



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:38 PM UTC

PDB ID : 8BYX / pdb_00008byx
Title : HOXB13-homodimer bound to DNA
Authors : Morgunova, E.; Popov, A.; Yin, Y.; Taipale, J.
Deposited on : 2022-12-14
Resolution : 3.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

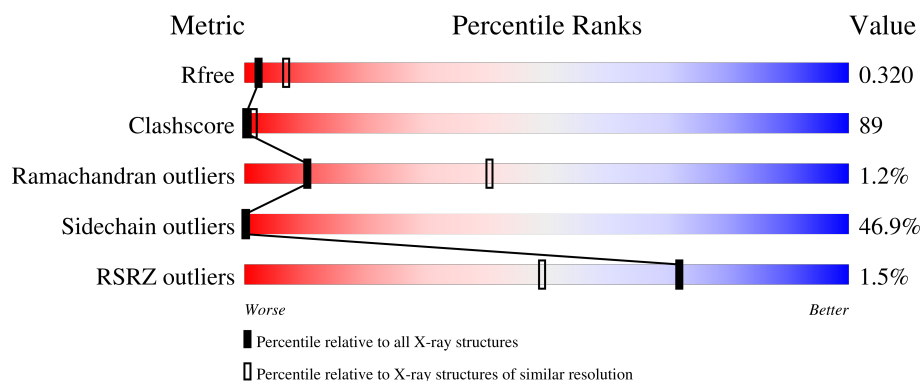
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	C	18	
1	D	18	
1	H	18	
2	E	18	
2	F	18	

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Mol	Chain	Length	Quality of chain
2	I	18	28%61%11%
3	A	63	2%13%40%32%10%6%
3	B	63	37%32%29%. .
3	G	63	2%16%46%35%. .
3	J	63	21%35%27%8%10%
3	K	63	2%22%35%38%. .
3	L	63	5%5%30%40%11%14%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5225 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 DNA chain called DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	17	Total	C	N	O	P	0	0	0
			347	168	51	111	17			
1	C	18	Total	C	N	O	P	0	0	0
			369	178	56	117	18			
1	H	18	Total	C	N	O	P	0	0	0
			369	178	56	117	18			

- Molecule 2 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	18	Total	C	N	O	P	0	0	0
			371	176	76	101	18			
2	F	18	Total	C	N	O	P	0	0	0
			371	176	76	101	18			
2	I	18	Total	C	N	O	P	0	0	0
			371	176	76	101	18			

- Molecule 3 is a protein called Homeobox protein Hox-B13.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	B	62	Total	C	N	O	0	0	0
			525	331	106	88			
3	A	59	Total	C	N	O	0	0	0
			501	317	99	85			
3	G	61	Total	C	N	O	0	0	0
			521	329	105	87			
3	J	57	Total	C	N	O	0	0	0
			481	305	93	83			
3	K	61	Total	C	N	O	0	0	0
			521	329	105	87			
3	L	54	Total	C	N	O	0	0	0
			459	290	89	80			

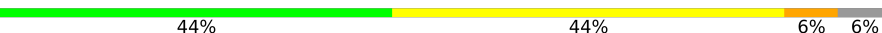
- Molecule 4 is water.

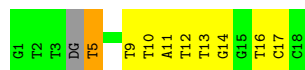
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	4	Total O 4 4	0	0
4	E	1	Total O 1 1	0	0
4	B	2	Total O 2 2	0	0
4	C	2	Total O 2 2	0	0
4	F	3	Total O 3 3	0	0
4	A	1	Total O 1 1	0	0
4	H	2	Total O 2 2	0	0
4	I	2	Total O 2 2	0	0
4	G	2	Total O 2 2	0	0

3 Residue-property plots [i](#)

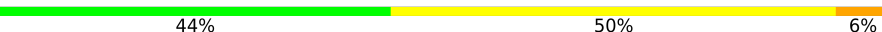
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

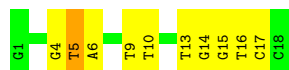
- Molecule 1: DNA

Chain D: 

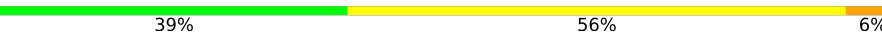


- Molecule 1: DNA

Chain C: 



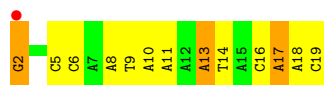
- Molecule 1: DNA

Chain H: 

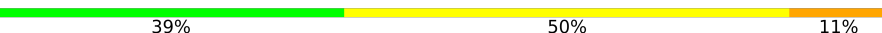


- Molecule 2: DNA

Chain E: 



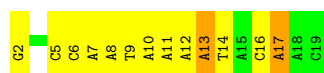
- Molecule 2: DNA

Chain F: 



- Molecule 2: DNA

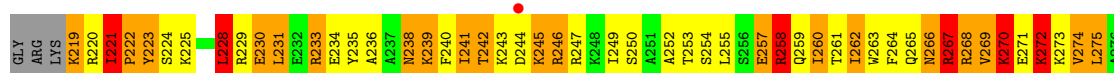
Chain I: 



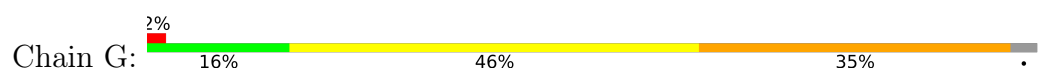
• Molecule 3: Homeobox protein Hox-B13



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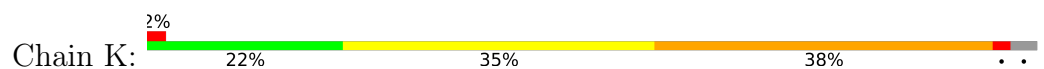
• Molecule 3: Homeobox protein Hox-B13



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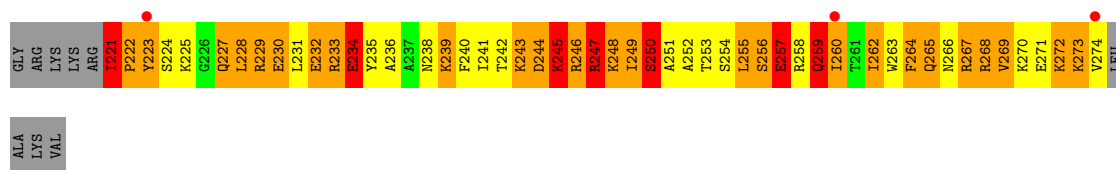


• Molecule 3: Homeobox protein Hox-B13



• Molecule 3: Homeobox protein Hox-B13





4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	116.78Å 116.78Å 118.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.00 30.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (30.00-3.00) 99.8 (30.00-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.254 , 0.304 0.280 , 0.320	Depositor DCC
R_{free} test set	941 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	72.3	Xtriage
Anisotropy	0.625	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 49.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.039 for -h,l,k 0.010 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5225	wwPDB-VP
Average B, all atoms (Å ²)	119.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.97% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	C	0.43	0/410	1.04	1/630 (0.2%)
1	D	0.45	0/384	1.07	1/587 (0.2%)
1	H	0.46	0/410	1.02	1/630 (0.2%)
2	E	0.50	0/418	1.04	4/640 (0.6%)
2	F	0.40	0/418	0.89	3/640 (0.5%)
2	I	0.38	0/418	0.94	3/640 (0.5%)
3	A	1.16	1/507 (0.2%)	1.93	16/672 (2.4%)
3	B	1.26	2/531 (0.4%)	1.70	5/702 (0.7%)
3	G	1.13	1/527 (0.2%)	1.67	3/697 (0.4%)
3	J	1.15	1/487 (0.2%)	1.84	7/647 (1.1%)
3	K	1.25	2/527 (0.4%)	1.75	5/697 (0.7%)
3	L	1.24	1/465 (0.2%)	2.00	13/618 (2.1%)
All	All	0.94	8/5502 (0.1%)	1.48	62/7800 (0.8%)

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
3	A	0	1
3	J	0	1
3	K	0	1
3	L	0	3
All	All	0	6

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	222	PRO	N-CA	19.23	1.69	1.47
3	B	222	PRO	N-CA	19.07	1.69	1.47
3	L	222	PRO	N-CA	18.01	1.70	1.47
3	A	222	PRO	N-CA	17.61	1.69	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	222	PRO	N-CA	17.56	1.69	1.47
3	J	222	PRO	N-CA	16.88	1.69	1.47
3	B	221	ILE	C-N	9.50	1.44	1.33
3	K	221	ILE	C-N	9.02	1.45	1.33

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	221	ILE	CA-C-N	17.90	138.16	119.90
3	K	221	ILE	C-N-CA	17.90	138.16	119.90
3	J	221	ILE	CA-C-N	16.65	140.65	119.84
3	J	221	ILE	C-N-CA	16.65	140.65	119.84
3	B	221	ILE	CA-C-N	16.56	137.65	119.93
3	B	221	ILE	C-N-CA	16.56	137.65	119.93
3	A	221	ILE	CA-C-N	14.80	138.34	119.84
3	A	221	ILE	C-N-CA	14.80	138.34	119.84
3	L	221	ILE	CA-C-N	14.48	137.94	119.84
3	L	221	ILE	C-N-CA	14.48	137.94	119.84
3	G	221	ILE	CA-C-N	14.06	137.41	119.84
3	G	221	ILE	C-N-CA	14.06	137.41	119.84
3	A	267	ARG	CB-CA-C	-12.39	91.88	110.96
3	J	222	PRO	CA-N-CD	-11.20	96.32	112.00
1	H	5	DT	C2'-C3'-O3'	10.97	127.96	111.50
1	D	5	DT	C2'-C3'-O3'	10.91	127.86	111.50
1	C	5	DT	C2'-C3'-O3'	10.76	127.64	111.50
3	L	250	SER	O-C-N	-8.56	112.39	122.15
3	A	222	PRO	CA-N-CD	-7.49	101.52	112.00
2	I	17	DA	C4'-C3'-O3'	7.46	121.19	110.00
2	E	13	DA	C2'-C3'-O3'	7.37	122.55	111.50
3	L	222	PRO	CA-N-CD	-7.26	101.84	112.00
3	K	222	PRO	CA-N-CD	-7.21	101.91	112.00
3	G	222	PRO	CA-N-CD	-7.15	102.00	112.00
3	B	222	PRO	CA-N-CD	-7.07	102.11	112.00
3	L	268	ARG	CG-CD-NE	6.85	127.06	112.00
3	B	222	PRO	N-CA-C	-6.67	100.39	111.26
3	A	259	GLN	CB-CA-C	6.59	122.05	110.85
2	I	2	DG	C2'-C3'-O3'	6.54	121.31	111.50
3	L	259	GLN	O-C-N	-6.38	114.10	122.39
2	E	17	DA	C4'-C3'-O3'	-6.37	100.45	110.00
3	L	223	TYR	CB-CA-C	6.16	120.88	109.54
2	F	2	DG	C2'-C3'-O3'	6.15	120.73	111.50
3	L	234	GLU	O-C-N	6.13	126.23	120.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	270	LYS	O-C-N	6.08	128.33	122.07
2	I	13	DA	C2'-C3'-O3'	6.01	120.52	111.50
3	L	247	ARG	CB-CG-CD	5.97	125.03	111.30
2	E	2	DG	C2'-C3'-O3'	5.96	120.44	111.50
3	A	268	ARG	CB-CA-C	5.94	121.61	110.63
3	J	223	TYR	CB-CA-C	5.91	120.34	109.46
3	A	267	ARG	CG-CD-NE	5.90	124.98	112.00
2	F	17	DA	C4'-C3'-O3'	-5.84	101.23	110.00
3	L	247	ARG	CG-CD-NE	5.71	124.57	112.00
3	B	257	GLU	N-CA-C	-5.68	105.08	111.28
3	L	268	ARG	CB-CA-C	-5.62	102.06	110.88
3	A	272	LYS	O-C-N	5.56	128.01	122.12
3	J	248	LYS	O-C-N	5.55	128.02	122.08
3	J	247	ARG	O-C-N	5.54	129.95	122.59
3	L	258	ARG	N-CA-C	-5.40	105.29	111.07
2	F	13	DA	C2'-C3'-O3'	5.35	119.53	111.50
3	L	257	GLU	N-CA-C	-5.30	105.40	111.07
3	A	258	ARG	N-CA-C	-5.18	105.71	111.36
3	A	267	ARG	CA-C-N	5.18	127.74	120.28
3	A	267	ARG	C-N-CA	5.18	127.74	120.28
3	A	244	ASP	O-C-N	-5.15	116.46	122.03
3	A	268	ARG	N-CA-C	-5.14	105.80	111.71
3	J	248	LYS	N-CA-C	-5.12	104.78	111.02
2	E	13	DA	C4'-C3'-O3'	-5.11	102.34	110.00
3	K	271	GLU	CB-CG-CD	5.09	121.25	112.60
3	A	252	ALA	O-C-N	5.05	127.27	122.07
3	A	228	LEU	N-CA-C	-5.02	105.80	111.28
3	A	236	ALA	N-CA-C	-5.01	105.82	111.28

