:C	7:K:154:PRO:N	1.67	1.41
4:D:39:ALA:CB	4:D:60:MET:HE1	0.91	1.38
4:D:46:LEU:CD1	4:D:50:HIS:O	1.70	1.36
7:L:16:THR:CG2	7:L:21:ARG:O	1.76	1.31
2:F:19:ARG:HH12	6:J:-22:DA:C4'	1.45	1.29
7:L:1:ACE:CH3	7:L:142:TRP:NE1	1.97	1.27
7:L:15:ILE:HB	7:L:23:ILE:CD1	1.66	1.25
1:A:80:THR:OG1	7:L:140:GLU:OE1	1.53	1.24
7:L:155:GLU:OE1	7:L:174:ARG:NE	1.71	1.23
3:C:38:ASN:OD1	3:G:38:ASN:HB3	1.30	1.23
7:L:11:TRP:N	7:L:44:ILE:HD11	1.51	1.23
4:D:39:ALA:O	4:D:42:VAL:HG23	1.34	1.22
7:L:10:GLY:C	7:L:44:ILE:HD11	0.82	1.20
4:D:39:ALA:HB2	4:D:60:MET:HE1	1.22	1.19
7:L:10:GLY:O	7:L:44:ILE:CD1	1.88	1.18
7:L:10:GLY:O	7:L:44:ILE:HD11	1.39	1.17
4:D:46:LEU:HD11	4:D:50:HIS:O	1.21	1.15
7:L:1:ACE:H3	7:L:142:TRP:NE1	1.56	1.13
7:L:15:ILE:HB	7:L:23:ILE:CG1	1.81	1.10
4:D:110:HIS:O	4:D:113:SER:OG	1.67	1.10
4:D:47:LYS:HA	4:D:51:PRO:HA	1.29	1.09
2:F:19:ARG:HH12	6:J:-22:DA:H4'	1.11	1.08
3:C:32:ARG:HG3	3:C:33:LEU:HD23	1.33	1.08
3:C:25:PHE:CZ	4:D:41:TYR:CE2	2.41	1.08
2:F:26:ILE:HD11	2:F:55:ARG:HB3	1.09	1.07
2:F:26:ILE:HD11	2:F:55:ARG:CB	1.83	1.07
3:C:25:PHE:CE1	4:D:41:TYR:CD2	2.43	1.07
7:L:10:GLY:CA	7:L:44:ILE:HD11	1.85	1.06
3:C:50:TYR:OH	4:D:112:VAL:HG13	1.54	1.05
5:I:-70:DC:H2'	5:I:-69:DG:C8	1.91	1.05
7:K:66:TYR:CD2	7:K:92:ARG:NH2	2.24	1.05
5:I:-53:DA:H2"	5:I:-52:DC:H5'	1.38	1.05
6:J:61:DA:H2"	6:J:62:DT:C5	1.93	1.03
7:K:158:TRP:HA	7:K:160:ASP:OD1	1.59	1.03
7:L:16:THR:HG22	7:L:21:ARG:O	0.87	1.03
7:L:60:ASP:OD1	7:L:63:THR:N	1.90	1.03
4:D:43:TYR:OH	5:I:-53:DA:OP2	1.73	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:46:LEU:HD12	4:D:50:HIS:O	1.57	1.02
7:L:5:LEU:HA	7:L:8:LEU:HD11	1.35	1.02
4:D:110:HIS:C	4:D:113:SER:HG	1.63	1.02
2:F:26:ILE:CD1	2:F:55:ARG:HB3	1.88	1.02
5:I:-58:DC:H2"	5:I:-57:DT:H71	1.40	1.02
3:C:32:ARG:NH1	5:I:-44:DG:P	2.33	1.01
7:L:15:ILE:HB	7:L:23:ILE:HG12	1.40	1.01
1:A:79:LYS:HE3	2:B:74:GLU:OE2	1.62	0.99
7:L:11:TRP:N	7:L:44:ILE:CD1	2.16	0.99
3:C:32:ARG:HH12	5:I:-44:DG:P	1.86	0.98
3:C:32:ARG:NH1	5:I:-44:DG:OP2	1.96	0.98
3:C:25:PHE:CZ	4:D:41:TYR:CZ	2.52	0.98
3:C:25:PHE:CE1	4:D:41:TYR:CE2	2.52	0.98
7:L:8:LEU:O	7:L:11:TRP:HB2	1.64	0.98
2:B:62:LEU:O	2:B:66:ILE:HG13	1.61	0.98
2:F:26:ILE:CD1	2:F:55:ARG:HD3	1.95	0.97
4:D:110:HIS:C	4:D:113:SER:OG	2.02	0.97
1:E:97:GLU:HG2	2:F:37:LEU:HD11	1.47	0.96
4:D:46:LEU:HD11	4:D:53:THR:OG1	1.65	0.96
7:L:156:SER:O	7:L:160:ASP:HB3	1.65	0.95
5:I:-60:DA:H2'	5:I:-59:DT:H71	1.46	0.95
1:A:80:THR:CB	7:L:140:GLU:OE1	2.14	0.95
2:F:23:ARG:HD2	7:K:213:VAL:HG22	1.47	0.95
1:E:61:LEU:O	2:F:36:ARG:NH2	2.00	0.94
7:L:8:LEU:H	7:L:8:LEU:HD13	1.29	0.94
7:L:1:ACE:H2	7:L:142:TRP:NE1	1.80	0.94
2:F:92:ARG:NH2	4:H:102:LEU:HD13	1.82	0.94
7:L:1:ACE:CH3	7:L:142:TRP:HE1	1.80	0.93
3:G:50:TYR:CD2	4:H:92:SER:HB3	2.03	0.93
2:F:19:ARG:NH1	6:J:-22:DA:C4'	2.31	0.93
7:L:44:ILE:H	7:L:44:ILE:HD13	1.33	0.93
6:J:66:DC:H2"	6:J:67:DA:N7	1.84	0.92
5:I:-51:DG:H2"	5:I:-50:DT:H5'	1.48	0.92
3:C:38:ASN:OD1	3:G:38:ASN:CB	2.18	0.91
4:D:39:ALA:CB	4:D:60:MET:HE2	1.98	0.91
4:D:39:ALA:HB1	4:D:60:MET:SD	2.11	0.91
3:C:25:PHE:HE1	4:D:41:TYR:CD2	1.90	0.90
2:F:19:ARG:NH1	6:J:-22:DA:O5'	2.04	0.90
3:G:31:HIS:NE2	3:G:43:VAL:HG22	1.86	0.90
7:L:15:ILE:HB	7:L:23:ILE:HD11	1.51	0.90
5:I:-58:DC:H2"	5:I:-57:DT:C7	2.01	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:155:GLU:OE1	7:L:174:ARG:CD	2.20	0.90
5:I:-51:DG:N2	6:J:51:DC:O2	2.05	0.89
2:B:75:HIS:CD2	4:D:97:THR:HG21	2.07	0.89
4:D:39:ALA:O	4:D:42:VAL:CG2	2.20	0.89
5:I:-49:DG:H2"	5:I:-48:DC:C5	2.07	0.88
3:C:32:ARG:CG	3:C:33:LEU:HD23	2.02	0.88
5:I:-53:DA:H2"	5:I:-52:DC:C5'	2.03	0.88
7:K:88:PHE:HA	7:K:137:GLU:O	1.74	0.88
3:G:35:ARG:HG2	3:G:43:VAL:HG11	1.55	0.87
5:I:-47:DC:H4'	5:I:-46:DT:H5'	1.55	0.87
4:D:39:ALA:HB2	4:D:60:MET:CE	1.79	0.87
5:I:-62:DA:H2"	5:I:-61:DT:C6	2.09	0.87
2:F:19:ARG:NH1	6:J:-22:DA:H4'	1.88	0.87
6:J:50:DA:H2"	6:J:51:DC:H5'	1.58	0.86
1:A:85:GLN:NE2	5:I:-24:DT:OP1	2.08	0.86
7:L:15:ILE:HD12	7:L:23:ILE:HD13	1.58	0.86
4:D:110:HIS:HE1	7:L:28:ARG:HB3	1.40	0.86
7:L:87:VAL:HG21	7:L:141:ILE:HD13	1.58	0.85
5:I:-59:DT:H2"	5:I:-58:DC:H5	1.39	0.85
3:C:23:LEU:HD12	3:C:24:GLN:H	1.39	0.85
3:C:38:ASN:CG	3:G:38:ASN:HB3	1.96	0.85
7:K:66:TYR:HE2	7:K:168:ASP:OD2	1.57	0.85
2:F:75:HIS:HA	4:H:93:ARG:HH21	1.41	0.85
7:K:63:THR:HB	7:K:65:THR:HG22	1.58	0.85
4:D:46:LEU:O	4:D:46:LEU:HD12	1.77	0.85
4:D:39:ALA:C	4:D:42:VAL:HG23	1.97	0.85
2:B:30:THR:HG23	2:B:33:ALA:H	1.42	0.85
7:K:158:TRP:CD1	7:K:172:LEU:HB2	2.12	0.84
5:I:-63:DT:H1'	5:I:-62:DA:H5'	1.59	0.84
5:I:-62:DA:H2"	5:I:-61:DT:C5	2.13	0.84
3:C:24:GLN:OE1	4:D:48:GLN:OE1	1.94	0.84
5:I:-58:DC:H1'	5:I:-57:DT:C5	2.13	0.84
1:A:97:GLU:HG2	2:B:37:LEU:HD21	1.60	0.84
1:E:63:ARG:HH11	2:F:30:THR:HG22	1.43	0.84
3:C:24:GLN:CD	4:D:48:GLN:OE1	2.17	0.83
2:F:19:ARG:HH12	6:J:-22:DA:C3'	1.91	0.83
3:C:90:ASP:OD2	7:L:29:ARG:NH2	2.11	0.83
7:L:5:LEU:HA	7:L:8:LEU:CD1	2.09	0.83
7:K:194:ARG:NH2	7:K:198:GLU:OE1	2.12	0.83
7:L:15:ILE:CB	7:L:23:ILE:CD1	2.55	0.83
7:K:181:ALA:HB1	7:K:184:PHE:CZ	2.14	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:50:TYR:HH	4:D:112:VAL:HG13	1.41	0.82
2:F:23:ARG:CD	7:K:213:VAL:HG22	2.08	0.82
2:F:75:HIS:HA	4:H:93:ARG:NH2	1.94	0.82
2:F:26:ILE:O	2:F:26:ILE:HD13	1.79	0.82
7:L:10:GLY:O	7:L:44:ILE:HD13	1.80	0.82
5:I:-59:DT:H2"	5:I:-58:DC:C5	2.15	0.81
4:H:102:LEU:HD22	4:H:102:LEU:H	1.45	0.81
7:L:60:ASP:N	7:L:65:THR:O	2.12	0.81
1:A:42:ARG:HG3	5:I:70:DG:H5"	1.63	0.81
6:J:61:DA:H2"	6:J:62:DT:C4	2.15	0.81
4:D:110:HIS:CE1	7:L:28:ARG:HB3	2.15	0.81
3:C:104:GLN:HB2	4:D:58:LYS:HZ2	1.46	0.80
7:L:15:ILE:CB	7:L:23:ILE:HG12	2.11	0.80
1:A:119:ILE:HG12	2:B:43:VAL:HG11	1.64	0.80
7:K:162:SER:HA	7:K:163:ILE:HG23	1.64	0.80
1:E:97:GLU:O	1:E:101:VAL:HG23	1.81	0.79
7:K:202:LYS:O	7:K:205:ASP:HB2	1.83	0.79
2:F:19:ARG:HH12	6:J:-22:DA:C5'	1.94	0.79
2:F:23:ARG:HD2	7:K:213:VAL:CG2	2.12	0.79
3:G:50:TYR:OH	4:H:96:GLN:CB	2.31	0.79
7:K:161:SER:OG	7:K:162:SER:N	2.16	0.79
7:K:66:TYR:N	7:K:92:ARG:HH12	1.52	0.78
4:D:69:ASP:OD2	2:F:98:TYR:OH	2.01	0.78
3:C:32:ARG:O	3:C:35:ARG:N	2.16	0.78
7:K:58:PHE:HD2	7:K:146:PHE:HA	1.49	0.78
3:G:31:HIS:CD2	3:G:43:VAL:HG22	2.19	0.77
5:I:-58:DC:H1'	5:I:-57:DT:C6	2.17	0.77
4:D:39:ALA:HB3	4:D:60:MET:CE	2.12	0.77
7:L:155:GLU:CD	7:L:174:ARG:NE	2.37	0.77
3:G:31:HIS:CD2	3:G:43:VAL:CG2	2.67	0.77
3:G:92:GLU:HB3	4:H:107:LEU:HD11	1.67	0.77
7:L:97:LYS:HB2	7:L:100:LEU:HD12	1.67	0.77
5:I:-60:DA:H2'	5:I:-59:DT:C7	2.13	0.77
4:D:110:HIS:HA	4:D:113:SER:OG	1.84	0.77
4:H:38:TYR:O	4:H:41:TYR:N	2.16	0.77
7:K:66:TYR:HB2	7:K:92:ARG:NH2	1.99	0.77
5:I:-51:DG:H2"	5:I:-50:DT:C5'	2.14	0.77
5:I:-57:DT:H2"	5:I:-56:DG:N7	2.00	0.76
5:I:-59:DT:H4'	5:I:-58:DC:OP1	1.85	0.76
7:L:86:TRP:HE3	7:L:138:LEU:HD22	1.50	0.76
3:G:39:TYR:O	4:H:79:SER:OG	2.01	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:71:ILE:HA	7:K:87:VAL:HG12	1.68	0.76
3:C:20:ARG:HD3	3:C:21:ALA:H	1.50	0.76
1:E:101:VAL:HG11	2:F:40:ARG:HG2	1.68	0.76
5:I:-60:DA:C2'	5:I:-59:DT:H71	2.15	0.76
7:K:66:TYR:HD2	7:K:92:ARG:NH2	1.81	0.76
4:H:102:LEU:HD22	4:H:102:LEU:N	2.00	0.76
6:J:61:DA:H4'	6:J:62:DT:OP1	1.84	0.76
7:K:158:TRP:NE1	7:K:172:LEU:HB2	2.01	0.76
4:H:102:LEU:HB2	4:H:103:LEU:HD23	1.69	0.75
5:I:-59:DT:H1'	5:I:-58:DC:C5	2.21	0.75
7:L:156:SER:O	7:L:160:ASP:CB	2.35	0.75
3:C:25:PHE:HZ	4:D:41:TYR:CE2	1.99	0.75
5:I:-60:DA:C5	5:I:-59:DT:C4	2.74	0.75
1:E:63:ARG:HH11	2:F:30:THR:CG2	1.99	0.75
7:K:89:SER:O	7:K:135:THR:OG1	2.03	0.75
7:L:96:LEU:HD11	7:L:184:PHE:HZ	1.51	0.74
3:G:50:TYR:OH	4:H:96:GLN:HB2	1.87	0.74
7:L:61:ASN:HA	7:L:64:GLU:OE1	1.88	0.74
5:I:-50:DT:H2"	5:I:-49:DG:C8	2.21	0.74
2:F:19:ARG:NH1	6:J:-22:DA:C3'	2.50	0.74
4:D:110:HIS:CA	4:D:113:SER:OG	2.35	0.74
7:L:5:LEU:N	7:L:5:LEU:HD12	2.03	0.74
4:D:46:LEU:HD11	4:D:53:THR:HG1	1.51	0.74
2:F:19:ARG:NH1	6:J:-22:DA:C5'	2.51	0.74
7:L:60:ASP:O	7:L:64:GLU:N	2.21	0.74
7:L:5:LEU:HD12	7:L:6:LYS:H	1.53	0.73
2:F:26:ILE:HD12	2:F:55:ARG:HD3	1.68	0.73
2:F:92:ARG:HH22	4:H:102:LEU:HD13	1.48	0.73
3:C:20:ARG:HD3	3:C:21:ALA:N	2.04	0.73
4:H:103:LEU:HD23	4:H:103:LEU:N	2.04	0.73
7:L:17:ASP:OD1	7:L:21:ARG:HB3	1.89	0.73
7:L:44:ILE:N	7:L:44:ILE:HD13	2.04	0.72
6:J:62:DT:H2"	6:J:63:DA:OP2	1.88	0.72
7:L:155:GLU:OE1	7:L:174:ARG:CG	2.37	0.72
3:G:32:ARG:HE	3:G:33:LEU:HD13	1.55	0.72
1:E:121:PRO:HB3	2:F:53:GLU:HG3	1.72	0.72
6:J:71:DA:H1'	6:J:72:DT:H5'	1.72	0.71
7:L:15:ILE:HD12	7:L:23:ILE:CD1	2.19	0.71
3:C:51:LEU:HB2	4:D:95:ILE:HD12	1.73	0.71
7:L:71:ILE:HA	7:L:87:VAL:HG12	1.70	0.71
4:H:39:ALA:HA	4:H:60:MET:HE1	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:50:DA:C2'	6:J:51:DC:H5'	2.21	0.71
3:C:104:GLN:NE2	1:E:58:THR:O	2.23	0.71
3:C:23:LEU:CD1	3:C:24:GLN:H	2.04	0.71
7:L:155:GLU:CD	7:L:174:ARG:HE	1.93	0.70
7:L:17:ASP:OD1	7:L:20:GLY:O	2.08	0.70
7:K:66:TYR:N	7:K:92:ARG:NH1	2.33	0.70
7:L:8:LEU:N	7:L:8:LEU:HD13	2.03	0.70
4:D:47:LYS:HA	4:D:51:PRO:CA	2.14	0.70
2:B:98:TYR:CE2	3:G:100:VAL:HG11	2.26	0.70
4:H:107:LEU:HD12	4:H:107:LEU:H	1.55	0.70
3:C:20:ARG:CD	3:C:21:ALA:H	2.04	0.70
3:C:50:TYR:OH	4:D:112:VAL:CG1	2.34	0.70
3:G:46:GLY:C	4:H:92:SER:OG	2.29	0.70
3:C:104:GLN:OE1	4:D:58:LYS:NZ	2.24	0.70
7:L:8:LEU:CD1	7:L:8:LEU:H	2.02	0.70
4:D:110:HIS:CE1	7:L:26:ASN:O	2.45	0.70
7:L:1:ACE:H2	7:L:142:TRP:HE1	1.45	0.70
7:L:4:THR:O	7:L:7:ASP:N	2.25	0.70
3:G:39:TYR:HB3	4:H:79:SER:HB2	1.74	0.69
6:J:51:DC:H2"	6:J:52:DG:OP2	1.92	0.69
7:K:17:ASP:HB2	7:K:20:GLY:H	1.57	0.69
7:L:5:LEU:CA	7:L:8:LEU:HD11	2.19	0.69
2:F:78:ARG:NH2	2:F:82:THR:OG1	2.24	0.69
3:G:37:GLY:HA3	3:G:39:TYR:CE1	2.27	0.69
7:K:3:LYS:C	7:K:3:LYS:HD3	2.13	0.69
7:K:66:TYR:HB2	7:K:92:ARG:CZ	2.23	0.69
1:A:61:LEU:HD12	2:B:37:LEU:HD23	1.75	0.68
1:A:85:GLN:HG3	2:B:82:THR:HA	1.74	0.68
5:I:-60:DA:C2	5:I:-59:DT:C2	2.81	0.68
7:K:158:TRP:O	7:K:160:ASP:N	2.25	0.68
6:J:50:DA:H1'	6:J:51:DC:C5'	2.23	0.68
7:K:160:ASP:O	7:K:162:SER:N	2.26	0.68
4:D:40:ILE:HG13	4:D:41:TYR:N	2.07	0.68
7:K:66:TYR:CB	7:K:92:ARG:HH22	2.06	0.68
4:D:100:ARG:NH2	7:L:77:ASN:O	2.27	0.68
3:C:78:ILE:N	4:D:54:GLY:O	2.25	0.68
2:F:56:GLY:O	2:F:60:VAL:HG23	1.94	0.68
7:L:200:GLU:N	7:L:200:GLU:OE1	2.26	0.68
7:K:66:TYR:H	7:K:92:ARG:HH12	1.41	0.68
5:I:-8:DG:H1	6:J:8:DC:H42	1.40	0.68
6:J:54:DG:H2'	6:J:54:DG:OP2	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:30:VAL:O	3:G:34:LEU:HD12	1.94	0.67
7:K:172:LEU:HD21	7:K:174:ARG:HD2	1.76	0.67
7:L:155:GLU:OE2	7:L:174:ARG:NH2	2.27	0.67
3:C:39:TYR:O	4:D:79:SER:OG	2.11	0.67
3:C:32:ARG:HG3	3:C:33:LEU:CD2	2.18	0.67
3:C:35:ARG:NH2	6:J:39:DA:OP2	2.18	0.67
7:L:15:ILE:CB	7:L:23:ILE:HD11	2.22	0.67
6:J:65:DA:C5	6:J:66:DC:C4	2.83	0.67
3:G:31:HIS:HD2	3:G:43:VAL:HG21	1.60	0.67
1:A:61:LEU:O	2:B:36:ARG:NH2	2.16	0.67
5:I:-32:DT:H2"	5:I:-31:DA:C8	2.29	0.67
1:A:69:ARG:NH2	6:J:17:DA:OP2	2.28	0.66
3:G:61:GLU:OE2	7:K:29:ARG:NH2	2.29	0.66
5:I:-51:DG:H2'	5:I:-50:DT:C6	2.30	0.66
7:K:72:HIS:O	7:K:72:HIS:ND1	2.28	0.66
6:J:61:DA:H2"	6:J:62:DT:C7	2.24	0.66
3:C:104:GLN:O	1:E:58:THR:OG1	2.12	0.66
7:K:8:LEU:HD23	7:K:8:LEU:C	2.16	0.66
6:J:35:DC:H1'	6:J:36:DC:C6	2.31	0.66
7:K:193:ILE:O	7:K:197:LYS:HG3	1.95	0.66
7:K:94:PHE:CE1	7:K:95:GLU:HG2	2.30	0.66
7:L:1:ACE:CH3	7:L:142:TRP:HD1	1.62	0.66
4:D:46:LEU:CD1	4:D:53:THR:OG1	2.41	0.66
7:K:94:PHE:CD1	7:K:95:GLU:N	2.63	0.66
5:I:47:DA:N6	6:J:-48:DC:H42	1.94	0.65
7:K:4:THR:HG23	7:K:7:ASP:HB3	1.77	0.65
1:A:80:THR:HB	7:L:140:GLU:OE1	1.95	0.65
4:D:99:VAL:HG13	4:D:103:LEU:HD12	1.77	0.65
2:F:26:ILE:CD1	2:F:55:ARG:CD	2.74	0.65
6:J:66:DC:H2"	6:J:67:DA:C8	2.30	0.65
7:K:13:VAL:HG22	7:K:41:LEU:HG	1.79	0.65
5:I:7:DC:H5"	5:I:7:DC:H6	1.62	0.65
7:K:58:PHE:CD2	7:K:146:PHE:HA	2.31	0.65
7:K:72:HIS:HE1	7:K:201:PRO:HA	1.61	0.65
7:L:27:ASN:O	7:L:29:ARG:N	2.30	0.65
6:J:15:DT:H2"	6:J:16:DA:C8	2.32	0.65
7:L:1:ACE:H3	7:L:142:TRP:HD1	0.83	0.65
2:B:52:GLU:OE1	2:B:53:GLU:N	2.30	0.64
2:F:25:ASN:O	2:F:28:GLY:N	2.30	0.64
6:J:59:DA:H2"	6:J:60:DT:O5'	1.97	0.64
3:G:88:ARG:HB3	3:G:108:LEU:HD11	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:91:LEU:HB2	7:K:95:GLU:OE1	1.96	0.64
4:D:46:LEU:C	4:D:46:LEU:HD12	2.16	0.64
7:K:109:LEU:O	7:K:119:TYR:OH	2.15	0.64
7:L:28:ARG:O	7:L:28:ARG:HG3	1.97	0.64
3:C:68:ASN:OD1	4:D:50:HIS:NE2	2.31	0.64