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	266	ASN	Mainchain
3	J	246	ARG	Mainchain
3	K	253	THR	Mainchain
3	L	245	LYS	Mainchain
3	L	250	SER	Mainchain
3	L	259	GLN	Mainchain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	369	0	209	30	0
1	D	347	0	199	32	0
1	H	369	0	209	17	0
2	E	371	0	201	19	4
2	F	371	0	201	27	0
2	I	371	0	201	23	0
3	A	501	0	541	143	0
3	B	525	0	571	90	0
3	G	521	0	567	121	0
3	J	481	0	515	102	0
3	K	521	0	566	128	4
3	L	459	0	484	214	0
4	A	1	0	0	1	0
4	B	2	0	0	0	0
4	C	2	0	0	1	0
4	D	4	0	0	0	0
4	E	1	0	0	0	0
4	F	3	0	0	0	0
4	G	2	0	0	0	0
4	H	2	0	0	0	0
4	I	2	0	0	1	0
All	All	5225	0	4464	859	4

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 89.

All (859) 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)
3:L:223:TYR:CE2	3:L:227:GLN:HB3	1.28	1.64
3:K:242:THR:HG23	3:K:245:LYS:CD	1.20	1.60
3:K:241:ILE:HD12	3:K:245:LYS:CD	1.28	1.59
3:L:223:TYR:CZ	3:L:227:GLN:HB3	1.31	1.58
3:G:228:LEU:HA	3:G:231:LEU:CD1	1.12	1.55
1:D:10:DT:C5'	3:B:223:TYR:CE1	1.86	1.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:263:TRP:CZ3	3:K:267:ARG:HG2	1.38	1.54
3:K:241:ILE:CD1	3:K:245:LYS:CE	1.82	1.52
1:D:10:DT:H5'	3:B:223:TYR:CD1	1.41	1.51
3:K:241:ILE:CD1	3:K:245:LYS:HE3	1.38	1.47
3:G:228:LEU:CA	3:G:231:LEU:HD12	1.44	1.46
3:J:222:PRO:N	3:J:222:PRO:CA	1.68	1.45
3:K:263:TRP:CH2	3:K:267:ARG:HD3	1.52	1.44
1:D:10:DT:H5'	3:B:223:TYR:CE1	1.47	1.43
3:K:263:TRP:CZ3	3:K:267:ARG:CG	2.03	1.42
3:K:222:PRO:N	3:K:222:PRO:CA	1.69	1.42
3:A:258:ARG:O	3:A:262:ILE:CG1	1.66	1.41
3:L:222:PRO:N	3:L:222:PRO:CA	1.70	1.39
3:L:235:TYR:CA	3:L:238:ASN:HD22	1.34	1.38
3:L:223:TYR:CE2	3:L:227:GLN:CB	2.06	1.38
3:G:222:PRO:N	3:G:222:PRO:CA	1.69	1.36
3:K:263:TRP:CH2	3:K:267:ARG:HG2	1.59	1.36
3:K:242:THR:HG23	3:K:245:LYS:CG	1.53	1.35
3:K:263:TRP:CH2	3:K:267:ARG:CD	2.10	1.33
1:H:4:DG:OP2	3:L:270:LYS:NZ	1.57	1.32
3:L:235:TYR:HA	3:L:238:ASN:ND2	1.03	1.31
3:K:263:TRP:CH2	3:K:267:ARG:CG	2.11	1.31
3:B:222:PRO:N	3:B:222:PRO:CA	1.69	1.31
3:K:242:THR:CG2	3:K:245:LYS:HD2	1.60	1.31
3:J:253:THR:OG1	3:J:255:LEU:CD1	1.77	1.30
1:C:6:DA:OP2	3:K:259:GLN:NE2	1.63	1.30
3:A:222:PRO:N	3:A:222:PRO:CA	1.69	1.29
3:K:242:THR:CG2	3:K:245:LYS:CD	2.11	1.28
3:G:228:LEU:O	3:G:231:LEU:HB2	1.24	1.28
3:L:223:TYR:CZ	3:L:227:GLN:CB	2.16	1.28
3:G:235:TYR:O	3:G:239:LYS:NZ	1.68	1.26
3:G:228:LEU:HD23	3:G:231:LEU:CD1	1.64	1.26
3:L:228:LEU:O	3:L:231:LEU:HB3	1.29	1.24
3:K:241:ILE:CD1	3:K:245:LYS:CD	2.05	1.24
1:H:5:DT:C7	3:L:266:ASN:HD22	1.50	1.23
3:L:235:TYR:HB3	3:L:238:ASN:CB	1.66	1.23
1:D:10:DT:C5'	3:B:223:TYR:HE1	1.30	1.22
3:L:223:TYR:HD2	3:L:228:LEU:CD1	1.52	1.21
3:A:253:THR:C	3:A:255:LEU:HD12	1.68	1.18
3:J:253:THR:OG1	3:J:255:LEU:HD13	1.35	1.17
3:G:228:LEU:CA	3:G:231:LEU:CD1	2.07	1.17
3:K:263:TRP:CZ3	3:K:267:ARG:CB	2.28	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:235:TYR:CA	3:L:238:ASN:ND2	1.96	1.16
3:L:235:TYR:CE2	3:L:245:LYS:HD2	1.81	1.16
3:G:228:LEU:HA	3:G:231:LEU:HD11	1.28	1.15
3:G:235:TYR:CE2	3:G:239:LYS:HE3	1.79	1.15
1:D:10:DT:C4'	3:B:223:TYR:HE1	1.58	1.15
3:K:263:TRP:CZ3	3:K:267:ARG:HB2	1.79	1.15
3:K:242:THR:CG2	3:K:245:LYS:HG3	1.77	1.14
3:L:267:ARG:HH12	3:L:270:LYS:HB3	1.06	1.14
2:I:7:DA:OP2	3:G:272:LYS:NZ	1.79	1.13
3:A:225:LYS:C	3:A:228:LEU:HD12	1.55	1.12
1:H:5:DT:H73	3:L:266:ASN:HD22	1.07	1.12
3:A:258:ARG:O	3:A:262:ILE:HG13	0.97	1.11
3:J:256:SER:HB3	3:J:259:GLN:HG3	1.12	1.11
3:L:235:TYR:OH	3:L:249:ILE:CD1	1.98	1.11
3:A:253:THR:CB	3:A:255:LEU:CD1	2.29	1.10
1:H:5:DT:C7	3:L:266:ASN:ND2	2.14	1.10
1:D:10:DT:H5''	3:B:223:TYR:CE1	1.71	1.09
3:K:247:ARG:HD2	3:K:257:GLU:OE2	1.53	1.08
3:A:267:ARG:NH1	3:A:270:LYS:HG3	1.66	1.08
3:K:242:THR:CG2	3:K:245:LYS:CG	2.28	1.08
3:J:258:ARG:O	3:J:262:ILE:HG12	1.54	1.07
3:G:228:LEU:O	3:G:231:LEU:CB	2.02	1.07
3:L:244:ASP:O	3:L:247:ARG:NH2	1.86	1.07
2:F:6:DC:H42	3:A:265:GLN:NE2	1.53	1.07
2:I:7:DA:P	3:G:272:LYS:NZ	2.28	1.07
3:G:230:GLU:O	3:G:233:ARG:HB3	1.52	1.06
3:G:249:ILE:HD13	3:G:249:ILE:H	1.18	1.06
3:J:231:LEU:HB3	3:J:263:TRP:CZ3	1.90	1.06
1:C:5:DT:O3'	3:K:223:TYR:OH	1.73	1.06
3:L:243:LYS:HA	3:L:246:ARG:HD2	1.31	1.06
3:L:247:ARG:HB3	3:L:247:ARG:HH21	1.20	1.06
3:L:247:ARG:HA	3:L:257:GLU:OE2	1.54	1.06
3:A:238:ASN:OD1	3:A:245:LYS:NZ	1.89	1.05
3:L:223:TYR:OH	3:L:255:LEU:HD11	1.55	1.05
3:A:253:THR:HB	3:A:255:LEU:HD11	1.32	1.05
3:A:253:THR:O	3:A:255:LEU:CD1	2.04	1.04
1:C:6:DA:P	3:K:223:TYR:OH	2.15	1.04
3:B:249:ILE:HD13	3:B:249:ILE:H	1.21	1.04
3:L:223:TYR:CD2	3:L:228:LEU:CD1	2.41	1.03
3:K:241:ILE:CD1	3:K:245:LYS:HD3	1.76	1.03
3:B:258:ARG:O	3:B:262:ILE:HG12	1.58	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:253:THR:HB	3:A:255:LEU:CD1	1.85	1.03
3:B:253:THR:O	3:B:255:LEU:HD12	1.58	1.02
3:G:253:THR:O	3:G:255:LEU:HD12	1.58	1.02
3:K:241:ILE:HD13	3:K:245:LYS:CE	1.82	1.02
2:F:6:DC:OP2	3:A:268:ARG:HD2	1.60	1.02
3:A:253:THR:C	3:A:255:LEU:CD1	2.32	1.01
3:K:242:THR:HG23	3:K:245:LYS:HD2	1.07	1.01
3:A:225:LYS:C	3:A:228:LEU:CD1	2.17	1.00
3:A:258:ARG:O	3:A:262:ILE:CD1	2.09	1.00
3:L:235:TYR:HB3	3:L:238:ASN:HB2	1.37	1.00
3:J:258:ARG:O	3:J:262:ILE:CG1	2.10	0.99
3:L:235:TYR:OH	3:L:249:ILE:HD11	1.63	0.99
3:L:270:LYS:O	3:L:273:LYS:HG2	1.62	0.99
3:K:241:ILE:HD11	3:K:245:LYS:CE	1.67	0.99
3:G:247:ARG:HH11	3:G:247:ARG:HB2	1.28	0.99
2:F:6:DC:OP1	3:A:268:ARG:HD3	1.63	0.97
3:L:223:TYR:OH	3:L:255:LEU:CD1	2.11	0.97
3:L:228:LEU:O	3:L:231:LEU:CB	2.13	0.96
3:L:223:TYR:CD2	3:L:228:LEU:HD13	2.00	0.96
3:L:241:ILE:HB	3:L:264:PHE:CE1	2.00	0.96
3:K:263:TRP:HH2	3:K:267:ARG:CD	1.65	0.96
3:B:273:LYS:NZ	3:B:273:LYS:HA	1.79	0.96
3:K:242:THR:OG1	3:K:245:LYS:HG3	1.65	0.95
3:B:246:ARG:HD3	3:B:257:GLU:OE2	1.64	0.95
3:B:246:ARG:O	3:B:249:ILE:HG12	1.65	0.94
2:E:5:DC:H5'	3:B:240:PHE:HE2	1.32	0.94
3:A:240:PHE:CD2	3:A:268:ARG:NH2	2.35	0.94
3:A:267:ARG:NH1	3:A:270:LYS:CG	2.30	0.94
3:K:242:THR:HG23	3:K:245:LYS:HD3	1.47	0.94
3:A:234:GLU:CD	3:A:249:ILE:HD11	1.93	0.93
3:G:228:LEU:HD23	3:G:231:LEU:HD11	1.47	0.93
1:C:6:DA:OP2	3:K:223:TYR:OH	1.87	0.93
1:D:10:DT:H5'	3:B:223:TYR:HD1	1.19	0.93
2:I:7:DA:P	3:G:272:LYS:HZ1	1.91	0.92
3:G:228:LEU:HA	3:G:231:LEU:CG	1.98	0.92
3:G:239:LYS:HD2	3:G:239:LYS:N	1.85	0.92
3:K:241:ILE:HD11	3:K:245:LYS:HB3	1.48	0.92
3:A:229:ARG:NH1	3:A:229:ARG:HB2	1.84	0.92
1:D:10:DT:C5'	3:B:223:TYR:CD1	2.27	0.91
3:G:228:LEU:CD2	3:G:231:LEU:CD1	2.47	0.91
3:K:263:TRP:CZ2	3:K:267:ARG:HD3	2.05	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:247:ARG:O	3:L:251:ALA:N	2.02	0.91
3:L:241:ILE:HG22	3:L:264:PHE:CE1	2.05	0.91
3:L:241:ILE:CG2	3:L:264:PHE:CE1	2.54	0.91
2:F:6:DC:H42	3:A:265:GLN:HE22	1.01	0.91
3:G:253:THR:O	3:G:255:LEU:CD1	2.19	0.91
3:G:253:THR:C	3:G:255:LEU:HD12	1.96	0.91
3:B:246:ARG:HA	3:B:249:ILE:CG1	2.00	0.91
3:B:273:LYS:HA	3:B:273:LYS:HZ2	1.34	0.91
1:H:5:DT:H71	3:L:266:ASN:ND2	1.83	0.90
3:G:227:GLN:O	3:G:231:LEU:HG	1.70	0.90
3:K:241:ILE:CD1	3:K:245:LYS:HE2	2.02	0.90
3:K:242:THR:CB	3:K:245:LYS:HG3	2.00	0.90
3:L:239:LYS:CE	3:L:239:LYS:HA	2.00	0.90
3:K:239:LYS:HD2	3:K:239:LYS:N	1.85	0.90
3:L:267:ARG:NH1	3:L:270:LYS:HB3	1.87	0.90
3:L:235:TYR:CB	3:L:238:ASN:HB2	2.01	0.89
2:F:6:DC:N4	3:A:265:GLN:NE2	2.20	0.89
2:F:6:DC:N3	3:A:265:GLN:NE2	2.21	0.89
2:F:6:DC:N4	3:A:265:GLN:HE22	1.71	0.89
3:A:242:THR:O	3:A:246:ARG:HG2	1.72	0.89
3:G:228:LEU:HD23	3:G:231:LEU:HD13	1.54	0.89
2:E:5:DC:H5"	3:B:240:PHE:CE2	2.07	0.88
1:D:11:DA:OP2	3:B:223:TYR:OH	1.90	0.88
3:A:249:ILE:O	3:A:253:THR:OG1	1.91	0.88
3:L:255:LEU:HD22	3:L:255:LEU:H	1.38	0.88
3:A:267:ARG:O	3:A:270:LYS:HB3	1.74	0.88
3:J:253:THR:CB	3:J:255:LEU:HD11	2.03	0.88
3:J:253:THR:C	3:J:255:LEU:HD12	1.98	0.88
3:K:241:ILE:HD13	3:K:245:LYS:HE2	1.56	0.88
3:B:273:LYS:HA	3:B:273:LYS:CE	2.00	0.88
2:I:7:DA:P	3:G:272:LYS:HZ3	1.90	0.88
3:J:231:LEU:HD13	3:J:263:TRP:CE3	2.08	0.88
3:L:247:ARG:HH21	3:L:247:ARG:CB	1.86	0.88
3:J:243:LYS:HA	3:J:246:ARG:NH1	1.89	0.87
3:J:253:THR:OG1	3:J:255:LEU:HD11	1.74	0.87
3:A:253:THR:O	3:A:255:LEU:HD11	1.73	0.87
3:K:263:TRP:HH2	3:K:267:ARG:HD3	1.14	0.87
3:J:243:LYS:HD2	3:J:246:ARG:NH1	1.90	0.87
3:L:249:ILE:HD13	3:L:249:ILE:H	1.38	0.87
3:J:269:VAL:O	3:J:273:LYS:HG2	1.75	0.87
3:L:245:LYS:O	3:L:248:LYS:HB2	1.74	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:223:TYR:OH	3:K:259:GLN:NE2	2.08	0.86
3:B:258:ARG:CB	3:B:258:ARG:HH21	1.88	0.86
3:G:230:GLU:O	3:G:233:ARG:CB	2.22	0.86
3:J:246:ARG:HG3	3:J:246:ARG:HH11	1.41	0.86
3:K:241:ILE:HD11	3:K:245:LYS:HE3	0.88	0.86
3:K:263:TRP:HZ3	3:K:267:ARG:HG2	1.06	0.86
3:L:235:TYR:CB	3:L:238:ASN:CB	2.52	0.86
3:A:223:TYR:O	3:A:228:LEU:HD21	1.75	0.86
3:L:235:TYR:OH	3:L:249:ILE:HD12	1.74	0.86
3:L:241:ILE:CB	3:L:264:PHE:CE1	2.58	0.86
3:A:253:THR:OG1	3:A:255:LEU:HD13	1.76	0.86
3:L:231:LEU:HD11	3:L:263:TRP:CD1	2.11	0.86
3:A:267:ARG:HH12	3:A:270:LYS:HG3	1.39	0.85
3:J:256:SER:CB	3:J:259:GLN:HG3	2.02	0.85
3:L:269:VAL:O	3:L:273:LYS:HD2	1.76	0.85
3:J:273:LYS:HE3	3:J:273:LYS:HA	1.55	0.85
3:K:263:TRP:CE3	3:K:267:ARG:HB2	2.11	0.85
3:A:253:THR:CB	3:A:255:LEU:HD13	2.07	0.85
3:K:247:ARG:CD	3:K:257:GLU:OE2	2.25	0.84
3:G:273:LYS:NZ	3:G:273:LYS:HA	1.91	0.84
3:K:241:ILE:CD1	3:K:245:LYS:CB	2.55	0.84
3:L:239:LYS:HA	3:L:239:LYS:HE3	1.59	0.84
3:L:223:TYR:CE2	3:L:227:GLN:HB2	2.12	0.84
1:C:4:DG:H1	2:F:16:DC:H5	1.25	0.84
3:L:245:LYS:O	3:L:248:LYS:CB	2.25	0.84
1:D:10:DT:C3'	3:B:223:TYR:HE1	1.91	0.84
1:D:10:DT:H3'	3:B:223:TYR:OH	1.78	0.84
3:G:230:GLU:OE2	3:G:253:THR:HG23	1.78	0.84
1:C:10:DT:H3'	3:A:223:TYR:OH	1.77	0.84
3:L:235:TYR:HA	3:L:238:ASN:CG	2.02	0.84
3:A:241:ILE:O	4:A:301:HOH:O	1.96	0.83
3:B:253:THR:O	3:B:255:LEU:CD1	2.26	0.83
3:L:223:TYR:HD2	3:L:228:LEU:HD12	1.43	0.83
3:L:243:LYS:HA	3:L:246:ARG:CD	2.08	0.83
3:B:247:ARG:CB	3:B:247:ARG:HH11	1.92	0.83
3:J:243:LYS:HA	3:J:246:ARG:HH11	1.43	0.83
3:L:268:ARG:O	3:L:272:LYS:NZ	2.12	0.82
3:A:267:ARG:O	3:A:270:LYS:CB	2.27	0.82
3:A:240:PHE:CG	3:A:268:ARG:NH2	2.46	0.82
3:L:273:LYS:CA	3:L:273:LYS:HE3	2.09	0.82
3:J:256:SER:HB3	3:J:259:GLN:CG	2.02	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:3:DT:O4	2:I:17:DA:N6	2.13	0.82
3:J:243:LYS:HD2	3:J:246:ARG:HH12	1.45	0.82
3:L:235:TYR:OH	3:L:245:LYS:CB	2.27	0.82
3:G:249:ILE:H	3:G:249:ILE:CD1	1.90	0.81
3:A:240:PHE:HA	3:A:268:ARG:NH2	1.95	0.81
3:G:219:LYS:HE3	3:G:221:ILE:HA	1.61	0.81
3:G:228:LEU:CB	3:G:231:LEU:HD12	2.11	0.81
3:L:249:ILE:O	3:L:255:LEU:HD23	1.81	0.81
3:J:249:ILE:HG22	3:J:260:ILE:HD13	1.62	0.80
3:L:231:LEU:HD21	3:L:263:TRP:CE2	2.16	0.80
3:L:273:LYS:HE3	3:L:273:LYS:HA	1.62	0.80
3:A:267:ARG:HH11	3:A:270:LYS:HB3	1.45	0.80
3:J:234:GLU:O	3:J:237:ALA:HB3	1.82	0.80
3:A:253:THR:CB	3:A:255:LEU:HD11	2.00	0.80
3:J:253:THR:CB	3:J:255:LEU:CD1	2.58	0.80
3:L:235:TYR:HB3	3:L:238:ASN:HB3	1.63	0.79
3:K:241:ILE:HG13	3:K:245:LYS:HB2	1.64	0.79
3:L:244:ASP:O	3:L:247:ARG:CZ	2.30	0.79
3:G:247:ARG:HH11	3:G:247:ARG:CB	1.95	0.79
3:K:241:ILE:CD1	3:K:245:LYS:HB3	2.13	0.79
3:L:223:TYR:CZ	3:L:227:GLN:CG	2.65	0.79
3:G:228:LEU:HA	3:G:231:LEU:HD12	0.81	0.79
1:C:5:DT:O3'	3:K:223:TYR:CZ	2.35	0.79
1:C:10:DT:H3'	3:A:223:TYR:CZ	2.17	0.79
3:K:241:ILE:HD12	3:K:245:LYS:HD3	0.79	0.78
3:L:223:TYR:OH	3:L:227:GLN:HB3	1.83	0.78
3:J:231:LEU:HD12	3:J:263:TRP:CD2	2.17	0.78
3:G:247:ARG:HB2	3:G:247:ARG:NH1	1.99	0.78
3:L:235:TYR:CE2	3:L:245:LYS:CD	2.65	0.77
1:C:5:DT:O4'	3:K:220:ARG:HD2	1.85	0.76
1:D:11:DA:H2''	1:D:12:DT:H72	1.67	0.76
3:J:245:LYS:O	3:J:249:ILE:HG12	1.85	0.76
3:K:241:ILE:HD11	3:K:245:LYS:CB	2.16	0.76
3:L:250:SER:HA	3:L:255:LEU:HD23	1.68	0.76
2:E:16:DC:H2'	2:E:16:DC:O2	1.84	0.76
1:C:10:DT:O4'	3:A:220:ARG:NH1	2.18	0.75
3:L:235:TYR:C	3:L:238:ASN:HD22	1.94	0.75
3:J:273:LYS:HE3	3:J:273:LYS:CA	2.09	0.75
3:K:225:LYS:H	3:K:225:LYS:HD2	1.50	0.75
3:A:270:LYS:O	3:A:273:LYS:HB3	1.86	0.75
3:K:242:THR:H	3:K:245:LYS:HD3	1.52	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:235:TYR:HB3	3:L:238:ASN:CG	2.11	0.75
1:D:10:DT:C3'	3:B:223:TYR:CE1	2.69	0.75
3:G:246:ARG:O	3:G:249:ILE:HG12	1.87	0.75
3:A:235:TYR:CE2	3:A:239:LYS:HD2	2.22	0.74
2:F:16:DC:H2'	2:F:16:DC:O2	1.86	0.74
3:L:247:ARG:CA	3:L:257:GLU:OE2	2.32	0.74
3:G:229:ARG:HG3	3:G:229:ARG:HH11	1.51	0.74
3:L:272:LYS:HB2	3:L:272:LYS:HZ2	1.52	0.74
3:K:228:LEU:HD23	3:K:228:LEU:N	2.02	0.74
3:L:235:TYR:OH	3:L:245:LYS:HB2	1.88	0.74
3:L:235:TYR:OH	3:L:245:LYS:HB3	1.86	0.74
3:K:242:THR:N	3:K:245:LYS:HD3	2.03	0.74
3:L:241:ILE:CB	3:L:264:PHE:HE1	2.00	0.74
3:B:253:THR:C	3:B:255:LEU:HD12	2.13	0.73
3:K:263:TRP:HZ3	3:K:267:ARG:CG	1.70	0.73
2:I:7:DA:H5'	3:J:247:ARG:HD3	1.70	0.73
3:L:223:TYR:HD2	3:L:228:LEU:HD13	1.34	0.73
3:L:241:ILE:HG22	3:L:264:PHE:CD1	2.22	0.73
3:A:229:ARG:HB2	3:A:229:ARG:HH11	1.48	0.73
3:A:260:ILE:HD13	3:A:260:ILE:C	2.13	0.73
3:K:238:ASN:N	3:K:238:ASN:HD22	1.86	0.73
3:L:223:TYR:CZ	3:L:227:GLN:HG3	2.23	0.73
1:D:10:DT:H3'	3:B:223:TYR:CE1	2.24	0.73
3:A:230:GLU:O	3:A:233:ARG:HB3	1.88	0.73
3:G:246:ARG:HH21	3:G:257:GLU:HB3	1.54	0.73
3:L:255:LEU:HD22	3:L:255:LEU:N	2.04	0.73
3:B:258:ARG:HH21	3:B:258:ARG:CA	2.02	0.73
1:C:5:DT:H3'	3:K:223:TYR:CZ	2.24	0.72
3:G:238:ASN:OD1	3:G:245:LYS:NZ	2.22	0.72
3:L:272:LYS:HE3	3:L:272:LYS:HA	1.70	0.72
3:A:257:GLU:O	3:A:261:THR:OG1	2.07	0.72
3:B:249:ILE:H	3:B:249:ILE:CD1	1.90	0.72
3:J:231:LEU:CD1	3:J:263:TRP:CE3	2.71	0.72
3:G:244:ASP:OD1	3:G:244:ASP:N	2.22	0.72
2:F:6:DC:C4	3:A:265:GLN:NE2	2.57	0.72
3:K:227:GLN:HE21	3:K:253:THR:HB	1.55	0.71
3:K:267:ARG:O	3:K:267:ARG:NH2	2.22	0.71
3:J:243:LYS:CD	3:J:246:ARG:HH12	2.03	0.71
3:L:241:ILE:HG22	3:L:264:PHE:HE1	1.55	0.71
3:G:228:LEU:C	3:G:231:LEU:HD12	2.15	0.71
3:B:246:ARG:C	3:B:249:ILE:CD1	2.62	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:232:GLU:C	3:L:234:GLU:H	1.98	0.71
3:B:222:PRO:N	3:B:222:PRO:C	2.47	0.71
2:F:6:DC:OP2	3:A:268:ARG:CD	2.38	0.71
3:B:246:ARG:HA	3:B:249:ILE:HG13	1.70	0.71
3:J:231:LEU:CD1	3:J:263:TRP:CD2	2.73	0.71
3:J:249:ILE:HG22	3:J:260:ILE:CD1	2.20	0.71
3:A:274:VAL:HG12	3:A:275:LEU:HD13	1.71	0.71
3:J:258:ARG:O	3:J:262:ILE:HG13	1.89	0.71
3:K:241:ILE:HD12	3:K:245:LYS:CG	2.20	0.71
3:G:257:GLU:HA	3:G:260:ILE:HG23	1.72	0.70
3:A:253:THR:OG1	3:A:255:LEU:CD1	2.34	0.70
1:D:11:DA:H2''	1:D:12:DT:C7	2.22	0.70
3:G:243:LYS:HA	3:G:246:ARG:HG2	1.74	0.70
3:A:243:LYS:O	3:A:246:ARG:HG3	1.92	0.70
3:G:217:ARG:HB2	3:G:218:LYS:HG3	1.74	0.70
3:J:250:SER:HA	3:J:260:ILE:HD11	1.73	0.70
3:G:273:LYS:HA	3:G:273:LYS:HZ2	1.54	0.70
3:L:235:TYR:HE2	3:L:245:LYS:HD2	1.50	0.70
3:L:247:ARG:C	3:L:247:ARG:HD2	2.17	0.70
3:G:231:LEU:HB3	3:G:263:TRP:CH2	2.27	0.69
3:B:239:LYS:HD2	3:B:239:LYS:N	2.06	0.69
1:D:10:DT:C4'	3:B:223:TYR:CE1	2.49	0.69
3:A:253:THR:O	3:A:255:LEU:HD12	1.75	0.69
3:A:238:ASN:ND2	3:A:238:ASN:O	2.25	0.69
3:K:244:ASP:HA	3:K:247:ARG:HG2	1.75	0.69
3:G:235:TYR:CE2	3:G:239:LYS:CE	2.68	0.69
3:J:253:THR:O	3:J:255:LEU:HD12	1.93	0.69
3:A:243:LYS:HA	3:A:246:ARG:HD2	1.75	0.68
3:L:235:TYR:CZ	3:L:249:ILE:CD1	2.76	0.68
2:E:10:DA:H2'	2:E:11:DA:C8	2.28	0.68
3:A:262:ILE:N	3:A:262:ILE:HD12	2.08	0.68
3:K:234:GLU:HA	3:K:234:GLU:OE1	1.90	0.68
3:L:241:ILE:CG2	3:L:264:PHE:HE1	2.06	0.68
3:L:249:ILE:HD13	3:L:249:ILE:N	2.07	0.68
1:D:11:DA:C2'	1:D:12:DT:H72	2.23	0.68
3:A:225:LYS:O	3:A:228:LEU:HD12	1.91	0.68
3:J:267:ARG:NH1	3:J:270:LYS:HB3	2.09	0.68