4:D:46:LEU:HD12	4:D:50:HIS:C	2.18	0.64
3:G:27:VAL:HG11	3:G:49:VAL:HG13	1.80	0.64
7:L:15:ILE:CD1	7:L:23:ILE:HD13	2.28	0.64
7:L:64:GLU:OE1	7:L:64:GLU:HA	1.96	0.64
5:I:-50:DT:H72	5:I:-49:DG:O6	1.98	0.64
3:G:31:HIS:CD2	3:G:43:VAL:HG21	2.33	0.64
7:K:24:ASP:O	7:K:26:ASN:ND2	2.30	0.64
7:L:63:THR:O	7:L:65:THR:HG22	1.97	0.64
3:C:32:ARG:HG3	3:C:33:LEU:N	2.12	0.64
4:D:47:LYS:O	4:D:51:PRO:HG3	1.97	0.64
7:K:77:ASN:C	7:K:77:ASN:HD22	2.01	0.64
7:L:191:GLN:OE1	7:L:194:ARG:NH1	2.30	0.64
3:C:51:LEU:HD23	4:D:95:ILE:HG23	1.80	0.63
4:D:120:THR:O	4:D:123:THR:N	2.30	0.63
7:K:154:PRO:O	7:K:158:TRP:CD1	2.51	0.63
1:A:79:LYS:HE3	2:B:74:GLU:CD	2.17	0.63
7:K:16:THR:HB	7:K:20:GLY:HA2	1.81	0.63
7:L:63:THR:HB	7:L:65:THR:CG2	2.29	0.63
2:F:26:ILE:HD11	2:F:55:ARG:CG	2.28	0.63
7:L:8:LEU:HD22	7:L:9:ASP:N	2.13	0.63
2:B:29:ILE:O	2:B:55:ARG:NH1	2.31	0.63
6:J:54:DG:H1'	6:J:55:DT:OP2	1.99	0.63
4:D:46:LEU:O	4:D:50:HIS:N	2.31	0.63
7:L:53:GLY:HA3	7:L:197:LYS:HE2	1.79	0.63
1:A:116:ARG:HD3	5:I:-3:DA:H3'	1.81	0.63
2:F:33:ALA:HA	2:F:36:ARG:CZ	2.29	0.63
6:J:50:DA:H1'	6:J:51:DC:H5'	1.79	0.63
7:K:158:TRP:C	7:K:160:ASP:H	2.02	0.63
7:K:80:ASN:O	7:K:81:ASN:ND2	2.31	0.62
3:G:82:HIS:HA	3:G:85:LEU:HD11	1.79	0.62
3:G:88:ARG:HB2	3:G:108:LEU:HD21	1.81	0.62
6:J:4:DC:H2"	6:J:5:DC:H6	1.64	0.62
7:L:97:LYS:HG3	7:L:181:ALA:HB3	1.81	0.62
7:K:58:PHE:HB2	7:K:145:ASP:O	1.99	0.62
7:K:166:ILE:HD12	7:K:166:ILE:H	1.63	0.62
7:L:11:TRP:CZ3	7:L:43:ARG:N	2.66	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:50:PHE:HB2	7:L:54:GLU:HG3	1.80	0.62
3:G:44:GLY:O	3:G:48:PRO:HD3	1.99	0.62
4:H:102:LEU:CB	4:H:103:LEU:HD23	2.30	0.62
7:K:41:LEU:HD23	7:K:143:LEU:HD11	1.82	0.62
5:I:-58:DC:C2'	5:I:-57:DT:H71	2.26	0.62
2:B:30:THR:HG23	2:B:33:ALA:N	2.12	0.62
5:I:21:DG:H1	6:J:-21:DC:H42	1.48	0.62
6:J:54:DG:H1'	6:J:55:DT:C6	2.35	0.61
2:F:32:PRO:HA	2:F:35:ARG:HB2	1.80	0.61
2:F:23:ARG:CZ	7:K:213:VAL:HG13	2.30	0.61
7:L:155:GLU:O	7:L:158:TRP:N	2.28	0.61
2:B:44:LYS:HG2	2:B:45:ARG:HG3	1.82	0.61
3:G:50:TYR:HD2	4:H:92:SER:HB3	1.61	0.61
7:L:46:ASP:OD1	7:L:48:LEU:N	2.16	0.61
3:G:31:HIS:O	3:G:35:ARG:HG3	2.00	0.61
5:I:-59:DT:C1'	5:I:-58:DC:C5	2.83	0.61
6:J:59:DA:H2'	6:J:60:DT:H71	1.83	0.61
7:L:15:ILE:O	7:L:23:ILE:HG12	2.00	0.61
7:L:63:THR:C	7:L:65:THR:HG22	2.21	0.61
2:F:26:ILE:HD13	2:F:55:ARG:HD3	1.81	0.61
3:G:64:GLU:HG2	4:H:49:VAL:HG11	1.81	0.61
5:I:-59:DT:C2'	5:I:-58:DC:C5	2.84	0.61
7:K:151:GLN:HB3	7:K:169:ARG:O	2.01	0.61
7:L:15:ILE:HB	7:L:23:ILE:HD13	1.76	0.61
7:L:173:VAL:HG11	7:L:189:ILE:HD13	1.83	0.61
7:L:3:LYS:O	7:L:82:VAL:HG23	2.00	0.61
2:B:73:THR:OG1	2:B:81:VAL:HG13	2.01	0.61
7:K:162:SER:HA	7:K:163:ILE:CG2	2.31	0.61
7:K:66:TYR:CB	7:K:92:ARG:NH2	2.62	0.61
3:C:29:ARG:HH22	6:J:49:DC:P	2.24	0.61
5:I:-63:DT:H2"	5:I:-62:DA:OP2	2.00	0.61
6:J:43:DT:H2"	6:J:44:DC:OP2	2.00	0.61
3:C:25:PHE:HZ	4:D:41:TYR:CZ	2.12	0.60
5:I:-4:DG:H1	6:J:4:DC:H42	1.49	0.60
7:L:4:THR:O	7:L:7:ASP:HB2	2.00	0.60
3:C:100:VAL:HG11	2:F:98:TYR:CE2	2.37	0.60
5:I:62:DG:N2	6:J:-62:DC:O2	2.30	0.60
7:K:181:ALA:HB1	7:K:184:PHE:HZ	1.66	0.60
7:L:2:ALA:O	7:L:82:VAL:HB	2.01	0.60
7:L:3:LYS:HA	7:L:81:ASN:HA	1.83	0.60
1:A:108:ASN:ND2	2:B:42:GLY:O	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:57:ILE:O	7:K:147:ILE:HB	2.01	0.60
4:D:39:ALA:HB1	4:D:42:VAL:HG21	1.83	0.60
7:L:46:ASP:OD1	7:L:47:GLY:N	2.35	0.60
5:I:-47:DC:C4'	5:I:-46:DT:H5'	2.30	0.60
1:E:72:ARG:NH2	6:J:-23:DC:OP1	2.34	0.60
5:I:46:DG:O6	6:J:-46:DC:N4	2.34	0.60
6:J:47:DG:H2"	6:J:48:DG:C8	2.36	0.60
7:K:172:LEU:HD11	7:K:174:ARG:HG3	1.84	0.60
3:C:24:GLN:NE2	4:D:48:GLN:OE1	2.35	0.60
3:G:50:TYR:CZ	4:H:96:GLN:HB2	2.36	0.60
3:C:32:ARG:NH1	5:I:-44:DG:OP1	2.33	0.60
3:G:47:ALA:N	4:H:92:SER:OG	2.34	0.59
6:J:67:DA:H2"	6:J:68:DT:OP2	2.00	0.59
1:A:121:PRO:HB3	2:B:53:GLU:HG3	1.85	0.59
4:D:41:TYR:O	4:D:44:LYS:HG3	2.02	0.59
1:E:63:ARG:NH1	6:J:-13:DA:H5"	2.16	0.59
5:I:-33:DG:H2"	5:I:-32:DT:OP2	2.02	0.59
4:D:38:TYR:C	4:D:64:ASN:HD21	2.05	0.59
6:J:63:DA:H2"	6:J:64:DT:OP2	2.00	0.59
6:J:60:DT:C2	6:J:61:DA:N7	2.70	0.59
2:F:26:ILE:C	2:F:26:ILE:HD13	2.23	0.59
3:G:27:VAL:HG21	3:G:49:VAL:HG12	1.84	0.59
4:H:117:LYS:HG2	4:H:121:LYS:HD2	1.85	0.59
5:I:-72:DA:H2"	5:I:-71:DT:O5'	2.02	0.59
7:L:11:TRP:CA	7:L:44:ILE:CD1	2.81	0.59
2:F:45:ARG:NH1	6:J:-4:DC:H4'	2.18	0.59
3:G:32:ARG:HE	3:G:33:LEU:CD1	2.16	0.59
5:I:-50:DT:C4	5:I:-49:DG:C6	2.91	0.59
2:B:14:GLY:HA3	7:L:63:THR:HG22	1.83	0.59
2:B:35:ARG:HH12	6:J:8:DC:P	2.26	0.59
4:H:116:THR:HG21	7:K:77:ASN:OD1	2.03	0.58
3:G:35:ARG:NH2	5:I:39:DA:OP2	2.34	0.58
5:I:-60:DA:C4	5:I:-59:DT:C4	2.90	0.58
7:K:8:LEU:HD23	7:K:8:LEU:O	2.03	0.58
3:C:55:LEU:O	3:C:59:THR:HG22	2.03	0.58
4:D:73:ARG:HB3	4:D:102:LEU:HD21	1.85	0.58
5:I:-58:DC:H4'	5:I:-57:DT:OP1	2.03	0.58
5:I:-71:DT:H2"	5:I:-70:DC:OP2	2.03	0.58
6:J:48:DG:H2"	6:J:49:DC:OP2	2.03	0.58
7:L:155:GLU:O	7:L:158:TRP:HB2	2.02	0.58
5:I:-62:DA:C2'	5:I:-61:DT:C5	2.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:29:ARG:NH2	6:J:49:DC:OP1	2.37	0.58
5:I:-50:DT:C2'	5:I:-49:DG:C8	2.86	0.58
6:J:51:DC:H1'	6:J:52:DG:C8	2.38	0.58
7:L:155:GLU:OE2	7:L:174:ARG:CZ	2.52	0.58
7:K:94:PHE:CE1	7:K:95:GLU:CG	2.86	0.58
1:A:58:THR:HB	3:G:104:GLN:O	2.03	0.58
4:H:102:LEU:H	4:H:102:LEU:CD2	2.15	0.58
3:C:69:ALA:O	3:C:73:ASN:ND2	2.37	0.58
2:B:98:TYR:CD1	4:H:65:SER:HB3	2.38	0.58
7:K:66:TYR:CB	7:K:92:ARG:NH1	2.66	0.58
3:C:51:LEU:HD13	3:C:55:LEU:HD11	1.85	0.57
1:E:63:ARG:CZ	6:J:-13:DA:H5"	2.34	0.57
7:K:66:TYR:CE2	7:K:168:ASP:OD2	2.48	0.57
3:C:32:ARG:O	3:C:35:ARG:HB2	2.05	0.57
3:G:90:ASP:OD1	3:G:93:LEU:N	2.30	0.57
7:K:158:TRP:CA	7:K:160:ASP:OD1	2.44	0.57
5:I:-57:DT:H3	6:J:57:DA:H61	1.51	0.57
7:K:11:TRP:CD2	7:K:143:LEU:HD13	2.39	0.57
7:L:5:LEU:CD1	7:L:6:LYS:H	2.16	0.57
3:C:32:ARG:HH12	5:I:-45:DG:H3'	1.70	0.57
1:A:76:GLN:O	1:A:78:PHE:N	2.37	0.57
5:I:-49:DG:H2"	5:I:-48:DC:C4	2.40	0.57
7:K:106:ARG:HH11	7:K:106:ARG:CG	2.18	0.57
3:C:83:LEU:HD11	4:D:63:MET:SD	2.45	0.57
3:G:84:GLN:CD	3:G:102:ILE:HD12	2.25	0.57
3:G:50:TYR:O	3:G:54:VAL:HG23	2.05	0.57
5:I:-59:DT:C2'	5:I:-58:DC:H5	2.16	0.57