3:L:245:LYS:HA	3:L:248:LYS:HB2	1.75	0.68
3:J:229:ARG:HB2	3:J:229:ARG:NH1	2.09	0.68
3:L:227:GLN:NE2	3:L:253:THR:HB	2.09	0.67
1:D:16:DT:H2''	1:D:17:DC:H5'	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:260:ILE:HD13	3:A:260:ILE:O	1.95	0.67
3:L:235:TYR:CB	3:L:238:ASN:CG	2.67	0.67
2:F:6:DC:P	3:A:268:ARG:HD3	2.34	0.67
3:K:245:LYS:O	3:K:248:LYS:HG3	1.93	0.67
3:G:228:LEU:O	3:G:231:LEU:CG	2.42	0.67
3:A:257:GLU:HA	3:A:260:ILE:HG22	1.76	0.67
3:J:253:THR:O	3:J:255:LEU:CD1	2.43	0.67
3:L:223:TYR:OH	3:L:255:LEU:HD12	1.95	0.67
3:L:224:SER:HB3	3:L:227:GLN:HG2	1.76	0.67
3:L:231:LEU:HD21	3:L:263:TRP:CZ2	2.29	0.67
3:L:244:ASP:O	3:L:247:ARG:NH1	2.27	0.67
3:K:234:GLU:HG3	3:K:249:ILE:CD1	2.24	0.66
3:K:248:LYS:HD3	3:K:249:ILE:HG12	1.78	0.66
1:D:10:DT:H3'	3:B:223:TYR:CZ	2.30	0.66
3:L:247:ARG:NH2	3:L:247:ARG:HB3	2.02	0.66
3:K:222:PRO:N	3:K:222:PRO:C	2.53	0.66
3:L:241:ILE:HB	3:L:264:PHE:CZ	2.30	0.66
3:A:240:PHE:HA	3:A:268:ARG:HH22	1.57	0.66
3:J:253:THR:HB	3:J:255:LEU:HD11	1.76	0.66
3:G:258:ARG:HD2	3:G:262:ILE:HG13	1.76	0.66
3:L:245:LYS:O	3:L:248:LYS:N	2.28	0.66
3:A:230:GLU:O	3:A:233:ARG:CB	2.44	0.66
3:G:246:ARG:HA	3:G:249:ILE:CG1	2.26	0.66
3:K:238:ASN:HD22	3:K:238:ASN:H	1.42	0.66
3:L:249:ILE:CD1	3:L:249:ILE:H	2.00	0.65
3:K:234:GLU:HG3	3:K:249:ILE:HD11	1.78	0.65
3:K:263:TRP:HH2	3:K:267:ARG:HG2	1.46	0.65
1:H:16:DT:H2''	1:H:17:DC:H5'	1.78	0.65
3:L:227:GLN:HE21	3:L:253:THR:HB	1.59	0.65
3:J:253:THR:C	3:J:255:LEU:CD1	2.70	0.65
3:J:231:LEU:HB3	3:J:263:TRP:CH2	2.32	0.65
3:K:241:ILE:CD1	3:K:245:LYS:CG	2.74	0.65
3:K:249:ILE:HA	3:K:252:ALA:HB3	1.78	0.65
3:L:235:TYR:CE1	3:L:249:ILE:CD1	2.78	0.65
3:L:272:LYS:HZ1	3:L:272:LYS:N	1.95	0.65
2:F:6:DC:P	3:A:268:ARG:CD	2.86	0.65
1:C:6:DA:H2'	4:C:101:HOH:O	1.96	0.64
1:C:16:DT:H2''	1:C:17:DC:H5'	1.79	0.64
3:L:223:TYR:CZ	3:L:255:LEU:HD12	2.32	0.64
3:L:235:TYR:HE2	3:L:245:LYS:CD	2.06	0.64
3:K:267:ARG:HH21	3:K:267:ARG:C	2.06	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:272:LYS:NZ	3:L:272:LYS:HB2	2.12	0.64
2:F:13:DA:H2''	2:F:14:DT:H5'	1.80	0.64
3:J:250:SER:HB2	3:J:260:ILE:HD12	1.79	0.64
3:B:258:ARG:HH21	3:B:258:ARG:HA	1.63	0.64
3:G:228:LEU:CA	3:G:231:LEU:CG	2.69	0.64
3:G:243:LYS:HA	3:G:246:ARG:CG	2.28	0.64
3:J:246:ARG:HH11	3:J:246:ARG:CG	2.10	0.64
3:L:235:TYR:CZ	3:L:245:LYS:HB2	2.33	0.64
3:L:235:TYR:CZ	3:L:249:ILE:HD12	2.32	0.64
3:L:245:LYS:C	3:L:248:LYS:HB2	2.23	0.63
3:J:239:LYS:HD3	3:J:239:LYS:N	2.13	0.63
3:L:223:TYR:HB3	3:L:228:LEU:HD11	1.80	0.63
3:L:245:LYS:O	3:L:249:ILE:CD1	2.46	0.63
3:G:222:PRO:N	3:G:222:PRO:C	2.53	0.63
3:G:245:LYS:HA	3:G:248:LYS:HG3	1.81	0.63
3:A:246:ARG:HH21	3:A:257:GLU:HB3	1.63	0.63
2:I:13:DA:H2''	2:I:14:DT:H5'	1.80	0.63
3:L:230:GLU:OE1	3:L:234:GLU:HG2	1.98	0.63
1:H:5:DT:C5	3:L:266:ASN:ND2	2.66	0.63
3:G:268:ARG:NH2	3:G:272:LYS:HD2	2.13	0.63
3:L:235:TYR:CA	3:L:238:ASN:HB2	2.28	0.63
3:J:230:GLU:OE1	3:J:230:GLU:HA	1.99	0.63
3:J:244:ASP:HA	3:J:247:ARG:HH22	1.63	0.63
3:L:235:TYR:CB	3:L:238:ASN:ND2	2.61	0.63
3:A:267:ARG:HH11	3:A:270:LYS:CB	2.12	0.62
3:L:239:LYS:HE2	3:L:271:GLU:OE1	1.99	0.62
3:K:224:SER:HB3	3:K:227:GLN:HG3	1.81	0.62
3:A:242:THR:HG23	3:A:245:LYS:HZ2	1.64	0.62
3:G:232:GLU:O	3:G:236:ALA:N	2.31	0.62
3:L:272:LYS:HE3	3:L:272:LYS:CA	2.29	0.62
1:D:10:DT:O4'	3:B:220:ARG:HD2	1.99	0.62
2:I:12:DA:H4'	3:G:219:LYS:HD2	1.81	0.62
2:F:10:DA:H2'	2:F:11:DA:C8	2.35	0.61
2:I:5:DC:H2'	2:I:6:DC:O2	2.01	0.61
3:J:229:ARG:HH11	3:J:229:ARG:CG	2.14	0.61
3:A:258:ARG:C	3:A:262:ILE:CD1	2.73	0.61
3:A:253:THR:HB	3:A:255:LEU:HD13	1.75	0.61
3:L:230:GLU:O	3:L:234:GLU:HB2	2.00	0.61
3:L:223:TYR:CE1	3:L:255:LEU:HD12	2.35	0.61
3:L:250:SER:CB	3:L:257:GLU:OE1	2.49	0.61
3:B:229:ARG:HG3	3:B:229:ARG:HH11	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:10:DA:H2'	2:I:11:DA:C8	2.36	0.61
3:K:263:TRP:HZ3	3:K:267:ARG:CB	1.95	0.60
3:L:241:ILE:CG2	3:L:264:PHE:CD1	2.83	0.60
2:F:16:DC:H2''	2:F:17:DA:OP2	2.01	0.60
3:B:229:ARG:HH11	3:B:229:ARG:CG	2.14	0.60
3:J:275:LEU:HD12	3:J:275:LEU:O	2.01	0.60
3:K:241:ILE:HD13	3:K:245:LYS:HE3	1.53	0.60
3:L:245:LYS:O	3:L:249:ILE:HD13	2.01	0.60
3:A:239:LYS:HD3	3:A:239:LYS:N	2.16	0.60
1:C:5:DT:C3'	3:K:223:TYR:CZ	2.85	0.60
3:G:268:ARG:NH2	3:G:272:LYS:HG3	2.15	0.60
3:B:258:ARG:HH21	3:B:258:ARG:CG	2.13	0.60
2:F:5:DC:H2'	2:F:6:DC:O2	2.01	0.60
3:K:241:ILE:HG13	3:K:245:LYS:CB	2.31	0.60
3:A:253:THR:CA	3:A:255:LEU:CD1	2.79	0.60
3:J:229:ARG:HH11	3:J:229:ARG:HG3	1.66	0.60
3:L:235:TYR:CZ	3:L:249:ILE:HD11	2.36	0.60
3:K:267:ARG:NH2	3:K:267:ARG:HG3	2.17	0.60
3:L:267:ARG:NH1	3:L:267:ARG:HG3	2.16	0.60
2:F:6:DC:O2	2:F:6:DC:O4'	2.19	0.59
2:I:16:DC:H2''	2:I:17:DA:OP2	2.02	0.59
3:K:246:ARG:HB2	3:K:257:GLU:HG3	1.84	0.59
3:A:262:ILE:HD12	3:A:262:ILE:H	1.66	0.59
3:L:267:ARG:HH11	3:L:267:ARG:CG	2.15	0.59
3:A:222:PRO:N	3:A:222:PRO:C	2.58	0.59
3:G:226:GLY:HA2	3:G:229:ARG:NH2	2.16	0.59
2:E:5:DC:H2'	2:E:6:DC:O2	2.02	0.59
3:G:273:LYS:HA	3:G:273:LYS:HZ3	1.66	0.59
3:B:221:ILE:HG22	3:B:221:ILE:O	2.02	0.59
3:G:229:ARG:HH11	3:G:229:ARG:CG	2.16	0.59
2:E:16:DC:H2''	2:E:17:DA:OP2	2.01	0.59
3:L:235:TYR:CE1	3:L:249:ILE:HD12	2.37	0.59
3:B:258:ARG:HA	3:B:258:ARG:NH2	2.16	0.59
3:J:234:GLU:HG3	3:J:249:ILE:CD1	2.32	0.59
3:B:247:ARG:HH11	3:B:247:ARG:CG	2.14	0.59
3:L:235:TYR:C	3:L:238:ASN:HB2	2.28	0.59
3:L:235:TYR:CA	3:L:238:ASN:CG	2.72	0.58
3:J:234:GLU:HG3	3:J:249:ILE:HD11	1.85	0.58
3:L:242:THR:O	3:L:246:ARG:HG2	2.04	0.58
3:A:231:LEU:HD13	3:A:231:LEU:C	2.28	0.58
3:K:268:ARG:O	3:K:271:GLU:HB3	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:241:ILE:HG12	3:L:246:ARG:HB3	1.86	0.58
3:B:258:ARG:CZ	3:B:262:ILE:HD11	2.33	0.58
1:H:5:DT:OP2	3:L:263:TRP:CZ3	2.56	0.58
3:A:234:GLU:OE1	3:A:249:ILE:HD11	2.04	0.58
3:L:235:TYR:O	3:L:238:ASN:HB2	2.04	0.58
1:H:5:DT:H73	3:L:266:ASN:ND2	1.91	0.58
3:G:245:LYS:HA	3:G:248:LYS:HE2	1.86	0.58
3:B:253:THR:HB	3:B:255:LEU:CD1	2.34	0.58
3:A:221:ILE:O	3:A:223:TYR:CE1	2.57	0.58
3:J:230:GLU:O	3:J:233:ARG:HB3	2.04	0.58
3:J:250:SER:HA	3:J:260:ILE:CD1	2.34	0.57
3:K:265:GLN:O	3:K:269:VAL:HG23	2.04	0.57
3:G:243:LYS:HA	3:G:246:ARG:HD2	1.86	0.57
3:B:246:ARG:CA	3:B:249:ILE:CG1	2.69	0.57
3:J:271:GLU:O	3:J:274:VAL:HG12	2.04	0.57
3:L:255:LEU:H	3:L:255:LEU:CD2	2.14	0.57
3:J:267:ARG:HD2	3:J:267:ARG:O	2.04	0.57
3:L:228:LEU:C	3:L:231:LEU:HB3	2.20	0.57
3:A:243:LYS:HA	3:A:246:ARG:CD	2.34	0.57
3:K:258:ARG:O	3:K:261:THR:OG1	2.22	0.57
3:G:268:ARG:HH22	3:G:272:LYS:HG3	1.68	0.57
3:K:242:THR:HG22	3:K:245:LYS:HD2	1.77	0.57
2:F:6:DC:O2	2:F:6:DC:O5'	2.22	0.57
3:G:253:THR:HB	3:G:255:LEU:CD1	2.35	0.57
3:G:228:LEU:CD2	3:G:231:LEU:HD12	2.31	0.57
3:G:228:LEU:CA	3:G:231:LEU:HG	2.34	0.57
3:J:244:ASP:O	3:J:248:LYS:HD3	2.03	0.57
3:L:223:TYR:CE1	3:L:227:GLN:HG3	2.40	0.57
3:A:242:THR:O	3:A:246:ARG:CG	2.50	0.56
3:K:227:GLN:O	3:K:231:LEU:HB2	2.05	0.56
2:I:7:DA:C5'	3:J:247:ARG:HD3	2.35	0.56
3:A:221:ILE:O	3:A:223:TYR:HE1	1.88	0.56
3:B:226:GLY:HA2	3:B:229:ARG:HH21	1.69	0.56
3:A:262:ILE:CD1	3:A:262:ILE:H	2.19	0.56
3:L:223:TYR:HE2	3:L:227:GLN:C	2.14	0.56
3:B:224:SER:HB3	3:B:227:GLN:HG3	1.88	0.56
3:G:271:GLU:O	3:G:274:VAL:HG22	2.06	0.56
3:K:241:ILE:HD12	3:K:245:LYS:CE	1.76	0.56
3:K:267:ARG:CG	3:K:267:ARG:HH21	2.18	0.56
2:I:6:DC:O2	2:I:6:DC:O5'	2.23	0.56
3:J:247:ARG:HB2	3:J:247:ARG:CZ	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:243:LYS:HA	3:A:246:ARG:CG	2.35	0.55
3:K:271:GLU:O	3:K:275:LEU:HG	2.06	0.55
3:A:240:PHE:CE2	3:A:268:ARG:NE	2.75	0.55
3:J:248:LYS:CD	3:J:248:LYS:H	2.19	0.55
2:E:6:DC:O2	2:E:6:DC:O4'	2.22	0.55
1:C:5:DT:C3'	3:K:223:TYR:OH	2.53	0.55
2:I:7:DA:H5'	3:J:247:ARG:CD	2.36	0.55
3:G:274:VAL:O	3:G:277:LYS:HG2	2.05	0.55
3:L:242:THR:HG23	3:L:245:LYS:HE2	1.88	0.55
2:E:6:DC:O2	2:E:6:DC:O5'	2.24	0.55
3:A:235:TYR:CE2	3:A:239:LYS:CD	2.90	0.55
3:A:243:LYS:HA	3:A:246:ARG:HG2	1.88	0.55
3:A:263:TRP:CE3	3:A:263:TRP:C	2.85	0.55
3:L:272:LYS:CA	3:L:272:LYS:CE	2.85	0.55
3:A:225:LYS:O	3:A:228:LEU:CD1	2.53	0.55
2:I:6:DC:O2	2:I:6:DC:O4'	2.21	0.55
3:G:246:ARG:C	3:G:249:ILE:CD1	2.79	0.55
3:L:243:LYS:HA	3:L:246:ARG:CG	2.36	0.55
3:L:241:ILE:N	3:L:264:PHE:HE1	2.04	0.55
3:L:260:ILE:C	3:L:262:ILE:HD12	2.31	0.55
3:B:246:ARG:C	3:B:249:ILE:HG12	2.32	0.55
3:A:258:ARG:C	3:A:262:ILE:CG1	2.71	0.54
3:K:241:ILE:CG1	3:K:245:LYS:HB2	2.36	0.54
3:L:243:LYS:CA	3:L:246:ARG:HD2	2.21	0.54
3:B:241:ILE:HD11	3:B:245:LYS:CB	2.38	0.54
3:G:243:LYS:O	3:G:246:ARG:HG3	2.07	0.54
3:G:253:THR:O	3:G:255:LEU:HD11	2.05	0.54
3:G:235:TYR:CD2	3:G:235:TYR:C	2.85	0.54
3:A:243:LYS:O	3:A:246:ARG:CG	2.56	0.54
3:J:269:VAL:O	3:J:273:LYS:CG	2.53	0.54
3:K:235:TYR:C	3:K:235:TYR:CD2	2.85	0.54
1:D:12:DT:H71	3:B:262:ILE:HD12	1.89	0.54
3:B:226:GLY:HA2	3:B:229:ARG:NH2	2.22	0.54
3:A:229:ARG:HB2	3:A:229:ARG:CZ	2.37	0.54
3:A:260:ILE:C	3:A:262:ILE:HD12	2.33	0.53
3:J:249:ILE:CG2	3:J:260:ILE:HD13	2.35	0.53
3:B:250:SER:HA	3:B:260:ILE:HD11	1.89	0.53
1:C:16:DT:H2'	1:C:17:DC:C6	2.43	0.53
1:D:11:DA:H2''	1:D:12:DT:C5	2.43	0.53
3:L:255:LEU:N	3:L:255:LEU:HD13	2.22	0.53
3:A:219:LYS:O	3:A:221:ILE:HD12	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:241:ILE:CG1	3:K:245:LYS:CB	2.86	0.53
3:G:250:SER:O	3:G:254:SER:N	2.41	0.53
3:K:238:ASN:OD1	3:K:245:LYS:HE2	2.07	0.53
3:L:231:LEU:HD11	3:L:263:TRP:NE1	2.24	0.53
3:A:235:TYR:HE2	3:A:239:LYS:HE3	1.73	0.53
3:J:250:SER:CA	3:J:260:ILE:CD1	2.87	0.53
3:L:222:PRO:N	3:L:222:PRO:C	2.62	0.53
3:L:232:GLU:O	3:L:236:ALA:HB2	2.09	0.53
3:A:235:TYR:CD2	3:A:239:LYS:HD2	2.43	0.53
3:L:253:THR:CB	3:L:255:LEU:HD11	2.39	0.53
3:L:262:ILE:HD12	3:L:262:ILE:N	2.23	0.53
3:L:267:ARG:HG3	3:L:267:ARG:HH11	1.74	0.53
1:H:16:DT:H2'	1:H:17:DC:C6	2.44	0.53
3:K:247:ARG:CD	3:K:247:ARG:N	2.72	0.53
3:L:245:LYS:CA	3:L:248:LYS:HB2	2.39	0.53
2:E:13:DA:H2''	2:E:14:DT:H5'	1.90	0.53
3:G:229:ARG:CG	3:G:229:ARG:NH1	2.72	0.53
1:C:10:DT:C3'	3:A:223:TYR:CZ	2.89	0.52
3:A:267:ARG:NH1	3:A:270:LYS:CB	2.70	0.52
3:B:229:ARG:NH1	3:B:229:ARG:CB	2.73	0.52
3:A:223:TYR:N	3:A:223:TYR:CD1	2.76	0.52
3:L:272:LYS:NZ	3:L:272:LYS:CB	2.72	0.52
3:B:258:ARG:HH21	3:B:258:ARG:HB2	1.73	0.52
3:K:228:LEU:N	3:K:228:LEU:CD2	2.72	0.52
1:C:4:DG:N1	2:F:16:DC:H5	2.01	0.52
3:J:229:ARG:NH1	3:J:229:ARG:CB	2.73	0.52
3:L:245:LYS:O	3:L:248:LYS:CA	2.57	0.52
3:L:247:ARG:HB2	3:L:257:GLU:OE2	2.09	0.52
3:B:246:ARG:CD	3:B:257:GLU:OE2	2.50	0.52
3:J:239:LYS:N	3:J:239:LYS:CD	2.73	0.52
3:K:238:ASN:HD21	3:K:245:LYS:HE2	1.74	0.52
1:D:16:DT:H2'	1:D:17:DC:C6	2.45	0.52
3:A:272:LYS:HB3	3:A:272:LYS:HZ2	1.75	0.52
3:A:235:TYR:CD2	3:A:235:TYR:C	2.88	0.51
3:A:253:THR:C	3:A:255:LEU:HD11	2.19	0.51
3:L:235:TYR:HD2	3:L:238:ASN:CG	2.18	0.51
3:K:217:ARG:O	3:K:217:ARG:HG3	2.04	0.51
3:A:247:ARG:O	3:A:250:SER:HB3	2.10	0.51
3:B:239:LYS:N	3:B:239:LYS:CD	2.72	0.51
3:B:246:ARG:O	3:B:249:ILE:CG1	2.50	0.51
3:B:229:ARG:CB	3:B:229:ARG:CZ	2.86	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:235:TYR:CD2	3:G:239:LYS:HE3	2.42	0.51
3:A:241:ILE:HD12	3:A:242:THR:H	1.75	0.51
3:K:231:LEU:HD13	3:K:231:LEU:C	2.36	0.51
1:C:9:DT:OP2	3:A:270:LYS:HE3	2.11	0.51
3:A:246:ARG:HH21	3:A:257:GLU:CB	2.24	0.51
3:J:229:ARG:CB	3:J:229:ARG:CZ	2.88	0.51
3:L:245:LYS:C	3:L:248:LYS:H	2.19	0.51
3:L:247:ARG:O	3:L:247:ARG:HD2	2.10	0.51
1:D:11:DA:N7	3:B:266:ASN:ND2	2.51	0.50
3:L:223:TYR:CE2	3:L:227:GLN:C	2.89	0.50
3:L:228:LEU:O	3:L:231:LEU:N	2.44	0.50
3:B:247:ARG:CG	3:B:247:ARG:NH1	2.72	0.50
3:K:267:ARG:CG	3:K:267:ARG:NH2	2.73	0.50
1:H:10:DT:HI'	3:G:220:ARG:CB	2.42	0.50
3:J:235:TYR:CE2	3:J:239:LYS:NZ	2.76	0.50
3:L:223:TYR:CZ	3:L:255:LEU:CD1	2.93	0.50
3:L:223:TYR:CD2	3:L:228:LEU:HD12	2.33	0.50
3:L:249:ILE:CD1	3:L:249:ILE:N	2.72	0.50
2:E:11:DA:P	3:J:268:ARG:HE	2.35	0.50
3:A:264:PHE:O	3:A:267:ARG:CB	2.59	0.50
3:G:238:ASN:N	3:G:238:ASN:ND2	2.59	0.50
3:L:244:ASP:C	3:L:247:ARG:HH22	2.15	0.50
3:L:256:SER:O	3:L:260:ILE:N	2.44	0.50
3:B:229:ARG:CZ	3:B:229:ARG:HB3	2.41	0.50
3:B:253:THR:HB	3:B:255:LEU:HD13	1.92	0.50
1:D:10:DT:OP1	3:B:223:TYR:HD1	1.95	0.50
3:G:228:LEU:C	3:G:231:LEU:HG	2.37	0.50
3:G:246:ARG:HE	3:G:257:GLU:HG2	1.77	0.50
3:K:247:ARG:N	3:K:247:ARG:HD3	2.27	0.50
3:L:236:ALA:C	3:L:238:ASN:H	2.20	0.50
3:L:265:GLN:O	3:L:269:VAL:HG13	2.11	0.50
3:L:267:ARG:HH11	3:L:267:ARG:HA	1.77	0.50
2:F:13:DA:H2''	2:F:14:DT:C5'	2.41	0.49
3:A:238:ASN:ND2	3:A:238:ASN:N	2.60	0.49
3:A:240:PHE:CA	3:A:268:ARG:NH2	2.72	0.49
3:K:235:TYR:O	3:K:239:LYS:HE3	2.11	0.49
2:E:5:DC:OP1	3:B:240:PHE:HD2	1.95	0.49
3:B:246:ARG:C	3:B:249:ILE:CG1	2.86	0.49
3:A:234:GLU:O	3:A:238:ASN:ND2	2.44	0.49
2:E:13:DA:H1'	2:E:14:DT:H5''	1.93	0.49
3:B:247:ARG:HH11	3:B:247:ARG:HB3	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:260:ILE:C	3:A:260:ILE:CD1	2.85	0.49
3:J:229:ARG:NH1	3:J:229:ARG:CG	2.73	0.49
3:L:235:TYR:HE1	3:L:249:ILE:CD1	2.24	0.49
2:F:8:DA:H1'	2:F:9:DT:H5'	1.95	0.49
3:A:243:LYS:C	3:A:246:ARG:HG3	2.37	0.49
3:A:255:LEU:HD12	3:A:255:LEU:N	2.28	0.49
3:J:247:ARG:CZ	3:J:247:ARG:CB	2.90	0.49
3:K:242:THR:H	3:K:245:LYS:CD	2.23	0.49
3:L:232:GLU:C	3:L:234:GLU:N	2.66	0.49
1:D:17:DC:OP1	3:L:242:THR:HG21	2.13	0.49
3:G:228:LEU:C	3:G:231:LEU:CG	2.85	0.49
3:K:263:TRP:HH2	3:K:267:ARG:CG	1.86	0.49
3:L:269:VAL:O	3:L:273:LYS:CD	2.54	0.49
3:G:217:ARG:HG3	3:G:218:LYS:HE3	1.95	0.49
3:K:263:TRP:CE3	3:K:263:TRP:C	2.90	0.49
3:B:250:SER:HB2	3:B:260:ILE:HD12	1.94	0.49
1:D:14:DG:H1	2:E:6:DC:H5	1.61	0.49
3:K:223:TYR:HH	3:K:259:GLN:NE2	2.09	0.49
3:L:241:ILE:HD11	3:L:246:ARG:N	2.27	0.49
3:L:249:ILE:O	3:L:255:LEU:CD2	2.57	0.49
3:A:239:LYS:N	3:A:239:LYS:CD	2.76	0.49
2:I:13:DA:H2''	2:I:14:DT:C5'	2.43	0.49
3:J:223:TYR:N	3:J:223:TYR:CD1	2.81	0.49
3:K:245:LYS:O	3:K:249:ILE:HG12	2.12	0.49
3:L:223:TYR:CD2	3:L:227:GLN:HB2	2.47	0.49
3:K:239:LYS:HD2	3:K:239:LYS:H	1.71	0.48
3:B:229:ARG:CG	3:B:229:ARG:NH1	2.73	0.48
3:J:248:LYS:O	3:J:252:ALA:N	2.34	0.48
3:J:250:SER:CB	3:J:260:ILE:HD12	2.42	0.48
3:L:241:ILE:HD11	3:L:246:ARG:H	1.78	0.48
3:A:275:LEU:HD22	3:A:275:LEU:H	1.76	0.48
3:G:243:LYS:C	3:G:246:ARG:HG3	2.38	0.48
3:G:258:ARG:O	3:G:262:ILE:HG13	2.13	0.48
3:J:267:ARG:NH1	3:J:267:ARG:O	2.39	0.48
3:K:241:ILE:HA	3:K:245:LYS:HD3	1.94	0.48
3:A:223:TYR:N	3:A:223:TYR:HD1	2.12	0.48
3:A:234:GLU:CD	3:A:249:ILE:CD1	2.76	0.48
3:G:230:GLU:OE2	3:G:253:THR:CG2	2.54	0.48
3:J:244:ASP:HA	3:J:247:ARG:NH2	2.29	0.48
3:L:235:TYR:CD2	3:L:238:ASN:CG	2.91	0.48
3:L:267:ARG:HH11	3:L:267:ARG:CA	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:229:ARG:O	3:L:233:ARG:HB3	2.14	0.48
3:L:233:ARG:O	3:L:233:ARG:HG2	2.14	0.48
3:B:241:ILE:HD11	3:B:245:LYS:HB3	1.96	0.48
2:I:13:DA:H1'	2:I:14:DT:H5''	1.96	0.48
3:L:231:LEU:O	3:L:234:GLU:CB	2.62	0.48
1:D:11:DA:O3'	3:B:218:LYS:HG2	2.14	0.48
2:E:16:DC:O2	2:E:16:DC:C2'	2.56	0.48
3:A:231:LEU:C	3:A:231:LEU:CD1	2.85	0.48
3:L:270:LYS:C	3:L:273:LYS:HG2	2.36	0.48
3:G:243:LYS:HA	3:G:246:ARG:CD	2.43	0.48
3:L:247:ARG:HD2	3:L:251:ALA:HB2	1.94	0.48
3:L:235:TYR:HE1	3:L:249:ILE:HG13	1.79	0.47
3:A:263:TRP:C	3:A:263:TRP:HE3	2.22	0.47
3:L:247:ARG:CB	3:L:257:GLU:OE2	2.61	0.47
3:L:247:ARG:C	3:L:247:ARG:CD	2.83	0.47
3:J:222:PRO:HD2	3:J:222:PRO:O	2.15	0.47
3:A:229:ARG:CZ	3:A:229:ARG:CB	2.92	0.47
3:B:258:ARG:CA	3:B:258:ARG:NH2	2.73	0.47
3:K:254:SER:O	3:K:254:SER:OG	2.12	0.47
3:A:241:ILE:HD11	3:A:245:LYS:HG3	1.97	0.47