6:J:65:DA:C5	6:J:66:DC:N4	2.73	0.57
7:K:23:ILE:O	7:K:26:ASN:ND2	2.38	0.57
3:G:55:LEU:O	3:G:59:THR:HG23	2.05	0.57
5:I:-53:DA:C5	5:I:-52:DC:N4	2.73	0.57
2:B:76:ALA:O	2:B:78:ARG:HG2	2.05	0.56
4:D:43:TYR:OH	5:I:-53:DA:P	2.62	0.56
3:G:77:ARG:HG2	4:H:54:GLY:HA3	1.87	0.56
7:L:10:GLY:HA2	7:L:44:ILE:CG1	2.35	0.56
4:D:38:TYR:O	4:D:39:ALA:HB3	2.05	0.56
6:J:-6:DT:H2"	6:J:-5:DA:C8	2.40	0.56
7:K:165:LYS:HA	7:K:165:LYS:HE2	1.86	0.56
5:I:-33:DG:H1'	5:I:-32:DT:H5'	1.87	0.56
2:B:75:HIS:HD2	4:D:97:THR:HG21	1.67	0.56
3:G:50:TYR:OH	4:H:96:GLN:CA	2.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:50:DA:H1'	6:J:51:DC:H5"	1.87	0.56
2:B:97:LEU:HD21	2:B:100:PHE:CD2	2.40	0.56
5:I:-32:DT:C4	5:I:-31:DA:N6	2.73	0.56
5:I:-52:DC:H2"	5:I:-51:DG:OP2	2.05	0.56
7:L:44:ILE:H	7:L:44:ILE:CD1	2.02	0.56
3:G:84:GLN:HE21	3:G:88:ARG:CG	2.18	0.56
1:A:83:ARG:NH2	5:I:-23:DT:H5'	2.20	0.56
5:I:-57:DT:H2"	5:I:-56:DG:C5	2.40	0.56
6:J:47:DG:C5	6:J:48:DG:C6	2.94	0.56
7:L:153:LEU:HB2	7:L:158:TRP:HE1	1.70	0.56
5:I:-11:DC:H2"	5:I:-10:DG:H8	1.70	0.56
5:I:-51:DG:O5'	5:I:-51:DG:H8	1.89	0.56
7:K:180:THR:O	7:K:182:GLU:N	2.38	0.56
7:L:166:ILE:HB	7:L:169:ARG:HB2	1.87	0.56
6:J:54:DG:H1'	6:J:55:DT:P	2.46	0.56
3:G:90:ASP:OD2	7:K:29:ARG:NH1	2.38	0.56
5:I:-58:DC:H4'	5:I:-57:DT:H5'	1.88	0.56
5:I:-61:DT:H2"	5:I:-60:DA:OP2	2.06	0.55
7:K:154:PRO:HB2	7:K:157:GLN:H	1.70	0.55
7:L:78:THR:OG1	7:L:81:ASN:HB2	2.06	0.55
5:I:3:DC:H2"	5:I:4:DG:C8	2.41	0.55
2:B:23:ARG:HB2	7:L:209:LYS:HG3	1.87	0.55
3:C:83:LEU:HD12	4:D:59:ALA:HB1	1.88	0.55
3:C:87:VAL:HG11	3:C:97:LEU:HD12	1.87	0.55
4:D:112:VAL:O	4:D:116:THR:N	2.31	0.55
6:J:50:DA:C1'	6:J:51:DC:H5'	2.35	0.55
7:L:178:GLU:O	7:L:180:THR:N	2.39	0.55
4:D:38:TYR:HB3	4:D:64:ASN:OD1	2.06	0.55
5:I:-53:DA:C6	5:I:-52:DC:N4	2.74	0.55
1:E:97:GLU:O	1:E:101:VAL:CG2	2.51	0.55
3:G:85:LEU:O	3:G:89:ASN:HB2	2.06	0.55
5:I:-53:DA:H2'	5:I:-52:DC:C6	2.42	0.55
6:J:60:DT:O4	6:J:61:DA:N6	2.39	0.55
3:G:50:TYR:OH	4:H:96:GLN:HA	2.07	0.55
7:K:200:GLU:HB3	7:K:201:PRO:CD	2.37	0.55
7:K:52:LYS:HA	7:K:71:ILE:HG22	1.88	0.55
7:K:153:LEU:C	7:K:154:PRO:CD	2.72	0.55
7:L:96:LEU:HD13	7:L:181:ALA:HB1	1.89	0.55
5:I:22:DT:H3	6:J:-22:DA:H61	1.55	0.55
6:J:63:DA:H8	6:J:63:DA:OP2	1.89	0.55
1:E:54:TYR:OH	2:F:36:ARG:HD2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:107:PRO:O	7:L:111:LYS:NZ	2.36	0.55
7:L:87:VAL:HG21	7:L:141:ILE:CD1	2.34	0.55
3:G:19:SER:O	3:G:22:GLY:N	2.41	0.54
7:K:201:PRO:HG2	7:K:202:LYS:H	1.72	0.54
7:K:28:ARG:H	7:K:28:ARG:HD2	1.72	0.54
3:G:87:VAL:HG13	3:G:93:LEU:HB3	1.88	0.54
7:L:63:THR:CB	7:L:65:THR:CG2	2.86	0.54
2:F:73:THR:OG1	2:F:81:VAL:HG22	2.08	0.54
7:L:99:LYS:O	7:L:103:GLU:HG3	2.07	0.54
3:C:27:VAL:HG21	3:C:49:VAL:HG13	1.89	0.54
5:I:-34:DA:C5	5:I:-33:DG:O6	2.60	0.54
7:K:106:ARG:HG3	7:K:109:LEU:HD12	1.89	0.54
4:D:77:GLU:HG2	4:D:80:ARG:HH12	1.73	0.54
3:G:32:ARG:NH2	4:H:36:GLU:OE2	2.35	0.54
2:F:32:PRO:O	2:F:36:ARG:HG3	2.08	0.54
1:A:65:LEU:O	1:A:68:GLN:HB2	2.08	0.54
3:C:22:GLY:O	3:C:23:LEU:HD22	2.08	0.54
4:D:106:GLU:OE2	7:L:28:ARG:HG2	2.06	0.54
4:D:63:MET:O	4:D:67:VAL:HG23	2.07	0.54
5:I:-68:DA:N3	5:I:-67:DT:C2	2.76	0.54
7:L:27:ASN:C	7:L:29:ARG:H	2.12	0.54
7:L:10:GLY:HA2	7:L:44:ILE:HG13	1.88	0.54
2:F:35:ARG:HG3	2:F:51:TYR:HE1	1.73	0.54
5:I:-67:DT:C4	5:I:-66:DG:C6	2.95	0.54
6:J:35:DC:H4'	6:J:36:DC:H5'	1.90	0.54
2:F:73:THR:O	2:F:74:GLU:C	2.44	0.53
5:I:-27:DC:N4	6:J:26:DG:O6	2.41	0.53
4:D:41:TYR:OH	4:D:67:VAL:HG21	2.07	0.53
7:K:93:TRP:CE3	7:K:94:PHE:CA	2.91	0.53
3:C:78:ILE:HB	4:D:55:ILE:HA	1.90	0.53
4:D:110:HIS:NE2	7:L:28:ARG:NH1	2.57	0.53
5:I:-50:DT:C5	5:I:-49:DG:C6	2.96	0.53
6:J:-4:DC:H2"	6:J:-3:DG:C8	2.44	0.53
6:J:53:DT:H2"	6:J:54:DG:OP2	2.08	0.53
1:A:78:PHE:CZ	2:B:67:ARG:HG2	2.43	0.53
4:H:78:ALA:O	4:H:81:LEU:HB2	2.09	0.53
4:H:79:SER:HA	4:H:90:ILE:HD11	1.90	0.53
5:I:-55:DA:H2"	5:I:-54:DC:C6	2.44	0.53
7:K:48:LEU:HD23	7:K:49:SER:N	2.24	0.53
3:C:33:LEU:HD23	3:C:33:LEU:N	2.23	0.53
4:D:46:LEU:HD21	4:D:53:THR:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:97:THR:HG23	7:K:79:LEU:HD21	1.90	0.53
3:C:38:ASN:ND2	3:G:38:ASN:HB3	2.23	0.53
7:K:93:TRP:CE3	7:K:94:PHE:N	2.76	0.53
4:D:77:GLU:O	4:D:81:LEU:HB2	2.09	0.53
6:J:5:DC:H2"	6:J:6:DC:C5	2.44	0.53
7:K:93:TRP:CZ3	7:K:94:PHE:HB3	2.44	0.53
2:F:92:ARG:NH2	4:H:102:LEU:CD1	2.64	0.53
3:C:50:TYR:HD2	4:D:92:SER:HB2	1.74	0.53
6:J:-27:DC:H4'	6:J:-26:DT:H5'	1.90	0.53
7:K:201:PRO:O	7:K:204:SER:OG	2.25	0.53
2:B:75:HIS:NE2	4:D:94:GLU:HG3	2.23	0.52
3:G:27:VAL:HG11	3:G:49:VAL:CG1	2.39	0.52
5:I:-11:DC:H2"	5:I:-10:DG:C8	2.43	0.52
3:C:77:ARG:NH2	6:J:58:DG:H5'	2.24	0.52
7:K:106:ARG:HH11	7:K:106:ARG:HG3	1.73	0.52
5:I:-42:DG:H2"	5:I:-41:DA:H5'	1.91	0.52
6:J:60:DT:C2	6:J:61:DA:C8	2.97	0.52
7:K:50:PHE:CE1	7:K:56:VAL:HG11	2.44	0.52
7:K:68:VAL:HG12	7:K:90:TYR:CD2	2.43	0.52
7:L:138:LEU:C	7:L:139:SER:OG	2.46	0.52
3:C:25:PHE:CE1	4:D:41:TYR:CG	2.98	0.52
2:F:31:LYS:HE2	2:F:51:TYR:CE2	2.44	0.52
3:G:27:VAL:HG22	3:G:52:ALA:CB	2.39	0.52
5:I:-13:DA:H2"	5:I:-12:DA:H8	1.72	0.52
7:L:48:LEU:HD21	7:L:149:VAL:CG2	2.39	0.52
3:C:23:LEU:CD1	3:C:24:GLN:N	2.73	0.52
1:E:65:LEU:CB	1:E:66:PRO:HD3	2.40	0.52
7:K:94:PHE:HE1	7:K:95:GLU:HG2	1.73	0.52
7:L:156:SER:O	7:L:160:ASP:N	2.39	0.52
5:I:-61:DT:H1'	5:I:-60:DA:C8	2.45	0.52
7:K:116:LEU:HD11	7:K:120:LYS:HE3	1.91	0.52
3:G:32:ARG:NE	3:G:36:LYS:HZ3	2.08	0.52
4:H:74:ILE:O	4:H:77:GLU:N	2.43	0.52
7:K:4:THR:HG23	7:K:7:ASP:CB	2.39	0.52
7:L:90:TYR:CE1	7:L:134:LEU:HD13	2.45	0.52
7:L:5:LEU:CD1	7:L:6:LYS:N	2.73	0.52
1:A:119:ILE:HD12	2:B:50:ILE:HD12	1.91	0.52
1:A:84:PHE:CE1	2:B:81:VAL:HG21	2.45	0.52
7:K:201:PRO:CG	7:K:202:LYS:H	2.23	0.52
3:C:50:TYR:CE2	4:D:96:GLN:HB2	2.45	0.52
7:L:63:THR:HB	7:L:65:THR:HG22	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:21:VAL:HG12	2:F:22:LEU:N	2.24	0.51
6:J:12:DT:H2"	6:J:13:DT:H71	1.92	0.51
7:K:201:PRO:CG	7:K:202:LYS:N	2.73	0.51
7:L:13:VAL:C	7:L:14:ILE:HD12	2.30	0.51
2:F:92:ARG:HH21	4:H:102:LEU:HD13	1.69	0.51
6:J:46:DA:H4'	6:J:47:DG:OP1	2.10	0.51
4:H:35:LYS:HB2	5:I:50:DG:OP1	2.10	0.51