3:A:243:LYS:O	3:A:246:ARG:CD	2.63	0.47
3:G:253:THR:CB	3:G:255:LEU:CD1	2.92	0.47
3:J:241:ILE:HD11	3:J:245:LYS:HB3	1.96	0.47
3:A:258:ARG:C	3:A:262:ILE:HD11	2.13	0.47
3:G:229:ARG:CZ	3:G:229:ARG:HB3	2.45	0.47
3:B:241:ILE:HD11	3:B:245:LYS:HB2	1.97	0.47
3:A:267:ARG:O	3:A:270:LYS:N	2.48	0.47
1:H:14:DG:H1	2:I:6:DC:H5	1.62	0.47
3:J:273:LYS:CA	3:J:273:LYS:CE	2.85	0.47
3:K:267:ARG:HA	3:K:267:ARG:HD2	1.56	0.47
2:I:8:DA:H1'	2:I:9:DT:H5'	1.96	0.46
3:A:266:ASN:O	3:A:269:VAL:HG23	2.15	0.46
3:G:219:LYS:HZ2	3:G:220:ARG:HG3	1.80	0.46
2:E:8:DA:H1'	2:E:9:DT:H5'	1.97	0.46
2:I:6:DC:OP1	3:G:268:ARG:HG2	2.15	0.46
2:F:13:DA:H1'	2:F:14:DT:H5''	1.96	0.46
3:A:238:ASN:N	3:A:238:ASN:HD22	2.12	0.46
3:K:223:TYR:HB2	3:K:228:LEU:HD21	1.98	0.46
3:K:255:LEU:HD22	3:K:256:SER:H	1.80	0.46
3:L:223:TYR:HH	3:L:227:GLN:HB3	1.80	0.46
3:L:255:LEU:HB3	3:L:260:ILE:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:246:ARG:NH1	3:J:246:ARG:CG	2.73	0.46
3:K:231:LEU:HD11	3:K:263:TRP:CE3	2.51	0.46
1:D:5:DT:H3'	3:J:223:TYR:CE2	2.48	0.46
3:G:234:GLU:OE2	3:G:234:GLU:HA	2.15	0.46
3:B:220:ARG:NH1	3:B:222:PRO:HG3	2.31	0.46
3:B:249:ILE:HD13	3:B:249:ILE:N	2.06	0.46
3:A:243:LYS:O	3:A:246:ARG:HD3	2.15	0.46
3:L:250:SER:C	3:L:252:ALA:N	2.71	0.46
3:B:253:THR:CB	3:B:255:LEU:HD13	2.46	0.46
1:C:6:DA:P	3:K:259:GLN:HE22	2.38	0.46
3:A:234:GLU:CG	3:A:249:ILE:HD11	2.46	0.46
3:L:227:GLN:HE21	3:L:253:THR:CB	2.28	0.46
3:G:231:LEU:HB3	3:G:263:TRP:CZ2	2.51	0.46
3:L:223:TYR:OH	3:L:227:GLN:CB	2.53	0.45
3:L:235:TYR:HA	3:L:238:ASN:HD22	0.64	0.45
3:B:258:ARG:CG	3:B:258:ARG:NH2	2.72	0.45
1:C:5:DT:H3'	3:K:223:TYR:OH	2.15	0.45
3:G:228:LEU:CD2	3:G:231:LEU:HD13	2.32	0.45
1:H:13:DT:H2''	1:H:14:DG:C8	2.51	0.45
3:B:244:ASP:O	3:B:248:LYS:HG3	2.17	0.45
1:D:13:DT:H2''	1:D:14:DG:C8	2.51	0.45
3:B:247:ARG:HH11	3:B:247:ARG:HB2	1.76	0.45
3:A:253:THR:CA	3:A:255:LEU:HD11	2.44	0.45
1:C:13:DT:H2''	1:C:14:DG:C8	2.52	0.45
2:F:6:DC:P	3:A:268:ARG:HD2	2.51	0.45
3:A:267:ARG:O	3:A:267:ARG:HD2	2.15	0.45
3:L:229:ARG:O	3:L:233:ARG:CB	2.65	0.45
3:B:241:ILE:HD12	3:B:242:THR:H	1.82	0.45
2:I:10:DA:C2'	2:I:11:DA:C8	3.00	0.45
3:A:264:PHE:O	3:A:267:ARG:HB2	2.17	0.45
3:J:248:LYS:O	3:J:252:ALA:CB	2.65	0.45
3:J:250:SER:N	3:J:260:ILE:CD1	2.79	0.45
3:A:235:TYR:CD2	3:A:235:TYR:O	2.70	0.45
3:K:249:ILE:HG12	3:K:249:ILE:H	1.60	0.45
2:E:10:DA:H2'	2:E:11:DA:H8	1.78	0.44
3:J:231:LEU:HB3	3:J:263:TRP:CE3	2.47	0.44
3:K:277:LYS:HE3	3:K:277:LYS:HB3	1.38	0.44
3:L:235:TYR:CA	3:L:238:ASN:CB	2.90	0.44
3:L:248:LYS:HD2	3:L:248:LYS:HA	1.60	0.44
3:A:263:TRP:CE3	3:A:263:TRP:O	2.70	0.44
3:A:267:ARG:HA	3:A:267:ARG:HD3	1.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:271:GLU:O	3:A:275:LEU:HD22	2.18	0.44
3:L:273:LYS:CA	3:L:273:LYS:CE	2.88	0.44
3:G:232:GLU:O	3:G:236:ALA:HB2	2.17	0.44
3:G:235:TYR:O	3:G:235:TYR:CD2	2.70	0.44
3:G:243:LYS:CA	3:G:246:ARG:CG	2.95	0.44
3:B:275:LEU:HA	3:B:277:LYS:HZ3	1.82	0.44
3:J:250:SER:CA	3:J:260:ILE:HD11	2.43	0.44
3:L:230:GLU:CD	3:L:230:GLU:C	2.85	0.44
3:G:225:LYS:O	3:G:228:LEU:HB2	2.18	0.44
3:J:250:SER:CA	3:J:260:ILE:HD12	2.48	0.44
3:L:231:LEU:O	3:L:234:GLU:HB3	2.17	0.44
3:L:247:ARG:HH21	3:L:247:ARG:CG	2.28	0.44
2:E:17:DA:H2''	2:E:18:DA:H5''	2.00	0.44
3:G:275:LEU:O	3:G:276:ALA:C	2.60	0.44
1:C:14:DG:H1	2:F:6:DC:H5	1.66	0.44
3:A:243:LYS:C	3:A:246:ARG:CG	2.91	0.44
3:K:244:ASP:CA	3:K:247:ARG:HG2	2.47	0.44
3:L:243:LYS:O	3:L:246:ARG:HG3	2.18	0.44
2:E:10:DA:C2'	2:E:11:DA:C8	2.98	0.44
3:K:238:ASN:ND2	3:K:245:LYS:HE2	2.33	0.44
3:L:221:ILE:HG22	3:L:221:ILE:O	2.18	0.44
3:L:234:GLU:C	3:L:234:GLU:CD	2.84	0.44
2:F:16:DC:O2	2:F:16:DC:C2'	2.57	0.43
3:A:258:ARG:HA	3:A:258:ARG:HD3	1.44	0.43
3:L:241:ILE:HD12	3:L:245:LYS:HE3	1.99	0.43
3:G:249:ILE:HA	3:G:252:ALA:HB3	2.00	0.43
3:K:275:LEU:O	3:K:276:ALA:C	2.61	0.43
3:L:259:GLN:HA	3:L:262:ILE:HG12	1.72	0.43
1:C:5:DT:H5'	3:K:220:ARG:NH1	2.33	0.43
3:L:234:GLU:C	3:L:236:ALA:H	2.26	0.43
3:L:247:ARG:NE	3:L:248:LYS:HD3	2.34	0.43
3:G:243:LYS:HG3	3:G:246:ARG:HD2	2.01	0.43
3:J:243:LYS:CA	3:J:246:ARG:NH1	2.74	0.43
3:J:247:ARG:HB3	3:J:247:ARG:NH1	2.33	0.43
2:E:13:DA:H2''	2:E:14:DT:C5'	2.49	0.43
3:B:229:ARG:NH1	3:B:229:ARG:HB2	2.33	0.43
1:H:9:DT:H1'	3:G:220:ARG:HH21	1.83	0.43
3:G:242:THR:O	3:G:246:ARG:HG2	2.19	0.43
3:L:227:GLN:NE2	3:L:253:THR:CB	2.81	0.43
3:L:227:GLN:NE2	3:L:253:THR:CG2	2.82	0.43
1:H:11:DA:H5'	3:G:220:ARG:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:223:TYR:O	3:L:228:LEU:HD22	2.19	0.42
3:A:267:ARG:CD	3:A:267:ARG:C	2.84	0.42
2:I:11:DA:H2'	4:I:101:HOH:O	2.20	0.42
3:J:229:ARG:HB2	3:J:229:ARG:CZ	2.49	0.42
3:B:231:LEU:HG	3:B:263:TRP:CE3	2.54	0.42
1:C:10:DT:H5'	3:A:223:TYR:CD1	2.54	0.42
3:G:245:LYS:CA	3:G:248:LYS:HG3	2.49	0.42
3:G:246:ARG:CB	3:G:260:ILE:HD11	2.49	0.42
3:G:257:GLU:HA	3:G:260:ILE:HD12	2.01	0.42
3:J:231:LEU:HD12	3:J:263:TRP:CE2	2.54	0.42
3:B:230:GLU:O	3:B:233:ARG:HB3	2.19	0.42
1:C:15:DG:H2'	1:C:16:DT:C6	2.54	0.42
2:F:10:DA:C2'	2:F:11:DA:C8	3.00	0.42
3:A:250:SER:O	3:A:254:SER:N	2.52	0.42
3:G:235:TYR:CZ	3:G:239:LYS:HE3	2.44	0.42
3:G:256:SER:O	3:G:260:ILE:HG23	2.18	0.42
3:G:273:LYS:NZ	3:G:273:LYS:CA	2.73	0.42
3:L:223:TYR:OH	3:L:227:GLN:HG3	2.19	0.42
3:L:252:ALA:O	3:L:255:LEU:CD2	2.67	0.42
3:A:235:TYR:C	3:A:235:TYR:HD2	2.27	0.42
1:C:5:DT:O3'	3:K:223:TYR:CE1	2.73	0.42
3:J:248:LYS:O	3:J:252:ALA:HB2	2.19	0.42
3:L:235:TYR:CZ	3:L:245:LYS:CB	3.01	0.42
3:G:258:ARG:HD2	3:G:262:ILE:CG1	2.49	0.42
3:K:259:GLN:HA	3:K:262:ILE:HD12	2.01	0.42
3:L:242:THR:C	3:L:244:ASP:N	2.76	0.42
3:K:246:ARG:HB2	3:K:257:GLU:CG	2.50	0.42
3:G:220:ARG:O	3:G:221:ILE:C	2.62	0.42
3:J:243:LYS:HA	3:J:246:ARG:HG3	2.01	0.42
3:J:263:TRP:O	3:J:267:ARG:N	2.46	0.42
3:B:250:SER:O	3:B:254:SER:N	2.54	0.41
1:C:10:DT:C3'	3:A:223:TYR:OH	2.51	0.41
1:C:15:DG:H2'	1:C:16:DT:H6	1.85	0.41
3:G:243:LYS:C	3:G:246:ARG:CG	2.93	0.41
3:J:258:ARG:C	3:J:262:ILE:HG13	2.45	0.41
2:I:12:DA:N3	3:G:220:ARG:HD2	2.35	0.41
3:K:255:LEU:HA	3:K:255:LEU:HD23	1.67	0.41
3:G:268:ARG:NH2	3:G:272:LYS:CG	2.83	0.41
3:K:241:ILE:HD12	3:K:242:THR:H	1.84	0.41
3:G:243:LYS:CA	3:G:246:ARG:HG2	2.45	0.41
3:J:243:LYS:CB	3:J:246:ARG:HH12	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:9:DT:OP2	3:B:270:LYS:NZ	2.52	0.41
1:H:15:DG:H2'	1:H:16:DT:C6	2.56	0.41
3:K:234:GLU:OE2	3:K:245:LYS:NZ	2.39	0.41
3:A:225:LYS:O	3:A:229:ARG:N	2.53	0.41
3:L:253:THR:OG1	3:L:254:SER:N	2.52	0.41
3:J:221:ILE:HA	3:J:222:PRO:HD3	1.89	0.41
3:K:238:ASN:N	3:K:238:ASN:ND2	2.59	0.41
1:D:11:DA:H2'	1:D:12:DT:H72	2.01	0.41
3:A:254:SER:O	3:A:254:SER:OG	2.31	0.41
3:G:219:LYS:HE3	3:G:221:ILE:CA	2.41	0.41
3:G:230:GLU:HA	3:G:233:ARG:HB2	2.02	0.41
3:J:247:ARG:CB	3:J:247:ARG:NH1	2.84	0.41
3:J:255:LEU:HD12	3:J:255:LEU:N	2.36	0.41
3:J:267:ARG:HD2	3:J:267:ARG:C	2.34	0.41
3:J:268:ARG:HG3	3:J:268:ARG:NH1	2.36	0.41
3:L:227:GLN:HE21	3:L:253:THR:CG2	2.34	0.41
3:L:260:ILE:HD12	3:L:260:ILE:HA	1.71	0.41
3:B:218:LYS:O	3:B:218:LYS:HG3	2.21	0.41
3:L:241:ILE:CG1	3:L:246:ARG:HB3	2.49	0.41
1:C:5:DT:H3'	3:K:223:TYR:CE2	2.56	0.40
3:A:234:GLU:HG3	3:A:249:ILE:CD1	2.51	0.40
3:G:229:ARG:CZ	3:G:229:ARG:CB	2.96	0.40
3:J:275:LEU:O	3:J:275:LEU:CG	2.70	0.40
3:L:223:TYR:O	3:L:228:LEU:CD2	2.69	0.40
3:G:233:ARG:O	3:G:236:ALA:HB3	2.21	0.40
3:J:234:GLU:HG3	3:J:249:ILE:HD12	2.02	0.40
3:J:253:THR:O	3:J:255:LEU:HD11	2.19	0.40
3:L:262:ILE:HD12	3:L:262:ILE:H	1.86	0.40
3:B:250:SER:CA	3:B:260:ILE:HD11	2.50	0.40
3:G:241:ILE:CD1	3:G:245:LYS:HB2	2.52	0.40
3:J:238:ASN:ND2	3:J:240:PHE:O	2.46	0.40
3:G:232:GLU:O	3:G:236:ALA:CB	2.70	0.40
3:L:250:SER:HB2	3:L:257:GLU:OE1	2.22	0.40