6:J:58:DG:H1'	6:J:59:DA:C8	2.45	0.51
7:K:208:LEU:O	7:K:211:VAL:HG22	2.10	0.51
3:G:38:ASN:O	3:G:40:ALA:N	2.43	0.51
7:K:68:VAL:O	7:K:90:TYR:HB2	2.10	0.51
4:H:102:LEU:N	4:H:102:LEU:CD2	2.73	0.51
5:I:41:DC:H2"	5:I:42:DA:C8	2.46	0.51
2:B:23:ARG:HH22	7:L:213:VAL:HG22	1.75	0.51
4:D:70:VAL:O	4:D:74:ILE:HG13	2.11	0.51
7:K:161:SER:HG	7:K:162:SER:H	1.56	0.51
7:K:93:TRP:CE3	7:K:94:PHE:HA	2.46	0.51
7:L:4:THR:HG23	7:L:7:ASP:H	1.76	0.51
3:G:77:ARG:NE	6:J:-54:DA:H4'	2.26	0.51
6:J:30:DT:H1'	6:J:31:DT:H5'	1.93	0.51
6:J:65:DA:C4	6:J:66:DC:C4	2.99	0.51
7:K:69:TYR:CE2	7:K:141:ILE:HG21	2.46	0.51
2:F:74:GLU:OE2	7:K:79:LEU:HB2	2.10	0.51
6:J:-8:DC:H2"	6:J:-7:DG:C8	2.45	0.51
7:K:57:ILE:HD11	7:K:171:PHE:HE1	1.76	0.51
7:L:10:GLY:CA	7:L:44:ILE:CD1	2.66	0.51
5:I:50:DG:H2"	5:I:51:DG:H8	1.76	0.50
7:K:77:ASN:ND2	7:K:77:ASN:O	2.44	0.50
4:D:38:TYR:C	4:D:64:ASN:ND2	2.64	0.50
6:J:4:DC:H2"	6:J:5:DC:C6	2.44	0.50
7:K:158:TRP:HE1	7:K:172:LEU:HA	1.75	0.50
4:D:40:ILE:HG13	4:D:41:TYR:H	1.73	0.50
5:I:49:DC:H2"	5:I:50:DG:C8	2.45	0.50
6:J:65:DA:C4	6:J:66:DC:C5	2.99	0.50
1:A:69:ARG:NH1	2:B:25:ASN:OD1	2.44	0.50
2:F:75:HIS:CA	4:H:93:ARG:NH2	2.71	0.50
7:L:63:THR:CB	7:L:65:THR:HG22	2.42	0.50
4:D:72:GLU:O	4:D:76:GLY:N	2.33	0.50
1:E:118:THR:HA	2:F:45:ARG:HB3	1.94	0.50
1:E:63:ARG:NH1	2:F:30:THR:HG22	2.21	0.50
7:K:91:LEU:HD22	7:K:135:THR:HG23	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:51:ILE:O	1:E:55:GLN:CG	2.59	0.50
5:I:16:DA:H1'	5:I:17:DA:C8	2.46	0.50
6:J:54:DG:C5	6:J:55:DT:C4	3.00	0.50
7:L:2:ALA:H	7:L:83:VAL:CG1	2.24	0.50
2:F:19:ARG:NH1	6:J:-22:DA:H3'	2.24	0.49
7:L:140:GLU:C	7:L:141:ILE:HG23	2.31	0.49
7:L:72:HIS:HB2	7:L:88:PHE:CE2	2.47	0.49
7:K:200:GLU:OE1	7:K:200:GLU:N	2.45	0.49
7:K:201:PRO:HG2	7:K:202:LYS:N	2.28	0.49
7:L:14:ILE:HD13	7:L:42:LYS:HB3	1.93	0.49
7:L:5:LEU:HD12	7:L:6:LYS:N	2.24	0.49
2:F:35:ARG:O	2:F:39:ARG:HG2	2.12	0.49
7:K:10:GLY:C	7:K:11:TRP:CD1	2.85	0.49
2:F:47:SER:OG	2:F:48:GLY:N	2.45	0.49
3:G:25:PHE:CD1	4:H:41:TYR:HB3	2.48	0.49
3:G:32:ARG:HD3	6:J:-44:DA:OP2	2.12	0.49
6:J:42:DC:H2'	6:J:43:DT:H72	1.93	0.49
3:C:96:LEU:O	3:C:97:LEU:HD23	2.13	0.49
4:H:63:MET:O	4:H:67:VAL:HG23	2.12	0.49
2:F:75:HIS:O	4:H:93:ARG:NH2	2.45	0.49
7:K:66:TYR:N	7:K:66:TYR:CD1	2.80	0.49
1:E:76:GLN:OE1	1:E:80:THR:HA	2.13	0.49
3:G:43:VAL:O	5:I:38:DG:H3'	2.13	0.49
1:E:128:ARG:HD2	1:E:133:GLU:OE1	2.12	0.48
4:H:117:LYS:HG2	4:H:121:LYS:CD	2.42	0.48
5:I:-13:DA:H2"	5:I:-12:DA:C8	2.47	0.48
1:A:63:ARG:HD3	6:J:18:DC:OP1	2.13	0.48
6:J:-61:DG:H2"	6:J:-60:DG:C8	2.48	0.48
7:K:91:LEU:HD21	7:K:133:TYR:HB2	1.95	0.48
7:K:72:HIS:CE1	7:K:204:SER:OG	2.66	0.48
7:K:66:TYR:HB2	7:K:92:ARG:NH1	2.25	0.48
7:L:5:LEU:CA	7:L:8:LEU:CD1	2.85	0.48
3:C:54:VAL:HG13	4:D:111:ALA:HB1	1.95	0.48
5:I:-46:DT:H2"	5:I:-45:DG:OP2	2.13	0.48
7:K:154:PRO:O	7:K:158:TRP:HD1	1.94	0.48
1:A:65:LEU:HD13	1:A:65:LEU:HA	1.70	0.48
4:D:71:PHE:C	4:D:71:PHE:HD1	2.16	0.48
4:H:98:ALA:O	4:H:101:LEU:HB2	2.13	0.48
5:I:47:DA:C5	5:I:48:DG:C6	3.01	0.48
6:J:69:DC:H2"	6:J:70:DG:C8	2.47	0.48
7:K:133:TYR:CD1	7:K:133:TYR:N	2.81	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:200:GLU:HB3	7:K:201:PRO:HD3	1.95	0.48
7:K:94:PHE:HD1	7:K:95:GLU:N	2.09	0.48
2:F:20:LYS:O	2:F:21:VAL:HB	2.14	0.48
2:F:59:LYS:HE2	2:F:63:GLU:OE2	2.13	0.48
5:I:21:DG:N2	6:J:-21:DC:N3	2.52	0.48
6:J:54:DG:C1'	6:J:55:DT:P	3.01	0.48
7:K:20:GLY:C	7:K:21:ARG:HD2	2.33	0.48
2:B:63:GLU:O	2:B:67:ARG:HG3	2.13	0.48
2:B:98:TYR:CD2	3:G:100:VAL:HG11	2.47	0.48
3:G:53:ALA:O	3:G:56:GLU:N	2.46	0.48
7:K:151:GLN:HG2	7:K:170:ASP:OD2	2.13	0.48
7:K:88:PHE:CE2	7:K:208:LEU:HD23	2.48	0.48
3:G:25:PHE:CE1	4:H:41:TYR:HB3	2.48	0.48
3:G:32:ARG:HG3	3:G:33:LEU:N	2.28	0.48
6:J:13:DT:C6	6:J:14:DT:H72	2.48	0.48
5:I:-69:DG:H1	6:J:69:DC:H42	1.62	0.48
2:F:26:ILE:CD1	2:F:55:ARG:CG	2.91	0.48
3:G:43:VAL:N	5:I:39:DA:OP1	2.30	0.48
4:D:108:ALA:O	4:D:112:VAL:HG23	2.14	0.48
4:D:87:ARG:NH1	4:D:94:GLU:OE2	2.46	0.48
5:I:35:DT:H2"	5:I:36:DA:C8	2.48	0.48
7:K:122:LYS:HG3	7:K:123:PHE:N	2.28	0.48
7:K:158:TRP:CE2	7:K:172:LEU:HB2	2.48	0.48
1:E:68:GLN:HE21	1:E:68:GLN:C	2.17	0.48
5:I:-60:DA:H2"	5:I:-59:DT:C6	2.48	0.48
7:L:5:LEU:H	7:L:5:LEU:HD12	1.75	0.48
3:C:80:PRO:HB3	4:D:62:ILE:CD1	2.43	0.48
3:G:100:VAL:HG12	3:G:101:THR:N	2.28	0.48
7:L:159:ASN:OD1	7:L:160:ASP:N	2.47	0.48
4:D:77:GLU:HG2	4:D:80:ARG:NH1	2.29	0.47
7:L:147:ILE:HG22	7:L:148:ALA:N	2.29	0.47
1:E:51:ILE:O	1:E:55:GLN:HG2	2.14	0.47
3:G:23:LEU:HD22	3:G:56:GLU:OE2	2.14	0.47
3:G:37:GLY:O	3:G:38:ASN:HB2	2.14	0.47
5:I:-31:DA:H2"	5:I:-30:DA:OP2	2.15	0.47
5:I:-53:DA:C2'	5:I:-52:DC:C5'	2.86	0.47
7:K:157:GLN:OE1	7:K:157:GLN:O	2.31	0.47
3:G:19:SER:O	3:G:20:ARG:C	2.50	0.47
3:G:79:ILE:HA	4:H:56:SER:OG	2.14	0.47
4:H:100:ARG:HD2	7:K:79:LEU:HD13	1.95	0.47
1:A:88:ALA:HB2	2:B:82:THR:C	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:71:PHE:CD1	4:D:71:PHE:C	2.88	0.47
4:H:95:ILE:O	4:H:98:ALA:HB3	2.15	0.47
7:K:134:LEU:H	7:K:176:ALA:HA	1.79	0.47
7:K:172:LEU:HD11	7:K:174:ARG:CG	2.43	0.47
3:C:25:PHE:CZ	3:C:59:THR:HG21	2.49	0.47
1:E:66:PRO:HB3	2:F:28:GLY:HA3	1.97	0.47
3:G:29:ARG:HG2	3:G:33:LEU:CD2	2.44	0.47
7:L:6:LYS:O	7:L:9:ASP:HB3	2.14	0.47
4:H:112:VAL:O	4:H:116:THR:HG22	2.13	0.47
4:H:62:ILE:O	4:H:65:SER:HB2	2.15	0.47
1:E:85:GLN:HA	6:J:-24:DG:OP1	2.15	0.47
4:D:41:TYR:OH	4:D:67:VAL:CG2	2.62	0.47
4:D:39:ALA:HB1	4:D:60:MET:HE1	0.47	0.47
4:H:102:LEU:C	4:H:103:LEU:HD23	2.35	0.47
5:I:-70:DC:O5'	5:I:-70:DC:H6	1.98	0.47
7:K:43:ARG:NH2	7:K:146:PHE:CE2	2.83	0.47
7:K:56:VAL:HA	7:K:150:GLY:H	1.80	0.47
7:L:92:ARG:HH12	7:L:94:PHE:HD2	1.63	0.47
3:G:47:ALA:HB2	4:H:91:THR:C	2.35	0.47
5:I:-8:DG:H1	6:J:8:DC:N4	2.12	0.47
6:J:-35:DA:H2"	6:J:-34:DG:C8	2.50	0.47
6:J:54:DG:C8	6:J:55:DT:C4	3.02	0.47
7:L:131:GLU:OE2	7:L:174:ARG:HB2	2.14	0.47
3:C:112:GLN:NE2	1:E:109:LEU:HD21	2.30	0.47
3:G:92:GLU:OE1	7:K:29:ARG:NE	2.48	0.47
7:K:96:LEU:O	7:K:98:PRO:HD3	2.15	0.47
1:A:107:THR:HG21	1:A:124:ILE:HG12	1.97	0.47
1:A:72:ARG:NH1	1:A:84:PHE:HD2	2.13	0.47
1:E:64:LYS:HG2	1:E:64:LYS:O	2.13	0.47