All (4) 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:E:19:DC:OP2	3:K:243:LYS:CE[4_665]	1.68	0.52
2:E:2:DG:C4'	3:K:243:LYS:CD[7_645]	1.81	0.39

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2:DG:O3'	3:K:243:LYS:CD[7_645]	1.92	0.28
2:E:2:DG:C3'	3:K:243:LYS:CD[7_645]	2.12	0.08

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	
3	A	57/63 (90%)	52 (91%)	4 (7%)	1 (2%)	6	31
3	B	60/63 (95%)	58 (97%)	2 (3%)	0	100	100
3	G	59/63 (94%)	53 (90%)	5 (8%)	1 (2%)	7	32
3	J	55/63 (87%)	49 (89%)	5 (9%)	1 (2%)	6	31
3	K	59/63 (94%)	55 (93%)	4 (7%)	0	100	100
3	L	52/63 (82%)	43 (83%)	8 (15%)	1 (2%)	6	30
All	All	342/378 (90%)	310 (91%)	28 (8%)	4 (1%)	10	40

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	231	LEU
3	L	233	ARG
3	A	270	LYS
3	J	222	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	
3	A	53/56 (95%)	28 (53%)	25 (47%)	0	0
3	B	55/56 (98%)	35 (64%)	20 (36%)	0	1
3	G	55/56 (98%)	33 (60%)	22 (40%)	0	1
3	J	51/56 (91%)	26 (51%)	25 (49%)	0	0
3	K	55/56 (98%)	28 (51%)	27 (49%)	0	0
3	L	49/56 (88%)	19 (39%)	30 (61%)	0	0
All	All	318/336 (95%)	169 (53%)	149 (47%)	0	0

All (149) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	220	ARG
3	B	221	ILE
3	B	229	ARG
3	B	230	GLU
3	B	231	LEU
3	B	233	ARG
3	B	239	LYS
3	B	241	ILE
3	B	244	ASP
3	B	246	ARG
3	B	247	ARG
3	B	249	ILE
3	B	254	SER
3	B	256	SER
3	B	258	ARG
3	B	265	GLN
3	B	273	LYS
3	B	274	VAL
3	B	275	LEU
3	B	277	LYS
3	A	219	LYS
3	A	221	ILE
3	A	223	TYR
3	A	224	SER
3	A	228	LEU
3	A	230	GLU
3	A	231	LEU
3	A	233	ARG
3	A	238	ASN
3	A	239	LYS

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Mol	Chain	Res	Type
3	A	241	ILE
3	A	242	THR
3	A	245	LYS
3	A	246	ARG
3	A	257	GLU
3	A	258	ARG
3	A	260	ILE
3	A	262	ILE
3	A	267	ARG
3	A	269	VAL
3	A	270	LYS
3	A	272	LYS
3	A	274	VAL
3	A	275	LEU
3	A	277	LYS
3	G	217	ARG
3	G	218	LYS
3	G	219	LYS
3	G	220	ARG
3	G	224	SER
3	G	229	ARG
3	G	230	GLU
3	G	232	GLU
3	G	234	GLU
3	G	238	ASN
3	G	239	LYS
3	G	244	ASP
3	G	246	ARG
3	G	247	ARG
3	G	249	ILE
3	G	256	SER
3	G	258	ARG
3	G	260	ILE
3	G	267	ARG
3	G	269	VAL
3	G	273	LYS
3	G	275	LEU
3	J	221	ILE
3	J	223	TYR
3	J	224	SER
3	J	225	LYS
3	J	229	ARG

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Mol	Chain	Res	Type
3	J	230	GLU
3	J	231	LEU
3	J	232	GLU
3	J	233	ARG
3	J	239	LYS
3	J	243	LYS
3	J	244	ASP
3	J	245	LYS
3	J	246	ARG
3	J	248	LYS
3	J	257	GLU
3	J	258	ARG
3	J	261	THR
3	J	262	ILE
3	J	267	ARG
3	J	269	VAL
3	J	271	GLU
3	J	273	LYS
3	J	274	VAL
3	J	275	LEU
3	K	217	ARG
3	K	219	LYS
3	K	221	ILE
3	K	222	PRO
3	K	225	LYS
3	K	228	LEU
3	K	230	GLU
3	K	234	GLU
3	K	238	ASN
3	K	239	LYS
3	K	241	ILE
3	K	242	THR
3	K	244	ASP
3	K	246	ARG
3	K	248	LYS
3	K	249	ILE
3	K	255	LEU
3	K	256	SER
3	K	257	GLU
3	K	260	ILE
3	K	261	THR
3	K	265	GLN

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Mol	Chain	Res	Type
3	K	267	ARG
3	K	269	VAL
3	K	270	LYS
3	K	273	LYS
3	K	277	LYS
3	L	221	ILE
3	L	225	LYS
3	L	227	GLN
3	L	228	LEU
3	L	229	ARG
3	L	230	GLU
3	L	232	GLU
3	L	234	GLU
3	L	239	LYS
3	L	240	PHE
3	L	243	LYS
3	L	244	ASP
3	L	245	LYS
3	L	246	ARG
3	L	247	ARG
3	L	248	LYS
3	L	249	ILE
3	L	250	SER
3	L	255	LEU
3	L	256	SER
3	L	257	GLU
3	L	260	ILE
3	L	262	ILE
3	L	264	PHE
3	L	265	GLN
3	L	267	ARG
3	L	269	VAL
3	L	272	LYS
3	L	273	LYS
3	L	274	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	265	GLN
3	J	265	GLN
3	K	227	GLN

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Mol	Chain	Res	Type
3	K	259	GLN
3	K	265	GLN
3	L	227	GLN
3	L	238	ASN
3	L	259	GLN
3	L	266	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	C	18/18 (100%)	-0.48	0	100	100	76, 96, 120, 145	0
1	D	17/18 (94%)	-0.37	0	100	100	49, 76, 104, 124	0
1	H	18/18 (100%)	-0.39	0	100	100	81, 109, 148, 167	0
2	E	18/18 (100%)	-0.37	1 (5%)	30	15	51, 78, 99, 116	0
2	F	18/18 (100%)	-0.35	0	100	100	89, 101, 126, 152	0
2	I	18/18 (100%)	-0.27	0	100	100	90, 104, 144, 149	0
3	A	59/63 (93%)	-0.01	1 (1%)	69	45	89, 140, 171, 200	0
3	B	62/63 (98%)	-0.19	0	100	100	59, 92, 132, 159	0
3	G	61/63 (96%)	-0.02	1 (1%)	70	47	82, 147, 184, 194	0
3	J	57/63 (90%)	-0.25	0	100	100	83, 132, 175, 196	0
3	K	61/63 (96%)	-0.14	1 (1%)	70	47	94, 139, 184, 221	0
3	L	54/63 (85%)	0.36	3 (5%)	30	15	115, 178, 233, 251	0
All	All	461/486 (94%)	-0.12	7 (1%)	72	49	49, 124, 193, 251	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	223	TYR	4.7
3	L	260	ILE	2.6
3	K	244	ASP	2.5
3	G	231	LEU	2.5
3	A	244	ASP	2.3
3	L	274	VAL	2.3
2	E	2	DG	2.2

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.