3:C:51:LEU:HD13	3:C:55:LEU:CD1	2.45	0.46
1:E:62:ILE:HB	1:E:93:GLN:HE21	1.79	0.46
7:L:65:THR:OG1	7:L:66:TYR:N	2.48	0.46
5:I:-30:DA:C4	5:I:-29:DT:C5	3.03	0.46
6:J:29:DA:C8	6:J:30:DT:H72	2.50	0.46
7:K:158:TRP:C	7:K:160:ASP:N	2.65	0.46
7:L:155:GLU:OE2	7:L:174:ARG:NE	2.48	0.46
2:B:56:GLY:O	2:B:60:VAL:HG23	2.16	0.46
4:H:40:ILE:HG23	4:H:41:TYR:CD1	2.50	0.46
7:K:201:PRO:CD	7:K:202:LYS:H	2.29	0.46
7:K:55:SER:OG	7:K:90:TYR:OH	2.32	0.46
4:D:38:TYR:CA	4:D:64:ASN:HD21	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:50:DG:H2"	5:I:51:DG:C8	2.50	0.46
7:L:15:ILE:CG1	7:L:23:ILE:HD11	2.44	0.46
7:L:97:LYS:HA	7:L:98:PRO:HD3	1.66	0.46
1:A:59:GLU:HG3	1:A:59:GLU:H	1.24	0.46
6:J:15:DT:H2"	6:J:16:DA:H8	1.78	0.46
7:K:50:PHE:HZ	7:K:146:PHE:CE1	2.33	0.46
1:A:92:LEU:HG	2:B:86:VAL:HG11	1.97	0.46
3:C:51:LEU:HD21	4:D:74:ILE:HG21	1.97	0.46
1:E:92:LEU:O	1:E:96:SER:OG	2.24	0.46
3:C:46:GLY:O	3:C:49:VAL:HG23	2.15	0.46
3:C:57:TYR:O	3:C:60:ALA:HB3	2.16	0.46
5:I:-5:DG:H2'	5:I:-5:DG:OP2	2.16	0.46
7:K:16:THR:HG22	7:K:21:ARG:H	1.81	0.46
2:B:49:LEU:HD12	2:B:49:LEU:H	1.80	0.46
4:D:75:ALA:O	4:D:78:ALA:HB3	2.15	0.46
2:B:97:LEU:HD21	2:B:100:PHE:HD2	1.81	0.46
1:A:61:LEU:HD13	2:B:36:ARG:O	2.15	0.46
3:C:64:GLU:OE2	3:C:68:ASN:ND2	2.47	0.46
4:D:38:TYR:CB	4:D:64:ASN:OD1	2.64	0.46
7:K:94:PHE:O	7:K:95:GLU:C	2.54	0.46
7:L:134:LEU:HA	7:L:134:LEU:HD12	1.57	0.46
3:C:50:TYR:O	3:C:53:ALA:HB3	2.15	0.46
1:E:88:ALA:HB2	2:F:83:ALA:HA	1.98	0.46
7:K:158:TRP:NE1	7:K:172:LEU:HA	2.31	0.46
1:E:84:PHE:CD1	2:F:81:VAL:HB	2.51	0.45
1:E:78:PHE:CE1	2:F:67:ARG:HB2	2.51	0.45
3:G:81:ARG:NH2	3:G:107:VAL:O	2.49	0.45
6:J:54:DG:C4	6:J:55:DT:C4	3.04	0.45
6:J:68:DT:H6	6:J:68:DT:H5"	1.81	0.45
7:K:140:GLU:O	7:K:142:TRP:CZ3	2.69	0.45
7:K:169:ARG:HA	7:K:169:ARG:HD3	1.64	0.45
2:B:78:ARG:NH2	2:B:85:ASP:OD2	2.41	0.45
4:D:42:VAL:HG21	4:D:60:MET:CE	2.46	0.45
7:L:10:GLY:C	7:L:44:ILE:CG1	2.73	0.45
1:E:69:ARG:O	1:E:72:ARG:N	2.49	0.45
3:C:77:ARG:NH1	5:I:-54:DC:H4'	2.32	0.45
7:L:169:ARG:HA	7:L:169:ARG:HD3	1.62	0.45
7:L:11:TRP:CZ3	7:L:42:LYS:C	2.90	0.45
7:L:60:ASP:OD1	7:L:62:VAL:N	2.49	0.45
7:L:2:ALA:H	7:L:83:VAL:HG13	1.81	0.45
5:I:22:DT:H3	6:J:-22:DA:N6	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:24:ASP:C	7:K:26:ASN:H	2.17	0.45
1:A:107:THR:HG23	1:A:123:ASP:C	2.36	0.45
4:H:105:GLY:O	4:H:108:ALA:HB3	2.16	0.45
7:L:199:MET:H	7:L:199:MET:HG2	1.58	0.45
2:F:61:PHE:O	2:F:65:VAL:HG23	2.17	0.45
2:F:90:LEU:HA	2:F:90:LEU:HD12	1.74	0.45
3:G:42:ARG:HA	5:I:39:DA:OP1	2.16	0.45
6:J:59:DA:C8	6:J:60:DT:C7	2.99	0.45
7:K:10:GLY:O	7:K:11:TRP:CD1	2.70	0.45
7:K:158:TRP:NE1	7:K:172:LEU:CB	2.78	0.45
7:L:156:SER:C	7:L:158:TRP:H	2.20	0.45
7:K:24:ASP:O	7:K:25:ASP:HB2	2.16	0.45
7:L:85:ILE:O	7:L:140:GLU:HA	2.17	0.45
3:C:20:ARG:CD	3:C:21:ALA:N	2.71	0.45
2:F:18:HIS:C	2:F:19:ARG:CG	2.86	0.45
2:F:35:ARG:HG3	2:F:51:TYR:CE1	2.51	0.45
4:H:35:LYS:HD3	4:H:35:LYS:HA	1.77	0.45
5:I:-60:DA:C6	5:I:-59:DT:N3	2.84	0.45
7:K:58:PHE:HB3	7:K:147:ILE:H	1.82	0.45
4:D:39:ALA:CA	4:D:42:VAL:CG2	2.94	0.45
6:J:31:DT:H2"	6:J:32:DA:H8	1.81	0.45
7:K:9:ASP:OD1	7:K:10:GLY:N	2.49	0.45
4:D:109:LYS:O	4:D:113:SER:OG	2.34	0.45
4:D:89:THR:OG1	5:I:-34:DA:OP1	2.25	0.45
5:I:-53:DA:C2'	5:I:-52:DC:H5'	2.29	0.45
5:I:-58:DC:O2	5:I:-57:DT:C2	2.70	0.45
6:J:59:DA:C5	6:J:60:DT:C4	3.05	0.45
7:L:11:TRP:CE3	7:L:42:LYS:C	2.90	0.45
7:L:43:ARG:HH22	7:L:146:PHE:HE2	1.64	0.45
7:L:60:ASP:OD1	7:L:62:VAL:HB	2.17	0.45
1:E:83:ARG:N	2:F:79:LYS:O	2.41	0.44
3:G:57:TYR:CE1	3:G:61:GLU:HG2	2.52	0.44
4:H:43:TYR:CE1	4:H:47:LYS:HE3	2.52	0.44
3:G:102:ILE:CG2	4:H:62:ILE:HD13	2.46	0.44
7:K:66:TYR:CB	7:K:92:ARG:CZ	2.94	0.44
7:L:17:ASP:OD1	7:L:21:ARG:CB	2.61	0.44
1:A:64:LYS:HG3	1:A:93:GLN:OE1	2.17	0.44
3:C:27:VAL:HG22	3:C:49:VAL:HA	1.98	0.44
3:G:79:ILE:HG12	3:G:82:HIS:CE1	2.53	0.44
7:K:86:TRP:HZ3	7:K:138:LEU:HD13	1.83	0.44
7:L:66:TYR:CD1	7:L:66:TYR:O	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:66:ALA:O	3:C:70:ALA:N	2.41	0.44
5:I:-70:DC:C6	5:I:-70:DC:O5'	2.71	0.44
7:L:110:ILE:HA	7:L:119:TYR:OH	2.17	0.44
4:D:79:SER:O	4:D:82:ALA:HB3	2.18	0.44
5:I:-34:DA:H1'	5:I:-33:DG:C8	2.52	0.44
5:I:-57:DT:H2"	5:I:-56:DG:C8	2.51	0.44
7:L:156:SER:C	7:L:158:TRP:N	2.70	0.44
7:L:19:GLN:N	7:L:19:GLN:OE1	2.51	0.44
5:I:-47:DC:O2	5:I:-46:DT:C2	2.71	0.44
7:K:76:LEU:HD12	7:K:77:ASN:H	1.82	0.44
3:C:81:ARG:O	3:C:81:ARG:HG3	2.15	0.44
3:C:45:ALA:N	6:J:38:DT:OP1	2.36	0.44
7:L:44:ILE:N	7:L:44:ILE:CD1	2.73	0.44
2:F:26:ILE:CD1	2:F:26:ILE:C	2.86	0.44
3:G:50:TYR:CE2	4:H:96:GLN:HB2	2.53	0.44
7:K:134:LEU:HB3	7:K:176:ALA:HB2	1.98	0.44
7:K:94:PHE:O	7:K:96:LEU:N	2.51	0.44
7:L:104:GLN:NE2	7:L:184:PHE:O	2.51	0.44
7:L:193:ILE:O	7:L:197:LYS:HG3	2.17	0.44
1:E:110:CYS:HB3	1:E:126:LEU:HD23	2.00	0.44
1:E:52:ARG:O	1:E:56:LYS:HD3	2.17	0.44
6:J:-47:DT:H2"	6:J:-46:DC:C5	2.53	0.44
3:G:38:ASN:C	3:G:40:ALA:N	2.69	0.44
6:J:5:DC:H2"	6:J:6:DC:C6	2.53	0.44
7:K:93:TRP:CD2	7:K:94:PHE:N	2.86	0.44
7:L:154:PRO:O	7:L:158:TRP:HD1	2.01	0.44
3:C:104:GLN:HB2	4:D:58:LYS:NZ	2.24	0.43
3:C:62:ILE:HD12	4:D:66:PHE:CE2	2.52	0.43
4:H:98:ALA:O	4:H:102:LEU:CD2	2.66	0.43
5:I:-65:DT:H2"	5:I:-64:DA:OP2	2.18	0.43
5:I:-68:DA:C2	5:I:-67:DT:N3	2.86	0.43
7:L:15:ILE:CD1	7:L:23:ILE:CD1	2.91	0.43
3:G:50:TYR:OH	4:H:96:GLN:CG	2.64	0.43
7:K:178:GLU:HA	7:K:179:PRO:HD2	1.69	0.43
7:L:128:ASN:OD1	7:L:131:GLU:N	2.51	0.43
4:D:93:ARG:O	4:D:96:GLN:HB3	2.18	0.43
4:D:95:ILE:O	4:D:98:ALA:HB3	2.19	0.43
1:E:95:ALA:CB	2:F:90:LEU:HD21	2.48	0.43
3:G:43:VAL:H	5:I:39:DA:P	2.37	0.43
3:G:21:ALA:HB2	4:H:122:TYR:HB2	2.01	0.43
5:I:-60:DA:C5	5:I:-59:DT:O4	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:42:DC:H2"	6:J:43:DT:O5'	2.19	0.43
6:J:55:DT:C6	6:J:55:DT:OP2	2.70	0.43
3:G:27:VAL:O	3:G:27:VAL:HG12	2.18	0.43
3:G:81:ARG:O	3:G:85:LEU:HG	2.17	0.43
3:G:77:ARG:HG2	4:H:55:ILE:N	2.33	0.43
7:K:154:PRO:HB2	7:K:157:GLN:HB2	1.99	0.43
7:K:200:GLU:O	7:K:203:GLN:HB3	2.19	0.43
7:L:56:VAL:O	7:L:68:VAL:HG13	2.18	0.43
1:A:99:TYR:OH	1:A:133:GLU:OE1	2.37	0.43
3:C:38:ASN:CG	3:G:38:ASN:CB	2.80	0.43
3:C:45:ALA:HB2	6:J:38:DT:OP2	2.19	0.43
3:G:35:ARG:HG2	3:G:43:VAL:CG1	2.37	0.43
4:H:121:LYS:HB2	4:H:121:LYS:HE2	1.88	0.43
7:K:131:GLU:OE2	7:K:174:ARG:HD3	2.19	0.43
1:A:44:GLY:O	1:A:48:LEU:HD22	2.19	0.43
3:C:88:ARG:O	3:C:108:LEU:HD11	2.19	0.43
3:C:32:ARG:HH12	5:I:-45:DG:C3'	2.31	0.43
2:F:71:THR:HG22	4:H:97:THR:CG2	2.49	0.43
3:G:67:GLY:HA2	3:G:70:ALA:HB3	2.01	0.43
6:J:50:DA:H2"	6:J:51:DC:OP2	2.19	0.43
6:J:60:DT:N3	6:J:61:DA:N7	2.67	0.43
7:K:113:ASP:N	7:K:113:ASP:OD1	2.50	0.43
7:L:5:LEU:O	7:L:8:LEU:HD13	2.19	0.43
3:C:83:LEU:O	3:C:87:VAL:HG23	2.19	0.43
1:E:78:PHE:CE1	2:F:67:ARG:HD2	2.54	0.43
4:H:71:PHE:C	4:H:71:PHE:CD1	2.92	0.43
6:J:14:DT:C2	6:J:15:DT:C5	3.06	0.43
6:J:23:DA:H2"	6:J:24:DA:OP2	2.17	0.43
6:J:58:DG:C2	6:J:59:DA:C6	3.07	0.43
7:K:27:ASN:HD22	7:K:27:ASN:N	2.16	0.43
1:E:68:GLN:HE22	1:E:72:ARG:NH1	2.17	0.43
1:E:83:ARG:O	2:F:80:THR:HA	2.19	0.43
2:F:60:VAL:O	2:F:64:ASN:ND2	2.52	0.43
7:K:97:LYS:HB2	7:K:100:LEU:HD12	1.99	0.43
7:L:10:GLY:CA	7:L:44:ILE:CG1	2.96	0.43
5:I:28:DA:H2"	5:I:29:DG:H8	1.83	0.43
6:J:58:DG:H1'	6:J:59:DA:N7	2.34	0.43
7:K:173:VAL:HG11	7:K:189:ILE:HD13	2.00	0.43
7:L:27:ASN:C	7:L:29:ARG:N	2.72	0.43
1:A:52:ARG:O	1:A:56:LYS:HG2	2.18	0.42
1:E:85:GLN:OE1	2:F:82:THR:HG22	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:27:GLN:NE2	2:F:27:GLN:C	2.72	0.42
4:H:106:GLU:HG3	4:H:110:HIS:CD2	2.54	0.42
5:I:-61:DT:O2	6:J:61:DA:H2	2.01	0.42
5:I:-18:DG:C8	5:I:-17:DT:H72	2.53	0.42
5:I:-60:DA:C5	5:I:-59:DT:N3	2.87	0.42
7:K:40:PHE:HA	7:K:50:PHE:O	2.18	0.42
7:L:58:PHE:O	7:L:66:TYR:HA	2.19	0.42
3:C:73:ASN:O	3:C:74:LYS:HG2	2.19	0.42
7:K:115:PRO:HG2	7:K:118:PHE:HB2	2.00	0.42
7:L:155:GLU:HA	7:L:172:LEU:HD13	2.01	0.42
3:G:38:ASN:O	3:G:39:TYR:C	2.58	0.42
6:J:49:DC:H2"	6:J:50:DA:OP2	2.19	0.42
7:K:58:PHE:HD2	7:K:146:PHE:CA	2.27	0.42
7:K:88:PHE:CZ	7:K:208:LEU:HD23	2.54	0.42
2:F:93:GLN:O	2:F:93:GLN:NE2	2.49	0.42
7:K:58:PHE:HB3	7:K:146:PHE:HA	2.02	0.42
7:L:58:PHE:O	7:L:67:SER:N	2.47	0.42
3:C:84:GLN:NE2	3:C:102:ILE:HB	2.34	0.42
3:G:27:VAL:HG22	3:G:52:ALA:HB3	2.01	0.42
3:G:66:ALA:O	3:G:70:ALA:N	2.53	0.42
1:A:83:ARG:HA	5:I:-23:DT:OP1	2.19	0.42
7:L:140:GLU:O	7:L:141:ILE:HG23	2.19	0.42
3:G:47:ALA:HB2	4:H:91:THR:HA	2.00	0.42
4:H:102:LEU:HB2	4:H:103:LEU:CD2	2.43	0.42
3:G:77:ARG:HA	4:H:54:GLY:C	2.40	0.42
4:H:71:PHE:HD1	4:H:71:PHE:C	2.23	0.42
6:J:51:DC:C2	6:J:52:DG:C5	3.07	0.42
7:K:162:SER:CA	7:K:163:ILE:HG23	2.44	0.42
3:C:57:TYR:CD1	3:C:57:TYR:C	2.93	0.42
2:F:18:HIS:C	2:F:19:ARG:HG3	2.40	0.42
1:E:61:LEU:HD13	2:F:36:ARG:HB3	2.02	0.42
3:G:26:PRO:HG3	4:H:41:TYR:CZ	2.55	0.42
5:I:-58:DC:O2	5:I:-57:DT:N3	2.53	0.42
6:J:-15:DA:H2"	6:J:-14:DA:C8	2.54	0.42
6:J:60:DT:C4	6:J:61:DA:N6	2.88	0.42
7:K:141:ILE:H	7:K:141:ILE:HG12	1.74	0.42
7:K:152:ILE:O	7:K:153:LEU:HD23	2.19	0.42
7:K:76:LEU:HD12	7:K:82:VAL:O	2.19	0.42
7:K:87:VAL:HG11	7:K:141:ILE:HD11	2.01	0.42
3:C:51:LEU:CD1	3:C:55:LEU:HD11	2.50	0.42
3:C:54:VAL:HG11	4:D:99:VAL:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:53:GLU:O	2:F:57:VAL:HG23	2.19	0.42
5:I:37:DC:H2"	5:I:38:DG:C8	2.54	0.42
7:K:106:ARG:HD3	7:K:106:ARG:HA	1.77	0.42
7:K:107:PRO:O	7:K:110:ILE:HG12	2.19	0.42
7:K:91:LEU:H	7:K:91:LEU:HD23	1.85	0.42
7:L:41:LEU:HA	7:L:41:LEU:HD23	1.80	0.42
4:D:103:LEU:HA	4:D:104:PRO:HD3	1.77	0.41
7:K:140:GLU:O	7:K:142:TRP:HZ3	2.02	0.41
7:L:66:TYR:C	7:L:66:TYR:CD1	2.89	0.41
1:A:72:ARG:HH11	1:A:84:PHE:HD2	1.69	0.41
4:D:42:VAL:HG21	4:D:60:MET:SD	2.60	0.41
6:J:59:DA:C8	6:J:60:DT:H73	2.55	0.41
3:C:83:LEU:HD21	4:D:63:MET:CE	2.51	0.41
4:D:103:LEU:HD22	4:D:107:LEU:HB3	2.02	0.41
4:D:39:ALA:C	4:D:42:VAL:CG2	2.80	0.41
4:H:38:TYR:CD1	4:H:38:TYR:N	2.88	0.41
6:J:57:DA:H2"	6:J:58:DG:OP2	2.20	0.41
7:K:194:ARG:HH11	7:K:195:ARG:NH1	2.18	0.41
7:L:11:TRP:N	7:L:44:ILE:HD12	2.21	0.41
3:C:77:ARG:HG3	4:D:54:GLY:HA3	2.02	0.41
7:K:58:PHE:HE1	7:K:141:ILE:HD12	1.86	0.41
1:E:73:GLU:C	1:E:75:ALA:H	2.23	0.41
4:H:98:ALA:O	4:H:102:LEU:HD22	2.21	0.41
5:I:-71:DT:H3	6:J:71:DA:H61	1.68	0.41
6:J:55:DT:H6	6:J:55:DT:OP2	2.03	0.41
6:J:60:DT:N3	6:J:61:DA:C5	2.89	0.41
6:J:64:DT:H2"	6:J:65:DA:OP2	2.20	0.41
7:L:206:GLU:HA	7:L:209:LYS:HB3	2.03	0.41
7:L:5:LEU:H	7:L:5:LEU:CD1	2.33	0.41
3:C:116:LEU:HB3	3:C:117:PRO:HD2	2.02	0.41
3:G:80:PRO:HG3	4:H:58:LYS:HB2	2.02	0.41
4:H:36:GLU:N	4:H:36:GLU:OE1	2.54	0.41
4:H:47:LYS:HE2	4:H:53:THR:O	2.21	0.41
6:J:34:DT:H2"	6:J:35:DC:OP2	2.21	0.41
2:B:68:ASP:O	2:B:69:ALA:C	2.57	0.41
4:D:71:PHE:O	4:D:71:PHE:HD1	2.04	0.41
2:F:62:LEU:O	2:F:66:ILE:HG13	2.21	0.41
3:G:77:ARG:NE	6:J:-53:DG:OP1	2.50	0.41
4:D:66:PHE:O	4:D:70:VAL:HG23	2.20	0.41
2:F:23:ARG:HG2	7:K:209:LYS:HE3	2.03	0.41
5:I:-34:DA:C4	5:I:-33:DG:C6	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:165:LYS:HB3	7:K:166:ILE:HD12	2.03	0.41
7:K:43:ARG:NH2	7:K:146:PHE:HE2	2.18	0.41
7:L:68:VAL:O	7:L:90:TYR:HB2	2.20	0.41
3:C:51:LEU:CD2	4:D:74:ILE:HG21	2.49	0.41
1:E:100:LEU:HD11	2:F:58:LEU:HD22	2.03	0.41
1:E:101:VAL:CG1	2:F:40:ARG:HG2	2.46	0.41
3:G:32:ARG:HA	3:G:35:ARG:HG3	2.02	0.41
3:G:92:GLU:OE1	4:H:107:LEU:HG	2.21	0.41
5:I:-60:DA:C2'	5:I:-59:DT:C7	2.86	0.41
6:J:65:DA:C6	6:J:66:DC:N4	2.90	0.41
5:I:-7:DG:C6	6:J:6:DC:N4	2.89	0.41
7:L:21:ARG:HD2	7:L:21:ARG:HA	1.55	0.41
7:L:15:ILE:CG1	7:L:23:ILE:CD1	2.99	0.41
1:A:73:GLU:OE1	2:B:25:ASN:HB2	2.20	0.40
3:C:93:LEU:HD23	3:C:93:LEU:HA	1.83	0.40
3:C:59:THR:HG21	4:D:41:TYR:HE2	1.86	0.40
7:K:77:ASN:C	7:K:77:ASN:ND2	2.73	0.40
2:B:90:LEU:HD23	2:B:90:LEU:HA	1.83	0.40
5:I:-44:DG:H2"	5:I:-43:DA:OP2	2.22	0.40
5:I:-47:DC:H2"	5:I:-46:DT:C5	2.56	0.40
6:J:29:DA:C5	6:J:30:DT:C4	3.09	0.40
6:J:65:DA:C6	6:J:66:DC:C4	3.09	0.40
7:L:104:GLN:HE21	7:L:184:PHE:HB2	1.86	0.40
3:C:51:LEU:CB	4:D:95:ILE:HD12	2.48	0.40
4:H:87:ARG:HA	4:H:87:ARG:HD2	1.89	0.40
5:I:-53:DA:C4	5:I:-52:DC:C4	3.09	0.40
6:J:60:DT:H2"	6:J:61:DA:OP2	2.20	0.40
1:A:114:ALA:O	1:A:115:LYS:HB2	2.21	0.40
2:B:68:ASP:OD2	2:B:93:GLN:NE2	2.54	0.40
3:C:79:ILE:H	3:C:82:HIS:CE1	2.38	0.40
2:F:68:ASP:OD2	2:F:92:ARG:HD3	2.20	0.40
4:H:103:LEU:CD2	4:H:103:LEU:N	2.73	0.40
6:J:65:DA:C2	6:J:66:DC:C2	3.09	0.40
7:L:23:ILE:H	7:L:23:ILE:HG13	1.45	0.40
4:D:86:LYS:HD3	4:D:86:LYS:HA	1.80	0.40
3:G:47:ALA:HB2	4:H:91:THR:CA	2.52	0.40
3:G:85:LEU:HD12	3:G:86:ALA:N	2.36	0.40
5:I:-38:DA:C2	6:J:39:DA:C2	3.10	0.40
7:K:3:LYS:O	7:K:3:LYS:HD3	2.21	0.40
7:K:53:GLY:HA3	7:K:197:LYS:HE2	2.04	0.40
7:L:153:LEU:HB2	7:L:158:TRP:NE1	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:17:ASP:N	7:L:17:ASP:OD1	2.55	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)
7:K:169:ARG:NH2	7:L:45:SER:O[6_545]	1.79	0.41

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	95/136 (70%)	89 (94%)	5 (5%)	1 (1%)	14 45
1	E	88/136 (65%)	78 (89%)	8 (9%)	2 (2%)	6 29
2	B	87/103 (84%)	72 (83%)	15 (17%)	0	100 100
2	F	81/103 (79%)	67 (83%)	10 (12%)	4 (5%)	2 14
3	C	96/130 (74%)	81 (84%)	12 (12%)	3 (3%)	4 23
3	G	98/130 (75%)	85 (87%)	12 (12%)	1 (1%)	15 46
4	D	84/126 (67%)	72 (86%)	10 (12%)	2 (2%)	6 28
4	H	86/126 (68%)	74 (86%)	11 (13%)	1 (1%)	13 42
7	K	205/236 (87%)	178 (87%)	25 (12%)	2 (1%)	15 46
7	L	202/236 (86%)	182 (90%)	18 (9%)	2 (1%)	15 46
All	All	1122/1462 (77%)	978 (87%)	126 (11%)	18 (2%)	9 36

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	77	ASP

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Mol	Chain	Res	Type
1	E	64	LYS
2	F	24	ASP
2	F	30	THR
4	H	105	GLY
7	K	161	SER
3	C	37	GLY
4	D	105	GLY
2	F	20	LYS
2	F	21	VAL
3	G	39	TYR
7	L	28	ARG
3	C	22	GLY
7	L	179	PRO
1	E	74	ILE
4	D	76	GLY
3	C	26	PRO
7	K	179	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	85/111 (77%)	75 (88%)	10 (12%)	5 21
1	E	77/111 (69%)	69 (90%)	8 (10%)	7 25
2	B	73/79 (92%)	61 (84%)	12 (16%)	2 10
2	F	70/79 (89%)	60 (86%)	10 (14%)	3 15
3	C	76/102 (74%)	59 (78%)	17 (22%)	1 3
3	G	79/102 (78%)	64 (81%)	15 (19%)	1 6
4	D	73/106 (69%)	55 (75%)	18 (25%)	0 2
4	H	75/106 (71%)	60 (80%)	15 (20%)	1 5
7	K	195/220 (89%)	149 (76%)	46 (24%)	1 3
7	L	194/220 (88%)	166 (86%)	28 (14%)	3 15
All	All	997/1236 (81%)	818 (82%)	179 (18%)	1 7

All (179) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	LEU
1	A	53	ARG
1	A	59	GLU
1	A	62	ILE
1	A	65	LEU
1	A	80	THR
1	A	115	LYS
1	A	117	VAL
1	A	119	ILE
1	A	129	ARG
2	B	18	HIS
2	B	19	ARG
2	B	22	LEU
2	B	23	ARG
2	B	35	ARG
2	B	52	GLU
2	B	80	THR
2	B	81	VAL
2	B	82	THR
2	B	84	MET
2	B	92	ARG
2	B	97	LEU
3	C	20	ARG
3	C	23	LEU
3	C	25	PHE
3	C	29	ARG
3	C	31	HIS
3	C	33	LEU
3	C	34	LEU
3	C	41	GLU
3	C	49	VAL
3	C	50	TYR
3	C	56	GLU
3	C	59	THR
3	C	61	GLU
3	C	81	ARG
3	C	84	GLN
3	C	99	ARG
3	C	107	VAL
4	D	38	TYR
4	D	42	VAL
4	D	43	TYR

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Mol	Chain	Res	Type
4	D	44	LYS
4	D	46	LEU
4	D	47	LYS
4	D	50	HIS
4	D	52	ASP
4	D	55	ILE
4	D	56	SER
4	D	61	SER
4	D	63	MET
4	D	71	PHE
4	D	81	LEU
4	D	90	ILE
4	D	102	LEU
4	D	113	SER
4	D	122	TYR
1	E	55	GLN
1	E	59	GLU
1	E	68	GLN
1	E	74	ILE
1	E	80	THR
1	E	93	GLN
1	E	101	VAL
1	E	128	ARG
2	F	18	HIS
2	F	26	ILE
2	F	27	GLN
2	F	30	THR
2	F	53	GLU
2	F	62	LEU
2	F	73	THR
2	F	82	THR
2	F	90	LEU
2	F	93	GLN
3	G	32	ARG
3	G	33	LEU
3	G	35	ARG
3	G	36	LYS
3	G	41	GLU
3	G	49	VAL
3	G	51	LEU
3	G	65	LEU
3	G	81	ARG

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Mol	Chain	Res	Type
3	G	85	LEU
3	G	90	ASP
3	G	99	ARG
3	G	111	ILE
3	G	113	SER
3	G	114	VAL
4	H	36	GLU
4	H	40	ILE
4	H	52	ASP
4	H	55	ILE
4	H	60	MET
4	H	64	ASN
4	H	71	PHE
4	H	72	GLU
4	H	87	ARG
4	H	91	THR
4	H	93	ARG
4	H	103	LEU
4	H	107	LEU
4	H	113	SER
4	H	116	THR
7	K	4	THR
7	K	7	ASP
7	K	8	LEU
7	K	18	ASP
7	K	21	ARG
7	K	23	ILE
7	K	28	ARG
7	K	29	ARG
7	K	30	ARG
7	K	37	GLU
7	K	39	VAL
7	K	49	SER
7	K	52	LYS
7	K	56	VAL
7	K	58	PHE
7	K	59	ASN
7	K	63	THR
7	K	64	GLU
7	K	66	TYR
7	K	67	SER
7	K	72	HIS

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Mol	Chain	Res	Type
7	K	75	ARG
7	K	77	ASN
7	K	81	ASN
7	K	83	VAL
7	K	101	TYR
7	K	106	ARG
7	K	108	ASP
7	K	112	GLU
7	K	113	ASP
7	K	121	ASP
7	K	130	SER
7	K	139	SER
7	K	141	ILE
7	K	144	LYS
7	K	157	GLN
7	K	160	ASP
7	K	162	SER
7	K	163	ILE
7	K	166	ILE
7	K	167	GLU
7	K	180	THR
7	K	183	LYS
7	K	194	ARG
7	K	202	LYS
7	K	210	ARG
7	L	3	LYS
7	L	5	LEU
7	L	7	ASP
7	L	8	LEU
7	L	17	ASP
7	L	19	GLN
7	L	21	ARG
7	L	23	ILE
7	L	28	ARG
7	L	42	LYS
7	L	44	ILE
7	L	49	SER
7	L	61	ASN
7	L	64	GLU
7	L	65	THR
7	L	66	TYR
7	L	87	VAL

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Mol	Chain	Res	Type
7	L	92	ARG
7	L	94	PHE
7	L	96	LEU
7	L	137	GLU
7	L	138	LEU
7	L	139	SER
7	L	163	ILE
7	L	174	ARG
7	L	183	LYS
7	L	203	GLN
7	L	208	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	GLN
3	C	73	ASN
2	F	27	GLN
3	G	84	GLN
7	K	72	HIS
7	K	151	GLN
7	L	26	ASN
7	L	38	ASN
7	L	61	ASN
7	L	81	ASN
7	L	104	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates 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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
7	K	2
7	L	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	K	153:LEU	C	154:PRO	N	1.67
1	K	182:GLU	C	183:LYS	N	1.64
1	L	18:ASP	C	19:GLN	N	1.62

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	97/136 (71%)	-0.03	0 100 100	29, 51, 106, 161	0
1	E	90/136 (66%)	-0.10	0 100 100	37, 69, 105, 120	0
2	B	89/103 (86%)	0.34	5 (5%) 24 23	29, 44, 121, 161	0
2	F	83/103 (80%)	-0.04	0 100 100	37, 65, 107, 129	0
3	C	98/130 (75%)	-0.00	2 (2%) 65 64	37, 71, 136, 172	0
3	G	100/130 (76%)	-0.15	0 100 100	32, 64, 104, 119	0
4	D	86/126 (68%)	-0.15	1 (1%) 79 78	36, 66, 128, 162	0
4	H	88/126 (69%)	-0.10	0 100 100	40, 70, 102, 160	0
5	I	143/167 (85%)	-0.99	0 100 100	68, 152, 199, 220	0
6	J	142/167 (85%)	-1.00	0 100 100	75, 157, 194, 206	0
7	K	210/236 (88%)	-0.05	3 (1%) 75 75	32, 75, 141, 170	0
7	L	205/236 (86%)	-0.20	1 (0%) 91 91	32, 71, 132, 156	0
All	All	1431/1796 (79%)	-0.25	12 (0%) 86 86	29, 74, 173, 220	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	12	LYS	11.4
2	B	13	GLY	8.2
2	B	14	GLY	6.7
7	K	34	ARG	5.9
2	B	19	ARG	3.8
2	B	15	ALA	3.4
7	K	215	VAL	2.9
7	K	124	PHE	2.8
4	D	90	ILE	2.7
7	L	124	PHE	2.3
3	C	63	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
3	C	41	GLU	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.